



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:29 AM UTC

PDB ID : 7SYQ / pdb_00007syq
EMDB ID : EMD-25537
Title : Structure of the wt IRES and 40S ribosome ternary complex, open conformation. Structure 11(wt)
Authors : Brown, Z.P.; Abaeva, I.S.; De, S.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on : 2021-11-25
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

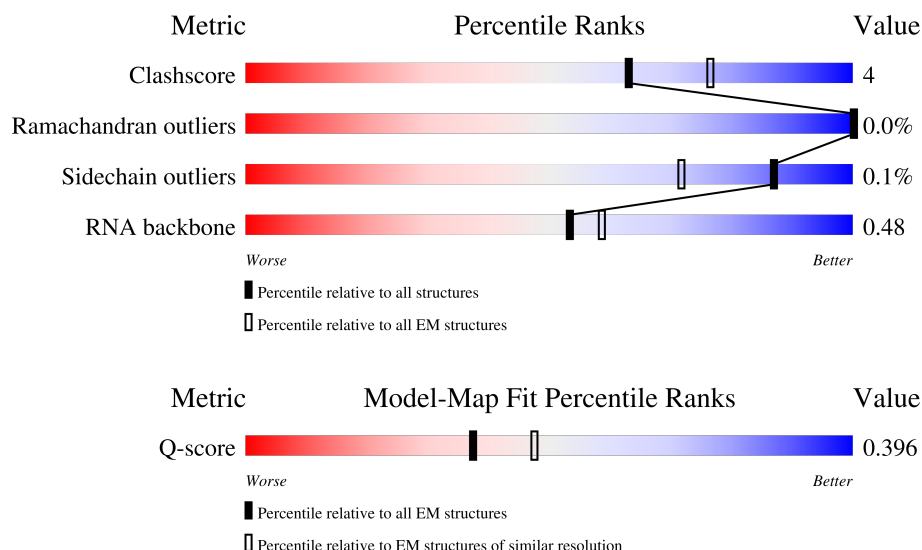
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



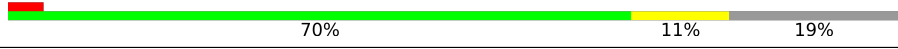
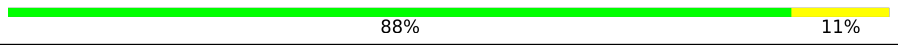
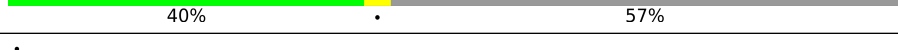
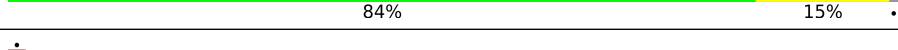
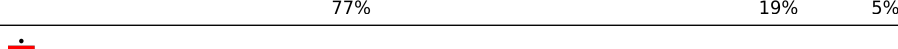
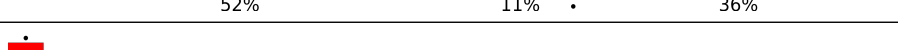
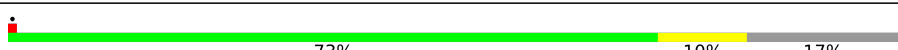
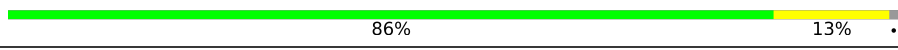
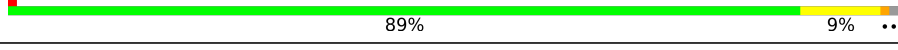
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	2	1870	
2	A	144	
3	B	295	

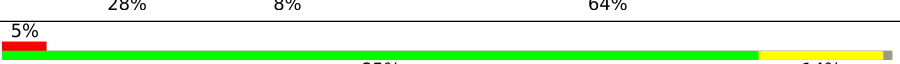
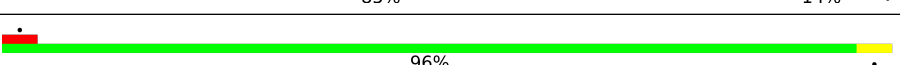
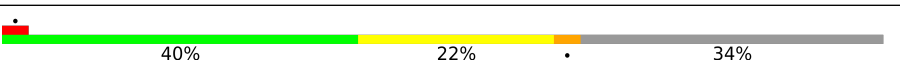
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Mol	Chain	Length	Quality of chain
4	C	264	
5	D	221	
6	E	281	
7	F	263	
8	G	204	
9	H	249	
10	I	432	
11	J	208	
12	K	194	
13	L	149	
14	M	158	
15	N	132	
16	O	151	
17	P	168	
18	Q	145	
19	R	172	
20	S	135	
21	T	152	
22	U	145	
23	V	119	
24	W	83	
25	X	130	
26	Y	143	
27	Z	131	
28	a	124	

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Mol	Chain	Length	Quality of chain
29	b	101	
30	c	84	
31	d	69	
32	e	56	
33	f	133	
34	g	188	
35	h	317	
36	n	25	
37	z	400	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 81427 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
1	2	1680	Total	C	N	O	P	0	0
			35864	16009	6439	11737	1679		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	101	Total	C	N	O	S	0	0
			816	514	146	152	4		

- Molecule 3 is a protein called uS2 (SA).

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is a protein called eS1.

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

- Molecule 5 is a protein called uS5.

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

- Molecule 6 is a protein called uS3.

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

- Molecule 7 is a protein called eS4 (S4 X isoform).

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

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 8 is a protein called uS7.

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

- Molecule 9 is a protein called eS6.

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

- Molecule 10 is a protein called eS7.

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

- Molecule 11 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 12 is a protein called uS4.

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

- Molecule 13 is a protein called eS10.

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

- Molecule 14 is a protein called uS17.

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

- Molecule 15 is a protein called eS12.

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

- Molecule 16 is a protein called uS15.

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

- Molecule 17 is a protein called uS11.

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

- Molecule 18 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 19 is a protein called uS9.

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

- Molecule 20 is a protein called eS17.

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

- Molecule 21 is a protein called uS13.

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

- Molecule 22 is a protein called eS19.

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

- Molecule 23 is a protein called uS10.

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

- Molecule 24 is a protein called eS21.

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

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
W	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 25 is a protein called uS8.

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

- Molecule 26 is a protein called uS12.

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

- Molecule 27 is a protein called eS24.

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

- Molecule 28 is a protein called eS25.

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

- Molecule 29 is a protein called eS26.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	28	ARG	CYS	conflict	UNP G1TFE8

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Chain	Residue	Modelled	Actual	Comment	Reference
b	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 30 is a protein called eS27.

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

- Molecule 31 is a protein called eS28.

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

- Molecule 32 is a protein called uS14.

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

- Molecule 33 is a protein called eS30.

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

- Molecule 34 is a protein called eS31.

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

- Molecule 35 is a protein called Receptor for Activated C Kinase 1 (RACK1).

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

- Molecule 36 is a protein called eL41.

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

- Molecule 37 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	z	264	Total	C	N	O	P	0	0
			5637	2512	1009	1852	264		

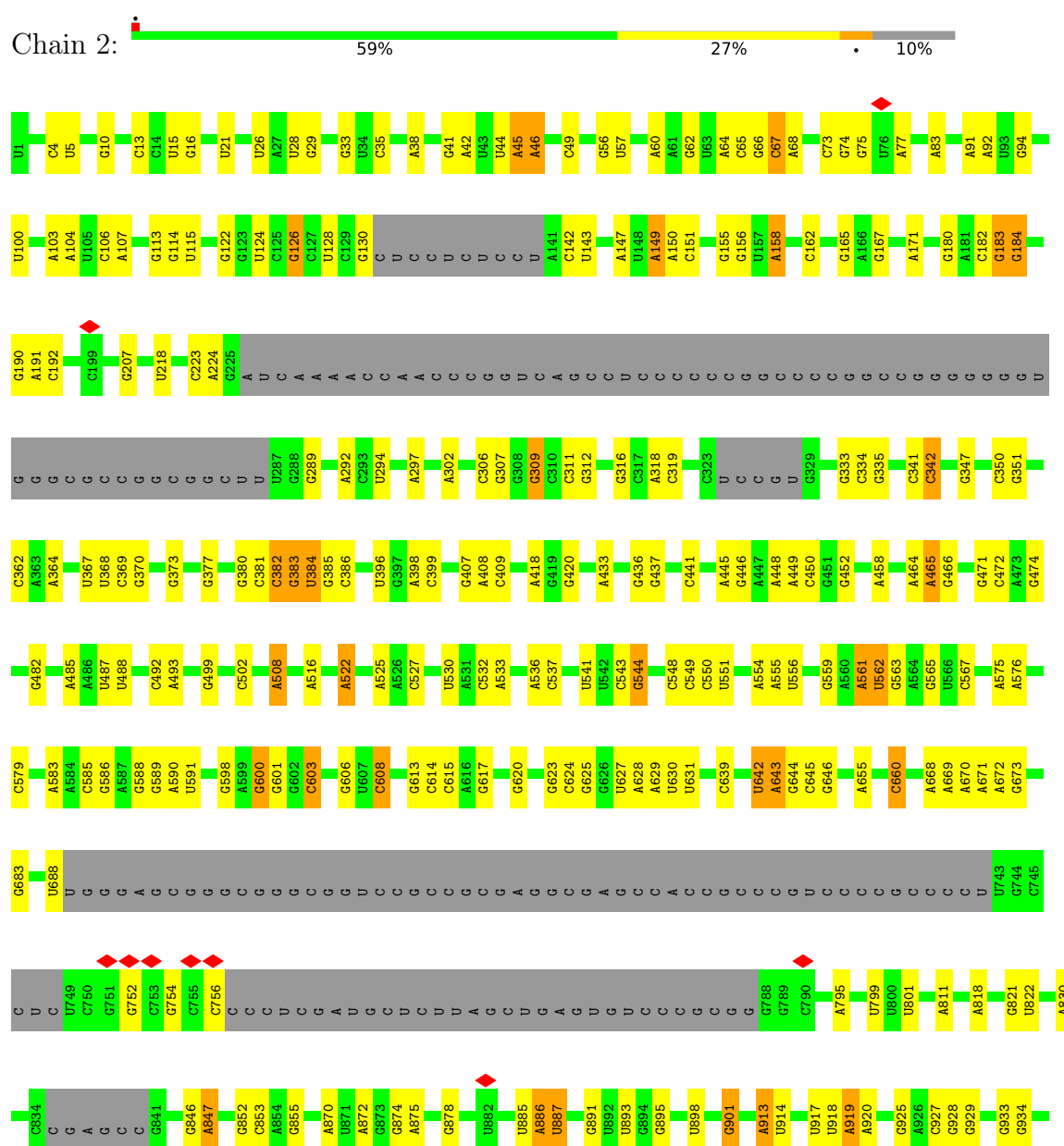
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

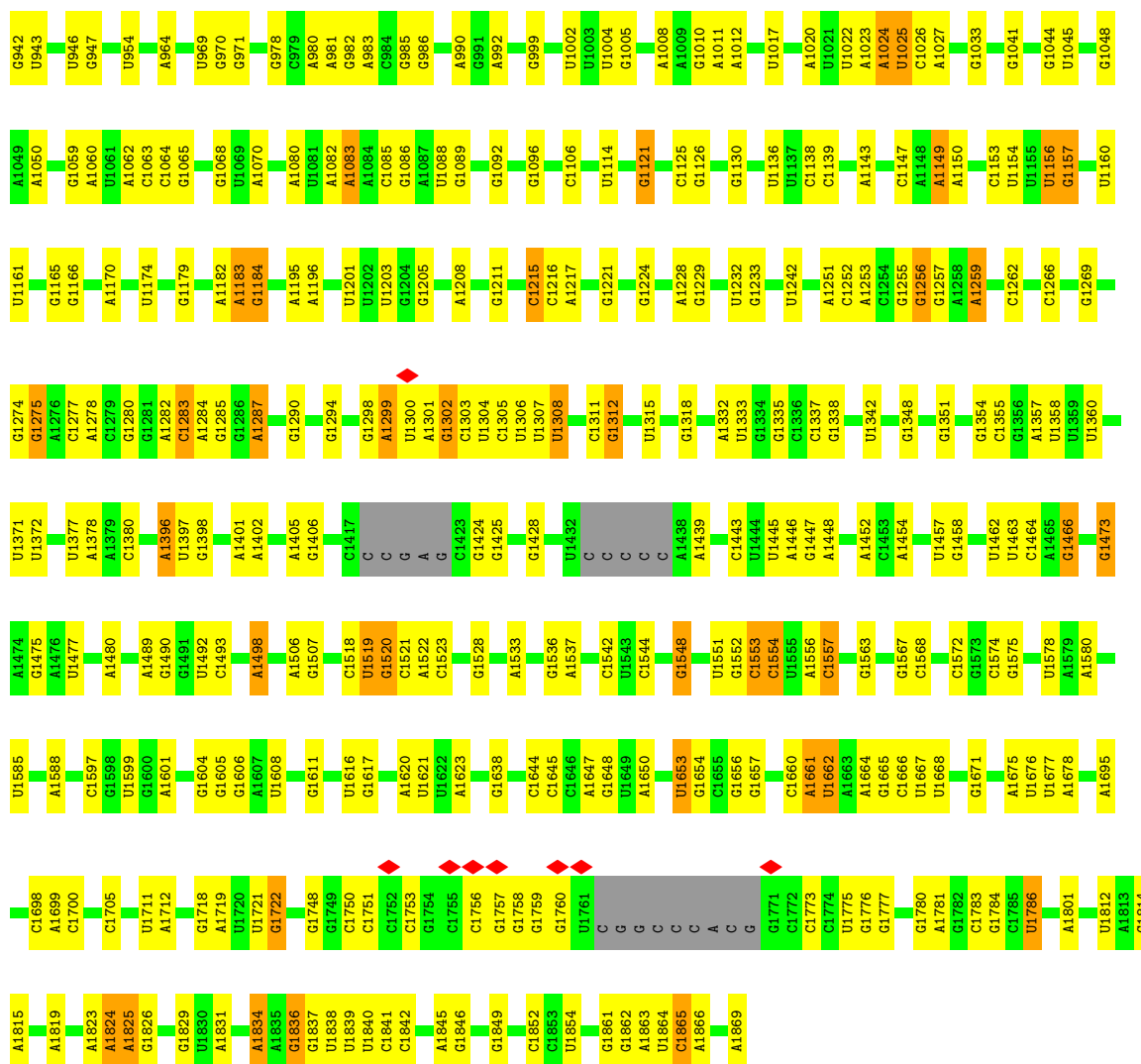
Mol	Chain	Residues	Atoms		AltConf
38	b	1	Total	Zn	0
			1	1	
38	g	1	Total	Zn	0
			1	1	

3 Residue-property plots

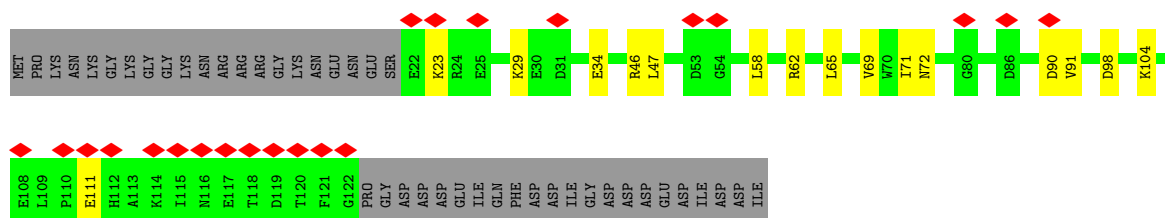
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



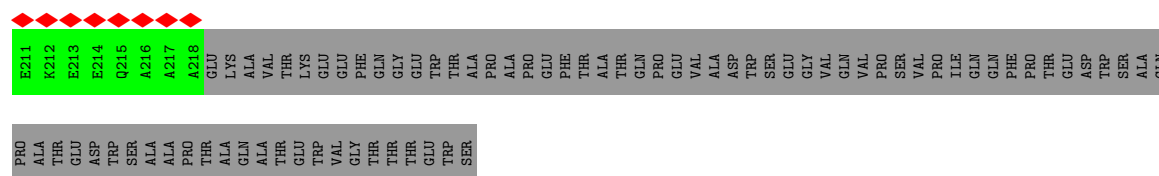


• Molecule 2: Eukaryotic translation initiation factor 1A, X-chromosomal

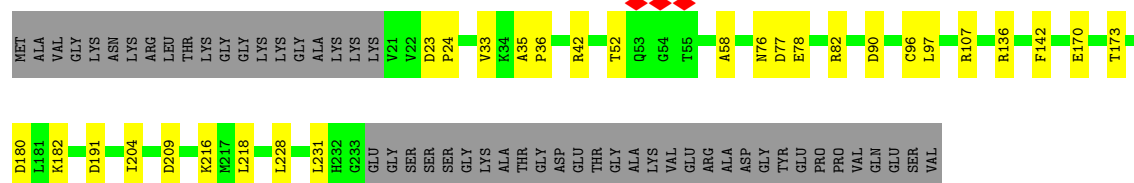


• Molecule 3: uS2 (SA)

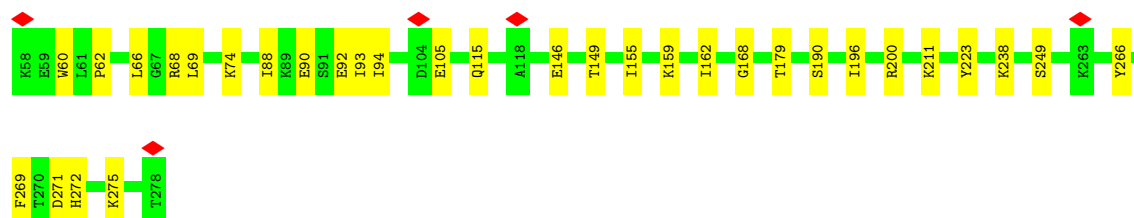
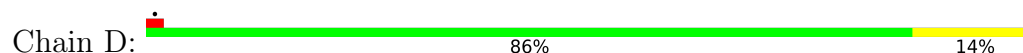




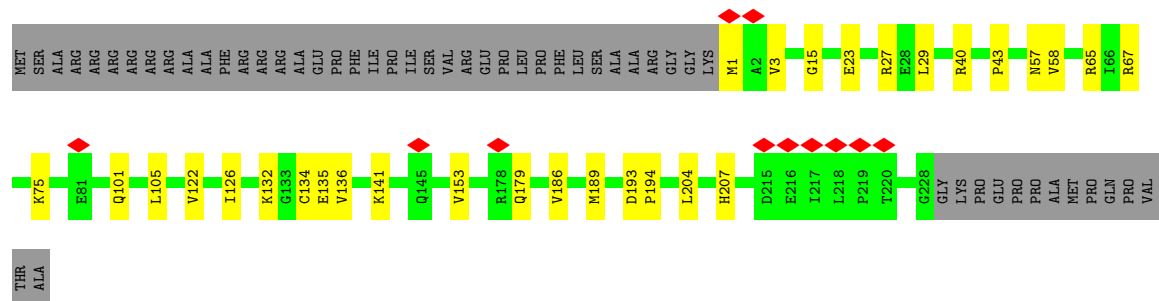
- Molecule 4: eS1



- Molecule 5: uS5



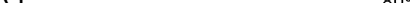
- Molecule 6: uS3



- Molecule 7: eS4 (S4 X isoform)



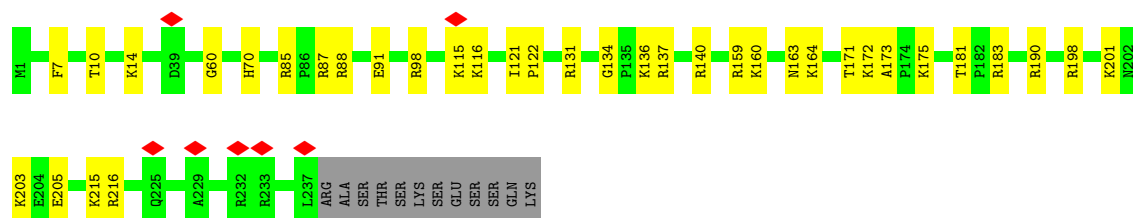
- Molecule 8: uS7

Chain G:  80% 14% 6%

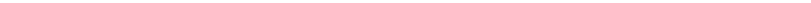


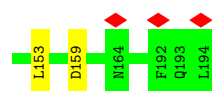
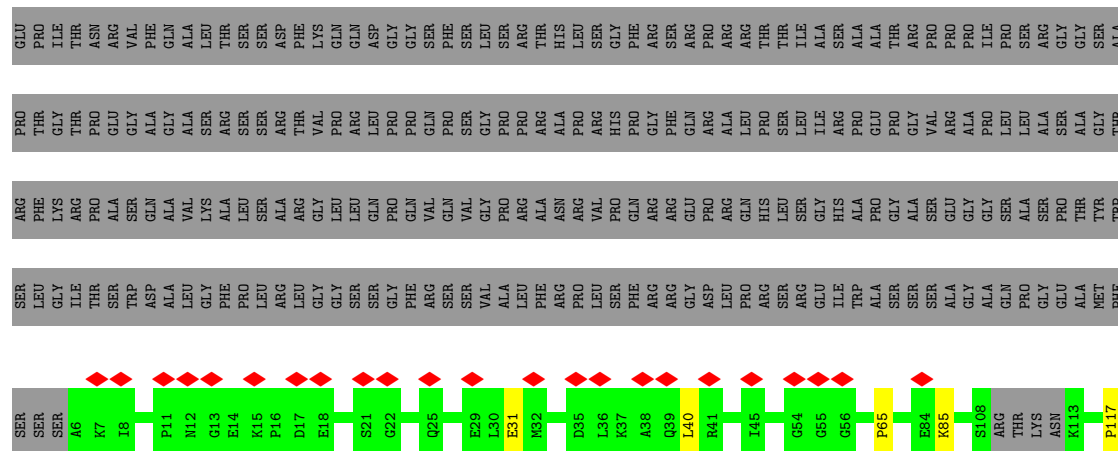
- Molecule 9: eS6

Chain H: 81% 14% 5%

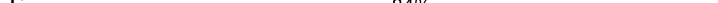


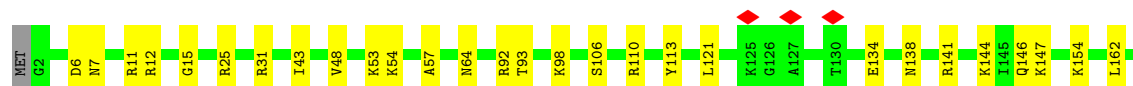
- Molecule 10: eS7

Chain I:  6% 40% 57%



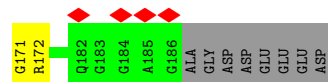
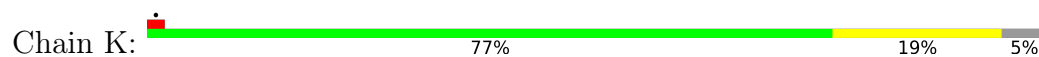
- Molecule 11: eS8

Chain J:  84% 15%

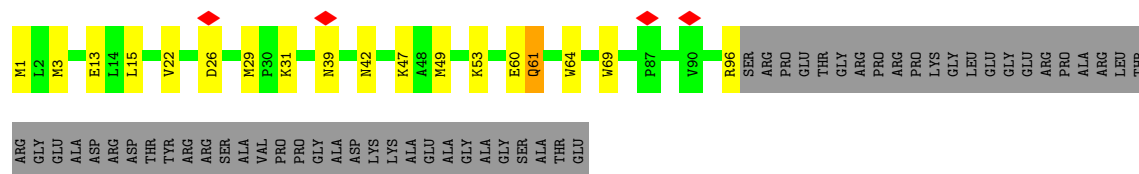




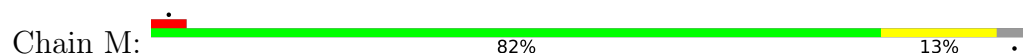
• Molecule 12: uS4



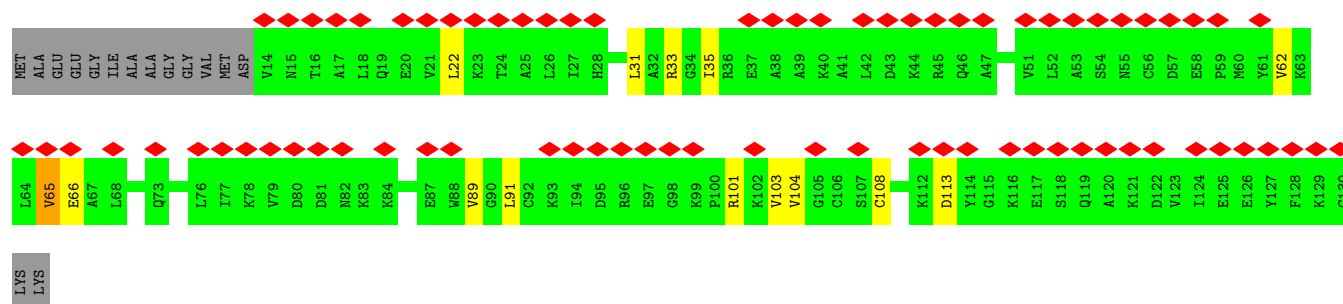
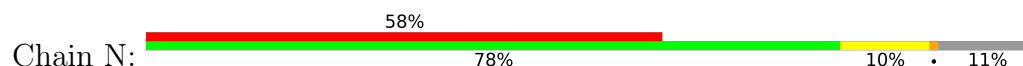
• Molecule 13: eS10



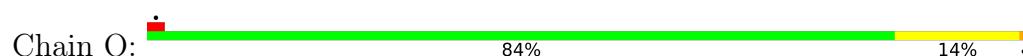
• Molecule 14: uS17



• Molecule 15: eS12

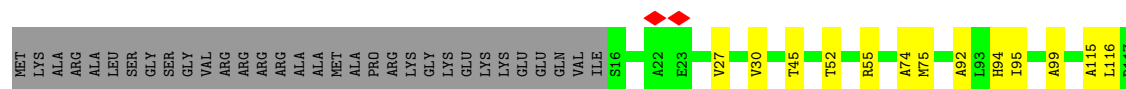


• Molecule 16: uS15

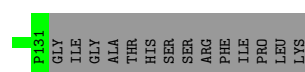
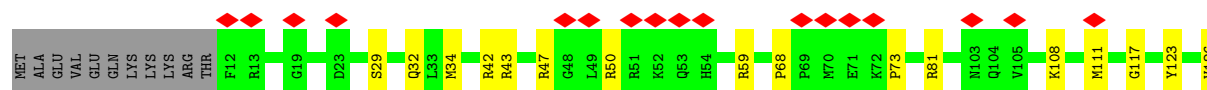
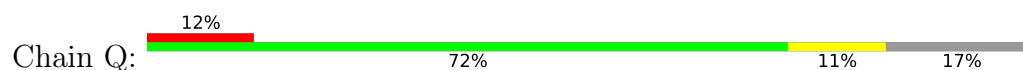




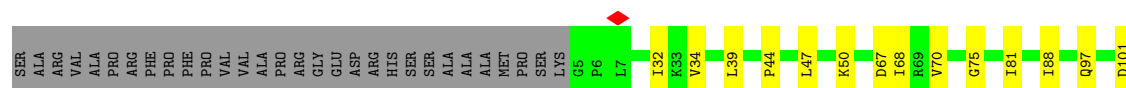
• Molecule 17: uS11



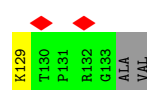
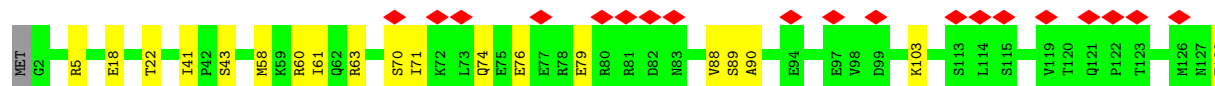
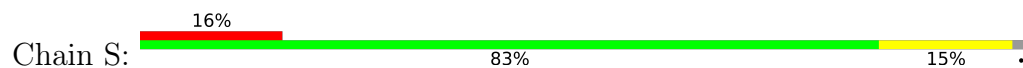
• Molecule 18: uS19



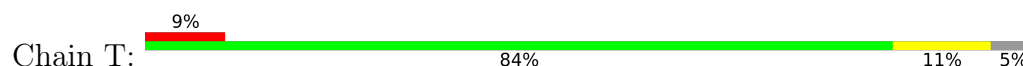
• Molecule 19: uS9

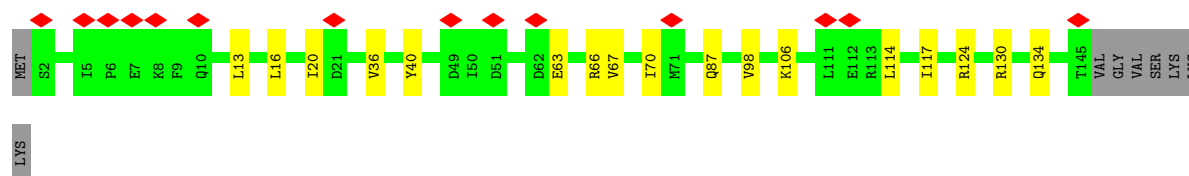


• Molecule 20: eS17

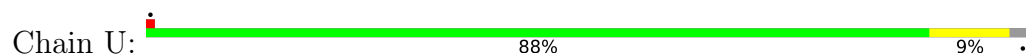


• Molecule 21: uS13

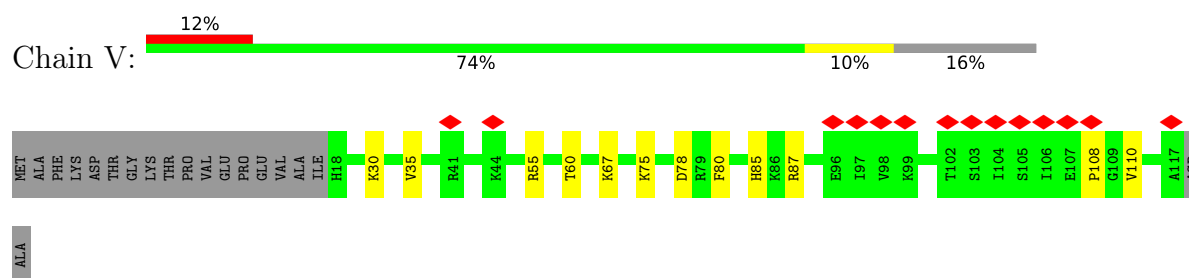




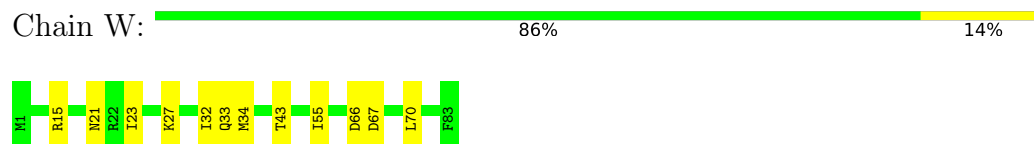
- Molecule 22: eS19



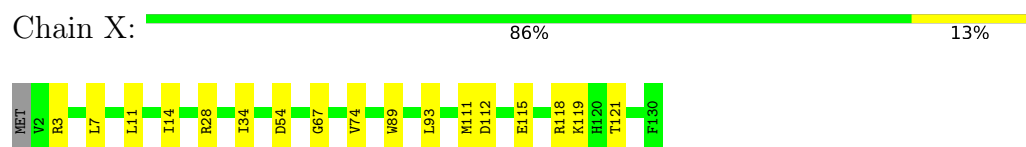
- Molecule 23: uS10



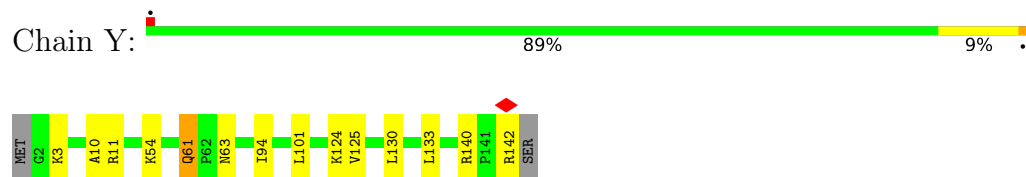
- Molecule 24: eS21



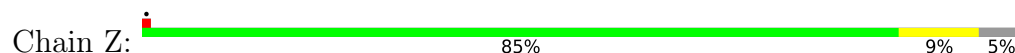
- Molecule 25: uS8



- Molecule 26: uS12

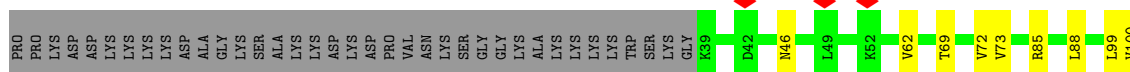


- Molecule 27: eS24

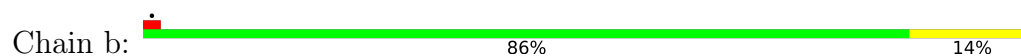




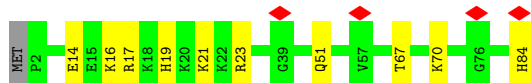
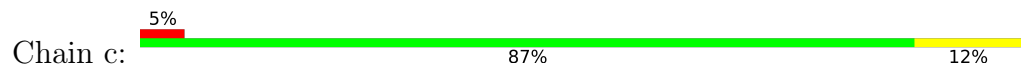
• Molecule 28: eS25



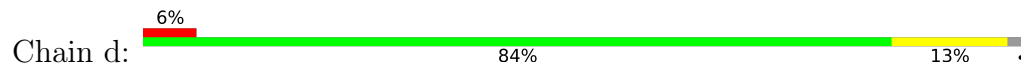
• Molecule 29: eS26



• Molecule 30: eS27



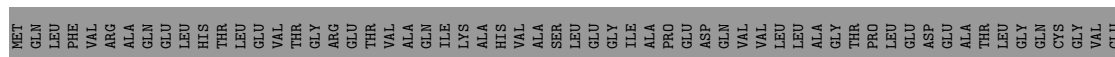
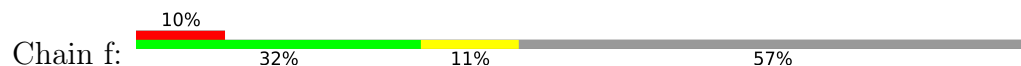
• Molecule 31: eS28

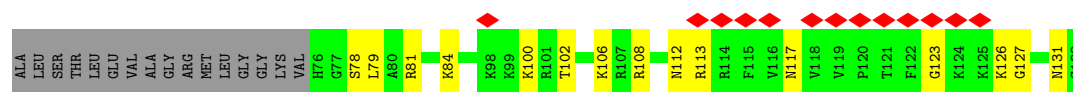


• Molecule 32: uS14

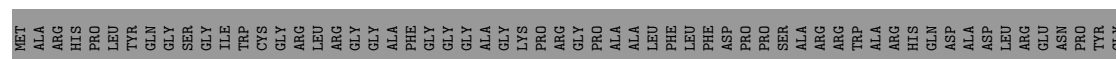


• Molecule 33: eS30

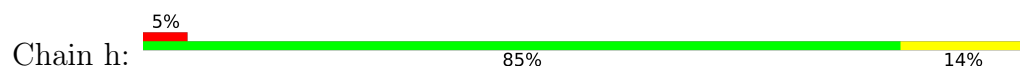




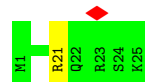
• Molecule 34: eS31



• Molecule 35: Receptor for Activated C Kinase 1 (RACK1)



• Molecule 36: eL41



• Molecule 37: HCV IRES





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	204782	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 ($e^-/\text{\AA}^2$)	70.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	56000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	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 ⓘ

5.1 Standard geometry ⓘ

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	0.14	0/40102	0.31	0/62495
2	A	0.37	0/827	0.67	0/1106
3	B	0.19	0/1747	0.49	0/2374
4	C	0.28	1/1756 (0.1%)	0.60	5/2350 (0.2%)
5	D	0.19	0/1753	0.53	0/2369
6	E	0.20	0/1796	0.49	3/2417 (0.1%)
7	F	0.16	0/2118	0.43	0/2849
8	G	0.21	0/1531	0.53	0/2059
9	H	0.16	0/1946	0.40	0/2590
10	I	0.19	0/1510	0.53	2/2022 (0.1%)
11	J	0.18	0/1715	0.45	0/2287
12	K	0.20	0/1550	0.48	0/2069
13	L	0.22	0/834	0.56	1/1125 (0.1%)
14	M	0.17	0/1254	0.46	0/1677
15	N	0.21	0/918	0.54	3/1233 (0.2%)
16	O	0.23	0/1226	0.55	1/1649 (0.1%)
17	P	0.17	0/1029	0.46	0/1380
18	Q	0.19	0/1017	0.49	0/1358
19	R	0.18	0/1146	0.45	0/1534
20	S	0.21	0/1082	0.57	0/1452
21	T	0.22	0/1208	0.59	2/1618 (0.1%)
22	U	0.16	0/1115	0.39	0/1493
23	V	0.17	0/805	0.41	0/1081
24	W	0.18	0/643	0.51	0/860
25	X	0.19	0/1051	0.47	0/1406
26	Y	0.18	0/1116	0.51	0/1490
27	Z	0.20	0/1028	0.56	2/1366 (0.1%)
28	a	0.37	1/620 (0.2%)	0.55	0/831
29	b	0.16	0/828	0.37	0/1109
30	c	0.16	0/665	0.39	0/891
31	d	0.15	0/532	0.41	0/712
32	e	0.15	0/470	0.38	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.16	0/462	0.47	0/607
34	g	0.10	0/567	0.29	0/753
35	h	0.17	0/2493	0.46	0/3394
36	n	0.18	0/240	0.48	0/305
37	z	0.15	0/6299	0.29	0/9818
All	All	0.17	2/86999 (0.0%)	0.40	19/126752 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	1
26	Y	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	62	VAL	C-N	7.75	1.41	1.33
4	C	36	PRO	CG-CD	-7.30	1.25	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	36	PRO	N-CD-CG	-9.55	88.87	103.20
4	C	24	PRO	CA-N-CD	-9.01	99.38	112.00
4	C	36	PRO	CA-N-CD	-7.05	102.14	112.00
27	Z	52	PRO	CA-N-CD	-6.75	102.55	112.00
10	I	65	PRO	CA-C-N	6.20	125.29	120.33
10	I	65	PRO	C-N-CA	6.20	125.29	120.33
13	L	13	GLU	N-CA-CB	5.92	120.05	110.40
4	C	78	GLU	CA-CB-CG	5.57	125.24	114.10
15	N	66	GLU	N-CA-CB	5.54	119.43	110.40
6	E	43	PRO	CA-C-N	5.39	131.02	122.61
6	E	43	PRO	C-N-CA	5.39	131.02	122.61
16	O	136	PRO	CA-N-CD	-5.34	104.53	112.00
4	C	24	PRO	N-CD-CG	-5.30	95.25	103.20
27	Z	42	GLU	N-CA-CB	5.30	119.03	110.40
21	T	16	LEU	CA-C-N	5.19	131.46	121.54
21	T	16	LEU	C-N-CA	5.19	131.46	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	194	PRO	CA-N-CD	-5.06	104.91	112.00
15	N	65	VAL	CA-C-N	-5.01	112.36	121.14
15	N	65	VAL	C-N-CA	-5.01	112.36	121.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	195	TRP	Peptide
26	Y	61	GLN	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	35864	0	18113	214	0
2	A	816	0	826	8	0
3	B	1710	0	1708	21	0
4	C	1729	0	1803	16	0
5	D	1716	0	1806	21	0
6	E	1768	0	1866	19	0
7	F	2076	0	2177	21	0
8	G	1509	0	1563	17	0
9	H	1923	0	2089	25	0
10	I	1488	0	1582	7	0
11	J	1686	0	1772	24	0
12	K	1525	0	1640	24	0
13	L	810	0	836	12	0
14	M	1233	0	1310	18	0
15	N	908	0	939	8	0
16	O	1202	0	1289	14	0
17	P	1016	0	1039	15	0
18	Q	997	0	1045	10	0
19	R	1128	0	1195	12	0
20	S	1068	0	1121	15	0
21	T	1190	0	1249	11	0
22	U	1097	0	1130	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	V	795	0	862	10	0
24	W	636	0	637	9	0
25	X	1034	0	1080	11	0
26	Y	1098	0	1167	11	0
27	Z	1011	0	1083	7	0
28	a	614	0	678	7	0
29	b	814	0	863	11	0
30	c	651	0	672	8	0
31	d	530	0	561	7	0
32	e	459	0	452	11	0
33	f	457	0	502	13	0
34	g	555	0	563	10	0
35	h	2436	0	2393	29	0
36	n	239	0	289	1	0
37	z	5637	0	2851	21	0
38	b	1	0	0	0	0
38	g	1	0	0	0	0
All	All	81427	0	62751	572	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 4.

All (572) 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)
1:2:1657:G:H1	1:2:1667:U:H3	1.26	0.83
1:2:16:G:H21	1:2:1195:A:H62	1.35	0.71
1:2:1048:G:H21	1:2:1070:A:H62	1.37	0.71
37:z:262:U:H3	37:z:271:G:H1	1.39	0.71
1:2:1563:G:H1	1:2:1572:C:H42	1.41	0.69
1:2:1656:G:H1	1:2:1668:U:H3	1.39	0.69
1:2:1033:G:H1	1:2:1080:A:HO2'	1.40	0.68
1:2:1287:A:N6	1:2:1312:G:H21	1.92	0.66
1:2:934:G:H1	1:2:1008:A:H2	1.42	0.65
1:2:1722:G:H1	1:2:1812:U:H3	1.45	0.64
19:R:34:VAL:HG12	19:R:70:VAL:HB	1.80	0.64
37:z:61:U:H3	37:z:107:G:H1	1.47	0.63
8:G:201:LYS:HA	8:G:204:ARG:HD3	1.81	0.63
1:2:1287:A:H62	1:2:1312:G:N2	1.96	0.62
1:2:318:A:N1	1:2:333:G:C6	2.67	0.62
17:P:30:VAL:HG12	17:P:94:HIS:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1287:A:H62	1:2:1312:G:H21	1.47	0.62
22:U:124:THR:HG23	22:U:127:GLY:H	1.65	0.61
25:X:3:ARG:HH12	25:X:28:ARG:HH21	1.48	0.61
24:W:32:ILE:HD12	24:W:55:ILE:HB	1.82	0.60
1:2:565:G:H22	1:2:586:G:H1'	1.67	0.60
1:2:1161:U:O4	26:Y:3:LYS:NZ	2.34	0.60
6:E:75:LYS:HZ2	13:L:22:VAL:H	1.48	0.60
12:K:18:ARG:O	12:K:24:ARG:NH2	2.34	0.59
1:2:1351:G:H1	1:2:1360:U:H3	1.50	0.58
9:H:137:ARG:HB3	9:H:140:ARG:HG3	1.85	0.58
1:2:1616:U:OP2	18:Q:43:ARG:NH2	2.36	0.58
1:2:1825:A:N6	2:A:65:LEU:O	2.37	0.58
1:2:1024:A:OP2	16:O:124:ARG:NH1	2.37	0.57
1:2:1653:U:H3	1:2:1671:G:H1	1.52	0.57
1:2:65:C:N4	9:H:134:GLY:O	2.37	0.57
1:2:1705:C:H42	1:2:1829:G:H1	1.52	0.57
1:2:10:G:H1'	5:D:115:GLN:HG2	1.86	0.57
6:E:15:GLY:HA3	32:e:50:ILE:HG23	1.86	0.57
15:N:91:LEU:HB2	15:N:103:VAL:HG13	1.85	0.57
35:h:166:VAL:HG23	35:h:176:VAL:HG22	1.87	0.57
1:2:383:G:H21	14:M:133:PRO:HG3	1.69	0.56
1:2:1174:U:OP1	36:n:21:ARG:NH1	2.38	0.56
14:M:103:GLU:HB2	26:Y:10:ALA:HB3	1.86	0.56
1:2:1308:U:H4'	34:g:118:ARG:HH22	1.69	0.56
1:2:1605:G:OP1	22:U:84:ARG:NH2	2.34	0.56
13:L:61:GLN:HE21	13:L:61:GLN:HA	1.71	0.56
1:2:1719:A:N6	1:2:1814:G:O2'	2.39	0.56
17:P:99:ALA:H	17:P:133:THR:HG22	1.71	0.56
1:2:60:A:HO2'	1:2:316:G:HO2'	1.51	0.56
1:2:818:A:OP1	12:K:80:ARG:NH2	2.38	0.56
29:b:22:ARG:HH21	29:b:27:ALA:HB1	1.70	0.56
1:2:16:G:N2	1:2:1195:A:H62	2.02	0.56
1:2:527:C:H4'	12:K:121:LYS:HD2	1.88	0.56
5:D:200:ARG:O	12:K:54:ARG:NH1	2.39	0.56
1:2:1396:A:O2'	1:2:1398:G:N7	2.39	0.56
1:2:1424:G:H2'	1:2:1425:G:H8	1.70	0.56
4:C:90:ASP:HB2	4:C:228:LEU:HD21	1.87	0.55
14:M:38:LYS:NZ	14:M:64:GLY:O	2.39	0.55
13:L:60:GLU:OE1	13:L:69:TRP:NE1	2.39	0.55
13:L:31:LYS:HE2	13:L:39:ASN:HA	1.88	0.55
35:h:107:ASP:O	35:h:124:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1280:G:OP2	15:N:101:ARG:NH2	2.39	0.55
2:A:104:LYS:NZ	2:A:111:GLU:OE2	2.40	0.55
10:I:31:GLU:HB3	10:I:40:LEU:HD22	1.89	0.55
20:S:71:ILE:HD12	20:S:74:GLN:HA	1.89	0.55
1:2:377:G:H5'	11:J:98:LYS:HB3	1.88	0.55
21:T:36:VAL:HG23	21:T:40:TYR:HD2	1.72	0.55
22:U:13:GLU:HA	22:U:16:ARG:HE	1.72	0.55
1:2:1542:C:OP1	22:U:62:ARG:NH1	2.40	0.55
23:V:80:PHE:HB3	32:e:52:PHE:HB3	1.89	0.55
1:2:603:C:N4	1:2:620:G:O6	2.40	0.55
1:2:1048:G:N2	1:2:1070:A:H62	2.05	0.55
1:2:1275:G:N2	1:2:1506:A:OP2	2.39	0.55
1:2:1553:C:H41	32:e:22:ARG:HH21	1.55	0.55
33:f:123:GLY:HA3	37:z:353:U:H4'	1.88	0.55
35:h:120:ILE:HB	35:h:132:TRP:HB2	1.88	0.54
3:B:198:MET:HE1	20:S:89:SER:HA	1.88	0.54
13:L:15:LEU:HD22	13:L:49:MET:HE1	1.89	0.54
17:P:142:ARG:NH2	29:b:26:CYS:O	2.40	0.54
8:G:59:LYS:HB2	8:G:62:ARG:HG3	1.89	0.54
1:2:927:C:O2	30:c:51:GLN:NE2	2.40	0.54
1:2:1475:G:OP2	1:2:1475:G:N2	2.38	0.54
15:N:22:LEU:HD21	15:N:89:VAL:HA	1.87	0.54
1:2:1447:G:OP1	23:V:85:HIS:ND1	2.41	0.54
30:c:16:LYS:HA	30:c:23:ARG:HH21	1.73	0.54
1:2:1147:C:OP1	29:b:6:ARG:NH1	2.41	0.54
14:M:104:LYS:O	26:Y:11:ARG:NH2	2.39	0.54
18:Q:68:PRO:HG2	18:Q:73:PRO:HA	1.89	0.54
1:2:1854:U:OP1	17:P:150:ARG:NH2	2.41	0.53
17:P:95:ILE:HD11	17:P:126:ILE:HD12	1.89	0.53
21:T:98:VAL:HG21	21:T:106:LYS:HD2	1.90	0.53
1:2:158:A:N6	1:2:466:G:N7	2.53	0.53
1:2:223:C:H2'	1:2:224:A:H8	1.74	0.53
25:X:11:LEU:HA	25:X:14:ILE:HG22	1.90	0.53
35:h:18:VAL:HA	35:h:35:SER:HA	1.91	0.53
1:2:218:U:O2	11:J:184:ARG:NH2	2.38	0.53
1:2:396:U:OP1	14:M:108:ASN:ND2	2.42	0.53
1:2:1083:A:N7	1:2:1841:C:O2'	2.39	0.53
1:2:913:A:N6	10:I:119:SER:O	2.41	0.53
35:h:9:GLY:O	35:h:308:ARG:NH1	2.42	0.53
1:2:21:U:O2	12:K:17:ARG:NH1	2.42	0.53
1:2:167:G:O2'	9:H:131:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:62:VAL:HA	15:N:65:VAL:HG12	1.91	0.53
26:Y:94:ILE:HG13	26:Y:125:VAL:HG21	1.91	0.53
34:g:149:CYS:SG	34:g:150:PHE:N	2.81	0.53
17:P:74:ALA:HB1	17:P:115:ALA:HB2	1.90	0.52
19:R:97:GLN:OE1	35:h:60:ARG:NH1	2.42	0.52
4:C:52:THR:HG22	4:C:58:ALA:H	1.74	0.52
4:C:107:ARG:NH1	17:P:131:ASP:O	2.42	0.52
1:2:1106:C:H5''	30:c:70:LYS:HD2	1.91	0.52
1:2:1599:U:OP2	28:a:46:ASN:ND2	2.42	0.52
10:I:117:PRO:HG2	10:I:120:ARG:HD3	1.92	0.52
1:2:954:U:O2	17:P:55:ARG:NH2	2.42	0.52
1:2:224:A:H61	1:2:297:A:H61	1.58	0.52
1:2:318:A:C2	1:2:333:G:C2	2.97	0.52
1:2:1299:A:O3'	18:Q:59:ARG:NH1	2.40	0.52
1:2:1608:U:OP1	21:T:130:ARG:NH2	2.42	0.52
1:2:334:C:OP2	9:H:190:ARG:NH2	2.42	0.52
5:D:146:GLU:HB3	5:D:149:THR:HG22	1.92	0.52
18:Q:81:ARG:NH2	18:Q:117:GLY:O	2.43	0.52
34:g:141:CYS:SG	34:g:144:CYS:HB2	2.49	0.52
16:O:69:ASN:HD22	16:O:73:ARG:HB2	1.74	0.52
35:h:292:SER:HB2	35:h:297:THR:H	1.75	0.52
1:2:67:C:H41	9:H:164:LYS:H	1.58	0.52
1:2:1012:A:OP1	16:O:3:ARG:NH1	2.43	0.52
1:2:1597:C:OP2	28:a:85:ARG:NH2	2.43	0.52
1:2:1834:A:H2	1:2:1837:G:H1	1.56	0.52
37:z:68:G:N7	37:z:100:G:N2	2.58	0.52
1:2:1156:U:H2'	1:2:1157:G:H21	1.76	0.51
1:2:124:U:OP1	9:H:201:LYS:NZ	2.43	0.51
1:2:1130:G:N2	1:2:1130:G:OP2	2.44	0.51
8:G:187:SER:OG	8:G:188:TYR:N	2.44	0.51
18:Q:108:LYS:HB2	18:Q:111:MET:HE3	1.92	0.51
1:2:516:A:N1	1:2:643:A:O2'	2.40	0.51
4:C:142:PHE:HB2	4:C:209:ASP:HB2	1.93	0.51
8:G:16:ASP:N	8:G:16:ASP:OD1	2.43	0.51
17:P:116:LEU:HD22	29:b:45:VAL:HG11	1.92	0.51
1:2:1302:G:N2	1:2:1305:C:OP2	2.44	0.51
29:b:38:LYS:HB3	29:b:71:LEU:HB2	1.91	0.51
1:2:289:G:OP1	7:F:155:LYS:NZ	2.42	0.51
1:2:683:G:N1	1:2:1022:U:OP2	2.41	0.51
14:M:112:HIS:HB3	14:M:141:ASN:ND2	2.26	0.51
26:Y:130:LEU:HA	26:Y:133:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1179:G:N2	1:2:1182:A:OP2	2.44	0.51
1:2:615:C:O2	33:f:84:LYS:NZ	2.43	0.51
12:K:21:GLU:OE1	12:K:23:SER:N	2.43	0.51
34:g:119:ARG:HH22	34:g:148:TYR:HB2	1.76	0.51
6:E:58:VAL:HA	6:E:65:ARG:HH21	1.76	0.51
6:E:135:GLU:HG3	6:E:153:VAL:HG12	1.92	0.51
6:E:136:VAL:HG22	6:E:186:VAL:HG23	1.92	0.51
1:2:151:C:OP1	27:Z:120:THR:OG1	2.29	0.51
5:D:94:ILE:HD12	5:D:162:ILE:HD11	1.93	0.51
1:2:126:G:OP1	9:H:198:ARG:NH1	2.43	0.50
1:2:1677:U:H2'	1:2:1678:A:H8	1.76	0.50
4:C:23:ASP:N	4:C:23:ASP:OD1	2.44	0.50
9:H:88:ARG:HB3	9:H:91:GLU:HB3	1.92	0.50
15:N:35:ILE:HG22	15:N:108:CYS:HB3	1.91	0.50
14:M:59:LYS:HG2	14:M:134:LEU:HD22	1.93	0.50
37:z:307:G:H1	37:z:329:U:H3	1.59	0.50
3:B:2:SER:N	3:B:56:GLU:OE1	2.44	0.50
7:F:45:ILE:HG13	7:F:61:VAL:HG11	1.92	0.50
35:h:158:PRO:HG2	35:h:202:PRO:HA	1.93	0.50
1:2:1050:A:H62	1:2:1068:G:H21	1.60	0.50
3:B:7:VAL:HG13	3:B:8:LEU:HG	1.94	0.50
8:G:88:MET:HG3	8:G:91:ARG:HH21	1.77	0.50
11:J:11:ARG:NH1	11:J:15:GLY:O	2.45	0.50
35:h:107:ASP:OD1	35:h:107:ASP:N	2.44	0.50
28:a:73:VAL:HG21	28:a:88:LEU:HD11	1.93	0.50
37:z:258:G:N2	37:z:274:A:OP2	2.44	0.50
1:2:600:G:H2'	1:2:601:G:H8	1.76	0.50
1:2:1304:U:O2	34:g:90:LYS:NZ	2.44	0.50
9:H:115:LYS:NZ	9:H:116:LYS:O	2.44	0.50
19:R:67:ASP:N	19:R:67:ASP:OD1	2.44	0.50
1:2:1866:A:OP1	29:b:95:ARG:NH2	2.44	0.50
37:z:135:G:O2'	37:z:297:U:OP1	2.30	0.50
1:2:1617:G:N2	1:2:1620:A:OP2	2.41	0.50
1:2:309:G:OP2	11:J:53:LYS:NZ	2.40	0.49
1:2:1121:G:O2'	4:C:204:ILE:O	2.30	0.49
3:B:41:ARG:HH21	20:S:128:PHE:HZ	1.58	0.49
8:G:68:ILE:HD11	8:G:116:ILE:HG13	1.93	0.49
11:J:110:ARG:HA	11:J:121:LEU:HD23	1.93	0.49
12:K:63:LEU:HD11	12:K:69:ARG:HH21	1.77	0.49
8:G:136:ARG:HB2	8:G:203:ASN:HD21	1.76	0.49
11:J:110:ARG:HG3	11:J:121:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:32:ILE:HD12	19:R:39:LEU:HD22	1.94	0.49
35:h:258:ILE:HD11	35:h:268:ASP:HB2	1.92	0.49
3:B:119:PRO:HG2	3:B:142:LEU:HD11	1.94	0.49
7:F:130:PHE:HB3	7:F:138:HIS:HB2	1.94	0.49
9:H:70:HIS:HA	9:H:98:ARG:HH12	1.77	0.49
31:d:29:GLN:HE22	37:z:332:A:H8	1.58	0.49
1:2:464:A:H3'	1:2:465:A:H8	1.77	0.49
1:2:1221:G:O2'	1:2:1676:U:O2	2.30	0.49
1:2:1722:G:O6	1:2:1812:U:O4	2.30	0.49
21:T:13:LEU:HB2	21:T:20:ILE:HB	1.93	0.49
26:Y:140:ARG:O	26:Y:142:ARG:NH1	2.46	0.49
3:B:174:MET:HA	3:B:177:MET:HG2	1.95	0.49
33:f:108:ARG:O	33:f:112:ASN:ND2	2.46	0.49
1:2:1355:C:O3'	5:D:238:LYS:NZ	2.45	0.49
15:N:113:ASP:OD1	15:N:113:ASP:N	2.44	0.49
1:2:64:A:H2	1:2:83:A:H62	1.60	0.49
18:Q:123:TYR:OH	21:T:124:ARG:NH1	2.45	0.49
1:2:351:G:OP1	11:J:7:ASN:ND2	2.45	0.49
1:2:399:C:N3	14:M:104:LYS:NZ	2.50	0.49
5:D:90:GLU:HB3	5:D:92:GLU:HG2	1.93	0.49
23:V:35:VAL:HG21	23:V:110:VAL:HG11	1.94	0.49
1:2:1473:G:H2'	1:2:1475:G:H22	1.78	0.49
1:2:350:C:O2'	1:2:383:G:N1	2.46	0.48
1:2:1528:G:O2'	1:2:1666:C:OP1	2.31	0.48
20:S:18:GLU:OE2	20:S:70:SER:OG	2.31	0.48
20:S:58:MET:HA	20:S:61:ILE:HG22	1.95	0.48
21:T:63:GLU:HA	21:T:66:ARG:HB3	1.95	0.48
2:A:23:LYS:NZ	2:A:98:ASP:OD2	2.46	0.48
7:F:148:ARG:NH2	9:H:205:GLU:OE2	2.44	0.48
7:F:184:THR:O	7:F:224:ASN:ND2	2.43	0.48
31:d:10:LYS:NZ	31:d:36:ASP:OD2	2.47	0.48
1:2:1864:U:O4	29:b:34:LYS:NZ	2.46	0.48
1:2:1025:U:O2'	1:2:1160:U:O2'	2.30	0.48
6:E:193:ASP:N	6:E:193:ASP:OD1	2.46	0.48
30:c:14:GLU:HA	30:c:17:ARG:HE	1.78	0.48
1:2:1143:A:H5'	5:D:190:SER:HB2	1.96	0.48
29:b:55:GLU:OE1	31:d:5:ARG:NH1	2.47	0.48
4:C:76:ASN:OD1	4:C:77:ASP:N	2.46	0.48
7:F:185:GLY:H	7:F:189:LEU:HD13	1.77	0.48
14:M:112:HIS:HB3	14:M:141:ASN:HD22	1.79	0.48
16:O:84:LEU:HD21	16:O:92:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:60:LEU:HB3	12:K:94:LEU:HD21	1.94	0.48
1:2:1354:G:N2	1:2:1357:A:OP2	2.42	0.48
4:C:82:ARG:NH2	4:C:191:ASP:OD1	2.47	0.48
5:D:196:ILE:HB	5:D:223:TYR:HB2	1.95	0.48
35:h:124:SER:OG	35:h:125:ARG:N	2.47	0.48
3:B:198:MET:HB3	3:B:201:LEU:HB2	1.95	0.48
6:E:101:GLN:HG3	6:E:126:ILE:HD11	1.96	0.48
6:E:204:LEU:HB2	6:E:207:HIS:HB2	1.96	0.48
34:g:100:LEU:HD23	34:g:103:LEU:HD22	1.94	0.48
1:2:1262:C:O2	32:e:12:ARG:NH2	2.47	0.48
1:2:1675:A:O2'	8:G:74:ASN:O	2.32	0.48
37:z:72:A:H5''	37:z:93:A:H61	1.79	0.48
1:2:183:G:O2'	1:2:184:G:O4'	2.32	0.47
17:P:45:THR:HA	17:P:52:THR:HA	1.95	0.47
1:2:598:G:N2	1:2:639:C:N3	2.61	0.47
1:2:1568:C:OP1	22:U:96:SER:OG	2.31	0.47
4:C:33:VAL:HG12	4:C:96:CYS:HB2	1.96	0.47
8:G:184:SER:HB2	37:z:99:A:H4'	1.96	0.47
31:d:17:VAL:HA	31:d:30:VAL:HG23	1.96	0.47
1:2:1466:G:OP2	20:S:5:ARG:NH1	2.47	0.47
3:B:57:LYS:HE3	24:W:70:LEU:HD13	1.96	0.47
22:U:40:ALA:HB3	22:U:43:LYS:HG2	1.97	0.47
33:f:78:SER:O	33:f:81:ARG:NH1	2.47	0.47
1:2:847:A:OP1	7:F:108:ARG:NH2	2.46	0.47
1:2:925:G:OP1	16:O:121:ARG:NH1	2.47	0.47
35:h:41:ILE:HD11	35:h:55:PRO:HB3	1.96	0.47
37:z:290:U:O2'	37:z:315:C:OP2	2.32	0.47
1:2:156:G:N2	9:H:60:GLY:O	2.47	0.47
9:H:181:THR:HG22	9:H:183:ARG:H	1.79	0.47
1:2:384:U:OP1	14:M:132:ARG:NH1	2.46	0.47
1:2:1824:A:OP2	26:Y:61:GLN:NE2	2.40	0.47
32:e:12:ARG:HH21	32:e:17:GLY:HA3	1.80	0.47
1:2:855:G:O2'	14:M:71:ARG:NH1	2.44	0.47
1:2:1096:G:H1	1:2:1136:U:H3	1.62	0.47
5:D:249:SER:HA	24:W:23:ILE:HD11	1.96	0.47
10:I:159:ASP:OD1	10:I:159:ASP:N	2.47	0.47
13:L:26:ASP:N	13:L:26:ASP:OD1	2.47	0.47
18:Q:29:SER:OG	18:Q:32:GLN:OE1	2.30	0.47
34:g:141:CYS:SG	34:g:142:GLY:N	2.86	0.47
35:h:244:ASN:ND2	35:h:294:ASP:O	2.47	0.47
1:2:65:C:OP1	9:H:136:LYS:NZ	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:184:ARG:HD3	3:B:191:ARG:HG2	1.97	0.47
8:G:99:ILE:HD13	8:G:171:GLU:HB3	1.95	0.47
13:L:53:LYS:HD2	13:L:60:GLU:HB2	1.97	0.47
27:Z:54:VAL:HB	27:Z:76:TYR:HB2	1.97	0.47
1:2:1748:G:H1	1:2:1786:U:H3	1.63	0.47
11:J:162:LEU:HD11	11:J:191:GLU:HG2	1.95	0.47
18:Q:47:ARG:O	18:Q:50:ARG:NH2	2.47	0.47
34:g:137:ASP:OD1	34:g:137:ASP:N	2.47	0.47
7:F:64:ILE:HG23	27:Z:17:LEU:HD21	1.96	0.47
7:F:137:PRO:HB2	7:F:150:PRO:HD2	1.97	0.47
10:I:142:LYS:HG3	25:X:54:ASP:HB3	1.97	0.47
11:J:134:GLU:OE2	11:J:138:ASN:ND2	2.47	0.47
24:W:21:ASN:HB3	25:X:67:GLY:HA3	1.96	0.47
37:z:156:C:N4	37:z:228:U:O4	2.49	0.47
1:2:886:A:H61	1:2:901:G:H1'	1.80	0.46
1:2:1050:A:OP1	1:2:1846:G:N2	2.49	0.46
1:2:373:G:H4'	14:M:85:THR:HG21	1.98	0.46
1:2:1183:A:H2'	1:2:1184:G:H8	1.80	0.46
8:G:76:MET:O	8:G:159:ARG:NH2	2.48	0.46
1:2:77:A:H2	9:H:175:LYS:HG3	1.80	0.46
1:2:380:G:N1	1:2:383:G:OP2	2.40	0.46
31:d:36:ASP:OD1	31:d:36:ASP:N	2.48	0.46
1:2:38:A:H5''	12:K:5:ARG:HG3	1.97	0.46
1:2:433:A:OP1	11:J:25:ARG:NH2	2.47	0.46
12:K:111:GLN:HE22	12:K:127:ARG:HH11	1.64	0.46
14:M:127:THR:HB	14:M:144:LYS:HG2	1.97	0.46
24:W:15:ARG:NH1	24:W:33:GLN:OE1	2.48	0.46
6:E:105:LEU:HD12	6:E:122:VAL:HG11	1.96	0.46
9:H:85:ARG:HG3	9:H:87:ARG:HH12	1.80	0.46
13:L:1:MET:HB3	13:L:3:MET:HE1	1.97	0.46
32:e:43:PHE:O	32:e:47:ALA:HB2	2.15	0.46
1:2:886:A:O2'	1:2:887:U:O4'	2.33	0.46
1:2:1139:C:H41	1:2:1149:A:H62	1.62	0.46
12:K:67:ASP:HB3	12:K:70:ARG:HB3	1.98	0.46
5:D:60:TRP:NE1	5:D:92:GLU:OE2	2.48	0.46
16:O:64:ARG:HD3	16:O:70:LYS:HE2	1.97	0.46
20:S:76:GLU:HA	20:S:79:GLU:HB3	1.97	0.46
1:2:420:G:O2'	1:2:660:C:N3	2.49	0.46
1:2:1059:G:N2	1:2:1829:G:O3'	2.49	0.46
3:B:25:LEU:HD12	3:B:46:ILE:HG21	1.97	0.46
4:C:90:ASP:HB3	4:C:97:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:132:LYS:HD2	6:E:189:MET:HE2	1.98	0.46
1:2:645:C:H2'	1:2:646:G:H8	1.81	0.46
1:2:1548:G:OP1	23:V:60:THR:OG1	2.32	0.46
6:E:23:GLU:OE1	13:L:64:TRP:NE1	2.45	0.46
8:G:28:VAL:HG12	8:G:110:GLN:HB2	1.98	0.46
12:K:12:THR:HG22	12:K:45:ARG:HG3	1.97	0.46
37:z:145:G:H1	37:z:248:U:H3	1.64	0.46
37:z:257:A:N6	37:z:275:A:N7	2.63	0.46
1:2:15:U:H3	1:2:1196:A:H61	1.63	0.46
3:B:104:THR:O	3:B:107:THR:OG1	2.31	0.46
27:Z:104:ARG:HA	27:Z:107:ARG:HD3	1.98	0.46
1:2:522:A:O2'	12:K:131:ARG:NH2	2.49	0.45
11:J:141:ARG:HB2	11:J:146:GLN:HG2	1.98	0.45
17:P:75:MET:HG2	17:P:118:ALA:HB2	1.99	0.45
7:F:60:GLU:OE1	27:Z:20:ARG:NH1	2.49	0.45
22:U:28:LEU:HB3	22:U:53:PHE:HE2	1.81	0.45
24:W:27:LYS:HA	24:W:27:LYS:HD2	1.81	0.45
35:h:213:ASP:N	35:h:213:ASP:OD1	2.49	0.45
37:z:132:G:H2'	37:z:133:G:H8	1.81	0.45
1:2:846:G:OP2	7:F:108:ARG:NH1	2.43	0.45
5:D:88:ILE:HD11	5:D:93:ILE:HD13	1.96	0.45
16:O:25:TRP:HE1	30:c:84:HIS:HB3	1.81	0.45
3:B:198:MET:HE3	3:B:200:ASP:HB2	1.97	0.45
1:2:223:C:H2'	1:2:224:A:C8	2.52	0.45
1:2:1252:C:OP1	23:V:75:LYS:NZ	2.37	0.45
12:K:81:LEU:HB3	12:K:87:LEU:HD13	1.98	0.45
24:W:66:ASP:OD2	24:W:67:ASP:N	2.50	0.45
1:2:1498:A:OP2	6:E:27:ARG:NH2	2.44	0.45
5:D:62:PRO:HG3	5:D:68:ARG:HE	1.81	0.45
1:2:1004:U:H2'	1:2:1005:G:H8	1.82	0.45
25:X:115:GLU:HA	25:X:118:ARG:HG2	1.99	0.45
3:B:17:LYS:HB3	3:B:173:LEU:HD11	1.99	0.45
6:E:141:LYS:NZ	6:E:179:GLN:O	2.44	0.45
7:F:46:ILE:O	7:F:50:ASN:HB2	2.17	0.45
9:H:216:ARG:HD3	9:H:216:ARG:HA	1.78	0.45
16:O:119:GLU:HA	16:O:122:ILE:HG22	1.99	0.45
33:f:84:LYS:HE2	33:f:84:LYS:HB3	1.78	0.45
6:E:126:ILE:HG21	6:E:134:CYS:HB2	1.99	0.44
21:T:130:ARG:HG2	21:T:134:GLN:HB2	1.98	0.44
30:c:67:THR:OG1	30:c:70:LYS:O	2.33	0.44
1:2:1445:U:O4	1:2:1446:A:N6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:45:ILE:HB	7:F:80:ILE:HG13	2.00	0.44
1:2:45:A:H4'	1:2:46:A:H5'	1.98	0.44
2:A:62:ARG:HE	33:f:79:LEU:HD11	1.81	0.44
7:F:180:LEU:HD21	7:F:192:ILE:HD12	1.99	0.44
11:J:144:LYS:HA	11:J:147:LYS:HG2	1.98	0.44
16:O:55:ARG:NH2	30:c:51:GLN:OE1	2.45	0.44
28:a:100:VAL:HB	28:a:108:ILE:HG13	1.98	0.44
1:2:380:G:OP1	11:J:31:ARG:NH1	2.41	0.44
1:2:1845:A:H2'	1:2:1846:G:H8	1.82	0.44
3:B:34:MET:HE2	3:B:154:LEU:HD21	2.00	0.44
4:C:170:GLU:HA	4:C:173:THR:HG22	1.99	0.44
5:D:272:HIS:HA	5:D:275:LYS:HE2	2.00	0.44
7:F:29:PRO:HG2	7:F:46:ILE:HD11	1.98	0.44
11:J:57:ALA:HB2	11:J:183:GLY:HA2	1.99	0.44
35:h:20:GLN:HB3	35:h:69:VAL:HG12	1.98	0.44
1:2:1337:C:H2'	1:2:1338:G:H8	1.83	0.44
1:2:1553:C:O2'	1:2:1554:C:O4'	2.36	0.44
11:J:92:ARG:HE	11:J:93:THR:HG23	1.82	0.44
27:Z:30:PRO:O	27:Z:32:LYS:NZ	2.51	0.44
1:2:1259:A:H62	1:2:1518:C:H3'	1.83	0.44
1:2:1518:C:H5'	1:2:1519:U:H5''	2.00	0.44
4:C:136:ARG:HB2	4:C:218:LEU:HD11	2.00	0.44
8:G:20:PHE:N	8:G:23:TRP:O	2.48	0.44
10:I:85:LYS:HA	10:I:85:LYS:HD3	1.89	0.44
20:S:41:ILE:HG22	20:S:43:SER:H	1.83	0.44
23:V:67:LYS:O	32:e:44:ARG:NH2	2.40	0.44
33:f:113:ARG:HA	33:f:117:ASN:HB2	1.99	0.44
35:h:39:THR:HG22	35:h:60:ARG:HG2	1.99	0.44
1:2:57:U:O2	1:2:499:G:O2'	2.36	0.44
1:2:982:G:H2'	1:2:983:A:H8	1.82	0.44
1:2:1138:C:OP1	3:B:155:ARG:NH2	2.43	0.44
12:K:136:ARG:HH11	12:K:139:LYS:HA	1.83	0.44
1:2:311:C:H5''	1:2:312:G:H5''	1.99	0.44
1:2:543:C:H3'	1:2:544:G:H8	1.83	0.44
1:2:986:G:H22	17:P:135:ILE:HD12	1.83	0.44
1:2:1010:G:H2'	1:2:1011:A:H8	1.83	0.44
6:E:57:ASN:O	6:E:65:ARG:NH2	2.51	0.44
7:F:141:THR:OG1	7:F:143:ASP:OD1	2.34	0.44
35:h:99:ARG:NE	35:h:135:LEU:O	2.42	0.44
1:2:165:G:OP2	1:2:165:G:N2	2.50	0.44
1:2:1157:G:O2'	25:X:74:VAL:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1448:A:OP1	23:V:30:LYS:NZ	2.50	0.44
1:2:1520:G:H21	18:Q:126:VAL:HG11	1.83	0.44
2:A:90:ASP:HB3	33:f:79:LEU:HD12	2.00	0.44
4:C:35:ALA:O	4:C:42:ARG:NE	2.48	0.44
7:F:11:ARG:HA	7:F:28:ALA:HB2	2.00	0.44
9:H:121:ILE:HD12	9:H:122:PRO:HD2	1.99	0.44
32:e:15:GLY:O	32:e:19:ARG:NH1	2.51	0.44
1:2:1064:C:H2'	1:2:1065:G:H8	1.83	0.43
1:2:1255:G:OP1	1:2:1256:G:O2'	2.34	0.43
1:2:1480:A:H5'	19:R:131:LYS:HD2	2.00	0.43
1:2:1657:G:O3'	32:e:33:LYS:NZ	2.51	0.43
1:2:1711:U:H2'	1:2:1712:A:C8	2.53	0.43
3:B:80:ARG:HA	3:B:80:ARG:HD2	1.82	0.43
4:C:182:LYS:HE3	4:C:231:LEU:HD13	1.99	0.43
9:H:160:LYS:O	9:H:171:THR:OG1	2.30	0.43
9:H:215:LYS:HE2	9:H:216:ARG:HH12	1.82	0.43
20:S:22:THR:O	35:h:212:LYS:NZ	2.51	0.43
35:h:251:ALA:HB2	35:h:289:LEU:HD22	1.99	0.43
1:2:1092:G:OP1	16:O:2:GLY:N	2.50	0.43
1:2:1536:G:H2'	1:2:1537:A:C8	2.53	0.43
4:C:180:ASP:OD1	4:C:180:ASP:N	2.43	0.43
5:D:155:ILE:O	5:D:159:LYS:HB2	2.19	0.43
5:D:211:LYS:HB3	5:D:211:LYS:HE3	1.83	0.43
7:F:31:PRO:HG3	7:F:43:PRO:HG3	1.99	0.43
18:Q:34:MET:HB2	18:Q:42:ARG:HG2	1.99	0.43
35:h:40:ILE:HD11	35:h:66:VAL:HG21	2.00	0.43
1:2:1660:C:O2'	1:2:1662:U:OP2	2.31	0.43
7:F:77:ARG:HD3	7:F:77:ARG:HA	1.84	0.43
12:K:111:GLN:HE21	12:K:145:PRO:HB2	1.83	0.43
19:R:47:LEU:HB3	19:R:50:LYS:HB2	2.01	0.43
37:z:351:A:H2'	37:z:352:A:H4'	2.01	0.43
5:D:168:GLY:N	5:D:179:THR:O	2.47	0.43
24:W:34:MET:HE2	24:W:34:MET:HB2	1.90	0.43
26:Y:101:LEU:HB3	26:Y:124:LYS:HB2	2.00	0.43
33:f:81:ARG:HE	33:f:84:LYS:HD3	1.83	0.43
11:J:48:VAL:HG11	11:J:54:LYS:HD3	1.99	0.43
14:M:135:SER:O	14:M:139:ARG:NH1	2.50	0.43
20:S:60:ARG:HG3	20:S:63:ARG:HH22	1.83	0.43
20:S:88:VAL:HG22	20:S:90:ALA:H	1.84	0.43
34:g:133:ALA:HB3	34:g:140:TYR:HB3	2.00	0.43
1:2:149:A:H3'	1:2:150:A:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1536:G:H2'	1:2:1537:A:H8	1.84	0.43
22:U:13:GLU:HB3	22:U:16:ARG:HH21	1.84	0.43
1:2:562:U:H2'	1:2:563:G:H8	1.83	0.43
6:E:67:ARG:HH12	13:L:96:ARG:HD3	1.84	0.43
7:F:61:VAL:HG22	7:F:80:ILE:HD11	2.00	0.43
11:J:113:TYR:HD2	11:J:121:LEU:HB2	1.84	0.43
12:K:3:VAL:HG21	12:K:5:ARG:HH11	1.82	0.43
14:M:96:ILE:HD12	26:Y:10:ALA:HB1	2.01	0.43
17:P:27:VAL:O	17:P:92:ALA:HB3	2.19	0.43
1:2:1277:C:H2'	1:2:1278:A:H8	1.83	0.43
8:G:40:ALA:HB1	8:G:45:TYR:HD2	1.84	0.43
11:J:6:ASP:N	11:J:6:ASP:OD1	2.49	0.43
21:T:114:LEU:HA	21:T:117:ILE:HG22	1.99	0.43
35:h:153:CYS:SG	35:h:154:VAL:N	2.92	0.43
1:2:1405:A:H2	1:2:1443:C:H42	1.65	0.43
2:A:47:LEU:HD21	2:A:71:ILE:HG21	2.01	0.43
3:B:18:PHE:HD2	3:B:51:LEU:HD21	1.83	0.43
37:z:49:G:H2'	37:z:50:A:H8	1.84	0.43
1:2:104:A:OP1	11:J:12:ARG:NH1	2.44	0.43
1:2:1718:G:H21	1:2:1815:A:H62	1.66	0.43
13:L:29:MET:SD	13:L:42:ASN:ND2	2.92	0.43
16:O:98:VAL:HG12	16:O:115:LEU:HD12	2.01	0.43
26:Y:54:LYS:NZ	26:Y:94:ILE:O	2.39	0.43
30:c:19:HIS:HD2	30:c:21:LYS:H	1.65	0.43
33:f:126:LYS:NZ	33:f:127:GLY:O	2.51	0.43
37:z:154:A:OP1	37:z:228:U:O2'	2.34	0.43
37:z:262:U:O4	37:z:271:G:O6	2.37	0.43
1:2:13:C:O2'	1:2:1355:C:N3	2.47	0.42
1:2:94:G:O2'	1:2:508:A:O2'	2.33	0.42
1:2:919:A:O2'	1:2:1020:A:N1	2.46	0.42
1:2:562:U:O4	12:K:172:ARG:NH2	2.52	0.42
3:B:120:ARG:HH11	5:D:266:TYR:HB3	1.84	0.42
11:J:106:SER:HB3	11:J:171:LEU:HD13	2.00	0.42
25:X:119:LYS:HG3	25:X:121:THR:HG22	2.00	0.42
1:2:436:G:O6	1:2:458:A:N6	2.52	0.42
2:A:46:ARG:HD2	2:A:58:LEU:HD21	2.01	0.42
13:L:47:LYS:HA	13:L:47:LYS:HD3	1.80	0.42
25:X:111:MET:HE1	25:X:119:LYS:HD2	2.01	0.42
35:h:8:ARG:HD2	35:h:311:GLN:HB2	2.01	0.42
1:2:1082:A:O2'	1:2:1842:C:O2'	2.34	0.42
16:O:136:PRO:HA	16:O:137:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:981:A:H2'	1:2:982:G:C8	2.54	0.42
11:J:43:ILE:HG22	11:J:57:ALA:HA	2.01	0.42
19:R:101:ASP:OD1	19:R:101:ASP:N	2.52	0.42
20:S:128:PHE:CD1	20:S:129:LYS:HG3	2.54	0.42
23:V:78:ASP:OD2	32:e:54:LYS:NZ	2.49	0.42
28:a:99:LEU:HA	28:a:109:TYR:HD1	1.84	0.42
1:2:1544:C:O2'	19:R:75:GLY:O	2.37	0.42
12:K:114:VAL:HG21	12:K:130:ILE:HD11	2.00	0.42
19:R:68:ILE:HG21	19:R:88:ILE:HG22	2.01	0.42
29:b:32:LYS:O	29:b:37:LYS:NZ	2.53	0.42
35:h:8:ARG:HH11	35:h:311:GLN:HB2	1.84	0.42
35:h:12:LYS:HE3	35:h:12:LYS:HB2	1.87	0.42
1:2:482:G:N2	1:2:485:A:OP2	2.48	0.42
7:F:123:LEU:HD23	7:F:236:ILE:HD11	2.02	0.42
15:N:31:LEU:HD13	15:N:33:ARG:HG3	2.00	0.42
35:h:152:SER:OG	35:h:196:ASN:O	2.32	0.42
1:2:1660:C:OP2	32:e:32:ARG:NH2	2.53	0.42
11:J:154:LYS:HB3	11:J:154:LYS:HE3	1.83	0.42
1:2:1557:C:H1'	1:2:1661:A:H4'	2.02	0.42
1:2:1650:A:H5''	19:R:139:ALA:HB2	2.02	0.42
27:Z:101:LYS:HB2	27:Z:101:LYS:HE2	1.87	0.42
1:2:561:A:H5'	12:K:171:GLY:HA3	2.01	0.41
1:2:885:U:H3	1:2:901:G:H22	1.68	0.41
3:B:10:MET:SD	3:B:10:MET:N	2.93	0.41
35:h:154:VAL:HB	35:h:165:ILE:HD11	2.02	0.41
6:E:1:MET:SD	6:E:3:VAL:N	2.91	0.41
1:2:91:A:H5''	1:2:92:A:H5''	2.01	0.41
1:2:1335:G:H1	1:2:1492:U:H3	1.68	0.41
12:K:65:GLU:HG3	12:K:66:LYS:HG2	2.01	0.41
1:2:302:A:N3	11:J:64:ASN:ND2	2.69	0.41
1:2:942:G:OP1	4:C:216:LYS:NZ	2.43	0.41
5:D:271:ASP:N	5:D:271:ASP:OD1	2.51	0.41
9:H:7:PHE:HD2	9:H:10:THR:HG22	1.85	0.41
12:K:132:GLN:HG2	12:K:134:HIS:HE1	1.85	0.41
25:X:112:ASP:OD1	25:X:112:ASP:N	2.53	0.41
1:2:122:G:H1	1:2:342:C:H42	1.68	0.41
1:2:1283:C:H3'	15:N:104:VAL:HG21	2.03	0.41
1:2:1611:G:O2'	21:T:87:GLN:O	2.39	0.41
35:h:66:VAL:HA	35:h:82:SER:HA	2.03	0.41
1:2:1215:C:O2'	1:2:1645:C:OP2	2.36	0.41
1:2:1644:C:H4'	19:R:140:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:382:C:H2'	1:2:383:G:C8	2.56	0.41
5:D:66:LEU:HD23	5:D:69:LEU:HD12	2.01	0.41
6:E:40:ARG:HA	23:V:108:PRO:HB3	2.02	0.41
16:O:62:GLN:HB3	16:O:65:PHE:HD2	1.86	0.41
1:2:1232:U:H2'	1:2:1233:G:H8	1.86	0.41
1:2:1845:A:H2'	1:2:1846:G:C8	2.55	0.41
8:G:92:ILE:HD13	8:G:169:ILE:HD13	2.03	0.41
9:H:159:ARG:HG3	9:H:173:ALA:HB2	2.03	0.41
16:O:63:VAL:HG11	16:O:71:ILE:HG13	2.03	0.41
1:2:67:C:OP2	9:H:172:LYS:NZ	2.44	0.41
1:2:106:C:H2'	1:2:107:A:C8	2.55	0.41
1:2:642:U:O4	33:f:106:LYS:NZ	2.50	0.41
1:2:1457:U:H2'	1:2:1458:G:H8	1.86	0.41
1:2:1865:C:H1'	29:b:7:ASN:HD21	1.86	0.41
3:B:191:ARG:NH1	24:W:43:THR:O	2.53	0.41
6:E:29:LEU:HD21	6:E:58:VAL:HG23	2.03	0.41
8:G:99:ILE:HD11	28:a:106:GLN:HE22	1.86	0.41
10:I:145:ARG:HB3	10:I:153:LEU:HB3	2.03	0.41
17:P:119:LEU:HD12	17:P:119:LEU:HA	1.95	0.41
37:z:64:U:N3	37:z:104:C:O2	2.54	0.41
1:2:155:G:H2'	1:2:156:G:H8	1.86	0.41
1:2:928:G:H2'	1:2:929:G:C8	2.56	0.41
1:2:1464:C:OP1	20:S:63:ARG:NH2	2.54	0.41
5:D:105:GLU:N	5:D:105:GLU:OE2	2.54	0.41
8:G:127:ARG:HD2	8:G:127:ARG:HA	1.90	0.41
9:H:14:LYS:HD3	9:H:14:LYS:HA	1.86	0.41
11:J:191:GLU:O	14:M:19:ASN:ND2	2.51	0.41
14:M:108:ASN:OD1	14:M:108:ASN:N	2.54	0.41
17:P:139:SER:OG	17:P:140:THR:N	2.54	0.41
22:U:75:MET:HA	22:U:78:ILE:HB	2.03	0.41
25:X:7:LEU:HD13	25:X:34:ILE:HG12	2.03	0.41
29:b:33:ASP:N	29:b:33:ASP:OD1	2.49	0.41
31:d:20:ARG:HE	31:d:20:ARG:HB3	1.69	0.41
9:H:203:LYS:HA	9:H:203:LYS:HD2	1.87	0.40
12:K:81:LEU:HD23	12:K:81:LEU:HA	1.95	0.40
19:R:44:PRO:HD2	19:R:81:ILE:HD11	2.03	0.40
1:2:28:U:H2'	1:2:29:G:H8	1.86	0.40
1:2:608:C:O4'	33:f:131:ASN:ND2	2.54	0.40
1:2:645:C:H2'	1:2:646:G:C8	2.56	0.40
1:2:980:A:H2'	1:2:981:A:C8	2.56	0.40
1:2:1062:A:H2'	1:2:1063:C:H6	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1125:C:O3'	3:B:41:ARG:NH2	2.53	0.40
1:2:1228:A:H2'	1:2:1229:G:C8	2.56	0.40
1:2:1290:G:O6	34:g:95:ARG:NH2	2.46	0.40
21:T:67:VAL:HA	21:T:70:ILE:HG22	2.03	0.40
28:a:69:THR:HG22	28:a:72:VAL:HG12	2.03	0.40
37:z:81:A:N7	37:z:82:G:N2	2.70	0.40
1:2:35:C:H5''	1:2:579:C:H5''	2.03	0.40
1:2:624:C:N4	26:Y:63:ASN:OD1	2.40	0.40
20:S:103:LYS:HA	20:S:103:LYS:HD2	1.90	0.40
25:X:89:TRP:O	25:X:93:LEU:HB2	2.21	0.40
31:d:37:ASP:OD2	31:d:39:SER:OG	2.38	0.40
1:2:1700:C:H5	1:2:1836:G:H1	1.69	0.40
2:A:29:LYS:HE3	2:A:34:GLU:HA	2.03	0.40
20:S:128:PHE:HD1	20:S:129:LYS:HG3	1.87	0.40
21:T:124:ARG:HA	21:T:124:ARG:HD2	1.78	0.40
33:f:100:LYS:HG2	33:f:102:THR:H	1.87	0.40
35:h:32:LEU:HD12	35:h:32:LEU:HA	1.94	0.40
35:h:116:ASP:OD1	35:h:116:ASP:N	2.51	0.40
1:2:946:U:H2'	1:2:947:G:C8	2.56	0.40
5:D:74:LYS:HD3	5:D:269:PHE:CG	2.56	0.40
12:K:88:ASP:OD1	12:K:89:GLU:N	2.55	0.40
14:M:78:THR:HG22	14:M:79:LYS:HG3	2.02	0.40
23:V:55:ARG:HE	23:V:87:ARG:HE	1.70	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	A	99/144 (69%)	96 (97%)	2 (2%)	1 (1%)	12 43
3	B	215/295 (73%)	199 (93%)	16 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	211/264 (80%)	199 (94%)	12 (6%)	0	100	100
5	D	219/221 (99%)	208 (95%)	11 (5%)	0	100	100
6	E	226/281 (80%)	218 (96%)	8 (4%)	0	100	100
7	F	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
8	G	189/204 (93%)	181 (96%)	8 (4%)	0	100	100
9	H	235/249 (94%)	230 (98%)	5 (2%)	0	100	100
10	I	181/432 (42%)	175 (97%)	6 (3%)	0	100	100
11	J	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
12	K	183/194 (94%)	178 (97%)	5 (3%)	0	100	100
13	L	94/149 (63%)	88 (94%)	6 (6%)	0	100	100
14	M	149/158 (94%)	136 (91%)	13 (9%)	0	100	100
15	N	115/132 (87%)	107 (93%)	8 (7%)	0	100	100
16	O	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
17	P	134/168 (80%)	127 (95%)	7 (5%)	0	100	100
18	Q	118/145 (81%)	108 (92%)	10 (8%)	0	100	100
19	R	140/172 (81%)	133 (95%)	7 (5%)	0	100	100
20	S	130/135 (96%)	119 (92%)	11 (8%)	0	100	100
21	T	142/152 (93%)	132 (93%)	10 (7%)	0	100	100
22	U	139/145 (96%)	133 (96%)	6 (4%)	0	100	100
23	V	98/119 (82%)	95 (97%)	3 (3%)	0	100	100
24	W	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
25	X	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
26	Y	139/143 (97%)	130 (94%)	9 (6%)	0	100	100
27	Z	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
28	a	75/124 (60%)	73 (97%)	2 (3%)	0	100	100
29	b	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
30	c	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
31	d	65/69 (94%)	62 (95%)	3 (5%)	0	100	100
32	e	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
33	f	55/133 (41%)	50 (91%)	5 (9%)	0	100	100
34	g	66/188 (35%)	62 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	h	311/317 (98%)	294 (94%)	17 (6%)	0	100	100
36	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	4925/5965 (83%)	4686 (95%)	238 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	91	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	86/123 (70%)	84 (98%)	2 (2%)	44	63
3	B	180/245 (74%)	180 (100%)	0	100	100
4	C	194/231 (84%)	194 (100%)	0	100	100
5	D	187/187 (100%)	187 (100%)	0	100	100
6	E	190/232 (82%)	190 (100%)	0	100	100
7	F	224/225 (100%)	224 (100%)	0	100	100
8	G	161/170 (95%)	161 (100%)	0	100	100
9	H	207/218 (95%)	206 (100%)	1 (0%)	81	81
10	I	165/360 (46%)	165 (100%)	0	100	100
11	J	178/180 (99%)	178 (100%)	0	100	100
12	K	161/168 (96%)	161 (100%)	0	100	100
13	L	87/125 (70%)	86 (99%)	1 (1%)	65	73
14	M	136/142 (96%)	136 (100%)	0	100	100
15	N	99/108 (92%)	99 (100%)	0	100	100
16	O	130/131 (99%)	130 (100%)	0	100	100
17	P	106/130 (82%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Q	109/130 (84%)	109 (100%)	0	100	100
19	R	117/140 (84%)	117 (100%)	0	100	100
20	S	119/121 (98%)	119 (100%)	0	100	100
21	T	125/132 (95%)	125 (100%)	0	100	100
22	U	111/116 (96%)	111 (100%)	0	100	100
23	V	92/107 (86%)	92 (100%)	0	100	100
24	W	67/67 (100%)	67 (100%)	0	100	100
25	X	112/113 (99%)	112 (100%)	0	100	100
26	Y	113/115 (98%)	113 (100%)	0	100	100
27	Z	107/113 (95%)	107 (100%)	0	100	100
28	a	68/102 (67%)	68 (100%)	0	100	100
29	b	88/88 (100%)	88 (100%)	0	100	100
30	c	75/76 (99%)	75 (100%)	0	100	100
31	d	60/62 (97%)	60 (100%)	0	100	100
32	e	48/49 (98%)	48 (100%)	0	100	100
33	f	47/106 (44%)	47 (100%)	0	100	100
34	g	61/154 (40%)	61 (100%)	0	100	100
35	h	272/275 (99%)	272 (100%)	0	100	100
36	n	24/24 (100%)	24 (100%)	0	100	100
All	All	4306/5065 (85%)	4302 (100%)	4 (0%)	87	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	69	VAL
2	A	72	ASN
9	H	163	ASN
13	L	61	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	33	GLN
2	A	44	ASN

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Mol	Chain	Res	Type
2	A	116	ASN
3	B	29	ASN
3	B	50	ASN
4	C	43	ASN
4	C	124	HIS
4	C	177	GLN
5	D	172	ASN
5	D	235	ASN
5	D	267	GLN
6	E	74	GLN
7	F	201	HIS
8	G	203	ASN
10	I	163	GLN
12	K	111	GLN
13	L	42	ASN
13	L	61	GLN
16	O	62	GLN
16	O	69	ASN
17	P	20	GLN
19	R	8	GLN
19	R	11	GLN
20	S	62	GLN
20	S	83	ASN
20	S	93	GLN
21	T	125	HIS
22	U	42	HIS
22	U	126	GLN
24	W	35	ASN
24	W	47	ASN
26	Y	23	HIS
28	a	45	ASN
28	a	46	ASN
30	c	26	GLN
33	f	112	ASN
33	f	117	ASN
34	g	91	ASN
35	h	76	GLN
35	h	215	GLN
35	h	226	HIS
35	h	244	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1669/1870 (89%)	351 (21%)	6 (0%)
37	z	262/400 (65%)	80 (30%)	0
All	All	1931/2270 (85%)	431 (22%)	6 (0%)

All (431) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	4	C
1	2	5	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	49	C
1	2	56	G
1	2	62	G
1	2	66	G
1	2	67	C
1	2	68	A
1	2	73	C
1	2	74	G
1	2	75	G
1	2	100	U
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	126	G
1	2	128	U
1	2	130	G
1	2	142	C
1	2	143	U
1	2	147	A
1	2	149	A
1	2	158	A
1	2	162	C
1	2	171	A
1	2	180	G
1	2	182	C
1	2	183	G

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Mol	Chain	Res	Type
1	2	184	G
1	2	190	G
1	2	191	A
1	2	192	C
1	2	207	G
1	2	292	A
1	2	294	U
1	2	306	C
1	2	307	G
1	2	309	G
1	2	319	C
1	2	335	G
1	2	341	C
1	2	342	C
1	2	347	G
1	2	362	C
1	2	364	A
1	2	367	U
1	2	368	U
1	2	369	C
1	2	370	G
1	2	381	C
1	2	382	C
1	2	383	G
1	2	384	U
1	2	385	G
1	2	386	C
1	2	398	A
1	2	407	G
1	2	408	A
1	2	409	C
1	2	418	A
1	2	437	G
1	2	441	C
1	2	446	G
1	2	448	A
1	2	449	A
1	2	450	C
1	2	452	G
1	2	465	A
1	2	471	G
1	2	472	C

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Mol	Chain	Res	Type
1	2	474	G
1	2	487	U
1	2	488	U
1	2	492	C
1	2	493	A
1	2	502	C
1	2	508	A
1	2	522	A
1	2	525	A
1	2	530	U
1	2	532	C
1	2	533	A
1	2	536	A
1	2	537	C
1	2	541	U
1	2	544	G
1	2	548	C
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	559	G
1	2	561	A
1	2	562	U
1	2	567	C
1	2	575	A
1	2	576	A
1	2	583	A
1	2	585	C
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	600	G
1	2	603	C
1	2	606	G
1	2	608	C
1	2	613	G
1	2	614	C
1	2	617	G

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Mol	Chain	Res	Type
1	2	623	G
1	2	625	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	630	U
1	2	631	U
1	2	642	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	660	C
1	2	668	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	688	U
1	2	752	G
1	2	754	G
1	2	756	C
1	2	795	A
1	2	799	U
1	2	801	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	847	A
1	2	852	G
1	2	853	C
1	2	870	A
1	2	872	A
1	2	874	G
1	2	875	A
1	2	878	G
1	2	887	U
1	2	891	G
1	2	893	U
1	2	895	G
1	2	898	U

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Mol	Chain	Res	Type
1	2	901	G
1	2	913	A
1	2	914	U
1	2	917	U
1	2	918	U
1	2	919	A
1	2	920	A
1	2	933	G
1	2	943	U
1	2	964	A
1	2	969	U
1	2	970	G
1	2	971	G
1	2	978	G
1	2	985	G
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1024	A
1	2	1025	U
1	2	1026	C
1	2	1027	A
1	2	1041	G
1	2	1044	G
1	2	1045	U
1	2	1060	A
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1088	U
1	2	1089	G
1	2	1114	U
1	2	1121	G
1	2	1126	G
1	2	1149	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1156	U

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Mol	Chain	Res	Type
1	2	1157	G
1	2	1165	G
1	2	1166	G
1	2	1170	A
1	2	1183	A
1	2	1184	G
1	2	1201	U
1	2	1203	U
1	2	1205	G
1	2	1208	A
1	2	1211	G
1	2	1215	C
1	2	1216	C
1	2	1217	A
1	2	1224	G
1	2	1242	U
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1266	C
1	2	1269	G
1	2	1274	G
1	2	1275	G
1	2	1282	A
1	2	1283	C
1	2	1284	A
1	2	1285	G
1	2	1287	A
1	2	1294	G
1	2	1298	G
1	2	1299	A
1	2	1300	U
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

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Mol	Chain	Res	Type
1	2	1315	U
1	2	1318	G
1	2	1332	A
1	2	1333	U
1	2	1342	U
1	2	1348	G
1	2	1358	U
1	2	1371	U
1	2	1372	U
1	2	1377	U
1	2	1378	A
1	2	1380	C
1	2	1396	A
1	2	1397	U
1	2	1401	A
1	2	1402	A
1	2	1406	G
1	2	1428	G
1	2	1439	A
1	2	1452	A
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1466	G
1	2	1473	G
1	2	1477	U
1	2	1489	A
1	2	1490	G
1	2	1493	C
1	2	1498	A
1	2	1507	G
1	2	1519	U
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1523	C
1	2	1533	A
1	2	1548	G
1	2	1551	U
1	2	1552	G
1	2	1553	C
1	2	1554	C

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Mol	Chain	Res	Type
1	2	1556	A
1	2	1557	C
1	2	1567	G
1	2	1574	C
1	2	1575	G
1	2	1578	U
1	2	1580	A
1	2	1585	U
1	2	1588	A
1	2	1601	A
1	2	1604	G
1	2	1606	G
1	2	1621	U
1	2	1623	A
1	2	1638	G
1	2	1647	A
1	2	1648	G
1	2	1653	U
1	2	1654	G
1	2	1661	A
1	2	1662	U
1	2	1664	A
1	2	1665	G
1	2	1695	A
1	2	1698	C
1	2	1699	A
1	2	1721	U
1	2	1722	G
1	2	1750	C
1	2	1751	C
1	2	1753	C
1	2	1756	C
1	2	1757	G
1	2	1758	G
1	2	1760	G
1	2	1773	C
1	2	1775	U
1	2	1776	G
1	2	1777	G
1	2	1780	G
1	2	1781	A
1	2	1783	C

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Mol	Chain	Res	Type
1	2	1784	G
1	2	1786	U
1	2	1801	A
1	2	1819	A
1	2	1823	A
1	2	1824	A
1	2	1825	A
1	2	1826	G
1	2	1831	A
1	2	1834	A
1	2	1836	G
1	2	1838	U
1	2	1839	U
1	2	1840	U
1	2	1849	G
1	2	1852	C
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
1	2	1869	A
37	z	45	C
37	z	48	U
37	z	49	G
37	z	50	A
37	z	57	A
37	z	82	G
37	z	83	C
37	z	85	A
37	z	86	U
37	z	94	G
37	z	100	G
37	z	106	U
37	z	107	G
37	z	111	C
37	z	121	C
37	z	123	C
37	z	128	C
37	z	134	A
37	z	137	G
37	z	150	G
37	z	153	G

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Mol	Chain	Res	Type
37	z	154	A
37	z	156	C
37	z	157	C
37	z	161	G
37	z	162	A
37	z	163	G
37	z	164	U
37	z	165	A
37	z	166	C
37	z	168	C
37	z	172	A
37	z	173	A
37	z	229	G
37	z	232	C
37	z	234	U
37	z	237	C
37	z	244	A
37	z	253	G
37	z	258	G
37	z	265	U
37	z	266	G
37	z	269	U
37	z	270	C
37	z	274	A
37	z	281	U
37	z	282	U
37	z	283	G
37	z	284	U
37	z	288	A
37	z	295	G
37	z	297	U
37	z	306	U
37	z	323	G
37	z	324	U
37	z	330	A
37	z	331	G
37	z	332	A
37	z	333	C
37	z	334	C
37	z	335	G
37	z	336	U
37	z	337	G

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Mol	Chain	Res	Type
37	z	338	C
37	z	339	A
37	z	340	C
37	z	341	C
37	z	342	A
37	z	343	U
37	z	344	G
37	z	345	A
37	z	346	G
37	z	347	C
37	z	348	A
37	z	349	C
37	z	350	G
37	z	352	A
37	z	353	U
37	z	354	C
37	z	355	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	383	G
1	2	445	A
1	2	532	C
1	2	561	A
1	2	886	A
1	2	1759	G

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](#)

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

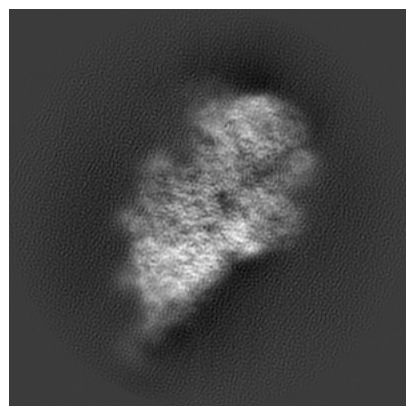
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25537. These allow visual inspection of the internal detail of the map and identification of artifacts.

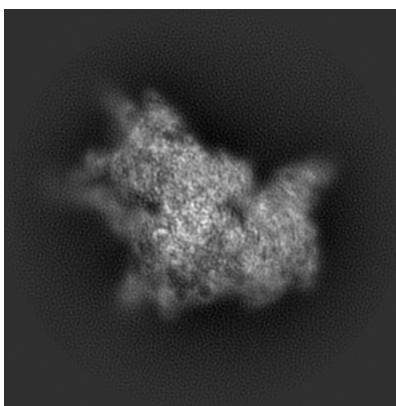
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

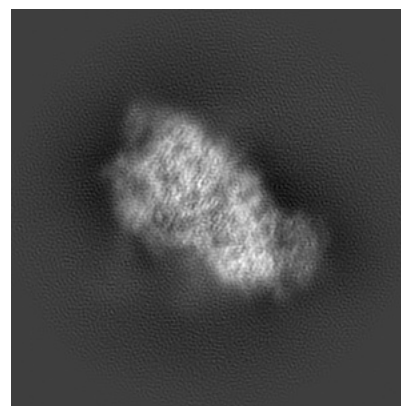
6.1.1 Primary map



X

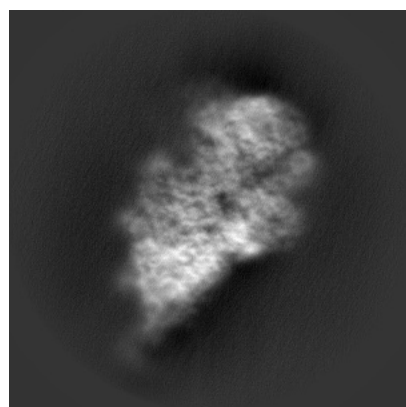


Y

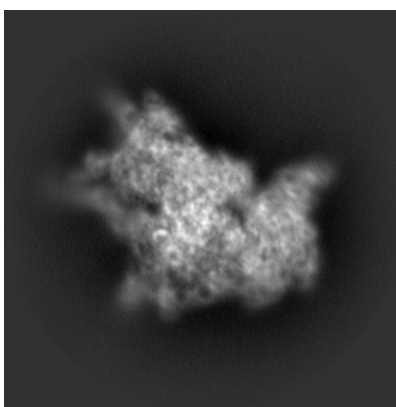


Z

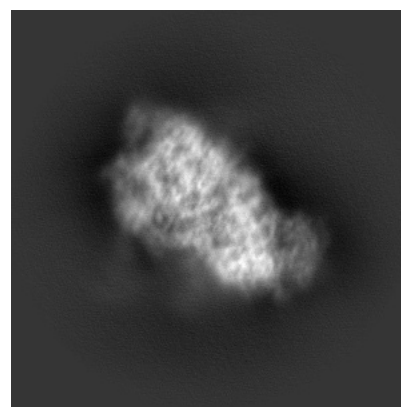
6.1.2 Raw map



X



Y

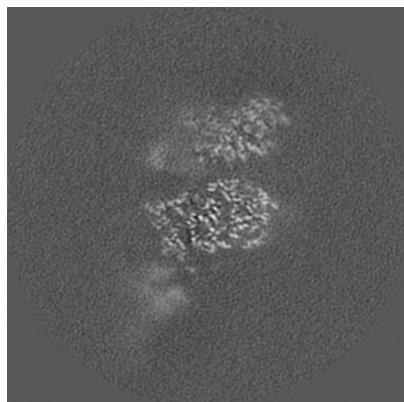


Z

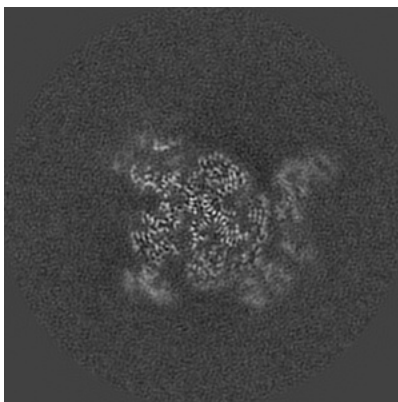
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

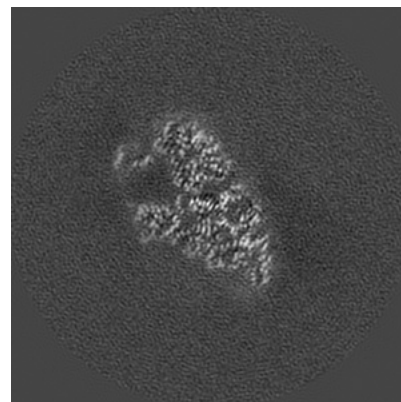
6.2.1 Primary map



X Index: 200

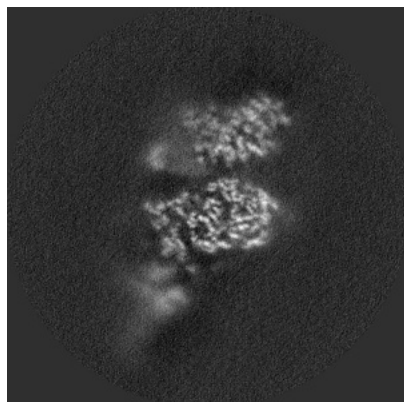


Y Index: 200

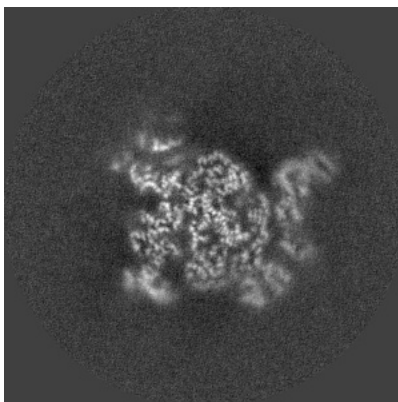


Z Index: 200

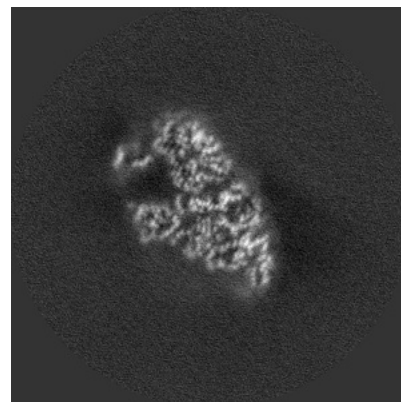
6.2.2 Raw map



X Index: 200



Y Index: 200

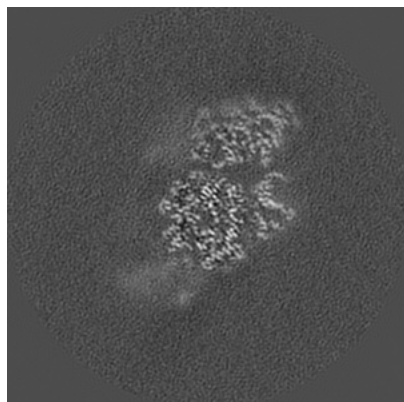


Z Index: 200

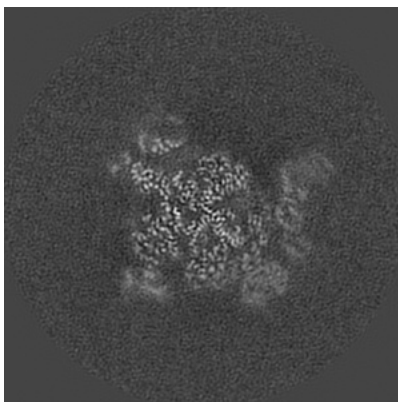
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

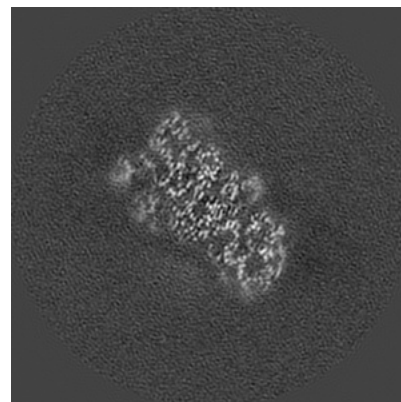
6.3.1 Primary map



X Index: 188

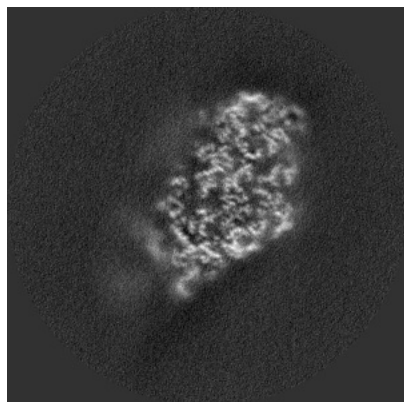


Y Index: 197

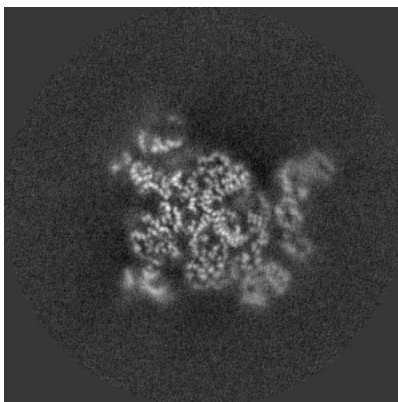


Z Index: 186

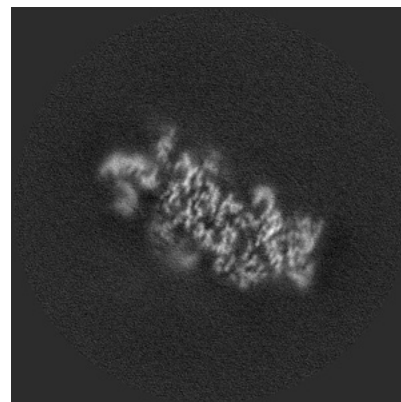
6.3.2 Raw map



X Index: 176



Y Index: 198

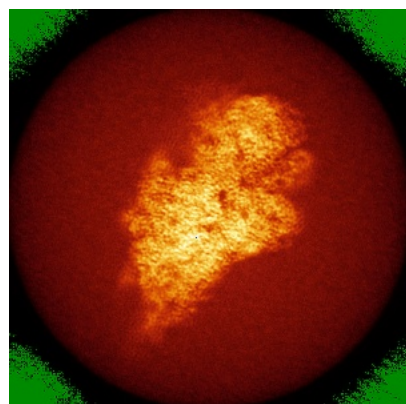


Z Index: 160

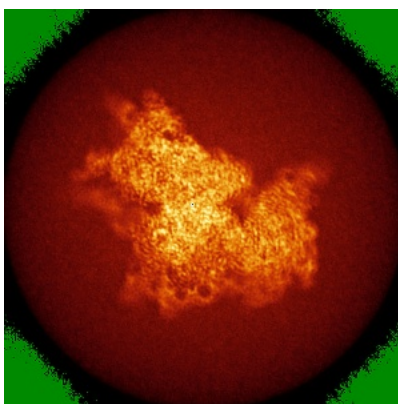
The images above show the largest variance slices of the map in three orthogonal directions.

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

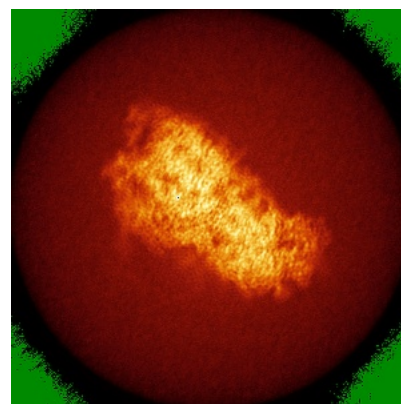
6.4.1 Primary map



X

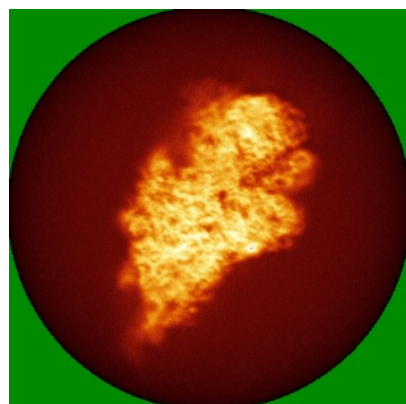


Y

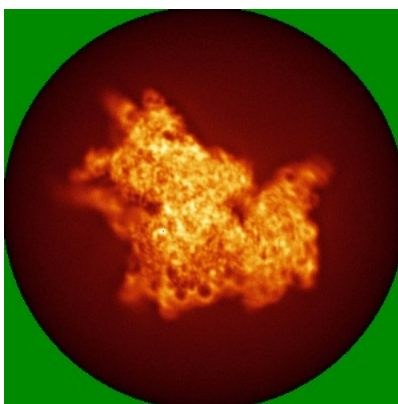


Z

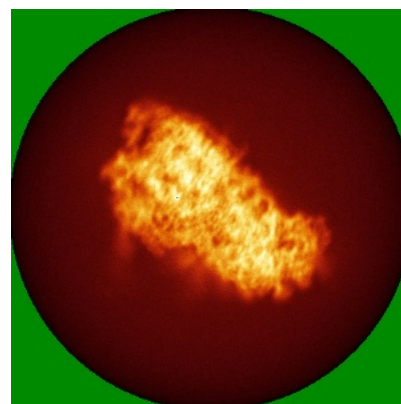
6.4.2 Raw map



X



Y

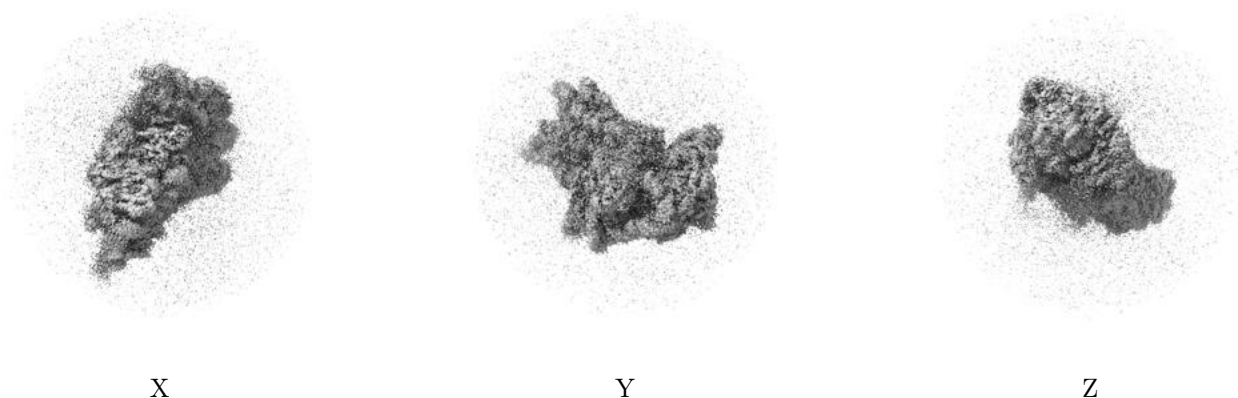


Z

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.

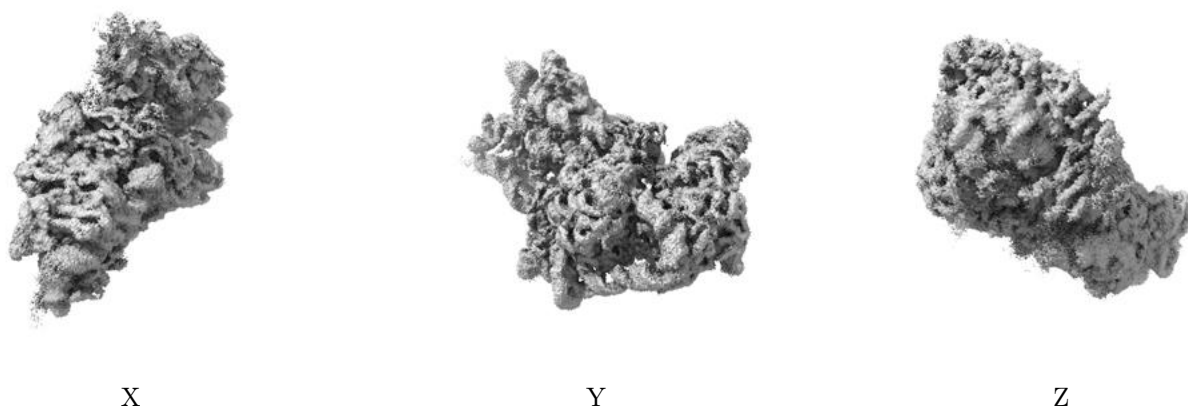
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

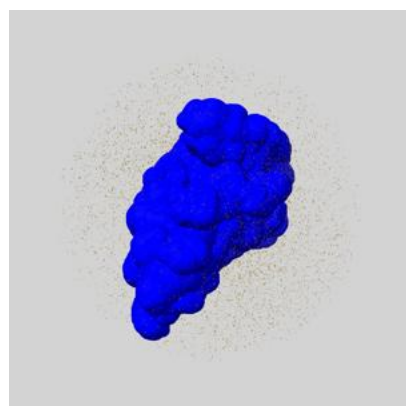
6.6 Mask visualisation [i](#)

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

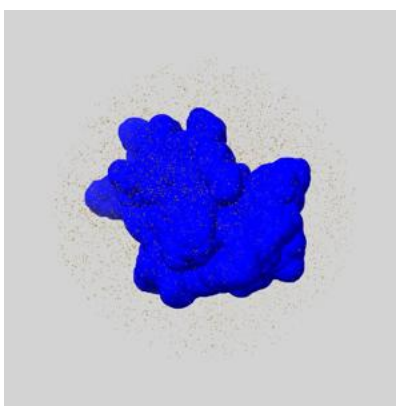
A mask typically either:

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

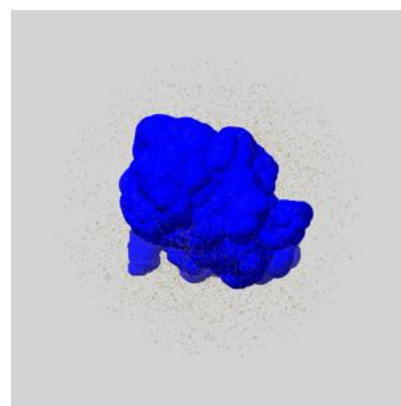
6.6.1 emd_25537_msk_1.map [i](#)



X



Y

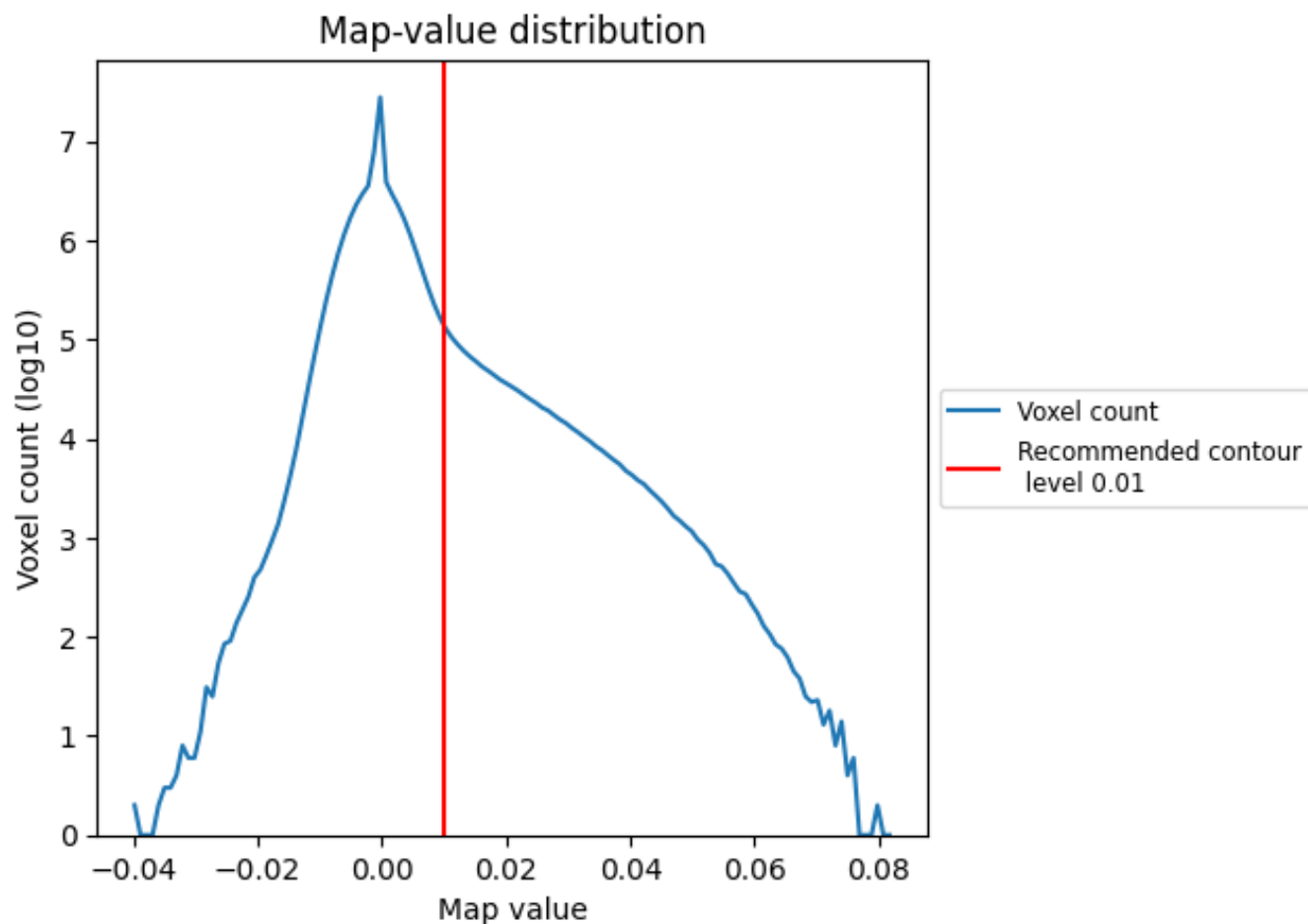


Z

7 Map analysis [i](#)

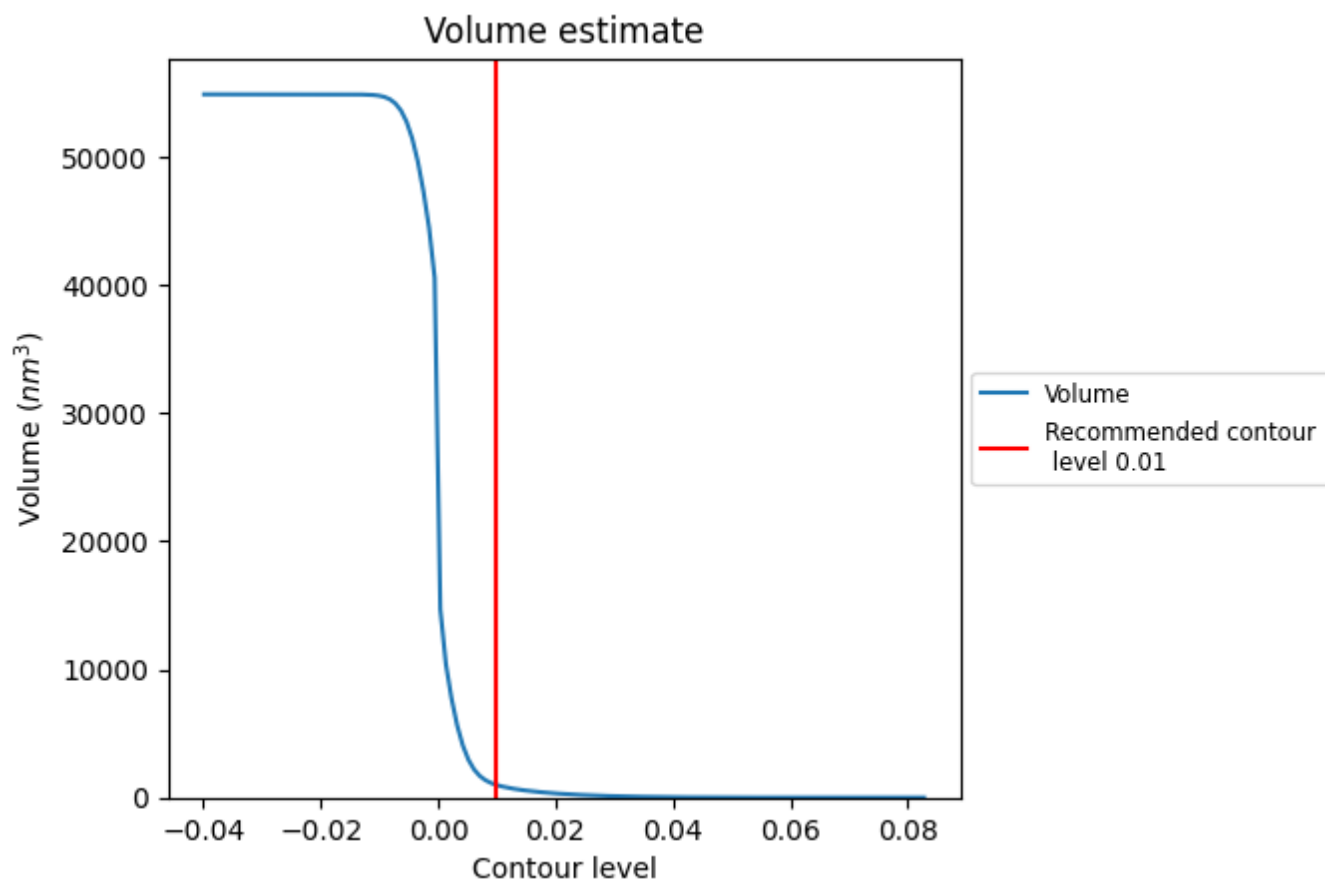
This section contains the results of statistical analysis of the map.

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.

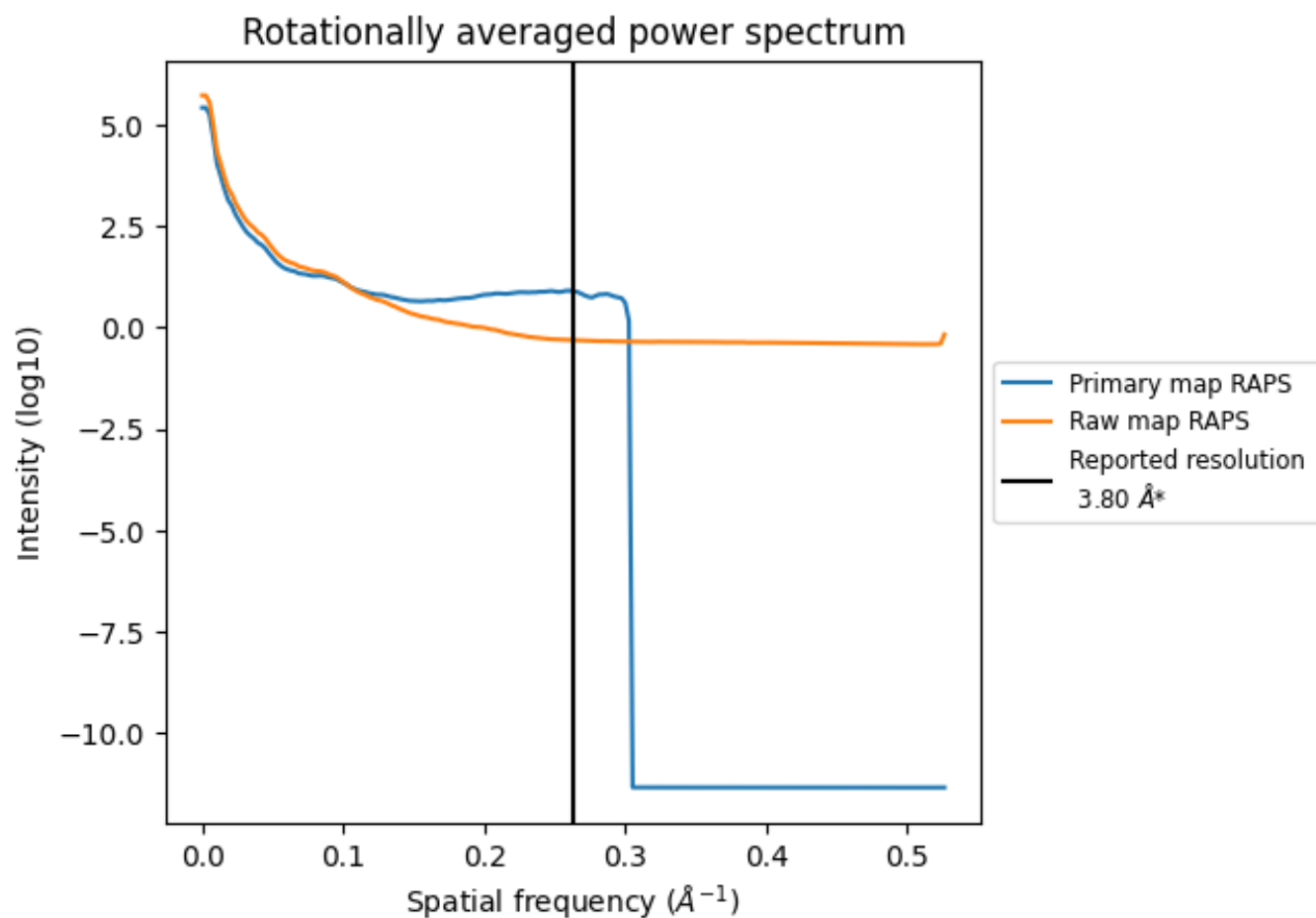
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 976 nm³; this corresponds to an approximate mass of 882 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 ⓘ

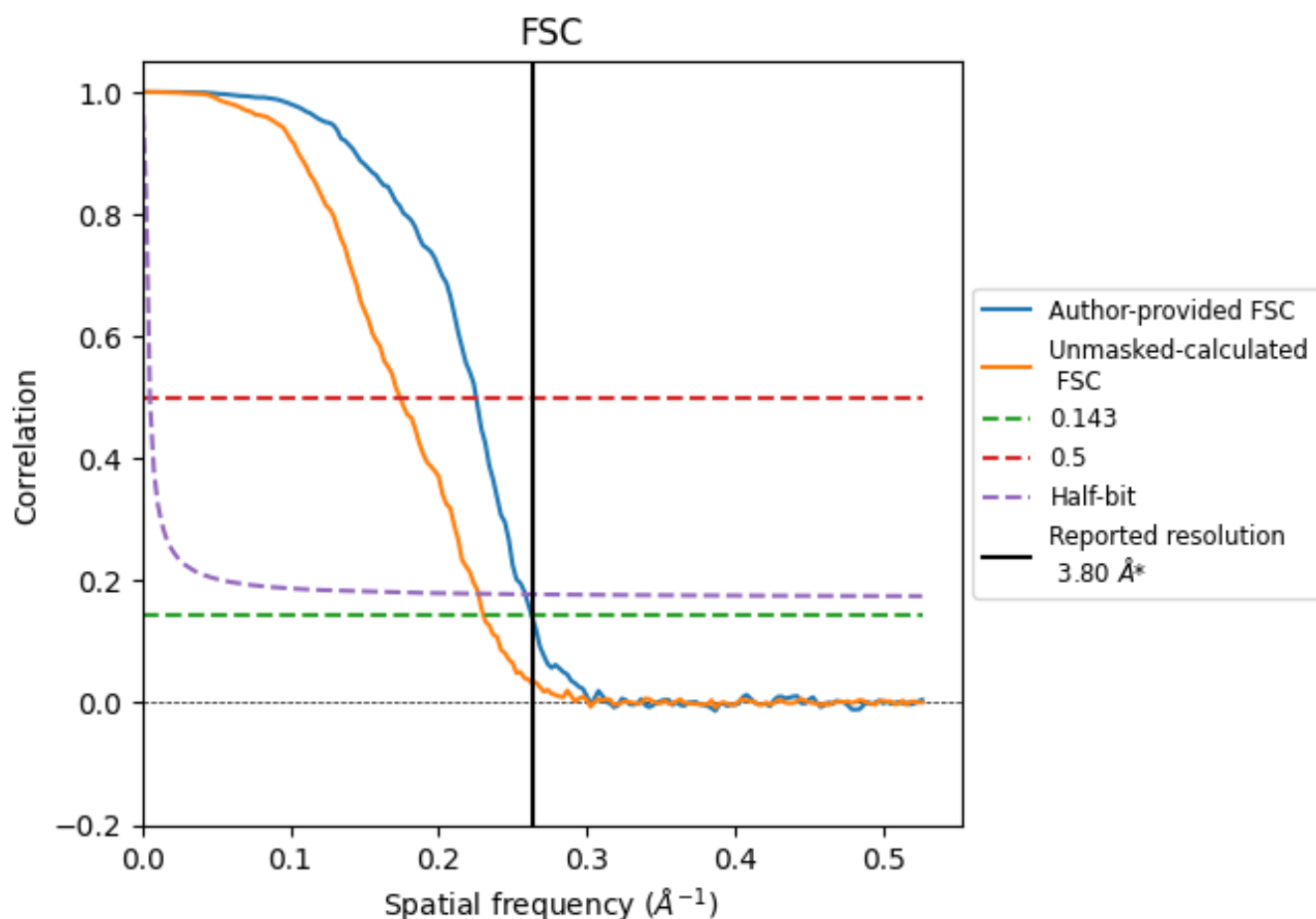


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

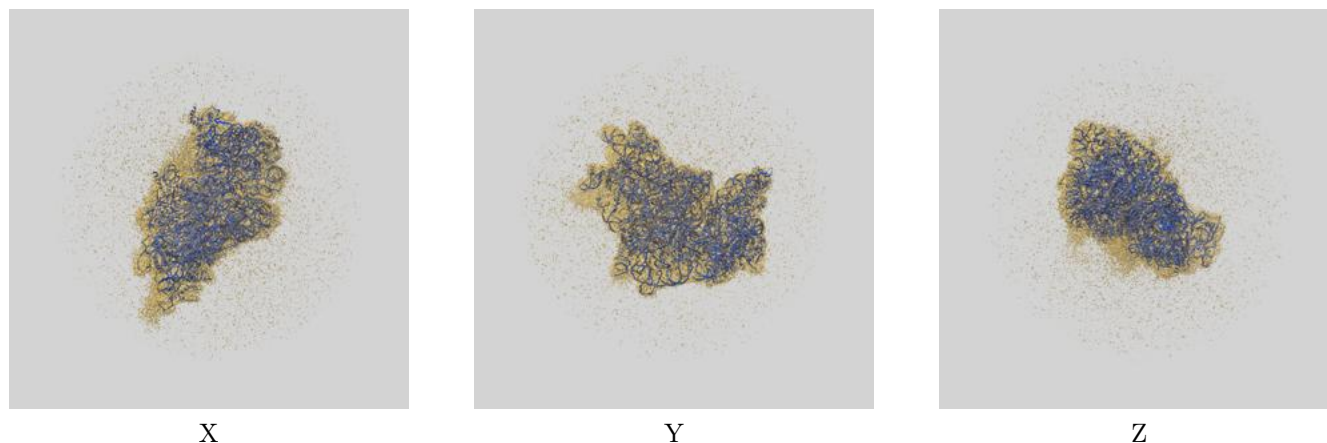
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	4.44	3.87
Unmasked-calculated*	4.34	5.75	4.41

*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 4.34 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

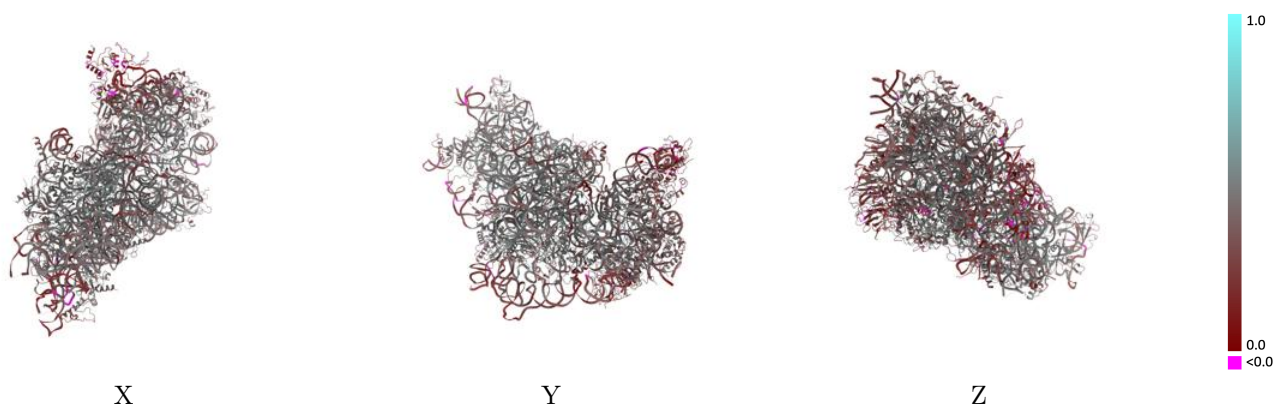
This section contains information regarding the fit between EMDB map EMD-25537 and PDB model 7SYQ. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



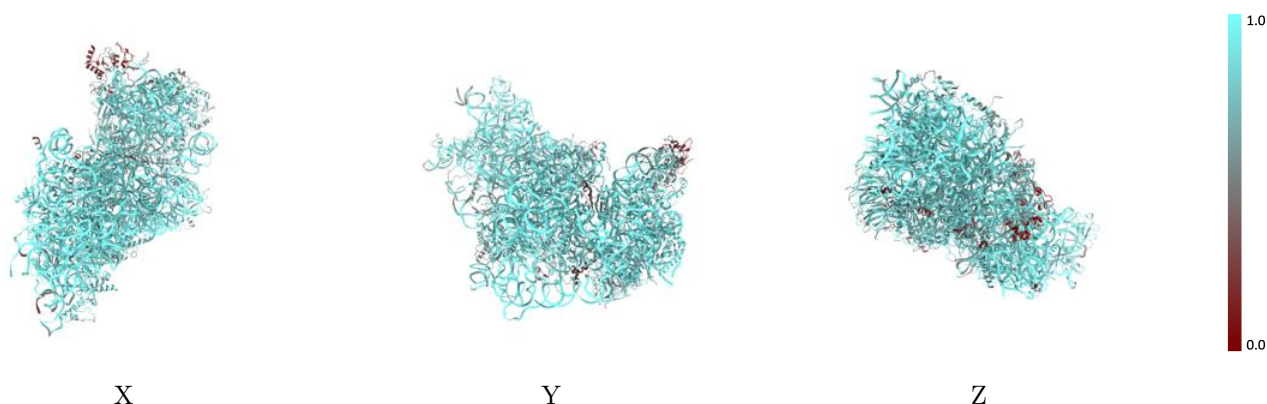
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



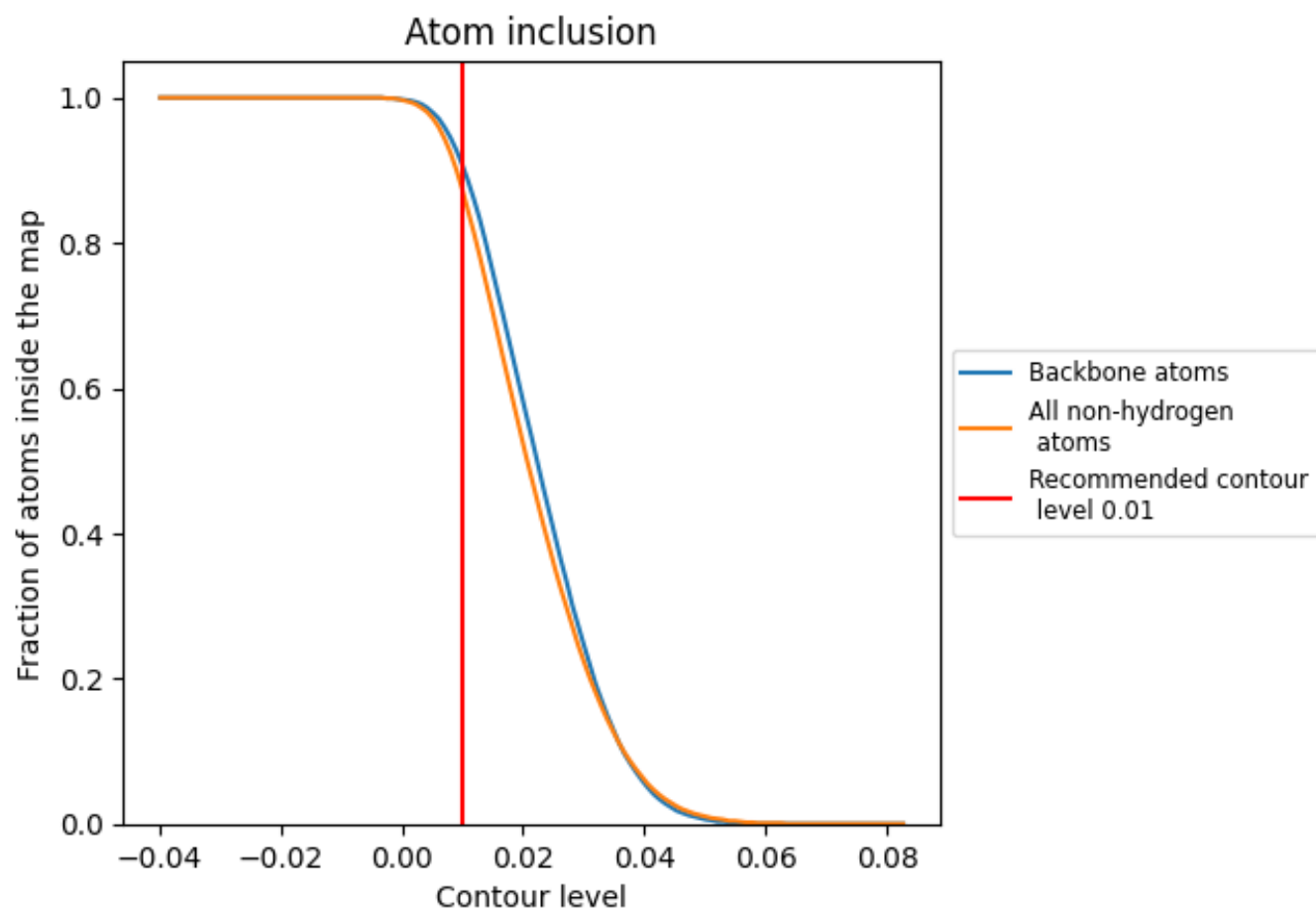
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.3960
2	 0.9400	 0.4090
A	 0.5860	 0.3260
B	 0.8410	 0.4250
C	 0.8920	 0.4510
D	 0.8660	 0.4440
E	 0.7810	 0.3730
F	 0.9160	 0.4680
G	 0.8620	 0.4480
H	 0.8580	 0.3750
I	 0.6970	 0.3830
J	 0.8840	 0.4240
K	 0.8880	 0.4530
L	 0.8130	 0.3260
M	 0.8510	 0.4700
N	 0.2940	 0.1950
O	 0.8750	 0.4430
P	 0.9150	 0.4620
Q	 0.7160	 0.3080
R	 0.8880	 0.4110
S	 0.6800	 0.3500
T	 0.7640	 0.3600
U	 0.9010	 0.4000
V	 0.7180	 0.3450
W	 0.8860	 0.4520
X	 0.8930	 0.4930
Y	 0.8680	 0.4720
Z	 0.9350	 0.4540
a	 0.7680	 0.3800
b	 0.8770	 0.4770
c	 0.8220	 0.4430
d	 0.7910	 0.4400
e	 0.8500	 0.3990
f	 0.6450	 0.2750
g	 0.3050	 0.1850



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Chain	Atom inclusion	Q-score
h	 0.7870	 0.2790
n	 0.8760	 0.4610
z	 0.8630	 0.2920