Full wwPDB EM Validation Report (i)

May 27, 2024 – 02:08 AM EDT

PDB ID	:	7SYK
EMDB ID	:	EMD-25531
Title	:	Structure of the HCV IRES binding to the 40S ribosomal subunit, closed conformation. Structure 5(delta dII)
Authors	:	Brown, Z.P.; Abaeva, I.S.; De, S.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on	:	2021-11-25
Resolution	:	4.20 Å(reported)
Based on initial models	:	5FLX, 6D9J

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

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

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

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

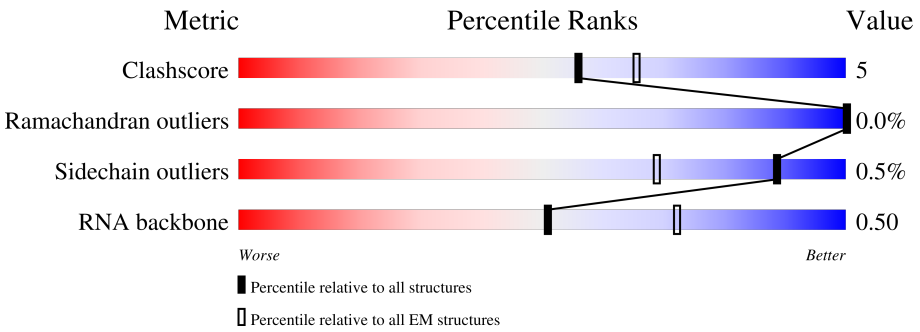
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 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
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	2	1870	• 53% 31% 6% 9%
2	B	295	5% 61% 13% 26%
3	C	264	• 66% 14% 19%
4	D	221	• 88% 12%
5	E	281	18% 72% 10% 19%
6	F	263	• 83% 17%
7	G	204	10% 78% 15% 6%

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Mol	Chain	Length	Quality of chain
8	H	249	84% 11% 5%
9	I	432	6% 37% 6% 57%
10	J	208	90% 9%
11	K	194	82% 13% 5%
12	L	149	18% 55% 7% 36%
13	M	158	8% 74% 22%
14	N	132	83% 74% 14% 11%
15	O	151	81% 17%
16	P	168	64% 17% 19%
17	Q	145	11% 69% 10% 21%
18	R	172	8% 66% 15% 17%
19	S	135	21% 79% 19%
20	T	152	12% 78% 17% 5%
21	U	145	78% 19%
22	V	119	44% 68% 16% 16%
23	W	83	95% 5%
24	X	130	86% 13%
25	Y	143	87% 11%
26	Z	131	82% 13% 5%
27	a	124	25% 62% 38%
28	b	101	5% 98%
29	c	84	6% 98%
30	d	69	19% 97%
31	e	56	7% 98%
32	f	133	11% 43% 57%

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Mol	Chain	Length	Quality of chain
33	g	188	30% 36% 64%
34	h	317	26% 98%
35	n	25	96%
36	z	400	30% 10% 60%

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 78761 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 RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1697	36227	16170	6504	11857	1696	0	0

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	217	1710	1086	300	316	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 3 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	213	1729	1098	309	308	14	0	0

- Molecule 4 is a protein called uS5 (S2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	221	1716	1111	295	301	9	0	0

- Molecule 5 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	228	1768	1126	318	316	8	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	262	2076	1324	386	358	8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17
F	51	ARG	LYS	conflict	UNP G1TK17
F	78	THR	ALA	conflict	UNP G1TK17
F	156	VAL	MET	conflict	UNP G1TK17

- Molecule 7 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	191	1509	943	286	273	7	0	0

- Molecule 8 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	237	1923	1200	387	329	7	0	0

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	185	1488	952	271	264	1	0	0

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	206	1686	1058	332	291	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 11 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	185	1525	969	306	248	2	0	0

- Molecule 12 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	96	810	530	143	131	6	0	0

- Molecule 13 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	151	1233	785	231	211	6	0	0

- Molecule 14 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	117	908	570	161	169	8	0	0

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	149	1202	770	228	203	1	0	0

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	136	1016	621	199	190	6	0	0

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	115	956	610	176	163	7	0	0

- Molecule 18 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	142	1128	717	213	195	3	0	0

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	132	1068	670	199	195	4	0	0

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	144	1190	746	241	202	1	0	0

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	141	1097	688	211	195	3	0	0

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	100	795	498	152	141	4	0	0

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	83	636	393	117	121	5	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	3	ASN	SER	conflict	UNP G1TM82
W	4	ASP	ASN	conflict	UNP G1TM82
W	33	GLN	PRO	conflict	UNP G1TM82
W	50	PHE	SER	conflict	UNP G1TM82
W	75	ALA	SER	conflict	UNP G1TM82
W	76	ASP	HIS	conflict	UNP G1TM82

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Chain	Residue	Modelled	Actual	Comment	Reference
W	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 24 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	129	1034	659	193	176	6	0	0

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	141	1098	693	219	183	3	0	0

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	124	1011	640	198	168	5	0	0

- Molecule 27 is a protein called eS25 (S25).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	a	77	614	393	114	106	1	0	0

- Molecule 28 is a protein called eS26 (S26).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	b	101	814	507	170	132	5	0	0

- Molecule 29 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	c	83	651	408	121	115	7	0	0

- Molecule 30 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	d	67	530	321	108	99	2	0	0

- Molecule 31 is a protein called eS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	e	55	459	286	94	74	5	0	0

- Molecule 32 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	f	57	457	282	101	73	1	0	0

- Molecule 33 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	g	68	555	351	103	94	7	0	0

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	h	313	2436	1535	424	465	12	0	0

- Molecule 35 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	n	25	239	145	64	27	3	0	0

- Molecule 36 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
36	z	162	3465	1542	621	1140	162	0	0

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

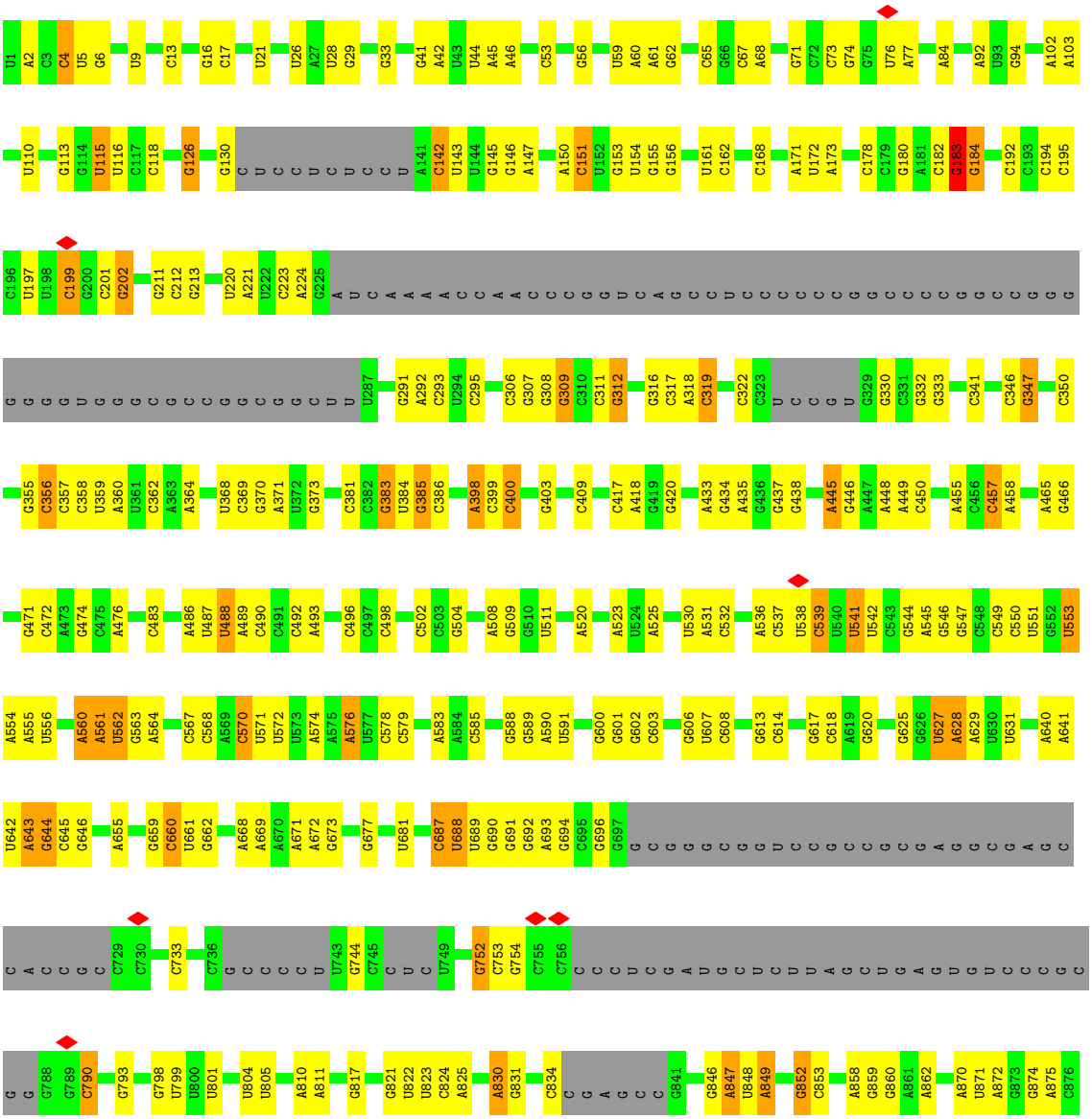
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
37	b	1	1	1	0
			Total	Zn	
37	g	1	1	1	0

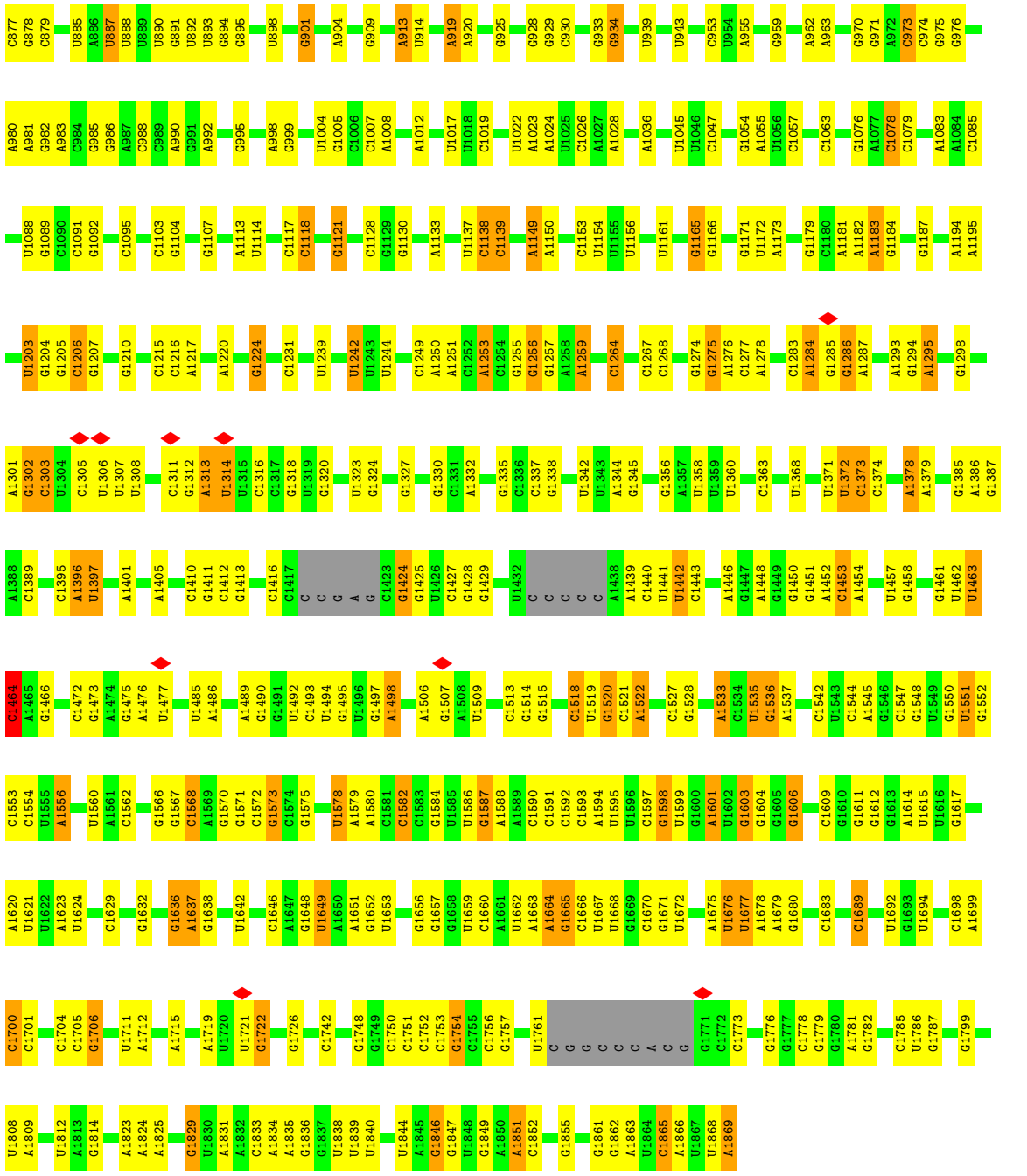
3 Residue-property plots (i)

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: 18S rRNA

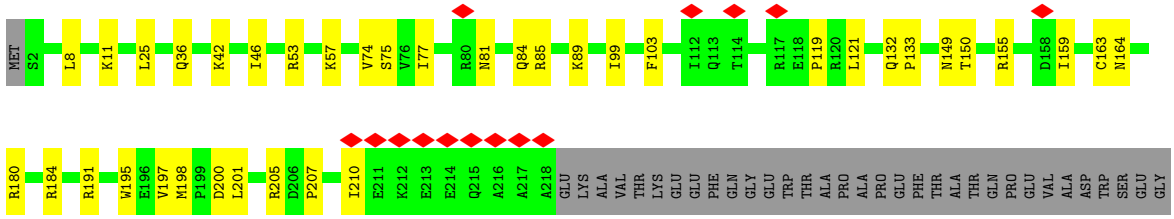
Chain 2:





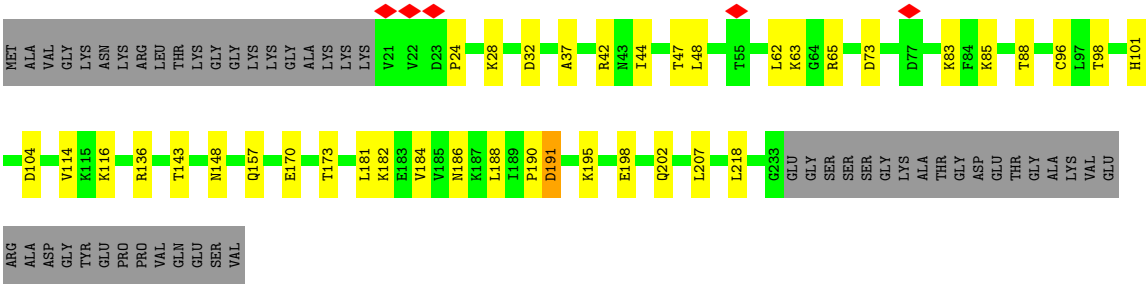
• Molecule 2: 40S ribosomal protein SA

Chain B:



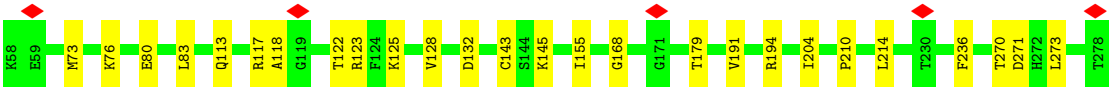
- Molecule 3: eS1

Chain C:



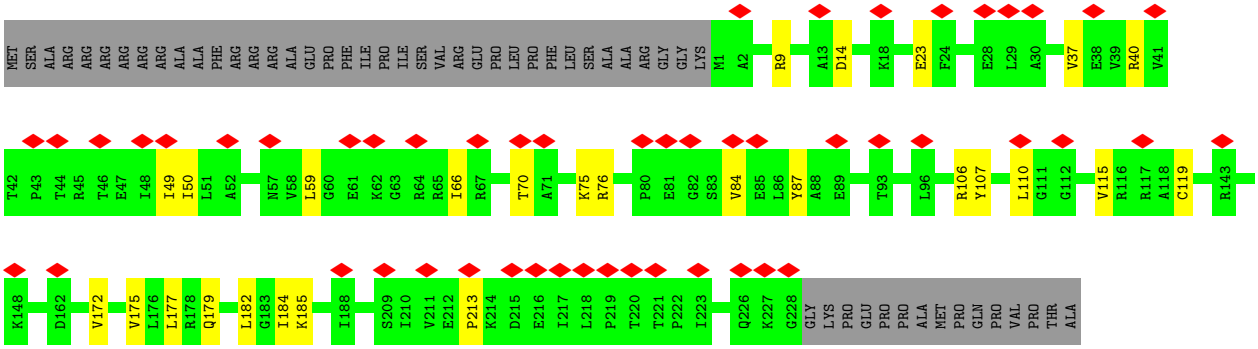
- Molecule 4: uS5 (S2)

Chain D:



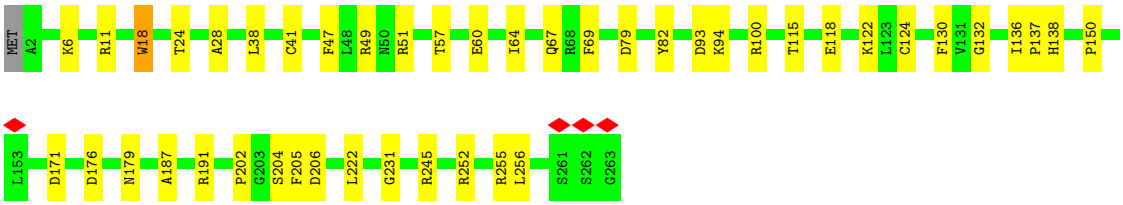
- Molecule 5: uS3

Chain E:



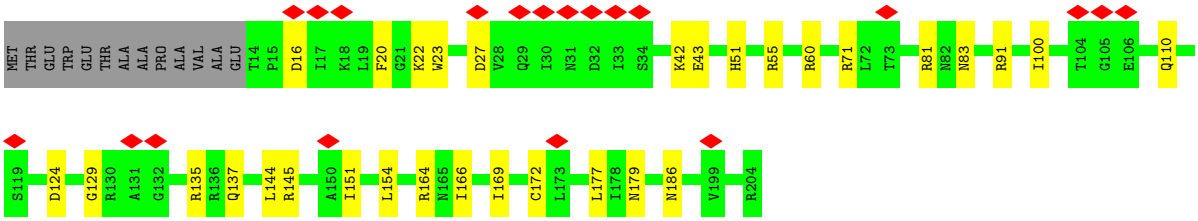
- Molecule 6: 40S ribosomal protein S4

Chain F:



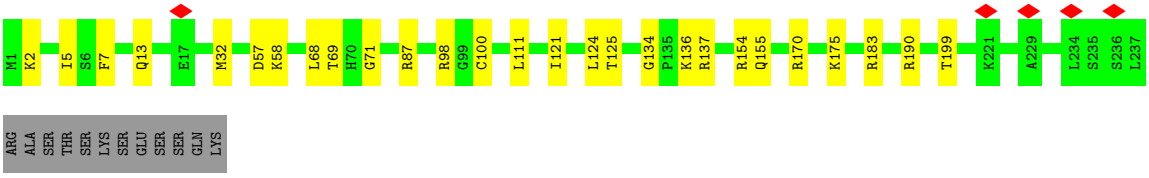
- Molecule 7: uS7

Chain G:



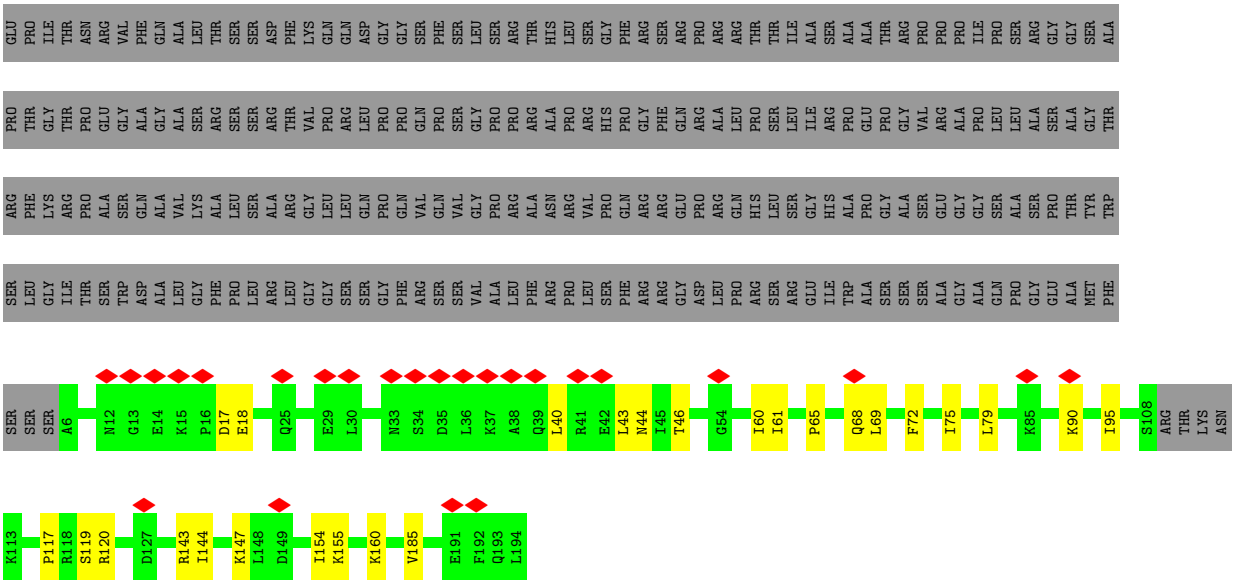
- Molecule 8: eS6

Chain H:



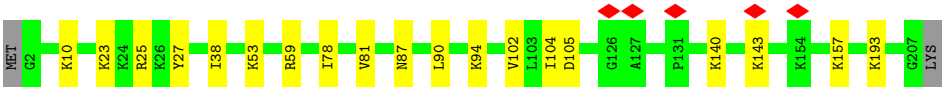
- Molecule 9: 40S ribosomal protein S7

Chain I:



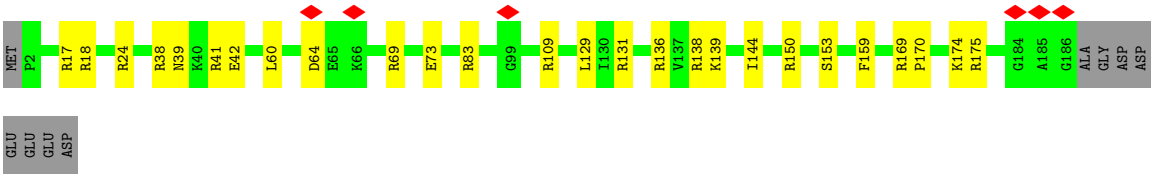
- Molecule 10: eS8

Chain J:



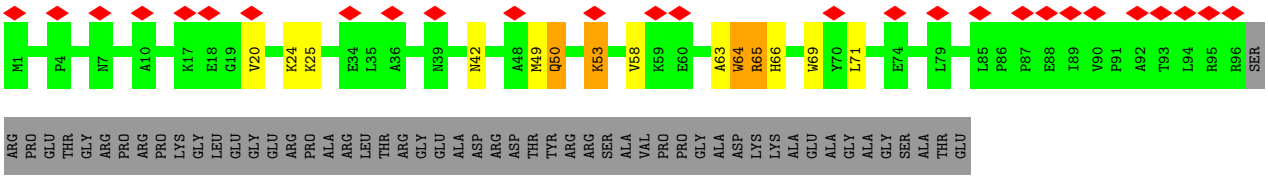
- Molecule 11: uS4

Chain K:



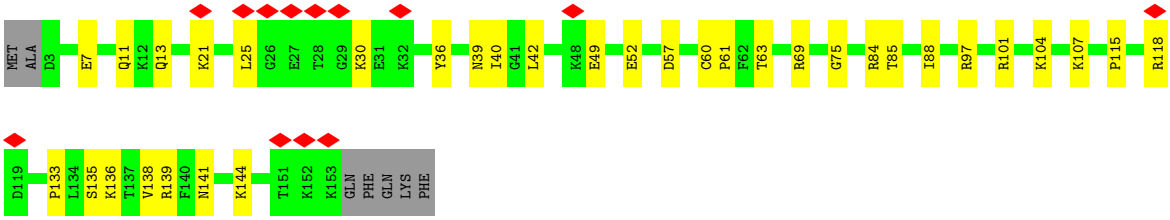
- Molecule 12: eS10

Chain L:



- Molecule 13: uS17

Chain M:

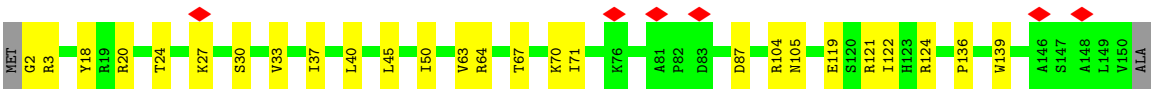


- Molecule 14: eS12

Chain N:

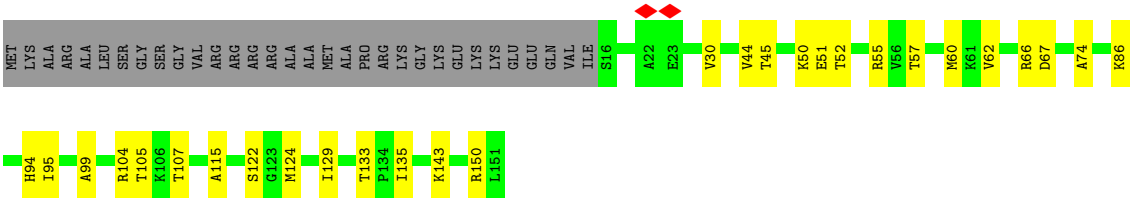
- Molecule 15: uS15

Chain O:



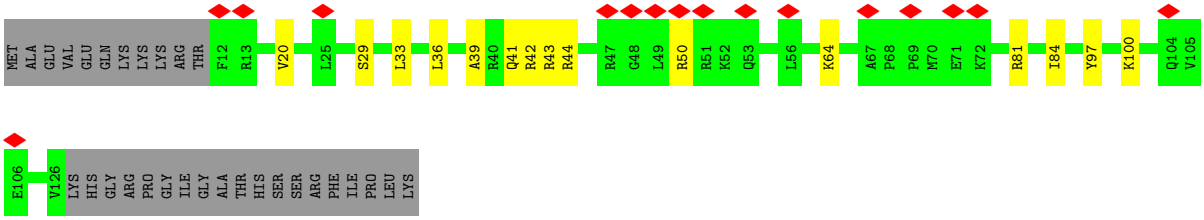
- Molecule 16: uS11

Chain P:



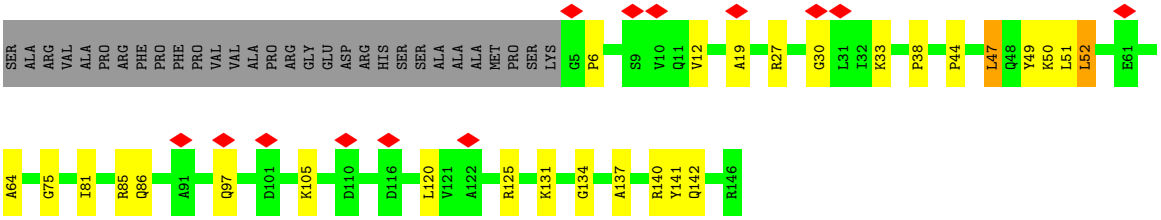
- Molecule 17: uS19

Chain Q:



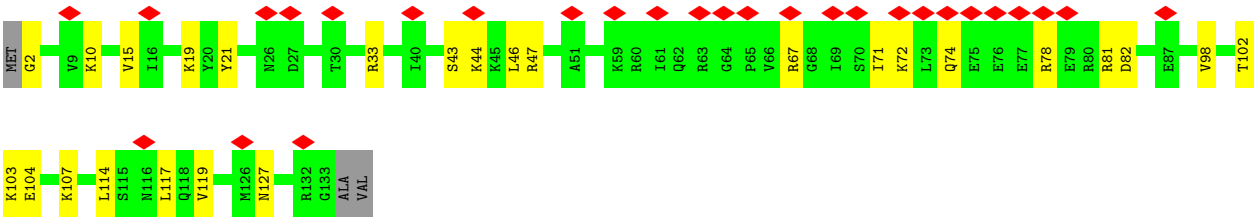
- Molecule 18: uS9

Chain R:



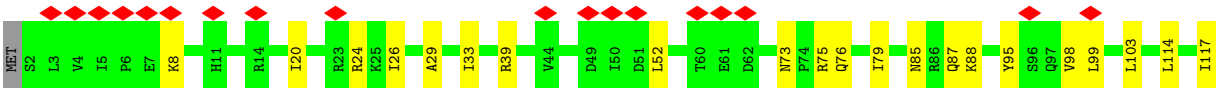
- Molecule 19: eS17

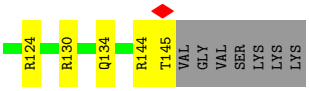
Chain S:



- Molecule 20: uS13

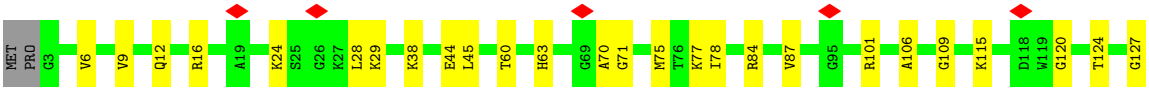
Chain T:

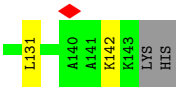




- Molecule 21: eS19

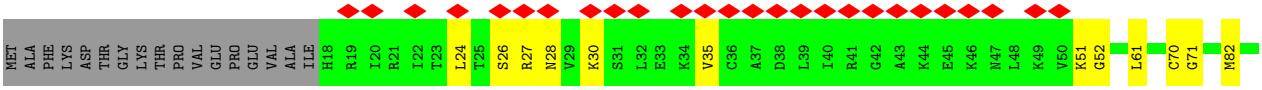
Chain U:





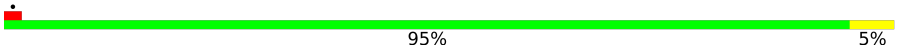
- Molecule 22: uS10

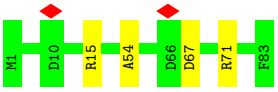
Chain V:



- Molecule 23: 40S ribosomal protein S21

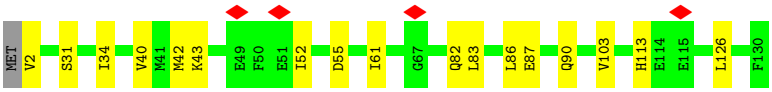
Chain W:





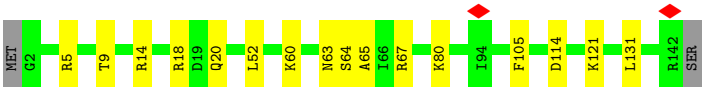
- Molecule 24: uS8

Chain X:



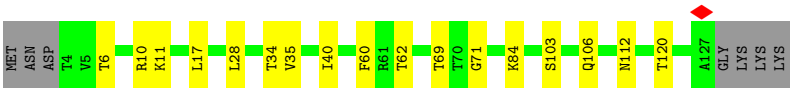
- Molecule 25: uS12

Chain Y:



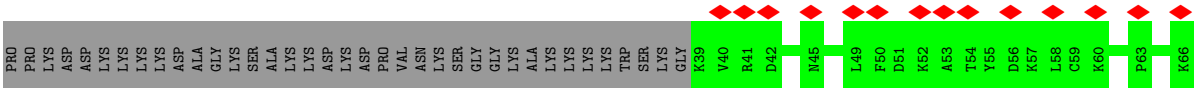
- Molecule 26: 40S ribosomal protein S24

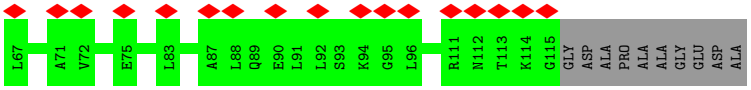
Chain Z:



• Molecule 27: eS25 (S25)

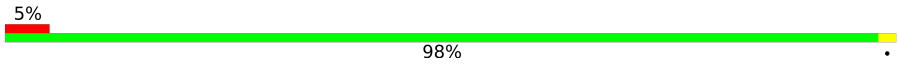
Chain a:

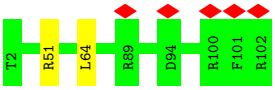




• Molecule 28: eS26 (S26)

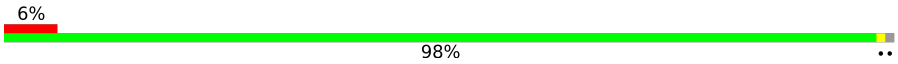
Chain b:

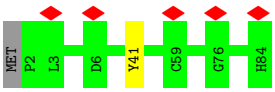




• Molecule 29: eS27

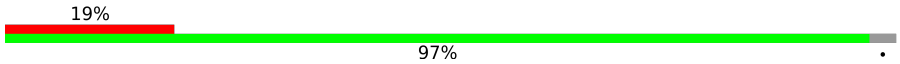
Chain c:

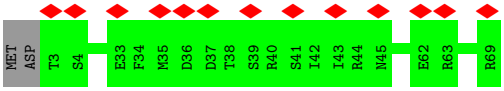




• Molecule 30: eS28

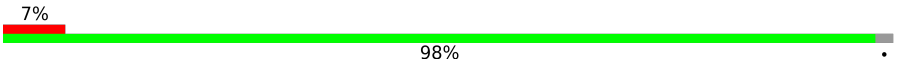
Chain d:

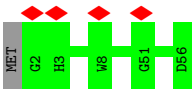




• Molecule 31: eS29

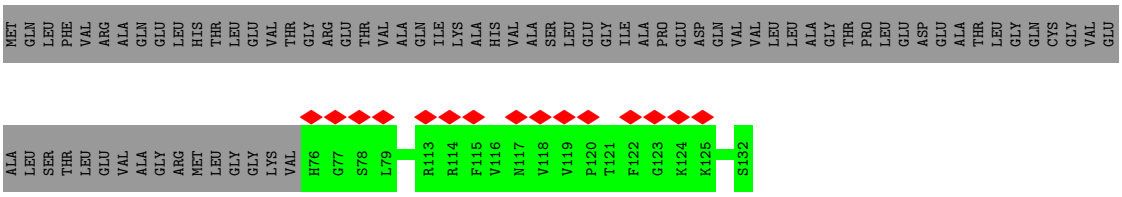
Chain e:





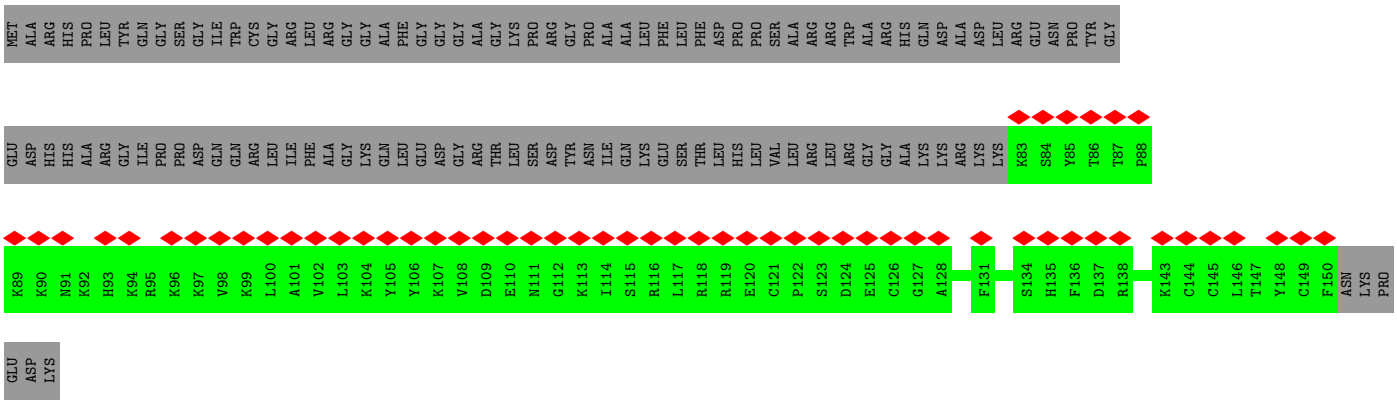
• Molecule 32: eS30

Chain f:



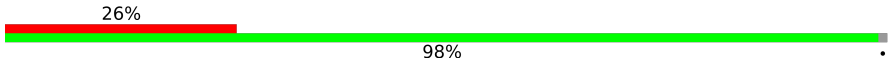
• Molecule 33: 40S ribosomal protein S27a

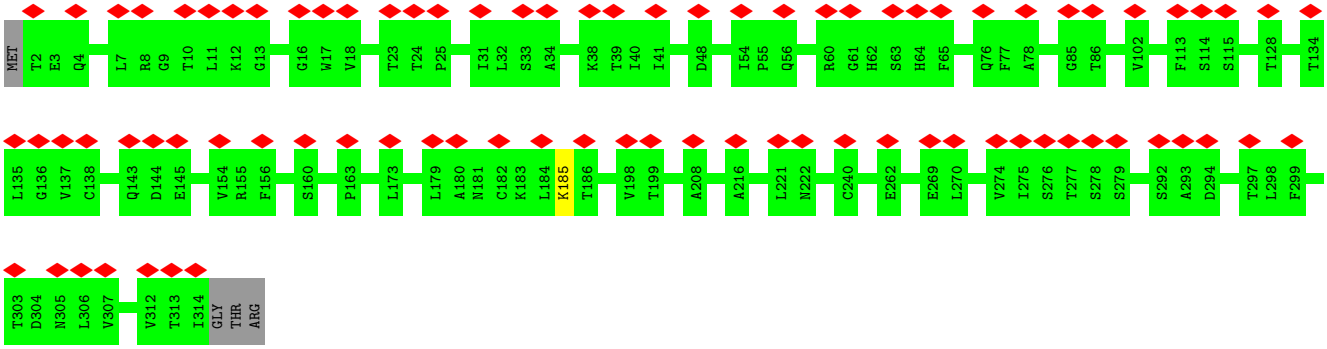
Chain g:



• Molecule 34: RACK1

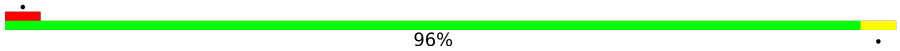
Chain h:





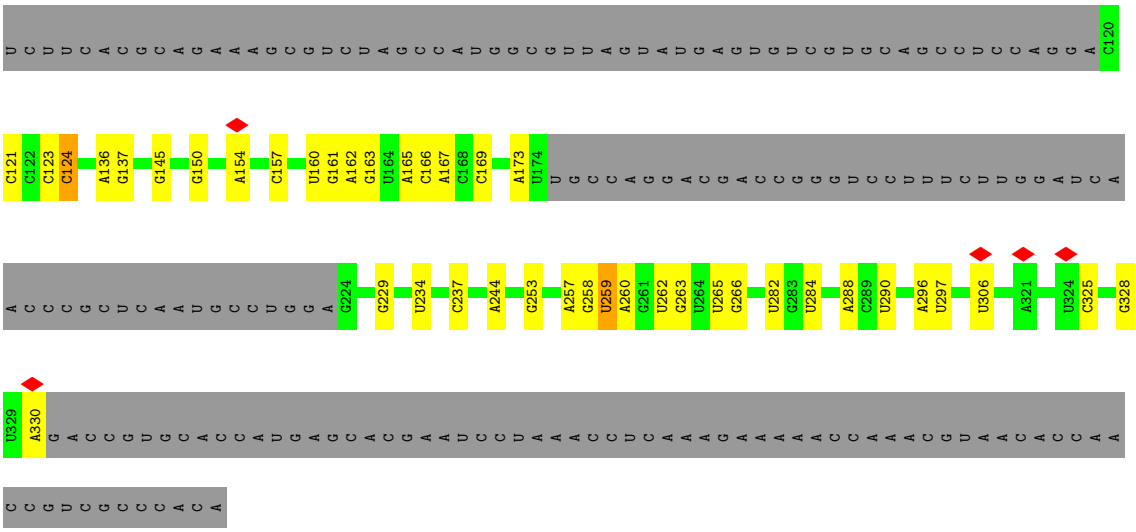
• Molecule 35: 60s ribosomal protein l41

Chain n:



• Molecule 36: HCV IRES

Chain z:


C120
C121
C122
C123
C124
A136
G137
G145
G150
A154
C157
U160
G161
A162
G163
U164
A165
C166
A167
C168
C169
A173
U174
G224
G229
U234
C237
A244
G253
A257
G258
U259
A260
G261
U262
G263
U264
U265
G266
U282
G283
U284
A288
C289
U290
A296
U297
U306
A321
U324
C325
G328
U329
A330

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48757	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	52000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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

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	2	0.29	1/40506 (0.0%)	1.03	196/63123 (0.3%)
2	B	0.27	0/1747	0.62	0/2374
3	C	0.27	0/1756	0.60	1/2350 (0.0%)
4	D	0.28	0/1753	0.65	1/2369 (0.0%)
5	E	0.29	0/1796	0.67	0/2417
6	F	0.27	0/2118	0.64	1/2849 (0.0%)
7	G	0.26	0/1531	0.62	0/2059
8	H	0.26	0/1946	0.63	1/2590 (0.0%)
9	I	0.27	0/1510	0.61	0/2022
10	J	0.27	0/1715	0.61	0/2287
11	K	0.28	0/1550	0.65	0/2069
12	L	0.30	0/834	0.69	1/1125 (0.1%)
13	M	0.29	0/1254	0.68	1/1677 (0.1%)
14	N	0.27	0/918	0.60	0/1233
15	O	0.29	0/1226	0.64	1/1649 (0.1%)
16	P	0.27	0/1029	0.63	0/1380
17	Q	0.28	0/974	0.71	0/1301
18	R	0.29	0/1146	0.68	2/1534 (0.1%)
19	S	0.32	0/1082	0.71	0/1452
20	T	0.27	0/1208	0.66	1/1618 (0.1%)
21	U	0.27	0/1115	0.63	0/1493
22	V	0.26	0/805	0.62	0/1081
23	W	0.30	0/643	0.63	0/860
24	X	0.31	0/1051	0.69	0/1406
25	Y	0.28	0/1116	0.67	1/1490 (0.1%)
26	Z	0.26	0/1028	0.60	0/1366
27	a	0.26	0/620	0.60	0/831
28	b	0.28	0/828	0.64	1/1109 (0.1%)
29	c	0.29	0/665	0.62	0/891
30	d	0.24	0/532	0.67	0/712
31	e	0.29	0/470	0.63	0/623
32	f	0.27	0/462	0.63	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	g	0.25	0/567	0.57	0/753
34	h	0.26	0/2493	0.61	0/3394
35	n	0.27	0/240	0.75	0/305
36	z	0.31	0/3871	0.99	7/6034 (0.1%)
All	All	0.28	1/84105 (0.0%)	0.88	215/122433 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
6	F	0	1
12	L	0	1
29	c	0	1
35	n	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1556	A	N9-C4	5.04	1.40	1.37

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1022	U	C2-N1-C1'	11.80	131.86	117.70
1	2	1078	C	N3-C2-O2	-10.94	114.24	121.90
1	2	1078	C	N1-C2-O2	10.79	125.37	118.90
1	2	1700	C	C6-N1-C2	-10.40	116.14	120.30
1	2	1022	U	N1-C2-O2	10.38	130.07	122.80
1	2	1022	U	N3-C2-O2	-10.15	115.10	122.20
1	2	1453	C	C2-N1-C1'	10.07	129.88	118.80
1	2	1453	C	N1-C2-O2	10.03	124.92	118.90
1	2	1700	C	N1-C2-O2	9.90	124.84	118.90
1	2	1139	C	N1-C2-O2	9.88	124.83	118.90
1	2	1752	C	N1-C2-O2	9.75	124.75	118.90
1	2	1591	C	N1-C2-O2	9.43	124.56	118.90
1	2	1700	C	N3-C2-O2	-8.89	115.68	121.90
1	2	1139	C	C2-N1-C1'	8.86	128.55	118.80
1	2	1464	C	N1-C2-O2	8.79	124.18	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	457	C	N3-C2-O2	-8.76	115.77	121.90
1	2	1303	C	N1-C2-O2	8.63	124.08	118.90
1	2	1442	U	N1-C2-O2	8.46	128.72	122.80
1	2	1063	C	N1-C2-O2	8.38	123.93	118.90
1	2	1464	C	C2-N1-C1'	8.38	128.02	118.80
1	2	1752	C	C2-N1-C1'	8.36	127.99	118.80
1	2	1442	U	N3-C2-O2	-8.30	116.39	122.20
1	2	1303	C	C2-N1-C1'	8.27	127.89	118.80
13	M	57	ASP	CB-CG-OD1	8.23	125.70	118.30
1	2	1624	U	C2-N1-C1'	8.10	127.42	117.70
1	2	1752	C	N3-C2-O2	-8.09	116.24	121.90
1	2	1520	G	C4-N9-C1'	8.02	136.93	126.50
1	2	199	C	N1-C2-O2	7.96	123.68	118.90
1	2	1139	C	N3-C2-O2	-7.82	116.43	121.90
1	2	585	C	N1-C2-O2	7.78	123.57	118.90
1	2	1022	U	C6-N1-C1'	-7.72	110.40	121.20
1	2	1700	C	C2-N1-C1'	7.67	127.23	118.80
1	2	1453	C	N3-C2-O2	-7.66	116.54	121.90
1	2	887	U	N1-C2-O2	7.61	128.13	122.80
1	2	539	C	N1-C2-O2	7.60	123.46	118.90
1	2	887	U	C2-N1-C1'	7.60	126.81	117.70
1	2	1520	G	N3-C4-N9	7.50	130.50	126.00
1	2	1464	C	N3-C2-O2	-7.34	116.76	121.90
1	2	1591	C	N3-C2-O2	-7.33	116.77	121.90
1	2	1314	U	C2-N1-C1'	7.30	126.46	117.70
1	2	1078	C	C6-N1-C2	-7.27	117.39	120.30
1	2	1442	U	C2-N1-C1'	7.27	126.42	117.70
1	2	183	G	C2-N3-C4	7.26	115.53	111.90
1	2	1591	C	C2-N1-C1'	7.26	126.79	118.80
1	2	1778	C	C5-C6-N1	7.25	124.63	121.00
1	2	195	C	C2-N1-C1'	7.17	126.69	118.80
1	2	1676	U	N1-C2-O2	7.16	127.81	122.80
18	R	52	LEU	CA-CB-CG	7.15	131.74	115.30
1	2	688	U	P-O3'-C3'	7.14	128.27	119.70
1	2	1700	C	C5-C6-N1	7.14	124.57	121.00
1	2	183	G	N3-C4-C5	-7.12	125.04	128.60
1	2	1453	C	C6-N1-C1'	-7.10	112.28	120.80
1	2	578	C	N1-C2-O2	7.08	123.15	118.90
1	2	1485	U	N1-C2-O2	7.07	127.75	122.80
1	2	118	C	N1-C2-O2	7.01	123.11	118.90
1	2	1464	C	C6-N1-C2	-7.00	117.50	120.30
36	z	124	C	N1-C2-O2	6.97	123.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1314	U	N3-C2-O2	-6.91	117.36	122.20
1	2	790	C	N1-C2-O2	6.89	123.03	118.90
1	2	1520	G	C8-N9-C1'	-6.88	118.05	127.00
1	2	887	U	N3-C2-O2	-6.85	117.40	122.20
6	F	176	ASP	CB-CG-OD2	6.84	124.46	118.30
1	2	1520	G	N3-C4-C5	-6.83	125.19	128.60
1	2	1373	C	C2-N1-C1'	6.76	126.23	118.80
1	2	1752	C	C6-N1-C2	-6.76	117.60	120.30
1	2	1063	C	N3-C2-O2	-6.76	117.17	121.90
1	2	1753	C	N3-C2-O2	-6.72	117.20	121.90
1	2	1778	C	N1-C2-O2	6.70	122.92	118.90
1	2	1303	C	N3-C2-O2	-6.70	117.21	121.90
1	2	541	U	N1-C2-O2	6.67	127.47	122.80
1	2	168	C	N1-C2-O2	6.67	122.90	118.90
1	2	1689	C	N1-C2-O2	6.66	122.90	118.90
1	2	1676	U	C2-N1-C1'	6.63	125.65	117.70
1	2	894	G	C4-N9-C1'	6.62	135.11	126.50
1	2	752	G	P-O3'-C3'	6.62	127.64	119.70
1	2	1485	U	N3-C2-O2	-6.56	117.61	122.20
8	H	68	LEU	CA-CB-CG	6.56	130.38	115.30
1	2	195	C	C6-N1-C2	-6.55	117.68	120.30
1	2	1624	U	N1-C2-O2	6.50	127.35	122.80
1	2	1057	C	C2-N1-C1'	6.49	125.94	118.80
1	2	319	C	O5'-P-OP1	6.45	118.44	110.70
1	2	1022	U	C5-C6-N1	6.44	125.92	122.70
1	2	1676	U	N3-C2-O2	-6.41	117.71	122.20
36	z	160	U	N3-C2-O2	-6.40	117.72	122.20
1	2	199	C	N3-C2-O2	-6.39	117.43	121.90
1	2	553	U	P-O3'-C3'	6.36	127.33	119.70
1	2	437	G	C5-C6-O6	6.35	132.41	128.60
1	2	1063	C	C6-N1-C2	-6.34	117.76	120.30
1	2	1389	C	C6-N1-C2	-6.30	117.78	120.30
18	R	47	LEU	CA-CB-CG	6.26	129.71	115.30
1	2	853	C	C2-N1-C1'	6.24	125.66	118.80
1	2	1314	U	N1-C2-O2	6.24	127.17	122.80
20	T	8	LYS	CA-CB-CG	6.21	127.07	113.40
1	2	541	U	C2-N1-C1'	6.20	125.13	117.70
1	2	570	C	N1-C2-O2	6.20	122.62	118.90
1	2	585	C	N3-C2-O2	-6.19	117.56	121.90
4	D	73	MET	CB-CG-SD	6.17	130.91	112.40
1	2	1556	A	C2-N3-C4	6.17	113.68	110.60
1	2	457	C	C6-N1-C2	-6.16	117.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1453	C	C6-N1-C2	-6.15	117.84	120.30
1	2	578	C	N3-C2-O2	-6.15	117.60	121.90
1	2	199	C	C2-N1-C1'	6.14	125.55	118.80
1	2	1019	C	N1-C2-O2	6.14	122.58	118.90
1	2	1063	C	C2-N1-C1'	6.12	125.54	118.80
15	O	45	LEU	C-N-CA	6.12	136.99	121.70
1	2	1139	C	C6-N1-C1'	-6.11	113.47	120.80
1	2	322	C	N1-C2-O2	6.10	122.56	118.90
1	2	1624	U	N3-C2-O2	-6.09	117.94	122.20
1	2	1095	C	C6-N1-C2	-6.07	117.87	120.30
1	2	541	U	N3-C2-O2	-6.04	117.97	122.20
1	2	1373	C	C5-C6-N1	6.01	124.00	121.00
1	2	293	C	N1-C2-O2	6.00	122.50	118.90
1	2	585	C	C2-N1-C1'	6.00	125.40	118.80
1	2	1019	C	N3-C2-O2	-5.97	117.72	121.90
12	L	65	ARG	CA-CB-CG	5.96	126.51	113.40
1	2	539	C	C2-N1-C1'	5.96	125.36	118.80
1	2	627	U	P-O3'-C3'	5.94	126.83	119.70
1	2	437	G	N1-C6-O6	-5.92	116.35	119.90
1	2	1591	C	C6-N1-C2	-5.90	117.94	120.30
1	2	1389	C	N3-C2-O2	-5.86	117.80	121.90
1	2	974	C	N1-C2-O2	5.85	122.41	118.90
1	2	539	C	N3-C2-O2	-5.85	117.81	121.90
1	2	1139	C	C6-N1-C2	-5.84	117.96	120.30
1	2	1373	C	N1-C2-O2	5.82	122.39	118.90
1	2	1303	C	C6-N1-C1'	-5.80	113.84	120.80
1	2	183	G	C4-N9-C1'	5.79	134.03	126.50
1	2	531	A	C2-N3-C4	5.79	113.49	110.60
1	2	659	G	C4-N9-C1'	5.78	134.02	126.50
1	2	1518	C	C2-N1-C1'	5.76	125.14	118.80
1	2	356	C	C2-N1-C1'	5.75	125.12	118.80
1	2	1453	C	C5-C6-N1	5.70	123.85	121.00
3	C	188	LEU	CA-CB-CG	5.69	128.39	115.30
1	2	1535	U	N1-C2-O2	5.68	126.78	122.80
36	z	124	C	N3-C2-O2	-5.68	117.92	121.90
1	2	195	C	N1-C2-O2	5.67	122.30	118.90
1	2	1396	A	O5'-P-OP1	-5.67	100.60	105.70
1	2	1022	U	C6-N1-C2	-5.64	117.61	121.00
1	2	13	C	C2-N1-C1'	5.63	125.00	118.80
1	2	894	G	N3-C4-N9	5.62	129.37	126.00
1	2	118	C	N3-C2-O2	-5.60	117.98	121.90
1	2	1590	C	N1-C2-O2	5.60	122.26	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	z	160	U	N1-C2-O2	5.60	126.72	122.80
1	2	1754	G	C6-C5-N7	-5.59	127.05	130.40
1	2	894	G	C8-N9-C1'	-5.57	119.75	127.00
1	2	1754	G	N7-C8-N9	5.56	115.88	113.10
1	2	1440	C	N3-C2-O2	-5.55	118.01	121.90
1	2	1443	C	N1-C2-O2	5.55	122.23	118.90
1	2	1595	U	N1-C2-O2	5.55	126.68	122.80
36	z	124	C	C2-N1-C1'	5.55	124.90	118.80
1	2	1754	G	C4-C5-N7	5.54	113.02	110.80
1	2	1389	C	N1-C2-O2	5.54	122.22	118.90
25	Y	131	LEU	CA-CB-CG	5.52	128.00	115.30
1	2	445	A	P-O3'-C3'	5.51	126.31	119.70
1	2	687	C	N1-C2-O2	5.50	122.20	118.90
1	2	579	C	N1-C2-O2	5.50	122.20	118.90
36	z	259	U	N1-C2-O2	5.49	126.64	122.80
1	2	894	G	N3-C4-C5	-5.47	125.86	128.60
1	2	358	C	C2-N1-C1'	5.47	124.81	118.80
1	2	887	U	C5-C6-N1	5.45	125.42	122.70
1	2	1624	U	O4'-C1'-N1	5.44	112.55	108.20
1	2	1752	C	C6-N1-C1'	-5.42	114.29	120.80
1	2	790	C	C5-C6-N1	5.42	123.71	121.00
1	2	1464	C	C5-C6-N1	5.42	123.71	121.00
1	2	1689	C	N3-C2-O2	-5.41	118.11	121.90
1	2	1078	C	C2-N1-C1'	5.40	124.75	118.80
1	2	571	U	N3-C2-O2	-5.40	118.42	122.20
1	2	356	C	N1-C2-O2	5.39	122.13	118.90
1	2	1464	C	C6-N1-C1'	-5.38	114.34	120.80
1	2	1416	C	C5-C6-N1	5.37	123.68	121.00
1	2	1389	C	C2-N1-C1'	5.36	124.70	118.80
1	2	1591	C	C5-C6-N1	5.36	123.68	121.00
1	2	183	G	N3-C4-N9	5.36	129.22	126.00
1	2	1373	C	C6-N1-C2	-5.36	118.16	120.30
1	2	1742	C	N1-C2-O2	5.36	122.11	118.90
1	2	168	C	N3-C2-O2	-5.36	118.15	121.90
1	2	1206	C	N1-C2-O2	5.36	122.11	118.90
1	2	142	C	N1-C2-O2	5.35	122.11	118.90
1	2	1443	C	C2-N1-C1'	5.34	124.68	118.80
1	2	358	C	C6-N1-C2	-5.33	118.17	120.30
1	2	1535	U	C2-N1-C1'	5.32	124.09	117.70
36	z	124	C	C6-N1-C2	-5.30	118.18	120.30
1	2	1624	U	C6-N1-C1'	-5.30	113.78	121.20
1	2	571	U	N1-C2-O2	5.29	126.50	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1753	C	N1-C2-O2	5.28	122.07	118.90
1	2	194	C	C2-N1-C1'	5.28	124.61	118.80
1	2	973	C	C6-N1-C2	-5.28	118.19	120.30
1	2	151	C	C2-N1-C1'	5.27	124.60	118.80
1	2	823	U	C2-N1-C1'	5.27	124.02	117.70
1	2	199	C	C6-N1-C2	-5.22	118.21	120.30
1	2	168	C	C2-N1-C1'	5.19	124.51	118.80
1	2	659	G	N3-C4-N9	5.18	129.11	126.00
1	2	1442	U	C5-C6-N1	5.18	125.29	122.70
1	2	1079	C	N1-C2-O2	5.17	122.00	118.90
1	2	853	C	N1-C2-O2	5.16	122.00	118.90
1	2	295	C	N1-C2-O2	5.16	121.99	118.90
1	2	1865	C	N1-C2-O2	5.14	121.99	118.90
1	2	1063	C	C5-C6-N1	5.14	123.57	121.00
1	2	1689	C	C6-N1-C2	-5.13	118.25	120.30
1	2	4	C	N1-C2-O2	5.12	121.97	118.90
1	2	151	C	N1-C2-O2	5.11	121.97	118.90
1	2	341	C	N1-C2-O2	5.10	121.96	118.90
1	2	1595	U	N3-C2-O2	-5.10	118.63	122.20
1	2	659	G	N3-C4-C5	-5.09	126.05	128.60
28	b	64	LEU	CA-CB-CG	5.09	127.00	115.30
1	2	1303	C	C6-N1-C2	-5.08	118.27	120.30
1	2	1590	C	C6-N1-C2	-5.08	118.27	120.30
1	2	1689	C	C2-N1-C1'	5.08	124.39	118.80
1	2	570	C	N3-C2-O2	-5.07	118.35	121.90
1	2	585	C	C6-N1-C2	-5.07	118.27	120.30
1	2	939	U	N1-C2-O2	5.07	126.35	122.80
1	2	852	G	O4'-C1'-N9	5.06	112.25	108.20
1	2	1485	U	C2-N1-C1'	5.02	123.73	117.70
1	2	1518	C	N1-C2-O2	5.02	121.91	118.90
1	2	1057	C	N1-C2-O2	5.01	121.91	118.90
1	2	183	G	C8-N9-C4	-5.00	104.40	106.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	191	ASP	Peptide
6	F	18	TRP	Peptide
12	L	64	TRP	Peptide
29	c	41	TYR	Peptide
35	n	1	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	36227	0	18299	279	0
2	B	1710	0	1708	23	0
3	C	1729	0	1803	24	0
4	D	1716	0	1806	17	0
5	E	1768	0	1866	18	0
6	F	2076	0	2177	29	0
7	G	1509	0	1563	21	0
8	H	1923	0	2089	18	0
9	I	1488	0	1582	16	0
10	J	1686	0	1772	13	0
11	K	1525	0	1640	19	0
12	L	810	0	836	10	0
13	M	1233	0	1310	21	0
14	N	908	0	939	12	0
15	O	1202	0	1289	17	0
16	P	1016	0	1039	19	0
17	Q	956	0	1002	9	0
18	R	1128	0	1195	22	0
19	S	1068	0	1121	18	0
20	T	1190	0	1249	17	0
21	U	1097	0	1130	19	0
22	V	795	0	862	13	0
23	W	636	0	637	2	0
24	X	1034	0	1080	13	0
25	Y	1098	0	1167	11	0
26	Z	1011	0	1083	11	0
27	a	614	0	678	0	0
28	b	814	0	863	0	0
29	c	651	0	672	0	0
30	d	530	0	561	0	0
31	e	459	0	452	0	0
32	f	457	0	502	0	0
33	g	555	0	563	0	0
34	h	2436	0	2393	0	0
35	n	239	0	289	0	0
36	z	3465	0	1751	0	0
37	b	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	g	1	0	0	0	0
All	All	78761	0	60968	568	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 5.

All (568) 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)
1:2:1332:A:H62	1:2:1493:C:N4	1.61	0.99
1:2:1472:C:H42	1:2:1476:A:H62	1.09	0.97
1:2:1656:G:H1	1:2:1668:U:H3	1.10	0.95
1:2:318:A:C2	1:2:333:G:N1	2.37	0.92
1:2:1332:A:N6	1:2:1493:C:H42	1.67	0.91
1:2:1286:G:H21	1:2:1313:A:N6	1.67	0.91
1:2:1286:G:N2	1:2:1313:A:H62	1.68	0.91
1:2:16:G:H21	1:2:1195:A:H62	1.22	0.84
1:2:1652:G:H1	1:2:1672:U:H3	1.22	0.83
1:2:1224:G:H1	1:2:1642:U:H3	1.23	0.81
1:2:318:A:N1	1:2:333:G:C6	2.49	0.80
1:2:934:G:H1	1:2:1008:A:H2	1.26	0.79
1:2:1472:C:N4	1:2:1476:A:H62	1.80	0.78
1:2:1332:A:H62	1:2:1493:C:H42	0.85	0.78
1:2:1472:C:H42	1:2:1476:A:N6	1.81	0.78
1:2:1368:U:HO2'	19:S:2:GLY:N	1.82	0.77
1:2:1726:G:H1	1:2:1808:U:H3	1.36	0.73
1:2:1286:G:H21	1:2:1313:A:H62	0.84	0.72
1:2:1665:G:H22	21:U:87:VAL:HG22	1.56	0.71
19:S:44:LYS:HA	19:S:47:ARG:HD3	1.73	0.70
6:F:206:ASP:H	6:F:222:LEU:HD23	1.57	0.69
1:2:16:G:N2	1:2:1195:A:H62	1.90	0.68
1:2:318:A:C2	1:2:333:G:C6	2.82	0.67
1:2:1629:C:H5"	20:T:39:ARG:HG2	1.76	0.67
1:2:1091:C:HO2'	24:X:2:VAL:N	1.92	0.67
1:2:934:G:N1	1:2:1008:A:C2	2.60	0.66
1:2:399:C:N3	13:M:104:LYS:NZ	2.44	0.66
1:2:1210:G:H1	1:2:1689:C:H42	1.45	0.65
1:2:359:U:H3	1:2:403:G:H1	1.45	0.64
2:B:198:MET:HG2	2:B:200:ASP:H	1.61	0.64
1:2:116:U:H3	1:2:347:G:H1	1.46	0.63
1:2:1284:A:N6	14:N:91:LEU:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:318:A:C2	1:2:333:G:C2	2.87	0.62
1:2:1527:C:H5"	18:R:142:GLN:HB2	1.80	0.62
1:2:1401:A:H4'	22:V:52:GLY:HA3	1.82	0.62
1:2:1397:U:H3	18:R:12:VAL:HA	1.65	0.62
1:2:1679:A:H2'	7:G:60:ARG:HD3	1.83	0.61
1:2:1649:U:H3	1:2:1675:A:N6	1.99	0.61
4:D:128:VAL:HG11	4:D:155:ILE:HG22	1.83	0.61
7:G:27:ASP:O	7:G:110:GLN:NE2	2.33	0.60
4:D:270:THR:HA	4:D:273:LEU:HG	1.84	0.60
22:V:70:CYS:SG	22:V:71:GLY:N	2.74	0.60
20:T:20:ILE:HG13	20:T:33:ILE:HG12	1.84	0.60
4:D:123:ARG:NH1	4:D:143:CYS:SG	2.75	0.60
3:C:83:LYS:HB2	3:C:104:ASP:HB3	1.83	0.60
24:X:86:LEU:HD21	24:X:113:HIS:HB2	1.83	0.59
1:2:934:G:O6	1:2:1008:A:N1	2.36	0.59
1:2:1267:C:O2	17:Q:100:LYS:NZ	2.35	0.59
1:2:1657:G:H1	1:2:1667:U:H3	1.51	0.59
1:2:560:A:H5'	11:K:174:LYS:HB2	1.85	0.58
1:2:852:G:H8	13:M:97:ARG:HH22	1.50	0.58
9:I:40:LEU:HG	9:I:43:LEU:HD12	1.84	0.58
1:2:618:C:H41	25:Y:67:ARG:HH21	1.52	0.58
1:2:934:G:N1	1:2:1008:A:H2	1.99	0.58
1:2:1183:A:H2'	1:2:1184:G:H8	1.69	0.58
11:K:136:ARG:HD2	11:K:139:LYS:HA	1.86	0.58
15:O:64:ARG:HD3	15:O:70:LYS:HE2	1.86	0.58
1:2:976:G:H21	16:P:50:LYS:HE3	1.69	0.57
1:2:1649:U:O4	1:2:1675:A:N7	2.38	0.57
7:G:42:LYS:HG2	7:G:43:GLU:HG2	1.85	0.57
1:2:681:U:H4'	25:Y:9:THR:HB	1.86	0.57
16:P:74:ALA:HB1	16:P:115:ALA:HB2	1.85	0.57
1:2:1566:G:N7	21:U:101:ARG:NH2	2.52	0.57
1:2:153:G:N3	8:H:13:GLN:NE2	2.53	0.57
3:C:85:LYS:HB3	3:C:101:HIS:HB3	1.87	0.57
6:F:18:TRP:NE1	6:F:41:CYS:O	2.35	0.57
16:P:30:VAL:HG12	16:P:94:HIS:HB2	1.86	0.57
1:2:1649:U:N3	1:2:1675:A:N6	2.51	0.57
2:B:85:ARG:NH2	2:B:201:LEU:O	2.38	0.57
7:G:179:ASN:HD21	7:G:186:ASN:HB2	1.69	0.57
26:Z:10:ARG:HG2	26:Z:11:LYS:HG3	1.87	0.57
1:2:804:U:OP1	24:X:82:GLN:NE2	2.38	0.56
6:F:191:ARG:HH21	6:F:245:ARG:HE	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ASN:OD1	19:S:127:ASN:ND2	2.38	0.56
1:2:986:G:OP2	1:2:988:C:N4	2.39	0.56
1:2:383:G:H21	13:M:133:PRO:HG3	1.71	0.56
1:2:1579:A:O2'	1:2:1582:C:N4	2.39	0.56
1:2:953:C:H5"	3:C:24:PRO:HG2	1.88	0.56
1:2:1259:A:N6	1:2:1519:U:O5'	2.39	0.56
1:2:1277:C:H2'	1:2:1278:A:H8	1.71	0.56
1:2:1463:U:OP1	19:S:67:ARG:NH2	2.39	0.56
11:K:169:ARG:HG2	11:K:175:ARG:HH22	1.69	0.56
1:2:511:U:O2'	1:2:576:A:N6	2.38	0.55
1:2:817:G:H21	1:2:847:A:H62	1.52	0.55
9:I:17:ASP:OD1	9:I:18:GLU:N	2.38	0.55
18:R:6:PRO:O	18:R:27:ARG:NH2	2.39	0.55
1:2:973:C:O2	16:P:55:ARG:NH2	2.39	0.55
5:E:37:VAL:HG12	5:E:50:ILE:HA	1.88	0.55
13:M:75:GLY:HA3	13:M:88:ILE:HD12	1.87	0.55
9:I:117:PRO:HG2	9:I:120:ARG:HD3	1.87	0.55
25:Y:63:ASN:ND2	25:Y:114:ASP:OD2	2.40	0.55
6:F:130:PHE:HB3	6:F:138:HIS:HB2	1.88	0.55
16:P:62:VAL:HG11	16:P:67:ASP:HB3	1.89	0.55
9:I:143:ARG:HB2	9:I:155:LYS:HG3	1.88	0.55
13:M:60:CYS:HG	13:M:63:THR:HG1	1.53	0.54
6:F:47:PHE:O	6:F:51:ARG:HB2	2.06	0.54
22:V:51:LYS:HB2	22:V:90:ASP:HB3	1.88	0.54
24:X:87:GLU:OE1	24:X:90:GLN:NE2	2.36	0.54
1:2:1275:G:O4'	1:2:1506:A:N6	2.41	0.54
9:I:154:ILE:HB	9:I:185:VAL:HG22	1.88	0.54
1:2:919:A:OP2	15:O:20:ARG:NH2	2.40	0.54
1:2:1344:A:N1	1:2:1385:G:O2'	2.39	0.54
1:2:1786:U:H2'	1:2:1787:G:H8	1.73	0.54
1:2:677:G:OP1	15:O:124:ARG:NH2	2.39	0.54
1:2:1637:A:H61	7:G:81:ARG:HH12	1.55	0.54
5:E:23:GLU:OE1	12:L:64:TRP:NE1	2.38	0.54
9:I:144:ILE:HG23	24:X:52:ILE:HG13	1.90	0.54
1:2:959:G:OP1	16:P:104:ARG:NH2	2.41	0.54
1:2:1651:A:N3	7:G:83:ASN:ND2	2.56	0.54
18:R:131:LYS:HB2	18:R:140:ARG:HH22	1.73	0.54
3:C:47:THR:OG1	3:C:65:ARG:NH2	2.41	0.54
5:E:107:TYR:HA	5:E:110:LEU:HD23	1.90	0.54
16:P:86:LYS:NZ	16:P:124:MET:SD	2.80	0.54
1:2:318:A:N1	1:2:333:G:O6	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1584:G:OP1	21:U:77:LYS:NZ	2.41	0.54
1:2:694:G:N2	1:2:733:C:O2	2.41	0.53
6:F:100:ARG:HH12	6:F:122:LYS:HA	1.74	0.53
1:2:877:C:H42	1:2:909:G:H1	1.57	0.53
24:X:40:VAL:HA	24:X:43:LYS:HG2	1.90	0.53
18:R:86:GLN:NE2	18:R:120:LEU:O	2.38	0.53
1:2:1598:G:N2	7:G:166:ILE:O	2.40	0.53
1:2:1615:U:OP2	17:Q:43:ARG:NH2	2.41	0.53
3:C:28:LYS:HD2	3:C:48:LEU:HD23	1.89	0.53
15:O:136:PRO:HG2	15:O:139:TRP:HB2	1.90	0.53
1:2:643:A:OP1	11:K:41:ARG:NH2	2.42	0.53
1:2:171:A:OP2	8:H:137:ARG:NH2	2.42	0.53
1:2:1461:G:H22	1:2:1464:C:H5"	1.74	0.53
1:2:1268:C:H42	1:2:1514:G:H1	1.55	0.53
18:R:47:LEU:HB2	18:R:50:LYS:HB3	1.90	0.53
1:2:53:C:OP1	26:Z:112:ASN:ND2	2.38	0.53
1:2:988:C:OP1	3:C:116:LYS:NZ	2.42	0.53
21:U:75:MET:HA	21:U:78:ILE:HG12	1.90	0.53
1:2:60:A:HO2'	1:2:316:G:HO2'	1.50	0.52
1:2:1592:C:H4'	18:R:44:PRO:HB3	1.92	0.52
2:B:74:VAL:HG22	2:B:121:LEU:HB2	1.92	0.52
21:U:60:THR:HG23	21:U:75:MET:HG2	1.91	0.52
1:2:498:C:H42	1:2:504:G:H1	1.56	0.52
1:2:1566:G:O2'	1:2:1568:C:N4	2.43	0.52
3:C:170:GLU:HA	3:C:173:THR:HG22	1.92	0.52
4:D:113:GLN:HE21	4:D:122:THR:HG22	1.74	0.52
10:J:81:VAL:HG22	10:J:102:VAL:HG12	1.91	0.52
21:U:12:GLN:O	21:U:16:ARG:NH1	2.42	0.52
1:2:1694:U:O2'	1:2:1833:C:O2'	2.28	0.52
2:B:77:ILE:HG21	2:B:133:PRO:HG2	1.92	0.52
11:K:42:GLU:OE1	11:K:109:ARG:NH2	2.43	0.52
1:2:1092:G:OP1	15:O:2:GLY:N	2.43	0.52
1:2:1719:A:N6	1:2:1814:G:O2'	2.43	0.52
16:P:57:THR:H	16:P:60:MET:HG3	1.75	0.52
17:Q:20:VAL:HG21	17:Q:36:LEU:HD21	1.91	0.52
17:Q:81:ARG:NH2	17:Q:97:TYR:O	2.43	0.52
19:S:43:SER:OG	19:S:44:LYS:N	2.43	0.52
1:2:1374:C:O2'	1:2:1464:C:O2	2.27	0.52
25:Y:52:LEU:HD11	25:Y:80:LYS:HE3	1.91	0.52
14:N:23:LYS:NZ	14:N:88:TRP:O	2.43	0.51
2:B:8:LEU:HD23	2:B:191:ARG:HH22	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:PRO:HA	2:B:210:ILE:HG12	1.92	0.51
6:F:122:LYS:NZ	6:F:124:CYS:SG	2.84	0.51
1:2:420:G:O2'	1:2:660:C:N3	2.44	0.51
10:J:81:VAL:O	10:J:94:LYS:NZ	2.43	0.51
1:2:433:A:OP1	10:J:25:ARG:NH2	2.43	0.51
1:2:457:C:H2'	1:2:458:A:H8	1.74	0.51
1:2:600:G:H2'	1:2:601:G:H8	1.75	0.51
1:2:65:C:OP1	8:H:136:LYS:NZ	2.43	0.51
14:N:32:ALA:HB1	14:N:37:GLU:HG2	1.93	0.51
1:2:360:A:N6	1:2:400:C:O2	2.43	0.51
1:2:398:A:H5"	1:2:400:C:H5'	1.92	0.51
1:2:21:U:O2	11:K:17:ARG:NH2	2.44	0.51
1:2:563:G:H2'	1:2:564:A:H8	1.75	0.51
1:2:1337:C:H2'	1:2:1338:G:H8	1.76	0.51
1:2:1601:A:H61	1:2:1636:G:H5'	1.76	0.51
16:P:105:THR:HG22	16:P:107:THR:H	1.74	0.51
1:2:1533:A:OP2	7:G:164:ARG:NH1	2.44	0.51
1:2:1609:C:OP1	20:T:130:ARG:NH1	2.41	0.51
1:2:1653:U:O2	1:2:1671:G:N2	2.37	0.51
3:C:88:THR:HG22	3:C:98:THR:HG22	1.93	0.51
18:R:49:TYR:HA	18:R:52:LEU:HB3	1.93	0.51
1:2:1722:G:O6	1:2:1812:U:O2	2.28	0.51
2:B:89:LYS:NZ	19:S:82:ASP:O	2.36	0.51
21:U:124:THR:HG23	21:U:127:GLY:H	1.76	0.51
1:2:309:G:OP2	10:J:53:LYS:NZ	2.42	0.50
1:2:830:A:OP2	1:2:846:G:N2	2.45	0.50
1:2:28:U:H2'	1:2:29:G:H8	1.76	0.50
1:2:490:C:O2'	1:2:574:A:N1	2.43	0.50
1:2:1156:U:O4	4:D:194:ARG:NH1	2.43	0.50
1:2:1617:G:N1	1:2:1620:A:OP2	2.44	0.50
1:2:1047:C:H5"	16:P:143:LYS:HD2	1.93	0.50
1:2:1497:G:N7	12:L:25:LYS:NZ	2.58	0.50
2:B:163:CYS:SG	2:B:164:ASN:N	2.84	0.50
7:G:55:ARG:HH22	18:R:125:ARG:HD3	1.77	0.50
15:O:30:SER:HB3	15:O:67:THR:HG22	1.93	0.50
1:2:434:G:H5"	10:J:23:LYS:HE3	1.94	0.50
2:B:36:GLN:O	2:B:53:ARG:NH1	2.45	0.50
1:2:476:A:N3	1:2:488:U:O2'	2.40	0.50
1:2:1121:G:N2	3:C:202:GLN:O	2.43	0.50
1:2:1612:G:H5"	20:T:88:LYS:HD3	1.92	0.50
6:F:79:ASP:HB3	6:F:82:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:95:ILE:HB	16:P:129:ILE:HA	1.94	0.50
19:S:43:SER:HB3	19:S:46:LEU:HD13	1.94	0.50
1:2:925:G:OP1	15:O:121:ARG:NH1	2.44	0.50
1:2:1448:A:OP1	22:V:30:LYS:NZ	2.43	0.50
3:C:182:LYS:O	3:C:186:ASN:ND2	2.45	0.50
1:2:94:G:OP1	6:F:6:LYS:NZ	2.41	0.50
1:2:1179:G:N2	1:2:1182:A:OP2	2.45	0.50
1:2:1649:U:C2	1:2:1675:A:N6	2.80	0.49
19:S:21:TYR:HD2	19:S:72:LYS:HB3	1.76	0.49
1:2:16:G:H21	1:2:1195:A:N6	2.01	0.49
1:2:525:A:H2	1:2:561:A:H61	1.61	0.49
1:2:1172:U:H2'	1:2:1173:A:H8	1.76	0.49
1:2:1486:A:O2'	4:D:118:ALA:O	2.30	0.49
20:T:26:ILE:HD11	20:T:52:LEU:HA	1.94	0.49
21:U:44:GLU:HG2	21:U:45:LEU:HD12	1.93	0.49
1:2:943:U:O2'	16:P:135:ILE:O	2.30	0.49
6:F:187:ALA:O	6:F:245:ARG:NH2	2.44	0.49
1:2:1130:G:N2	1:2:1130:G:OP2	2.45	0.49
1:2:1220:A:H4'	7:G:145:ARG:HH22	1.77	0.49
1:2:1249:C:H5"	1:2:1250:A:H2'	1.94	0.49
10:J:157:LYS:O	13:M:21:LYS:NZ	2.45	0.49
20:T:144:ARG:HG2	20:T:145:THR:HG23	1.94	0.49
6:F:115:THR:HG23	6:F:118:GLU:H	1.77	0.49
15:O:63:VAL:HG21	15:O:71:ILE:HD11	1.94	0.49
1:2:1386:A:H3'	1:2:1387:G:H8	1.78	0.49
3:C:37:ALA:HA	3:C:42:ARG:HH12	1.78	0.49
3:C:191:ASP:O	3:C:195:LYS:N	2.43	0.49
9:I:61:ILE:HG23	9:I:95:ILE:HD13	1.93	0.49
19:S:98:VAL:HG13	19:S:102:THR:HB	1.94	0.49
1:2:975:G:N2	16:P:50:LYS:O	2.44	0.49
1:2:1649:U:H3	1:2:1675:A:H62	1.53	0.49
5:E:177:LEU:HD23	5:E:182:LEU:HD13	1.94	0.49
9:I:44:ASN:O	9:I:68:GLN:NE2	2.38	0.49
15:O:40:LEU:HB3	15:O:50:ILE:HD12	1.94	0.49
1:2:1551:U:H5"	1:2:1578:U:H3	1.78	0.49
7:G:135:ARG:O	7:G:137:GLN:NE2	2.46	0.49
14:N:31:LEU:HA	14:N:111:VAL:HA	1.94	0.49
1:2:1007:C:O2'	15:O:104:ARG:NH2	2.42	0.48
1:2:1139:C:H41	1:2:1149:A:H62	1.60	0.48
7:G:129:GLY:HA3	7:G:135:ARG:HH22	1.78	0.48
22:V:107:GLU:HG3	22:V:109:GLY:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:51:LEU:HD21	18:R:81:ILE:HD12	1.95	0.48
3:C:198:GLU:O	3:C:202:GLN:NE2	2.46	0.48
17:Q:41:GLN:HB3	17:Q:84:ILE:HD13	1.95	0.48
18:R:19:ALA:HB2	18:R:75:GLY:HA3	1.95	0.48
1:2:913:A:N6	9:I:119:SER:O	2.44	0.48
2:B:184:ARG:HH21	2:B:191:ARG:HE	1.62	0.48
6:F:64:ILE:HD12	26:Z:17:LEU:HG	1.96	0.48
1:2:1378:A:OP1	2:B:132:GLN:NE2	2.46	0.48
9:I:69:LEU:HA	9:I:72:PHE:HB2	1.95	0.48
19:S:103:LYS:HD3	19:S:119:VAL:HG11	1.94	0.48
20:T:130:ARG:HG2	20:T:134:GLN:HG2	1.96	0.48
1:2:311:C:H5"	1:2:312:G:H5"	1.95	0.48
1:2:1570:G:H2'	1:2:1571:G:H8	1.79	0.48
13:M:135:SER:OG	13:M:136:LYS:N	2.47	0.48
1:2:645:C:H2'	1:2:646:G:H8	1.79	0.48
24:X:31:SER:HB3	24:X:34:ILE:HG13	1.94	0.48
5:E:115:VAL:O	5:E:119:CYS:HB2	2.13	0.48
5:E:175:VAL:HG21	5:E:184:ILE:HD12	1.95	0.48
6:F:171:ASP:N	6:F:171:ASP:OD1	2.47	0.48
2:B:42:LYS:HE3	2:B:46:ILE:HB	1.95	0.48
1:2:373:G:H4'	13:M:85:THR:HG21	1.94	0.48
1:2:1427:C:H2'	1:2:1429:G:H8	1.79	0.48
1:2:1606:G:OP1	21:U:84:ARG:NH2	2.46	0.48
23:W:15:ARG:HH21	23:W:54:ALA:HB1	1.79	0.48
1:2:292:A:O2'	13:M:39:ASN:O	2.32	0.47
1:2:642:U:OP1	11:K:39:ASN:ND2	2.46	0.47
1:2:928:G:H2'	1:2:929:G:C8	2.49	0.47
5:E:75:LYS:NZ	12:L:20:VAL:O	2.38	0.47
1:2:1711:U:H2'	1:2:1712:A:C8	2.49	0.47
13:M:84:ARG:HD2	13:M:115:PRO:HG3	1.95	0.47
16:P:99:ALA:H	16:P:133:THR:HG22	1.79	0.47
7:G:100:ILE:HD13	7:G:177:LEU:HD22	1.97	0.47
10:J:87:ASN:HB3	10:J:90:LEU:HD13	1.96	0.47
14:N:89:VAL:HG11	14:N:109:VAL:HG21	1.96	0.47
1:2:1597:C:O2'	1:2:1603:G:N7	2.47	0.47
1:2:1522:A:H4'	20:T:144:ARG:HD2	1.96	0.47
1:2:1593:C:OP2	7:G:91:ARG:NH1	2.48	0.47
20:T:124:ARG:NE	20:T:130:ARG:O	2.45	0.47
1:2:1475:G:OP2	1:2:1475:G:N2	2.47	0.47
1:2:77:A:H2	8:H:175:LYS:HG3	1.80	0.47
1:2:930:C:O2'	1:2:1104:G:OP1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1103:C:OP1	3:C:157:GLN:NE2	2.42	0.47
1:2:1302:G:N2	1:2:1305:C:OP2	2.47	0.47
6:F:93:ASP:OD1	6:F:93:ASP:N	2.46	0.47
6:F:100:ARG:HH21	6:F:118:GLU:HG3	1.79	0.47
8:H:69:THR:HG22	8:H:71:GLY:H	1.80	0.47
21:U:9:VAL:HG13	21:U:142:LYS:HZ1	1.80	0.47
4:D:210:PRO:HD3	4:D:236:PHE:HE2	1.79	0.47
22:V:61:LEU:HB2	22:V:82:MET:HB3	1.97	0.47
1:2:570:C:O2'	26:Z:34:THR:O	2.31	0.47
1:2:858:A:H2'	1:2:859:G:H8	1.79	0.47
1:2:1138:C:OP1	2:B:155:ARG:NH1	2.48	0.47
6:F:179:ASN:HD22	6:F:231:GLY:H	1.63	0.47
13:M:13:GLN:NE2	13:M:36:TYR:O	2.47	0.47
1:2:17:C:O2'	1:2:1194:A:N1	2.47	0.47
1:2:350:C:O2'	1:2:383:G:N1	2.43	0.47
1:2:1206:C:H42	1:2:1692:U:H3	1.63	0.46
2:B:99:ILE:HG21	2:B:103:PHE:HD1	1.79	0.46
5:E:213:PRO:HA	19:S:19:LYS:HE3	1.98	0.46
1:2:71:G:OP2	8:H:170:ARG:NH2	2.47	0.46
1:2:21:U:O2'	11:K:18:ARG:NH1	2.48	0.46
1:2:562:U:H2'	1:2:563:G:H8	1.79	0.46
4:D:191:VAL:HG11	4:D:236:PHE:HA	1.97	0.46
6:F:11:ARG:HA	6:F:28:ALA:HB2	1.98	0.46
12:L:25:LYS:H	12:L:65:ARG:HB3	1.80	0.46
1:2:1165:G:N2	25:Y:20:GLN:OE1	2.37	0.46
1:2:1726:G:N2	1:2:1808:U:O2	2.38	0.46
2:B:11:LYS:HA	2:B:11:LYS:HD3	1.79	0.46
13:M:135:SER:HB3	13:M:138:VAL:HG22	1.97	0.46
15:O:24:THR:O	15:O:27:LYS:NZ	2.44	0.46
1:2:982:G:H2'	1:2:983:A:H8	1.80	0.46
1:2:1547:C:H1'	1:2:1670:C:H4'	1.98	0.46
1:2:1659:U:O2	1:2:1664:A:N7	2.49	0.46
12:L:58:VAL:HG23	12:L:71:LEU:HA	1.98	0.46
2:B:149:ASN:OD1	2:B:150:THR:N	2.46	0.46
1:2:1373:C:O3'	19:S:10:LYS:NZ	2.41	0.46
10:J:38:ILE:O	10:J:59:ARG:NH2	2.48	0.46
12:L:63:ALA:O	12:L:66:HIS:N	2.44	0.46
1:2:1036:A:N3	1:2:1844:U:O2'	2.45	0.46
1:2:1004:U:H2'	1:2:1005:G:H8	1.80	0.45
3:C:62:LEU:O	3:C:88:THR:OG1	2.26	0.45
26:Z:62:THR:HA	26:Z:69:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:848:U:O4	1:2:849:A:N6	2.49	0.45
5:E:106:ARG:HH11	5:E:175:VAL:HA	1.82	0.45
13:M:40:ILE:HD11	13:M:61:PRO:HB2	1.98	0.45
20:T:73:ASN:HB3	20:T:76:GLN:HB2	1.97	0.45
1:2:496:C:OP1	6:F:49:ARG:NH1	2.47	0.45
1:2:562:U:H2'	1:2:563:G:C8	2.51	0.45
1:2:642:U:H4'	1:2:644:G:H4'	1.98	0.45
1:2:934:G:C6	1:2:1008:A:N1	2.84	0.45
2:B:75:SER:HB2	2:B:119:PRO:HG3	1.98	0.45
4:D:168:GLY:N	4:D:179:THR:O	2.42	0.45
14:N:25:ALA:O	14:N:30:GLY:N	2.45	0.45
21:U:38:LYS:HD2	21:U:44:GLU:HA	1.98	0.45
26:Z:35:VAL:HG13	26:Z:40:ILE:HD11	1.97	0.45
1:2:1677:U:H2'	1:2:1678:A:H8	1.81	0.45
4:D:80:GLU:HA	4:D:83:LEU:HB3	1.99	0.45
11:K:138:ARG:HH21	11:K:153:SER:HA	1.81	0.45
1:2:1566:G:H21	1:2:1568:C:H6	1.64	0.45
11:K:170:PRO:O	11:K:175:ARG:NH2	2.49	0.45
19:S:71:ILE:O	19:S:78:ARG:NH1	2.41	0.45
22:V:24:LEU:HD21	22:V:35:VAL:HG12	1.99	0.45
1:2:1277:C:H2'	1:2:1278:A:C8	2.52	0.45
10:J:78:ILE:HA	10:J:104:ILE:HG22	1.98	0.45
14:N:26:LEU:HG	14:N:31:LEU:HD21	1.97	0.45
18:R:30:GLY:HA3	18:R:64:ALA:HA	1.98	0.45
1:2:625:G:O6	25:Y:64:SER:N	2.50	0.45
3:C:44:ILE:HD11	3:C:73:ASP:HB3	1.99	0.45
17:Q:29:SER:O	17:Q:33:LEU:HB2	2.16	0.45
1:2:1668:U:OP2	18:R:141:TYR:OH	2.35	0.45
20:T:75:ARG:NH1	20:T:95:TYR:O	2.49	0.45
20:T:85:ASN:HD21	20:T:98:VAL:HB	1.81	0.45
1:2:1255:G:OP1	1:2:1256:G:O2'	2.32	0.45
1:2:1611:G:O2'	20:T:87:GLN:O	2.34	0.45
1:2:1652:G:O6	1:2:1672:U:O4	2.35	0.45
7:G:16:ASP:N	7:G:16:ASP:OD1	2.49	0.45
8:H:7:PHE:HB2	8:H:124:LEU:HD23	1.99	0.45
1:2:1528:G:O2'	1:2:1666:C:OP1	2.34	0.45
1:2:1572:C:H2'	1:2:1573:G:C8	2.52	0.45
1:2:1660:C:H4'	1:2:1663:A:H62	1.82	0.45
9:I:75:ILE:HG12	9:I:79:LEU:HB2	1.98	0.45
1:2:5:U:H2'	1:2:6:G:H8	1.82	0.44
1:2:1705:C:H42	1:2:1829:G:H1	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:ASP:O	3:C:96:CYS:N	2.50	0.44
6:F:67:GLN:HG3	6:F:69:PHE:HD2	1.81	0.44
13:M:135:SER:O	13:M:139:ARG:NH1	2.47	0.44
1:2:5:U:H2'	1:2:6:G:C8	2.53	0.44
1:2:1425:G:O2'	18:R:33:LYS:NZ	2.45	0.44
10:J:105:ASP:N	10:J:105:ASP:OD1	2.50	0.44
11:K:18:ARG:O	11:K:24:ARG:NH2	2.50	0.44
16:P:45:THR:OG1	16:P:51:GLU:O	2.27	0.44
1:2:628:A:N6	5:E:179:GLN:O	2.43	0.44
1:2:643:A:OP1	11:K:38:ARG:NH2	2.43	0.44
1:2:1705:C:O2	1:2:1851:A:O2'	2.32	0.44
18:R:50:LYS:O	18:R:85:ARG:NH2	2.37	0.44
26:Z:84:LYS:HA	26:Z:84:LYS:HD3	1.83	0.44
1:2:355:G:OP2	13:M:107:LYS:NZ	2.46	0.44
1:2:572:U:H3	1:2:576:A:H5"	1.81	0.44
6:F:202:PRO:HB2	13:M:42:LEU:HD23	2.00	0.44
1:2:1497:G:H4'	1:2:1498:A:H5"	1.99	0.44
1:2:1869:A:N6	3:C:114:VAL:O	2.50	0.44
6:F:255:ARG:HG3	6:F:256:LEU:HD12	2.00	0.44
22:V:26:SER:OG	22:V:28:ASN:O	2.35	0.44
24:X:52:ILE:HG22	24:X:61:ILE:HG23	1.98	0.44
1:2:126:G:H8	8:H:199:THR:HG21	1.83	0.44
7:G:169:ILE:HA	7:G:172:CYS:HB2	1.99	0.44
9:I:147:LYS:HA	9:I:147:LYS:HD2	1.85	0.44
25:Y:14:ARG:O	25:Y:18:ARG:HB2	2.18	0.44
11:K:131:ARG:HA	11:K:131:ARG:HD2	1.88	0.44
13:M:25:LEU:HA	13:M:30:LYS:HE3	1.99	0.44
19:S:74:GLN:HB2	19:S:78:ARG:HG2	1.99	0.44
20:T:99:LEU:O	20:T:103:LEU:N	2.42	0.44
22:V:101:ILE:HA	22:V:104:ILE:HG22	2.00	0.44
1:2:1562:C:H5"	21:U:71:GLY:HA3	2.00	0.44
6:F:132:GLY:N	6:F:136:ILE:O	2.43	0.44
8:H:57:ASP:OD1	8:H:58:LYS:N	2.51	0.44
20:T:24:ARG:HB2	20:T:29:ALA:HB2	1.99	0.44
26:Z:103:SER:OG	26:Z:106:GLN:OE1	2.33	0.44
1:2:212:C:H2'	1:2:213:G:C8	2.54	0.43
1:2:1323:U:H2'	1:2:1324:G:H8	1.82	0.43
1:2:1337:C:H2'	1:2:1338:G:C8	2.53	0.43
1:2:1844:U:H3	1:2:1855:G:H1	1.66	0.43
12:L:49:MET:HG2	12:L:69:TRP:CD2	2.53	0.43
17:Q:39:ALA:HA	17:Q:42:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:65:C:N4	8:H:134:GLY:O	2.45	0.43
1:2:602:G:H3'	1:2:603:C:H2'	1.99	0.43
1:2:1313:A:OP2	14:N:33:ARG:NH2	2.51	0.43
21:U:29:LYS:HZ1	21:U:109:GLY:HA3	1.83	0.43
21:U:70:ALA:H	21:U:120:GLY:HA2	1.83	0.43
24:X:103:VAL:HG23	24:X:126:LEU:HB2	1.99	0.43
1:2:76:U:H4'	8:H:155:GLN:HE21	1.83	0.43
1:2:1427:C:H2'	1:2:1429:G:C8	2.54	0.43
5:E:40:ARG:HA	22:V:108:PRO:HB3	2.00	0.43
4:D:204:ILE:HD12	4:D:214:LEU:HD23	1.99	0.43
6:F:57:THR:HB	6:F:60:GLU:HG2	2.00	0.43
13:M:61:PRO:HD3	13:M:141:ASN:HD21	1.83	0.43
14:N:80:ASP:HB2	14:N:84:LYS:HE2	1.98	0.43
19:S:103:LYS:NZ	19:S:104:GLU:OE2	2.47	0.43
1:2:1283:C:H41	14:N:102:LYS:HG2	1.82	0.43
1:2:1335:G:O6	1:2:1492:U:O4	2.37	0.43
7:G:151:ILE:HD13	7:G:154:LEU:HD21	1.99	0.43
11:K:150:ARG:HG3	11:K:153:SER:HB3	2.00	0.43
1:2:381:C:H41	10:J:27:TYR:HB2	1.84	0.43
1:2:1587:G:OP1	1:2:1587:G:N2	2.46	0.43
4:D:76:LYS:HA	4:D:76:LYS:HD3	1.74	0.43
8:H:121:ILE:N	8:H:125:THR:OG1	2.51	0.43
10:J:193:LYS:HE2	10:J:193:LYS:HB2	1.88	0.43
1:2:1239:U:N3	1:2:1242:U:OP2	2.42	0.43
1:2:1662:U:O4	1:2:1663:A:N6	2.52	0.43
2:B:81:ASN:HA	2:B:84:GLN:HE21	1.84	0.43
26:Z:60:PHE:HD1	26:Z:71:GLY:HA3	1.83	0.43
3:C:181:LEU:HA	3:C:184:VAL:HG22	2.00	0.43
5:E:115:VAL:O	5:E:119:CYS:CB	2.67	0.43
6:F:11:ARG:NH1	6:F:24:THR:OG1	2.51	0.43
1:2:805:U:H5'	24:X:83:LEU:HD23	2.01	0.43
1:2:1410:C:H2'	1:2:1411:G:C8	2.54	0.43
1:2:1536:G:H2'	1:2:1537:A:H8	1.84	0.43
12:L:63:ALA:HB1	12:L:64:TRP:HD1	1.84	0.43
1:2:146:G:H1	1:2:173:A:H61	1.66	0.42
1:2:980:A:H2'	1:2:981:A:H8	1.84	0.42
1:2:1544:C:O2'	18:R:75:GLY:O	2.32	0.42
15:O:87:ASP:OD1	15:O:87:ASP:N	2.52	0.42
21:U:28:LEU:HG	21:U:106:ALA:HB1	2.00	0.42
1:2:1335:G:O6	1:2:1492:U:C4	2.73	0.42
3:C:63:LYS:HB3	3:C:63:LYS:HE3	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:32:MET:HG2	8:H:100:CYS:HB2	2.00	0.42
17:Q:44:ARG:O	17:Q:50:ARG:NH2	2.52	0.42
22:V:26:SER:HB3	22:V:110:VAL:HG12	2.01	0.42
1:2:539:C:H42	1:2:545:A:H61	1.68	0.42
4:D:132:ASP:OD1	4:D:132:ASP:N	2.51	0.42
9:I:60:ILE:HD11	9:I:90:LYS:HD3	2.01	0.42
16:P:44:VAL:O	16:P:52:THR:OG1	2.32	0.42
21:U:24:LYS:HA	21:U:24:LYS:HD2	1.81	0.42
1:2:1295:A:N6	1:2:1305:C:N3	2.67	0.42
1:2:1545:A:H2	1:2:1671:G:H1'	1.85	0.42
2:B:57:LYS:HZ1	2:B:159:ILE:HA	1.83	0.42
16:P:86:LYS:NZ	16:P:122:SER:O	2.45	0.42
25:Y:65:ALA:HB3	25:Y:67:ARG:HH12	1.83	0.42
1:2:62:G:O2'	1:2:172:U:OP1	2.38	0.42
1:2:962:A:H4'	16:P:66:ARG:HD2	2.01	0.42
1:2:1231:C:O2'	1:2:1253:A:N6	2.52	0.42
1:2:1513:C:H2'	1:2:1514:G:C8	2.54	0.42
1:2:1846:G:H2'	1:2:1847:G:C8	2.54	0.42
5:E:59:LEU:HA	5:E:66:ILE:HG13	2.02	0.42
6:F:94:LYS:HA	6:F:94:LYS:HD2	1.91	0.42
7:G:51:HIS:HB3	18:R:50:LYS:HE2	2.01	0.42
22:V:107:GLU:HG2	22:V:110:VAL:HG22	2.02	0.42
1:2:1808:U:H2'	1:2:1809:A:C8	2.55	0.42
1:2:691:G:H2'	1:2:692:G:H8	1.83	0.42
1:2:1536:G:H2'	1:2:1537:A:C8	2.55	0.42
21:U:115:LYS:HD2	21:U:115:LYS:HA	1.79	0.42
1:2:220:U:H2'	1:2:221:A:C8	2.55	0.42
1:2:640:A:H2'	1:2:641:A:C8	2.55	0.42
1:2:995:G:N2	1:2:998:A:OP2	2.47	0.42
1:2:1024:A:OP2	15:O:124:ARG:NH1	2.52	0.42
1:2:1171:G:O2'	1:2:1187:G:O6	2.37	0.42
25:Y:60:LYS:HA	25:Y:60:LYS:HD2	1.86	0.42
1:2:84:A:N3	1:2:150:A:O2'	2.52	0.42
1:2:1593:C:H2'	1:2:1594:A:C8	2.55	0.42
5:E:70:THR:HG23	5:E:84:VAL:HG23	2.02	0.42
11:K:64:ASP:OD1	11:K:64:ASP:N	2.53	0.42
1:2:1450:G:H2'	1:2:1451:G:H8	1.85	0.42
15:O:18:TYR:HE1	24:X:55:ASP:HA	1.85	0.42
23:W:67:ASP:O	23:W:71:ARG:HG3	2.20	0.42
3:C:143:THR:HA	3:C:207:LEU:HA	2.02	0.41
11:K:129:LEU:HD21	11:K:159:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:6:THR:HB	26:Z:28:LEU:HB2	2.02	0.41
1:2:201:C:H3'	1:2:202:G:H8	1.84	0.41
1:2:1514:G:H2'	1:2:1515:G:H8	1.85	0.41
1:2:1656:G:O6	1:2:1668:U:O4	2.37	0.41
1:2:1722:G:O6	1:2:1812:U:C2	2.73	0.41
3:C:136:ARG:HB2	3:C:218:LEU:HD11	2.02	0.41
5:E:14:ASP:OD2	22:V:27:ARG:NH2	2.52	0.41
9:I:43:LEU:HD13	9:I:72:PHE:HE1	1.84	0.41
18:R:134:GLY:HA3	18:R:140:ARG:HA	2.02	0.41
1:2:433:A:H2'	1:2:434:G:C8	2.55	0.41
1:2:885:U:H2'	1:2:901:G:H22	1.85	0.41
2:B:25:LEU:HD12	2:B:46:ILE:HG21	2.02	0.41
19:S:15:VAL:O	19:S:19:LYS:CB	2.67	0.41
1:2:115:U:O2'	1:2:381:C:O2	2.30	0.41
1:2:1360:U:O2'	1:2:1379:A:OP2	2.34	0.41
1:2:1424:G:H2'	1:2:1425:G:H8	1.85	0.41
1:2:1542:C:OP1	21:U:63:HIS:NE2	2.54	0.41
6:F:252:ARG:HA	6:F:255:ARG:HG2	2.03	0.41
7:G:71:ARG:HH12	7:G:144:LEU:HD11	1.85	0.41
1:2:223:C:H2'	1:2:224:A:H8	1.85	0.41
1:2:603:C:N4	1:2:620:G:O6	2.54	0.41
2:B:180:ARG:HG3	2:B:195:TRP:HE1	1.85	0.41
12:L:50:GLN:HA	12:L:53:LYS:HG3	2.02	0.41
1:2:145:G:H2'	1:2:146:G:C8	2.56	0.41
3:C:65:ARG:NH2	16:P:51:GLU:OE1	2.53	0.41
17:Q:64:LYS:HE2	17:Q:64:LYS:HB3	1.95	0.41
20:T:79:ILE:HD12	20:T:79:ILE:HA	2.00	0.41
1:2:1457:U:H2'	1:2:1458:G:H8	1.86	0.41
7:G:20:PHE:HD2	7:G:23:TRP:HD1	1.66	0.41
9:I:46:THR:HG23	9:I:65:PRO:HD3	2.02	0.41
11:K:60:LEU:HD23	11:K:60:LEU:HA	1.91	0.41
15:O:119:GLU:HA	15:O:122:ILE:HG22	2.02	0.41
1:2:457:C:H2'	1:2:458:A:C8	2.55	0.41
1:2:520:A:O2'	1:2:825:A:N3	2.52	0.41
1:2:1323:U:H2'	1:2:1324:G:C8	2.56	0.41
1:2:1356:G:O3'	4:D:125:LYS:NZ	2.54	0.41
4:D:271:ASP:OD1	4:D:271:ASP:N	2.53	0.41
13:M:101:ARG:HH21	25:Y:5:ARG:HA	1.85	0.41
1:2:161:U:O2'	8:H:87:ARG:NH1	2.39	0.41
1:2:317:C:OP2	8:H:183:ARG:NH2	2.54	0.41
1:2:1012:A:OP1	15:O:3:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1117:C:H2'	1:2:1118:C:C6	2.56	0.41
1:2:1172:U:H2'	1:2:1173:A:C8	2.56	0.41
1:2:1264:C:H42	1:2:1518:C:H41	1.68	0.41
1:2:1412:C:H2'	1:2:1413:G:H8	1.86	0.41
1:2:1550:G:H5"	5:E:9:ARG:HH12	1.86	0.41
2:B:205:ARG:NH2	19:S:81:ARG:O	2.54	0.41
8:H:5:ILE:HG22	8:H:111:LEU:HB2	2.03	0.41
9:I:160:LYS:HB3	9:I:160:LYS:HE3	1.81	0.41
12:L:24:LYS:O	12:L:42:ASN:ND2	2.53	0.41
25:Y:105:PHE:HD1	25:Y:121:LYS:HD2	1.84	0.41
1:2:346:C:H5"	6:F:38:LEU:HB2	2.03	0.41
1:2:804:U:H5"	24:X:82:GLN:HG3	2.02	0.41
7:G:124:ASP:OD1	7:G:124:ASP:N	2.53	0.41
13:M:7:GLU:HB2	13:M:11:GLN:HE22	1.85	0.41
14:N:92:CYS:HB2	14:N:103:VAL:HG22	2.03	0.41
15:O:33:VAL:O	15:O:37:ILE:HD12	2.21	0.41
18:R:131:LYS:HG3	18:R:137:ALA:HA	2.02	0.41
20:T:114:LEU:HD13	20:T:117:ILE:HD11	2.03	0.41
21:U:6:VAL:HG11	21:U:131:LEU:HB3	2.03	0.41
1:2:183:G:O2'	1:2:184:G:O4'	2.35	0.40
1:2:220:U:H2'	1:2:221:A:H8	1.85	0.40
1:2:385:G:O2'	10:J:10:LYS:NZ	2.54	0.40
8:H:190:ARG:HA	8:H:190:ARG:HD2	1.94	0.40
13:M:49:GLU:HA	13:M:52:GLU:HG2	2.02	0.40
18:R:81:ILE:HD13	18:R:81:ILE:HA	1.97	0.40
1:2:980:A:H2'	1:2:981:A:C8	2.55	0.40
4:D:145:LYS:HB3	4:D:145:LYS:HE2	1.88	0.40
14:N:23:LYS:HD3	14:N:23:LYS:HA	1.91	0.40
18:R:97:GLN:HB3	18:R:105:LYS:HG3	2.02	0.40
1:2:151:C:OP1	26:Z:120:THR:OG1	2.28	0.40
1:2:824:C:C2	11:K:144:ILE:HD13	2.56	0.40
1:2:1372:U:OP1	1:2:1385:G:N2	2.51	0.40
5:E:172:VAL:HG13	5:E:185:LYS:HE3	2.04	0.40
6:F:137:PRO:HB2	6:F:150:PRO:HD2	2.03	0.40
6:F:204:SER:OG	6:F:205:PHE:N	2.55	0.40
18:R:33:LYS:HA	18:R:38:PRO:HA	2.02	0.40
24:X:42:MET:HE3	24:X:42:MET:HB2	1.91	0.40
1:2:156:G:OP1	8:H:2:LYS:NZ	2.55	0.40
1:2:1203:U:O3'	4:D:117:ARG:NH1	2.55	0.40
2:B:197:VAL:HG23	2:B:198:MET:H	1.85	0.40
11:K:69:ARG:O	11:K:73:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1705:C:H2'	1:2:1706:G:C8	2.56	0.40
5:E:49:ILE:HG23	5:E:87:TYR:HB2	2.04	0.40
19:S:114:LEU:HB2	19:S:117:LEU:HG	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	215/295 (73%)	203 (94%)	12 (6%)	0	100	100
3	C	211/264 (80%)	196 (93%)	14 (7%)	1 (0%)	29	68
4	D	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
5	E	226/281 (80%)	217 (96%)	9 (4%)	0	100	100
6	F	260/263 (99%)	240 (92%)	20 (8%)	0	100	100
7	G	189/204 (93%)	180 (95%)	9 (5%)	0	100	100
8	H	235/249 (94%)	225 (96%)	10 (4%)	0	100	100
9	I	181/432 (42%)	174 (96%)	7 (4%)	0	100	100
10	J	204/208 (98%)	191 (94%)	13 (6%)	0	100	100
11	K	183/194 (94%)	175 (96%)	8 (4%)	0	100	100
12	L	94/149 (63%)	91 (97%)	3 (3%)	0	100	100
13	M	149/158 (94%)	138 (93%)	11 (7%)	0	100	100
14	N	115/132 (87%)	106 (92%)	9 (8%)	0	100	100
15	O	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
16	P	134/168 (80%)	124 (92%)	10 (8%)	0	100	100
17	Q	113/145 (78%)	100 (88%)	13 (12%)	0	100	100
18	R	140/172 (81%)	133 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	130/135 (96%)	113 (87%)	17 (13%)	0	100	100
20	T	142/152 (93%)	133 (94%)	9 (6%)	0	100	100
21	U	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
22	V	98/119 (82%)	93 (95%)	5 (5%)	0	100	100
23	W	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
24	X	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
25	Y	139/143 (97%)	131 (94%)	8 (6%)	0	100	100
26	Z	122/131 (93%)	116 (95%)	6 (5%)	0	100	100
27	a	75/124 (60%)	69 (92%)	6 (8%)	0	100	100
28	b	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
29	c	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
30	d	65/69 (94%)	60 (92%)	5 (8%)	0	100	100
31	e	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
32	f	55/133 (41%)	51 (93%)	4 (7%)	0	100	100
33	g	66/188 (35%)	63 (96%)	3 (4%)	0	100	100
34	h	311/317 (98%)	279 (90%)	32 (10%)	0	100	100
35	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	4821/5821 (83%)	4534 (94%)	286 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	190	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	
2	B	180/245 (74%)	180 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	194/231 (84%)	194 (100%)	0	100	100
4	D	187/187 (100%)	187 (100%)	0	100	100
5	E	190/232 (82%)	189 (100%)	1 (0%)	88	93
6	F	224/225 (100%)	224 (100%)	0	100	100
7	G	161/170 (95%)	160 (99%)	1 (1%)	86	92
8	H	207/218 (95%)	205 (99%)	2 (1%)	76	86
9	I	165/360 (46%)	165 (100%)	0	100	100
10	J	178/180 (99%)	176 (99%)	2 (1%)	73	84
11	K	161/168 (96%)	160 (99%)	1 (1%)	86	92
12	L	87/125 (70%)	85 (98%)	2 (2%)	50	70
13	M	136/142 (96%)	133 (98%)	3 (2%)	52	70
14	N	99/108 (92%)	98 (99%)	1 (1%)	76	86
15	O	130/131 (99%)	129 (99%)	1 (1%)	81	89
16	P	106/130 (82%)	105 (99%)	1 (1%)	78	87
17	Q	105/130 (81%)	105 (100%)	0	100	100
18	R	117/140 (84%)	117 (100%)	0	100	100
19	S	119/121 (98%)	117 (98%)	2 (2%)	60	78
20	T	125/132 (95%)	125 (100%)	0	100	100
21	U	111/116 (96%)	111 (100%)	0	100	100
22	V	92/107 (86%)	92 (100%)	0	100	100
23	W	67/67 (100%)	67 (100%)	0	100	100
24	X	112/113 (99%)	112 (100%)	0	100	100
25	Y	113/115 (98%)	113 (100%)	0	100	100
26	Z	107/113 (95%)	107 (100%)	0	100	100
27	a	68/102 (67%)	68 (100%)	0	100	100
28	b	88/88 (100%)	87 (99%)	1 (1%)	73	84
29	c	75/76 (99%)	75 (100%)	0	100	100
30	d	60/62 (97%)	60 (100%)	0	100	100
31	e	48/49 (98%)	48 (100%)	0	100	100
32	f	47/106 (44%)	47 (100%)	0	100	100
33	g	61/154 (40%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	h	272/275 (99%)	271 (100%)	1 (0%)	91	94
35	n	24/24 (100%)	24 (100%)	0	100	100
All	All	4216/4942 (85%)	4197 (100%)	19 (0%)	89	93

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	76	ARG
7	G	22	LYS
8	H	98	ARG
8	H	154	ARG
10	J	140	LYS
10	J	143	LYS
11	K	83	ARG
12	L	50	GLN
12	L	53	LYS
13	M	69	ARG
13	M	118	ARG
13	M	144	LYS
14	N	45	ARG
15	O	105	ASN
16	P	150	ARG
19	S	33	ARG
19	S	107	LYS
28	b	51	ARG
34	h	185	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	148	ASN
19	S	127	ASN
35	n	22	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1870 (90%)	389 (23%)	10 (0%)
36	z	160/400 (40%)	40 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	1845/2270 (81%)	429 (23%)	10 (0%)

All (429) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	9	U
1	2	26	U
1	2	33	G
1	2	41	G
1	2	42	A
1	2	44	U
1	2	45	A
1	2	46	A
1	2	56	G
1	2	59	U
1	2	61	A
1	2	67	C
1	2	68	A
1	2	73	C
1	2	74	G
1	2	92	A
1	2	102	A
1	2	103	A
1	2	110	U
1	2	113	G
1	2	115	U
1	2	126	G
1	2	130	G
1	2	142	C
1	2	143	U
1	2	147	A
1	2	154	U
1	2	155	G
1	2	162	C
1	2	178	C
1	2	180	G
1	2	182	C
1	2	183	G
1	2	184	G
1	2	192	C

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Mol	Chain	Res	Type
1	2	197	U
1	2	199	C
1	2	202	G
1	2	211	G
1	2	291	G
1	2	306	C
1	2	307	G
1	2	308	G
1	2	309	G
1	2	312	G
1	2	319	C
1	2	330	G
1	2	332	G
1	2	347	G
1	2	356	C
1	2	357	C
1	2	362	C
1	2	364	A
1	2	368	U
1	2	369	C
1	2	370	G
1	2	371	A
1	2	383	G
1	2	384	U
1	2	385	G
1	2	386	C
1	2	398	A
1	2	400	C
1	2	409	C
1	2	417	C
1	2	418	A
1	2	435	A
1	2	438	G
1	2	446	G
1	2	448	A
1	2	449	A
1	2	450	C
1	2	455	A
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C

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Mol	Chain	Res	Type
1	2	474	G
1	2	483	C
1	2	486	A
1	2	487	U
1	2	488	U
1	2	489	A
1	2	492	C
1	2	493	A
1	2	502	C
1	2	508	A
1	2	509	G
1	2	523	A
1	2	530	U
1	2	532	C
1	2	536	A
1	2	537	C
1	2	538	U
1	2	541	U
1	2	542	U
1	2	544	G
1	2	546	G
1	2	547	G
1	2	549	C
1	2	550	C
1	2	551	U
1	2	554	A
1	2	555	A
1	2	556	U
1	2	560	A
1	2	562	U
1	2	567	C
1	2	568	C
1	2	576	A
1	2	583	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	606	G
1	2	607	U
1	2	608	C
1	2	613	G

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Mol	Chain	Res	Type
1	2	614	C
1	2	617	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	631	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	660	C
1	2	661	U
1	2	662	G
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	687	C
1	2	688	U
1	2	689	U
1	2	690	G
1	2	693	A
1	2	696	G
1	2	744	G
1	2	752	G
1	2	753	C
1	2	754	G
1	2	790	C
1	2	793	G
1	2	798	G
1	2	799	U
1	2	801	U
1	2	810	A
1	2	811	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	831	G
1	2	834	C
1	2	847	A
1	2	849	A
1	2	860	G

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Mol	Chain	Res	Type
1	2	862	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	874	G
1	2	875	A
1	2	878	G
1	2	879	C
1	2	887	U
1	2	888	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	895	G
1	2	898	U
1	2	901	G
1	2	904	A
1	2	913	A
1	2	914	U
1	2	919	A
1	2	920	A
1	2	933	G
1	2	934	G
1	2	955	A
1	2	963	A
1	2	970	G
1	2	971	G
1	2	985	G
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1017	U
1	2	1023	A
1	2	1026	C
1	2	1028	A
1	2	1045	U
1	2	1054	G
1	2	1055	A
1	2	1076	G
1	2	1078	C
1	2	1083	A

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Mol	Chain	Res	Type
1	2	1085	C
1	2	1088	U
1	2	1089	G
1	2	1107	G
1	2	1113	A
1	2	1114	U
1	2	1118	C
1	2	1121	G
1	2	1128	C
1	2	1133	A
1	2	1138	C
1	2	1149	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1161	U
1	2	1165	G
1	2	1166	G
1	2	1181	A
1	2	1183	A
1	2	1203	U
1	2	1205	G
1	2	1207	G
1	2	1215	C
1	2	1216	C
1	2	1217	A
1	2	1224	G
1	2	1242	U
1	2	1244	U
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1264	C
1	2	1274	G
1	2	1275	G
1	2	1276	A
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1287	A

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Mol	Chain	Res	Type
1	2	1293	A
1	2	1294	G
1	2	1295	A
1	2	1298	G
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1306	U
1	2	1307	U
1	2	1308	U
1	2	1311	C
1	2	1312	G
1	2	1313	A
1	2	1314	U
1	2	1316	C
1	2	1318	G
1	2	1320	G
1	2	1327	G
1	2	1330	G
1	2	1342	U
1	2	1345	G
1	2	1358	U
1	2	1363	C
1	2	1371	U
1	2	1372	U
1	2	1378	A
1	2	1395	C
1	2	1396	A
1	2	1397	U
1	2	1405	A
1	2	1424	G
1	2	1428	G
1	2	1439	A
1	2	1441	U
1	2	1442	U
1	2	1446	A
1	2	1452	A
1	2	1453	C
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1464	C

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Mol	Chain	Res	Type
1	2	1466	G
1	2	1473	G
1	2	1477	U
1	2	1489	A
1	2	1490	G
1	2	1494	U
1	2	1495	G
1	2	1498	A
1	2	1507	G
1	2	1509	U
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1533	A
1	2	1535	U
1	2	1536	G
1	2	1548	G
1	2	1551	U
1	2	1552	G
1	2	1553	C
1	2	1554	C
1	2	1556	A
1	2	1560	U
1	2	1567	G
1	2	1568	C
1	2	1573	G
1	2	1575	G
1	2	1578	U
1	2	1580	A
1	2	1582	C
1	2	1586	U
1	2	1587	G
1	2	1588	A
1	2	1598	G
1	2	1599	U
1	2	1601	A
1	2	1603	G
1	2	1604	G
1	2	1606	G
1	2	1614	A
1	2	1621	U
1	2	1623	A

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Mol	Chain	Res	Type
1	2	1632	G
1	2	1636	G
1	2	1637	A
1	2	1638	G
1	2	1646	C
1	2	1648	G
1	2	1649	U
1	2	1664	A
1	2	1665	G
1	2	1676	U
1	2	1677	U
1	2	1680	G
1	2	1683	C
1	2	1698	C
1	2	1699	A
1	2	1700	C
1	2	1701	C
1	2	1704	C
1	2	1706	G
1	2	1715	A
1	2	1721	U
1	2	1722	G
1	2	1748	G
1	2	1750	C
1	2	1751	C
1	2	1754	G
1	2	1756	C
1	2	1757	G
1	2	1761	U
1	2	1773	C
1	2	1776	G
1	2	1779	G
1	2	1781	A
1	2	1782	G
1	2	1785	C
1	2	1799	G
1	2	1823	A
1	2	1824	A
1	2	1825	A
1	2	1829	G
1	2	1831	A
1	2	1834	A

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Mol	Chain	Res	Type
1	2	1835	A
1	2	1836	G
1	2	1838	U
1	2	1839	U
1	2	1840	U
1	2	1846	G
1	2	1849	G
1	2	1851	A
1	2	1852	C
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
1	2	1866	A
1	2	1868	U
1	2	1869	A
36	z	121	C
36	z	123	C
36	z	124	C
36	z	136	A
36	z	137	G
36	z	145	G
36	z	150	G
36	z	154	A
36	z	157	C
36	z	161	G
36	z	162	A
36	z	163	G
36	z	165	A
36	z	166	C
36	z	167	A
36	z	169	C
36	z	173	A
36	z	229	G
36	z	234	U
36	z	237	C
36	z	244	A
36	z	253	G
36	z	257	A
36	z	258	G
36	z	259	U
36	z	260	A

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Mol	Chain	Res	Type
36	z	262	U
36	z	263	G
36	z	265	U
36	z	266	G
36	z	282	U
36	z	284	U
36	z	288	A
36	z	290	U
36	z	296	A
36	z	297	U
36	z	306	U
36	z	325	C
36	z	328	G
36	z	330	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	383	G
1	2	445	A
1	2	553	U
1	2	561	A
1	2	627	U
1	2	688	U
1	2	752	G
1	2	1137	U
1	2	1204	G
1	2	1395	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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.

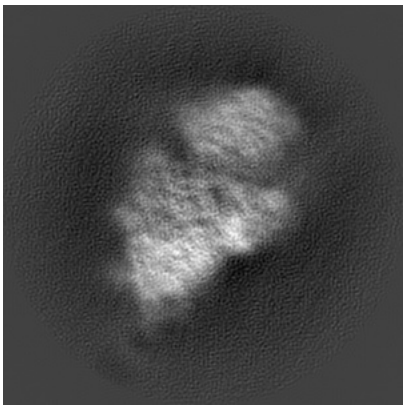
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25531. These allow visual inspection of the internal detail of the map and identification of artifacts.

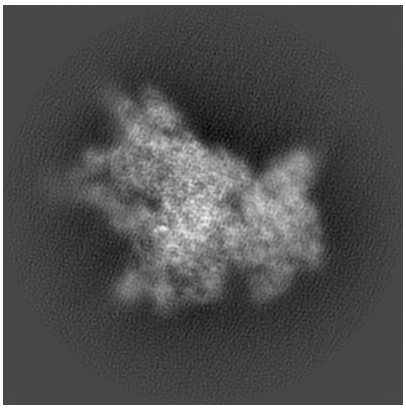
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

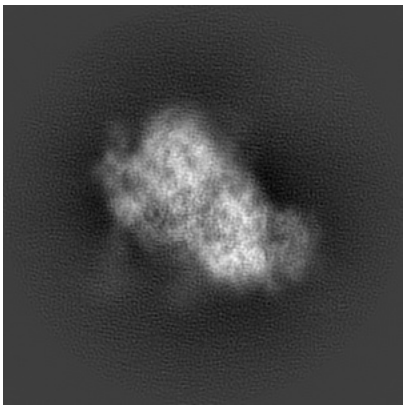
6.1.1 Primary map



X

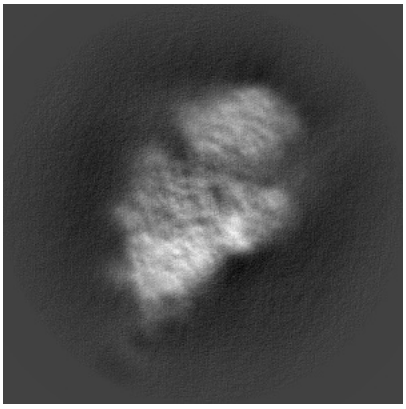


Y

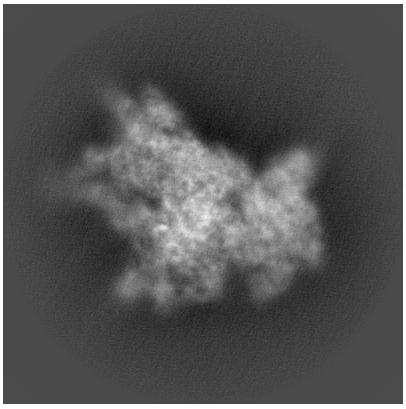


Z

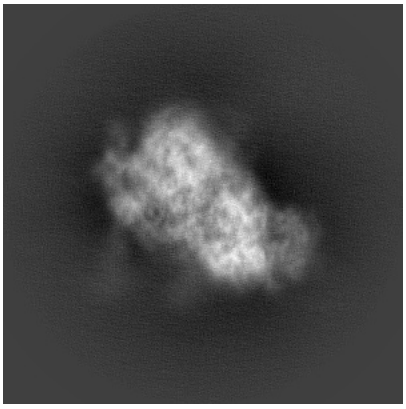
6.1.2 Raw map



X



Y

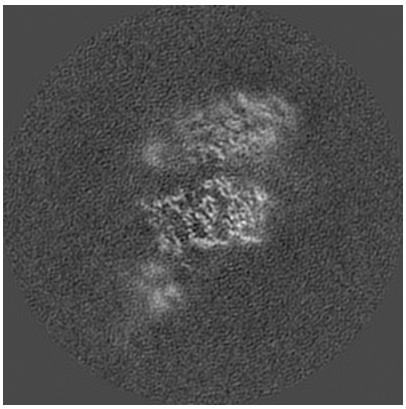


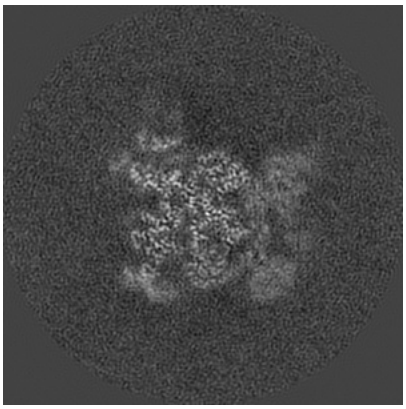
Z

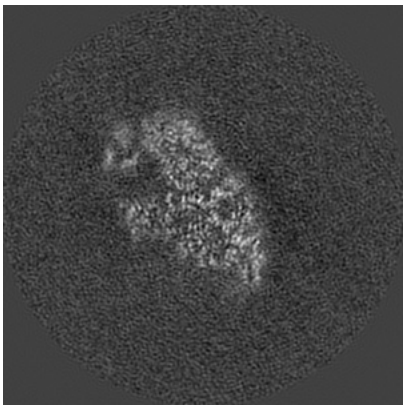
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

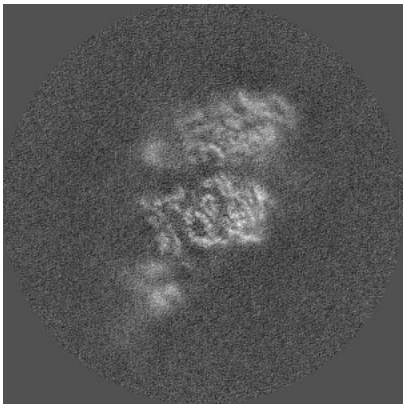
6.2.1 Primary map

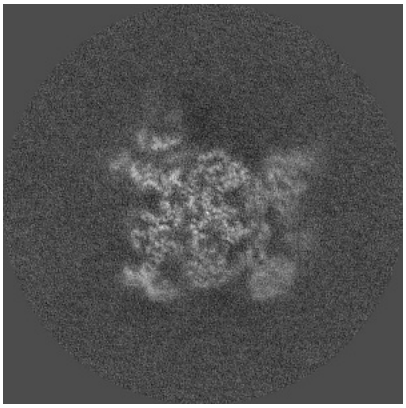

X Index: 200

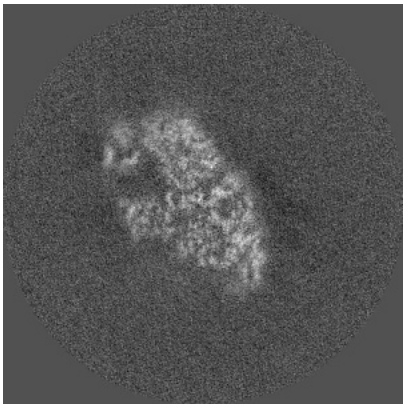

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

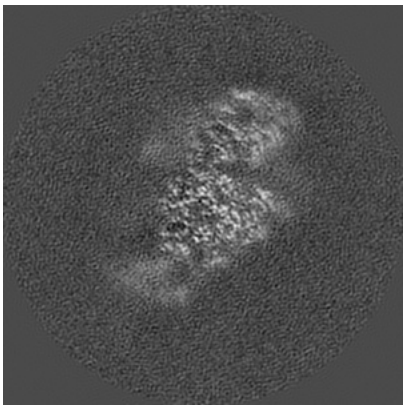

Y Index: 200

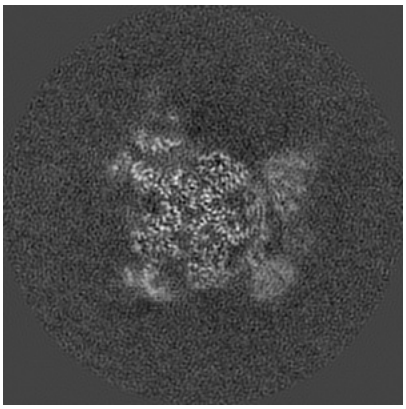

Z Index: 200

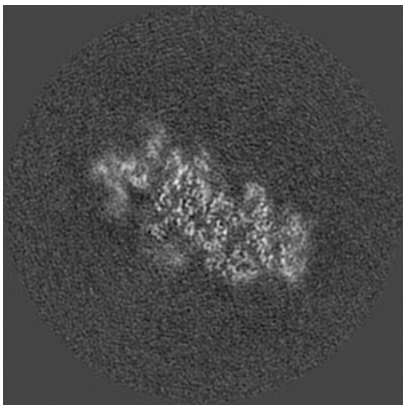
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

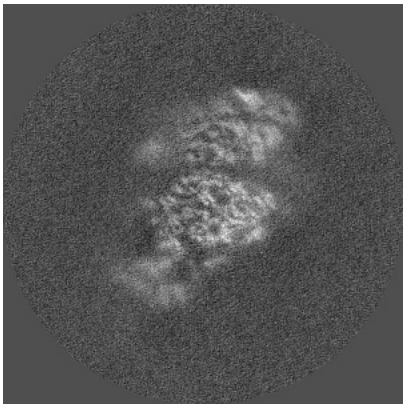
6.3.1 Primary map

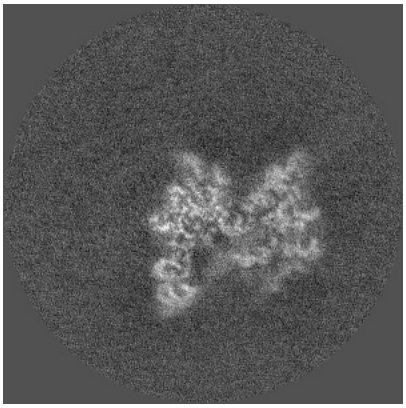

X Index: 192

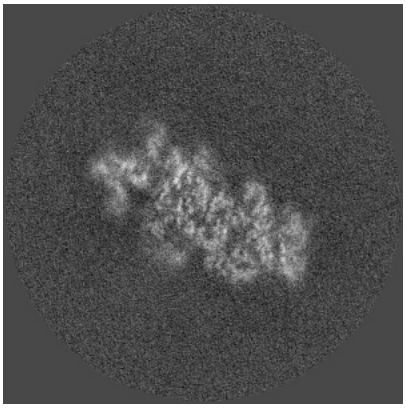

Y Index: 198


Z Index: 162

6.3.2 Raw map


X Index: 195

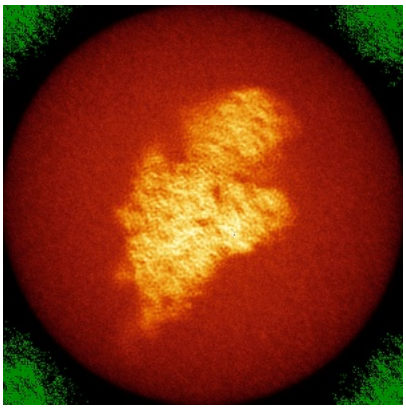

Y Index: 230

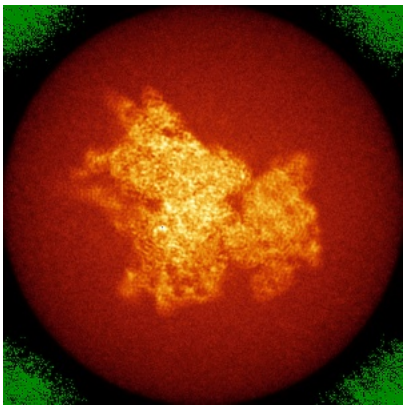

Z Index: 162

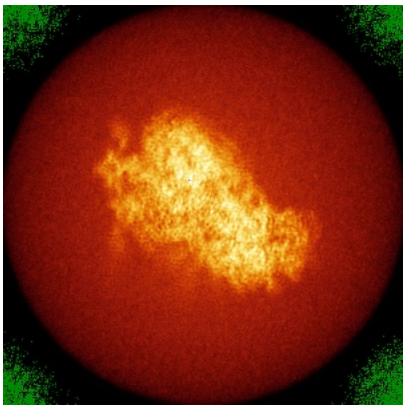
The images above show the largest variance slices of the map in three orthogonal directions.

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

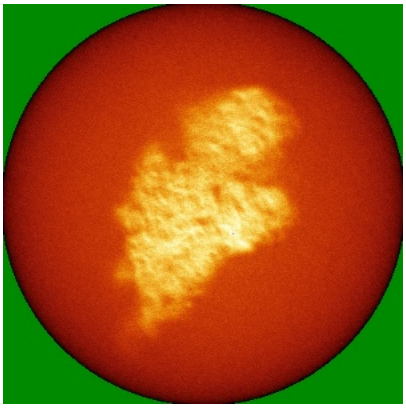
6.4.1 Primary map

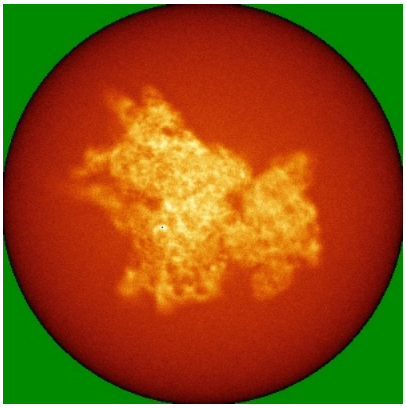

X

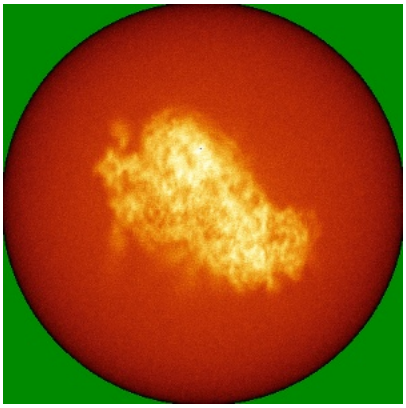

Y


Z

6.4.2 Raw map


X

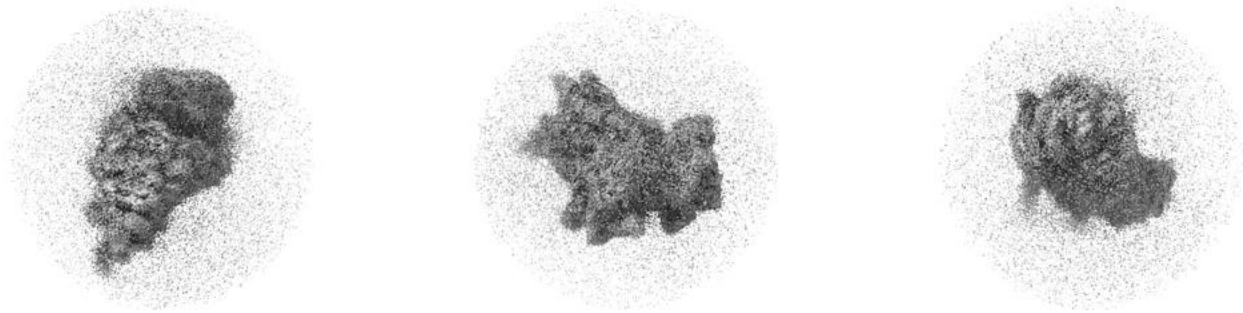

Y


Z

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

6.5 Orthogonal surface views (i)

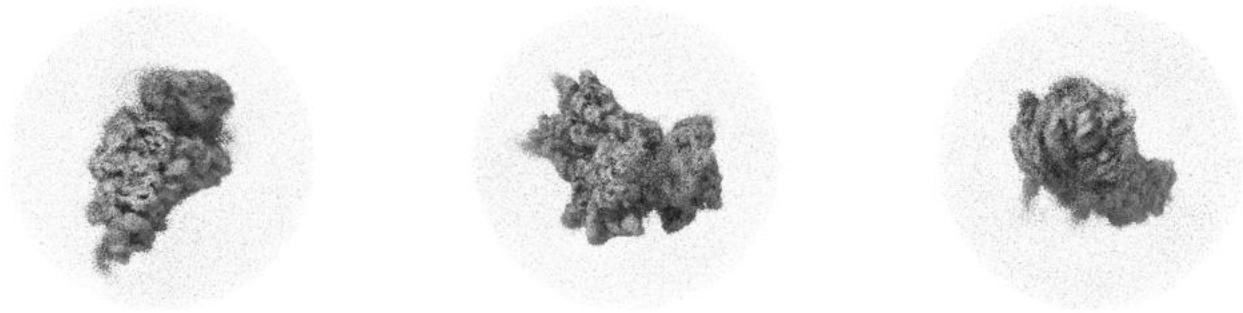
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

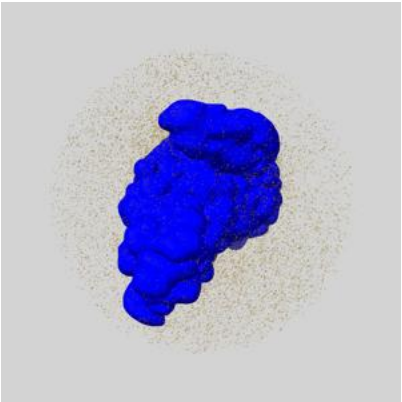
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

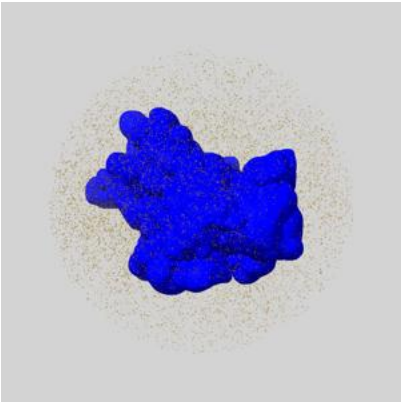
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

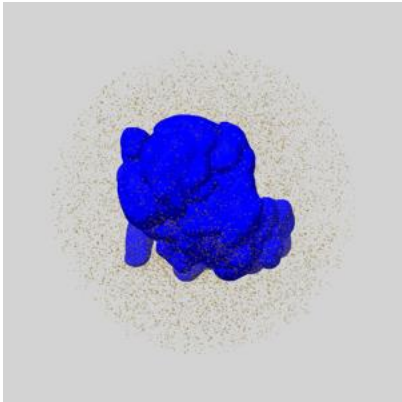
6.6.1 emd_25531_msk_1.map (i)



X



Y

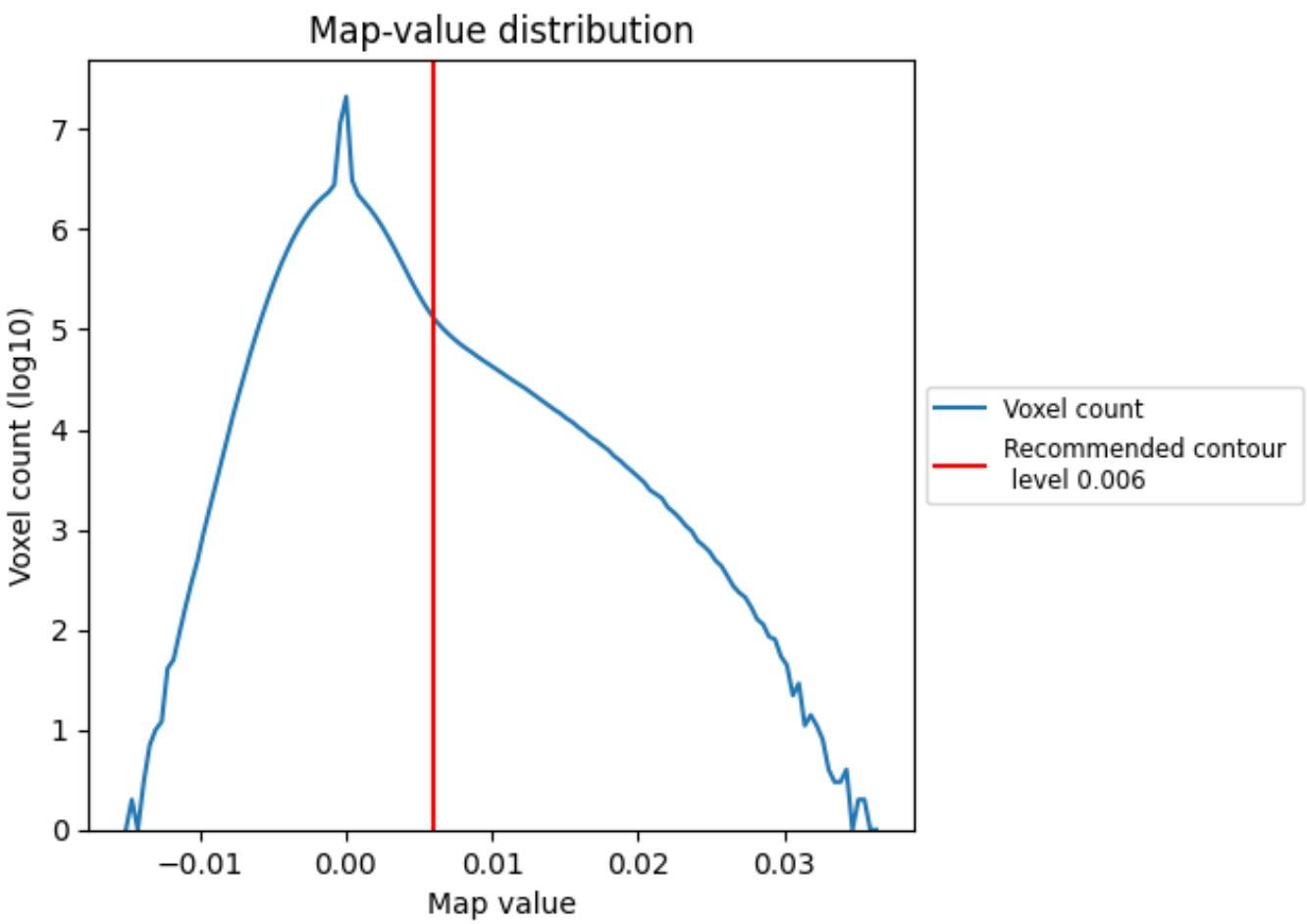


Z

7 Map analysis (i)

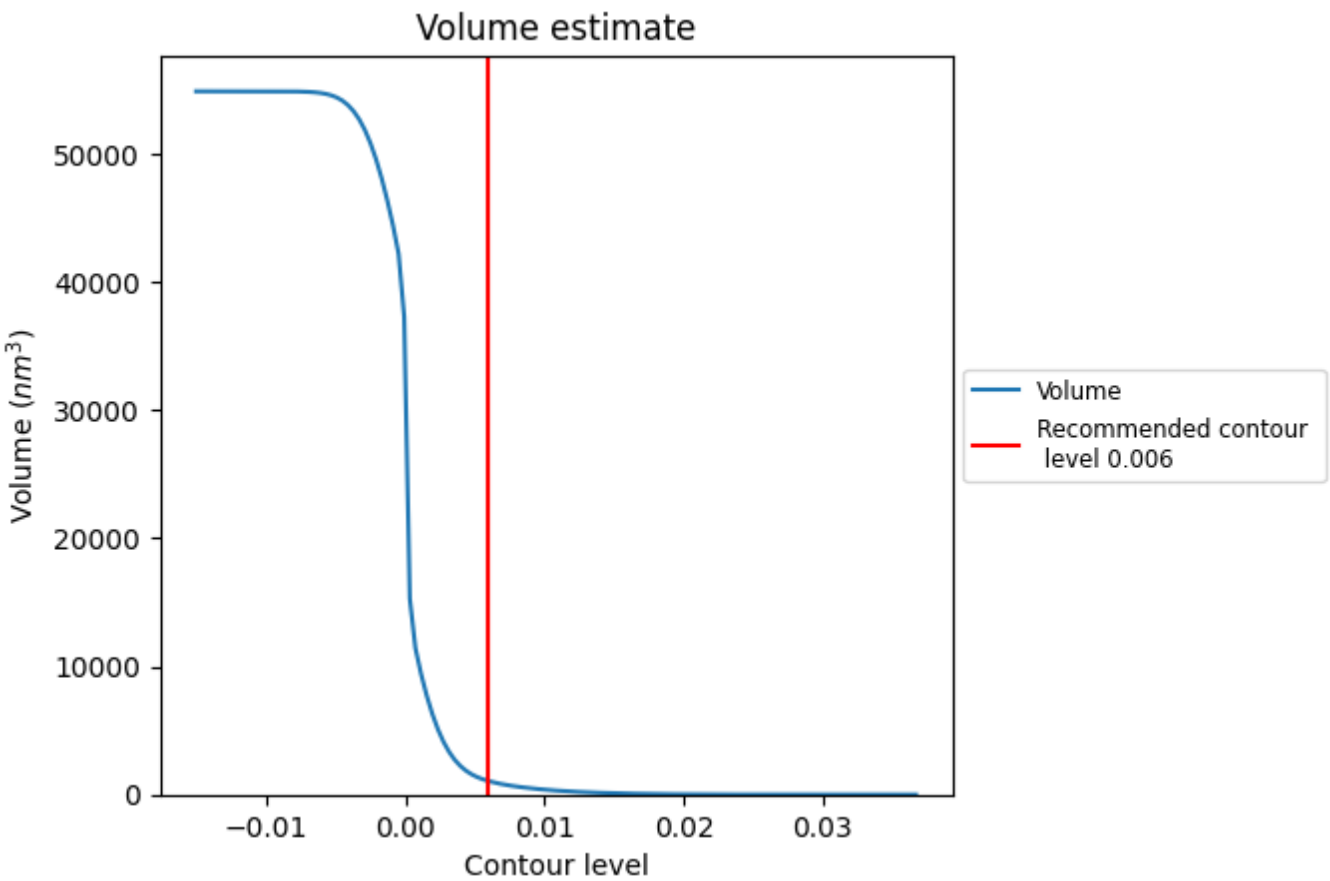
This section contains the results of statistical analysis of the map.

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.

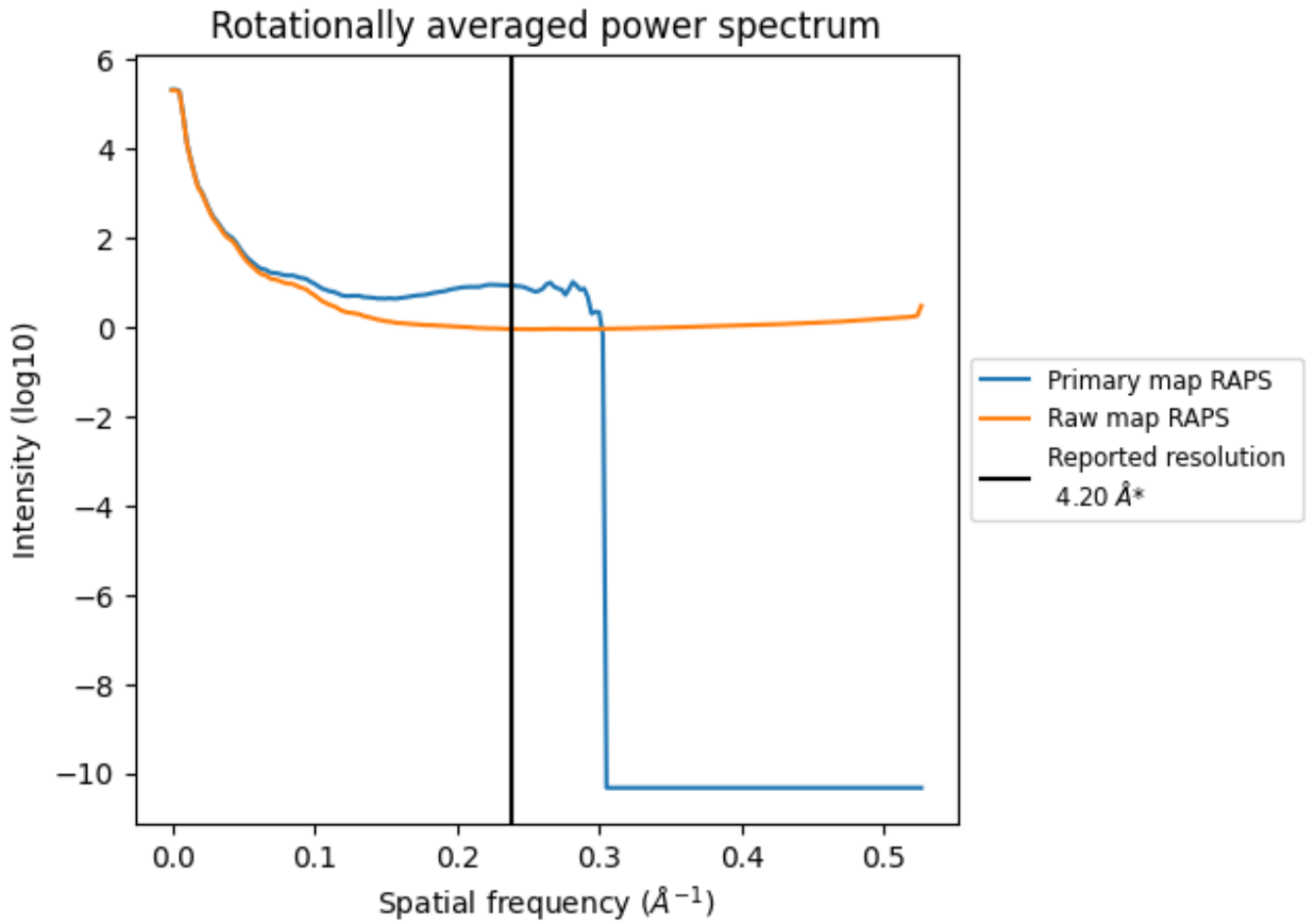
7.2 Volume estimate (i)



The volume at the recommended contour level is 1049 nm^3; this corresponds to an approximate mass of 947 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)

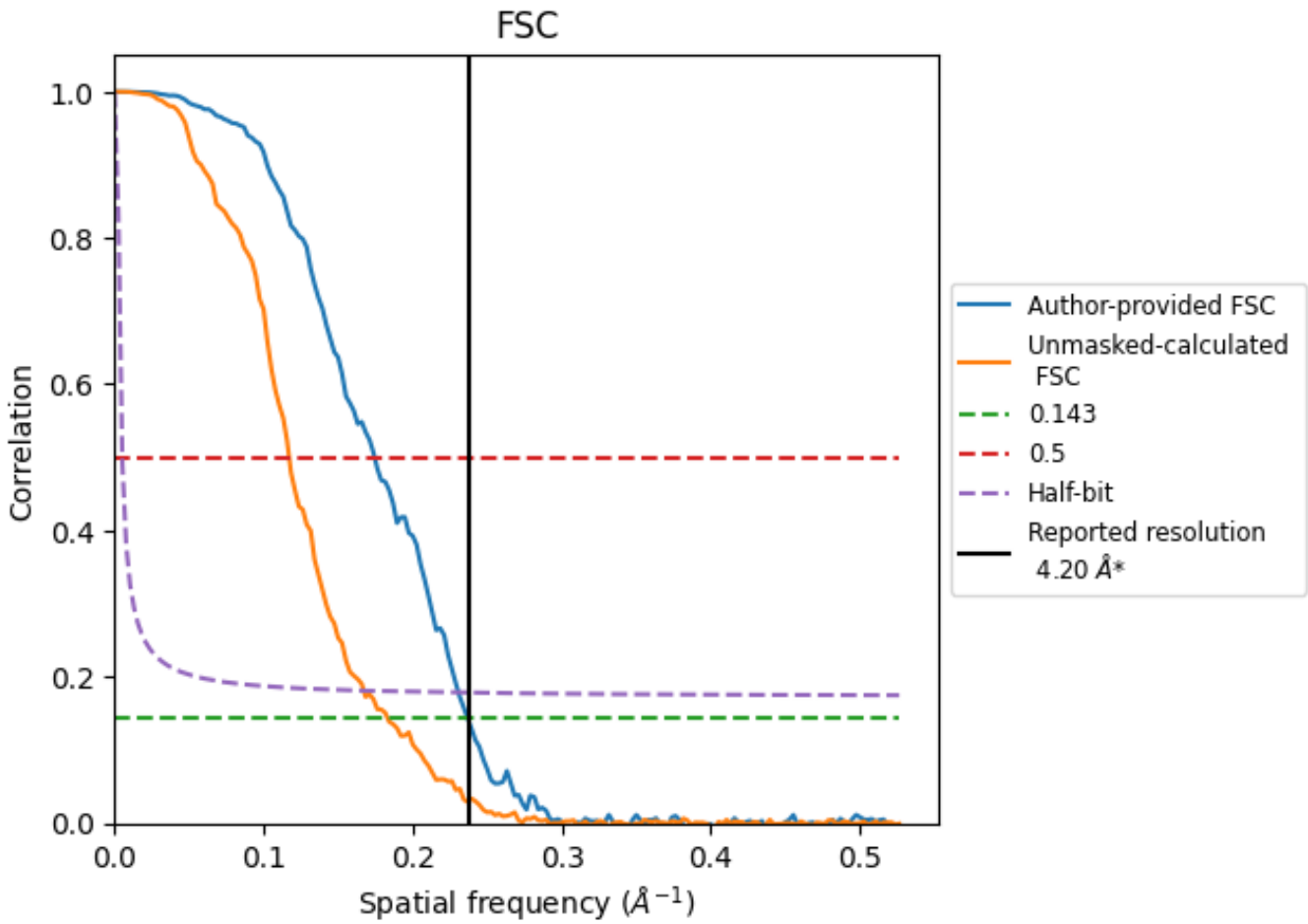


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

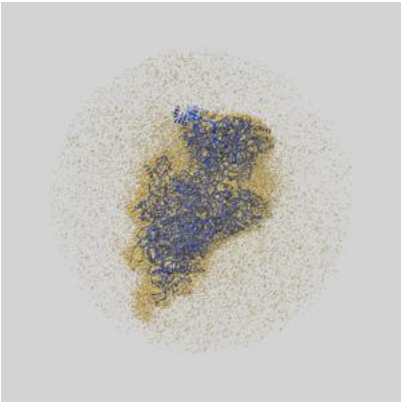
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.22	5.73	4.33
Unmasked-calculated*	5.46	8.54	5.98

*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 5.46 differs from the reported value 4.2 by more than 10 %

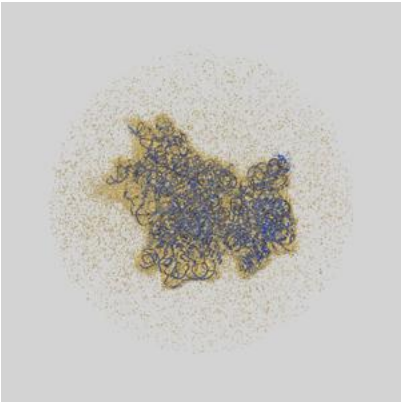
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25531 and PDB model 7SYK. Per-residue inclusion information can be found in section 3 on page 12.

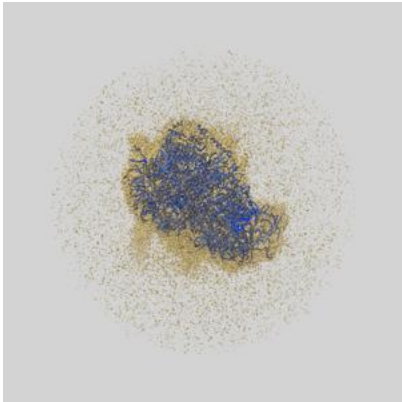
9.1 Map-model overlay (i)



X



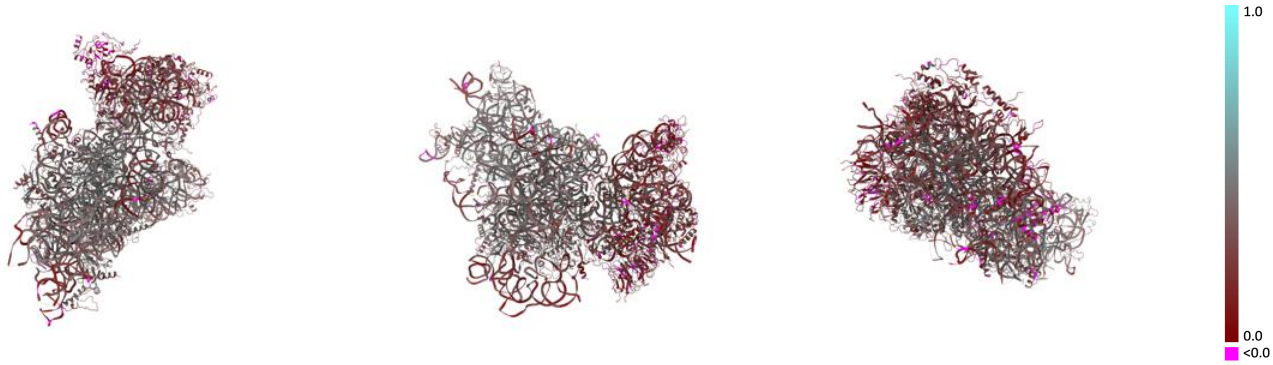
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

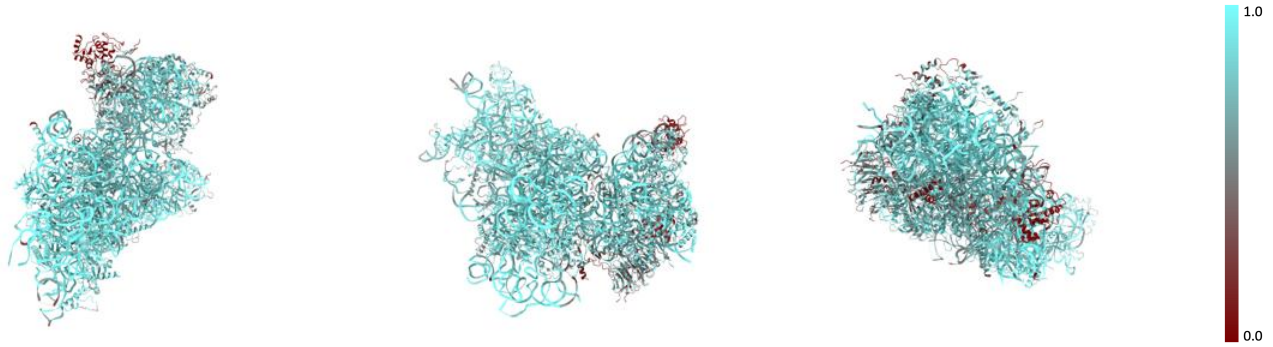
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

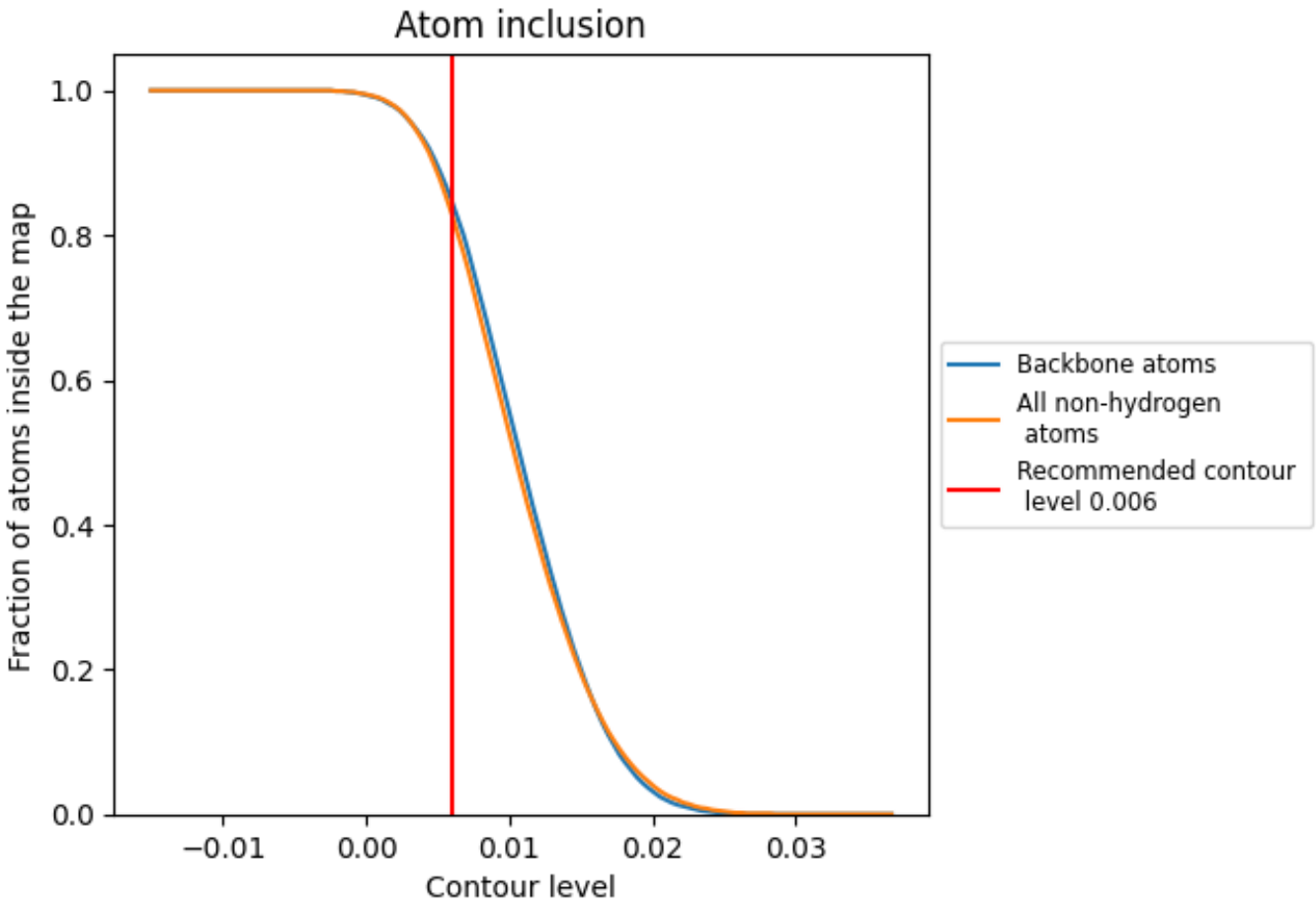
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.3360
2	0.9190	0.3530
B	0.7900	0.3880
C	0.8610	0.3700
D	0.7890	0.4020
E	0.6010	0.2660
F	0.8860	0.4310
G	0.7220	0.2370
H	0.8570	0.3670
I	0.7140	0.3730
J	0.8920	0.3990
K	0.8680	0.4080
L	0.5810	0.2100
M	0.8120	0.4230
N	0.0850	0.1010
O	0.8590	0.4120
P	0.9130	0.3740
Q	0.6890	0.2070
R	0.7380	0.2880
S	0.5850	0.2860
T	0.6910	0.2120
U	0.8240	0.2550
V	0.4250	0.2510
W	0.8170	0.4070
X	0.7990	0.4450
Y	0.8750	0.4400
Z	0.9310	0.4070
a	0.5330	0.1980
b	0.8520	0.4060
c	0.8090	0.4090
d	0.6100	0.2830
e	0.6960	0.2850
f	0.6390	0.2660
g	0.1590	0.1550
h	0.5790	0.1890

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
n	0.8210	0.3830
z	0.8600	0.2310