



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:09 PM UTC

PDB ID : 7SYV / pdb_00007syv
EMDB ID : EMD-25542
Title : Structure of the wt IRES eIF5B-containing pre-48S initiation complex, open conformation. Structure 14(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 : 3.90 Å(reported)
Based on initial models : 6D9J, 4UJD, 5K0Y, 5FLX

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:

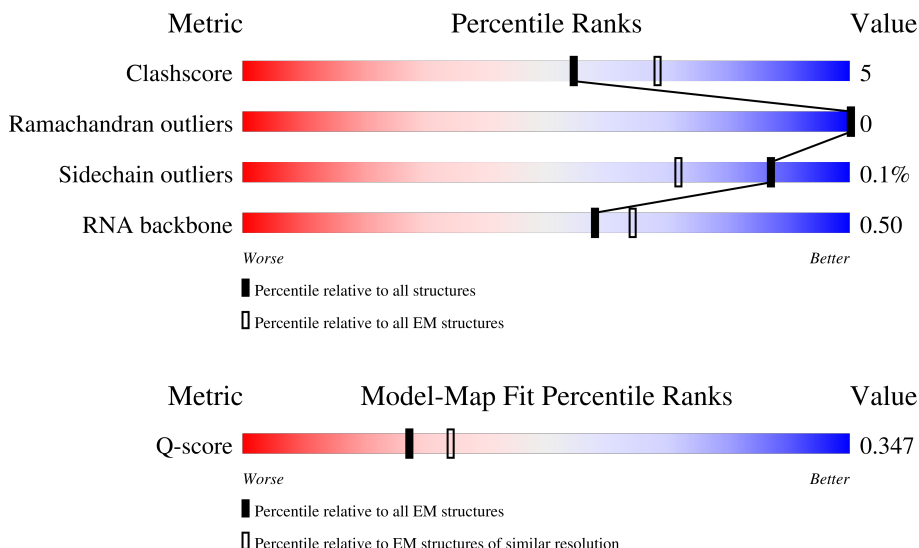
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

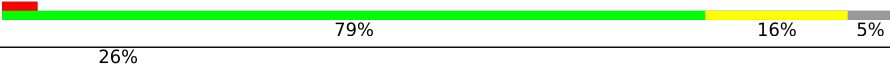
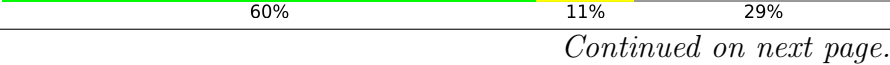
The reported resolution of this entry is 3.90 Å.

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	8855 (3.40 - 4.40)

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	Z	131	
3	A	144	

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Mol	Chain	Length	Quality of chain
4	a	124	
5	B	295	
6	b	101	
7	C	264	
8	c	84	
9	D	221	
10	d	69	
11	E	281	
12	e	56	
13	F	263	
14	f	133	
15	G	204	
16	g	188	
17	H	249	
18	h	317	
19	I	432	
20	i	75	
21	J	208	
22	n	25	
23	K	194	
24	x	627	
25	L	149	
26	z	400	
27	M	158	
28	N	132	

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Mol	Chain	Length	Quality of chain
29	O	151	
30	P	168	
31	Q	145	
32	R	172	
33	S	135	
34	T	152	
35	U	145	
36	V	119	
37	W	83	
38	X	130	
39	Y	143	

2 Entry composition [i](#)

There are 43 unique types of molecules in this entry. The entry contains 87912 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 40S ribosomal protein S24.

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

- Molecule 3 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	102	Total	C	N	O	S	0	0
			822	517	147	154	4		

- Molecule 4 is a protein called 40S ribosomal protein S25.

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

- Molecule 5 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	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 6 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	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
b	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 7 is a protein called eS1.

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

- Molecule 8 is a protein called eS27.

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

- Molecule 9 is a protein called 40S ribosomal protein S2.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	73	MET	VAL	conflict	UNP G1TUT9
D	101	SER	ALA	conflict	UNP G1TUT9
D	119	GLY	ALA	conflict	UNP G1TUT9
D	194	ARG	HIS	conflict	UNP G1TUT9
D	215	MET	LEU	conflict	UNP G1TUT9
D	227	ARG	TRP	conflict	UNP G1TUT9
D	228	GLY	SER	conflict	UNP G1TUT9

- Molecule 10 is a protein called eS28.

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

- Molecule 11 is a protein called uS3.

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

- Molecule 12 is a protein called eS29.

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

- Molecule 13 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	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 14 is a protein called eS30.

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

- Molecule 15 is a protein called uS7.

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

- Molecule 16 is a protein called 40S ribosomal protein S27a.

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

- Molecule 17 is a protein called eS6.

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

- Molecule 18 is a protein called RACK1.

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

- Molecule 19 is a protein called 40S ribosomal protein S7.

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

- Molecule 20 is a RNA chain called Met-tRNA-i-Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 21 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	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 22 is a protein called 60s ribosomal protein l41.

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

- Molecule 23 is a protein called uS4.

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

- Molecule 24 is a protein called Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	x	627	Total	C	N	O	S	0	0
			4965	3157	856	929	23		

- Molecule 25 is a protein called eS10.

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

- Molecule 26 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	z	258	Total	C	N	O	P	0	0
			5513	2456	989	1810	258		

- Molecule 27 is a protein called uS17.

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

- Molecule 28 is a protein called eS12.

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

- Molecule 29 is a protein called uS15.

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

- Molecule 30 is a protein called uS11.

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

- Molecule 31 is a protein called uS19.

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

- Molecule 32 is a protein called uS9.

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

- Molecule 33 is a protein called eS17.

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

- Molecule 34 is a protein called uS13.

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

- Molecule 35 is a protein called eS19.

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

- Molecule 36 is a protein called uS10.

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

- Molecule 37 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	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 38 is a protein called uS8.

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

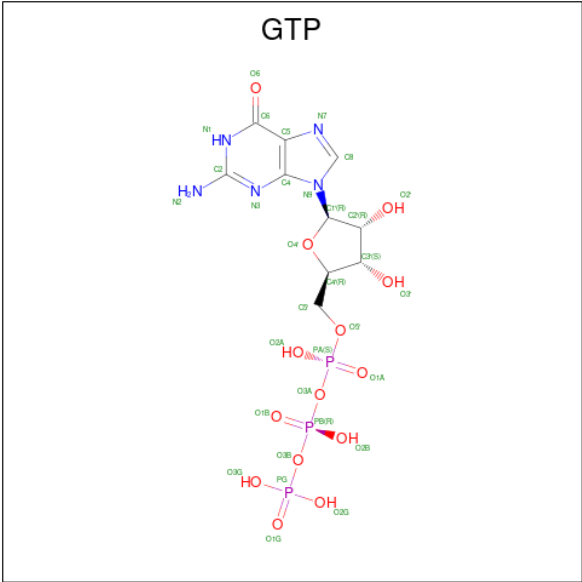
- Molecule 39 is a protein called uS12.

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

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 41 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
41	x	1	Total	C	N	O	P	0
			32	10	5	14	3	

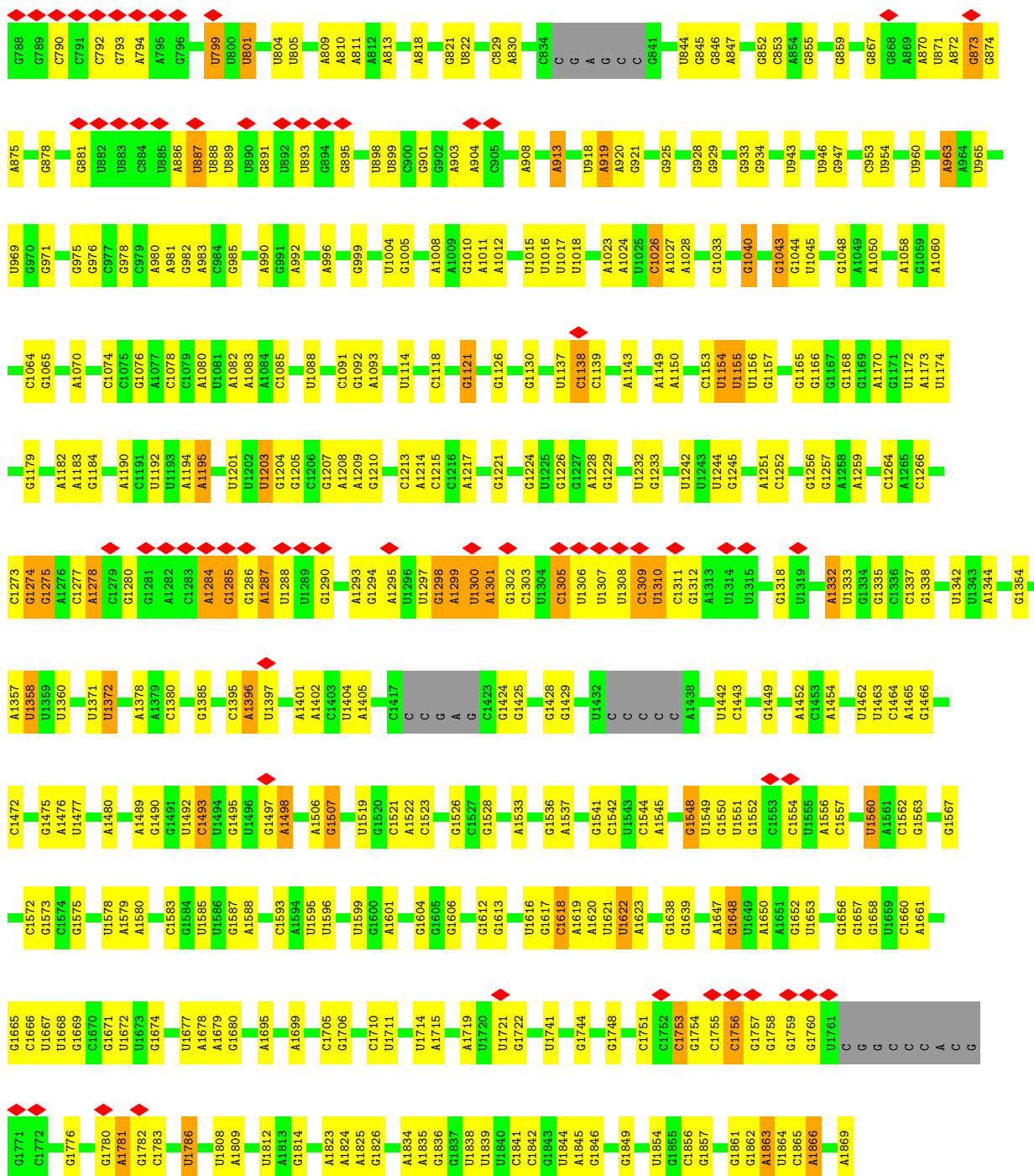
- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
42	x	1	Total	Mg	0
			1	1	

- Molecule 43 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
43	x	1	Total	Na	0
			1	1	



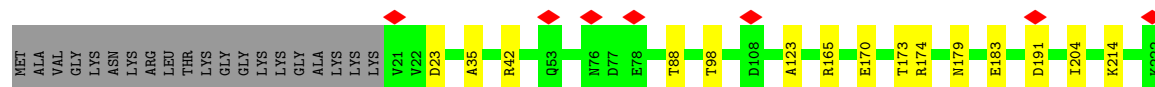


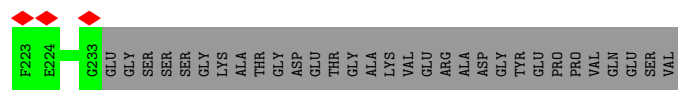
- Molecule 2: 40S ribosomal protein S24

Chain Z: 79% 16% 5%

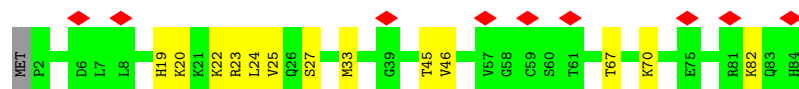
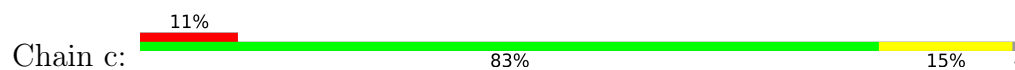


- Molecule 3: Eukaryotic translation initiation factor 1A, X-chromosomal

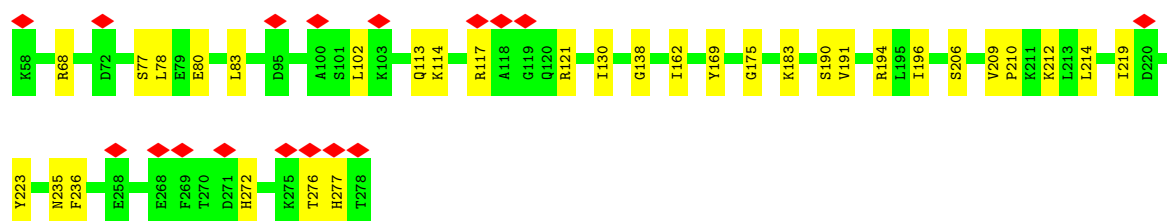
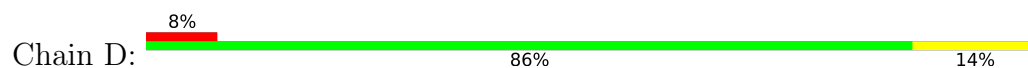




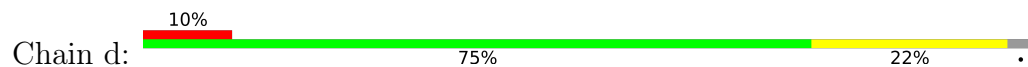
• Molecule 8: eS27



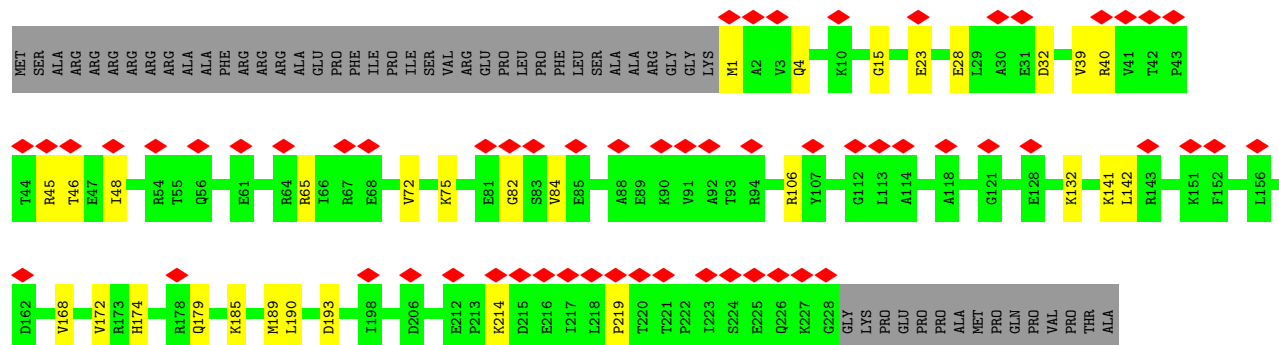
• Molecule 9: 40S ribosomal protein S2



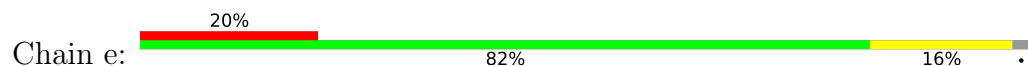
• Molecule 10: eS28

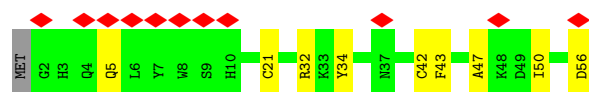


• Molecule 11: uS3



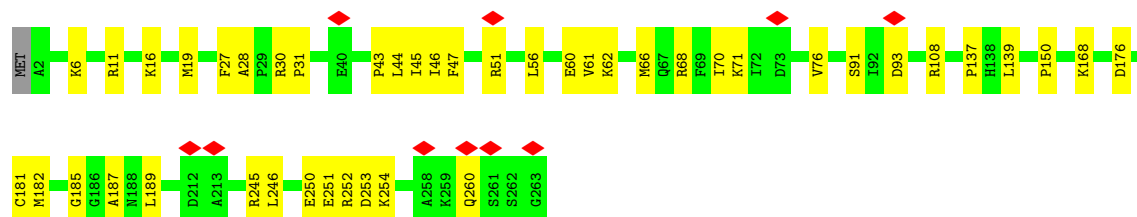
• Molecule 12: eS29





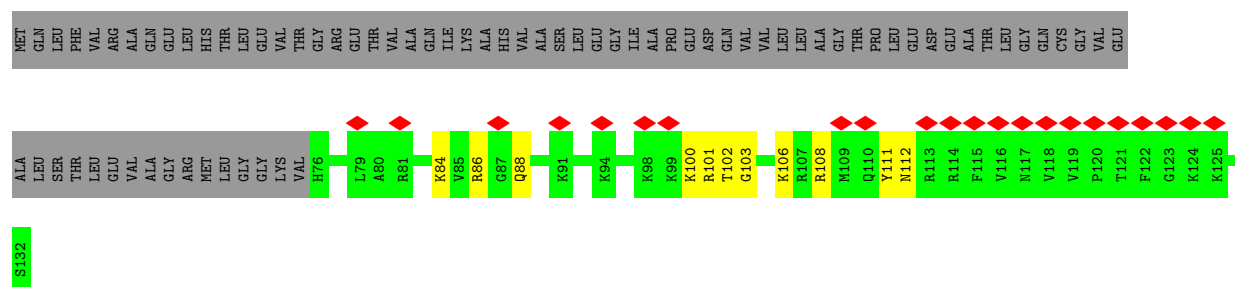
- Molecule 13: 40S ribosomal protein S4

Chain F: 83% 17%



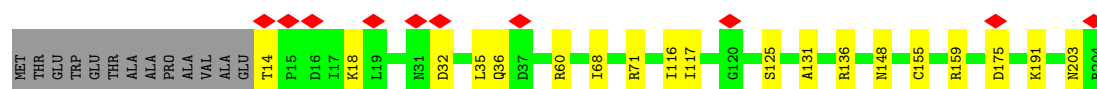
- Molecule 14: eS30

Chain f: 17% 35% 8% 57%



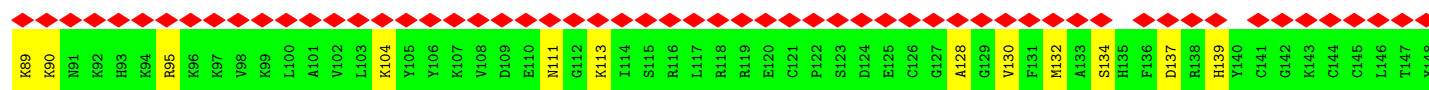
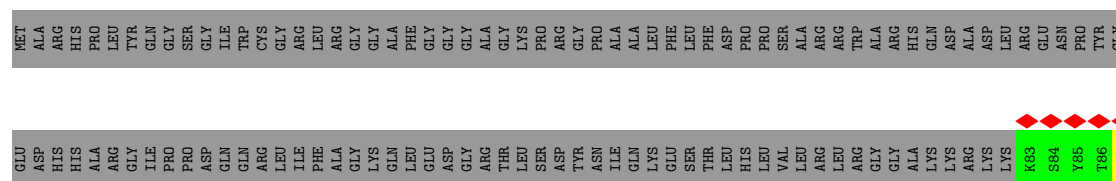
- Molecule 15: uS7

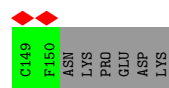
Chain G: 5% 84% 9% 6%



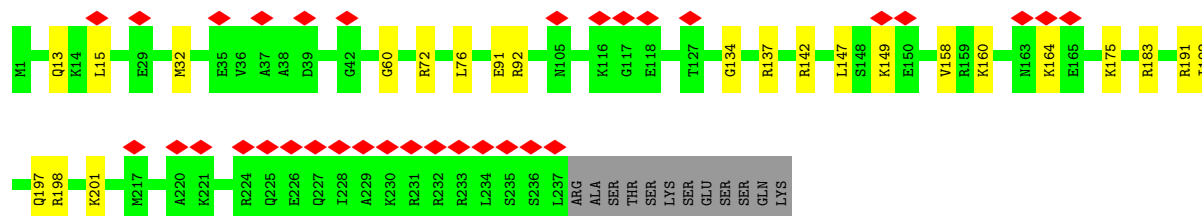
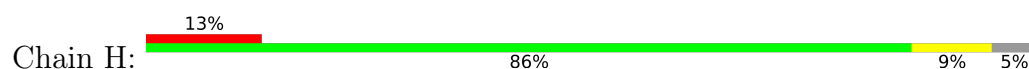
- Molecule 16: 40S ribosomal protein S27a

Chain g: 35% 29% 7% 64%

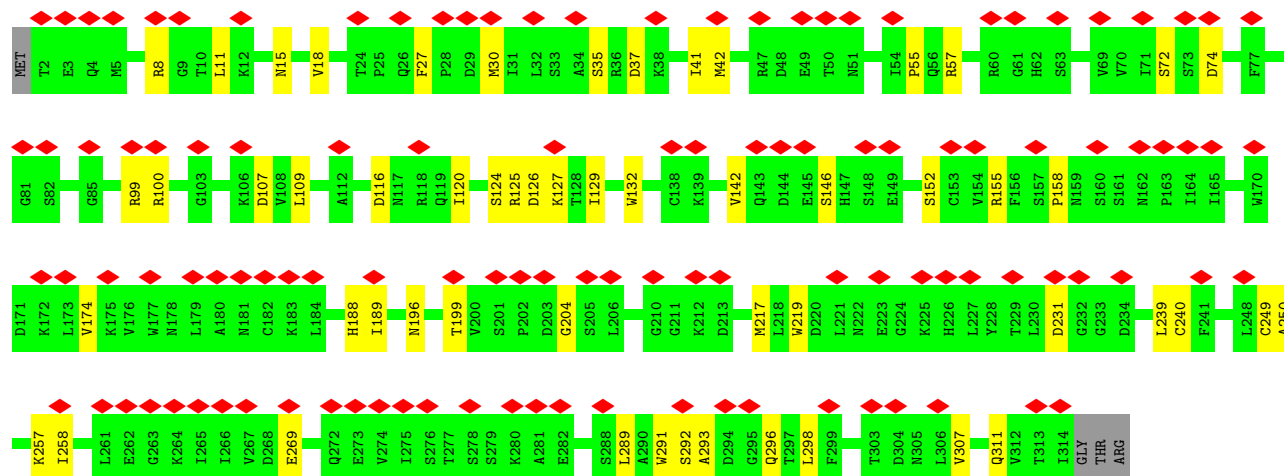
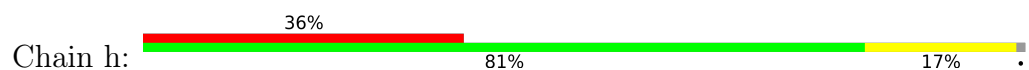




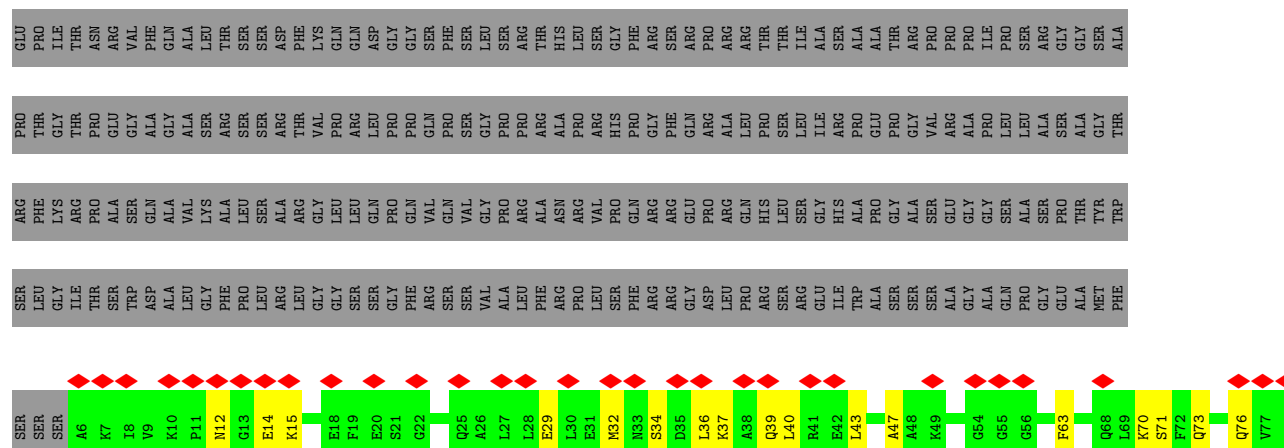
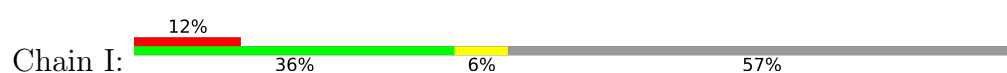
- Molecule 17: eS6



- Molecule 18: RACK1

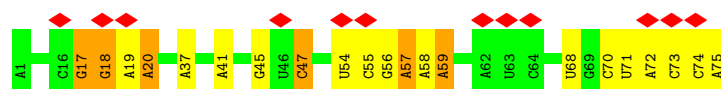


- Molecule 19: 40S ribosomal protein S7

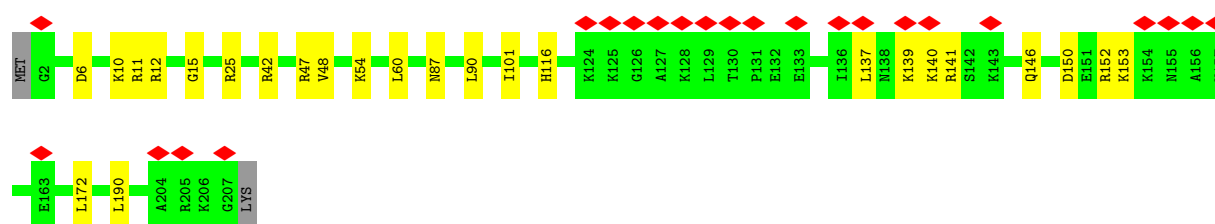
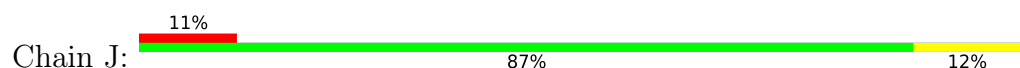




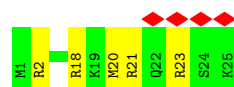
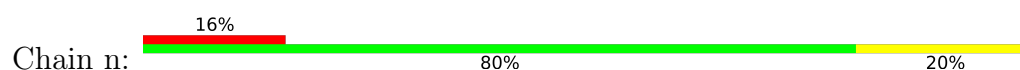
• Molecule 20: Met-tRNA-i-Met



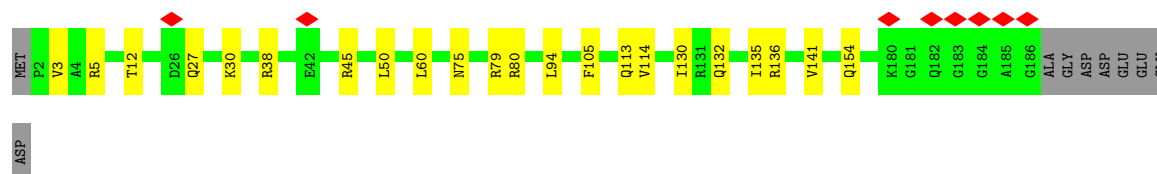
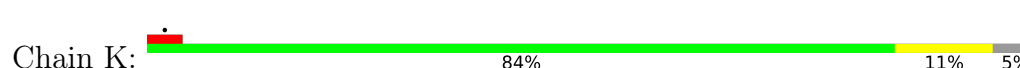
• Molecule 21: eS8



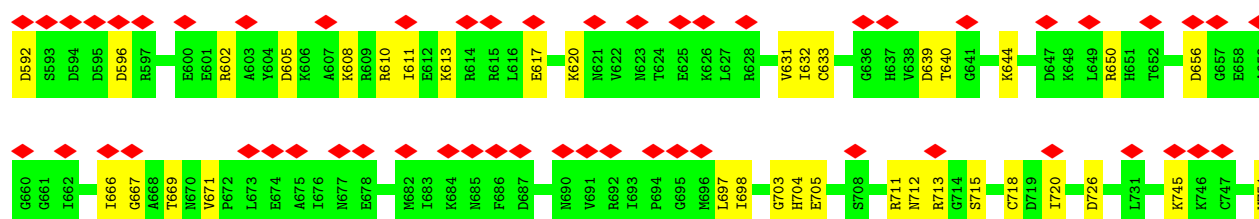
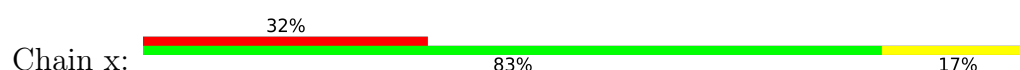
• Molecule 22: 60s ribosomal protein l41

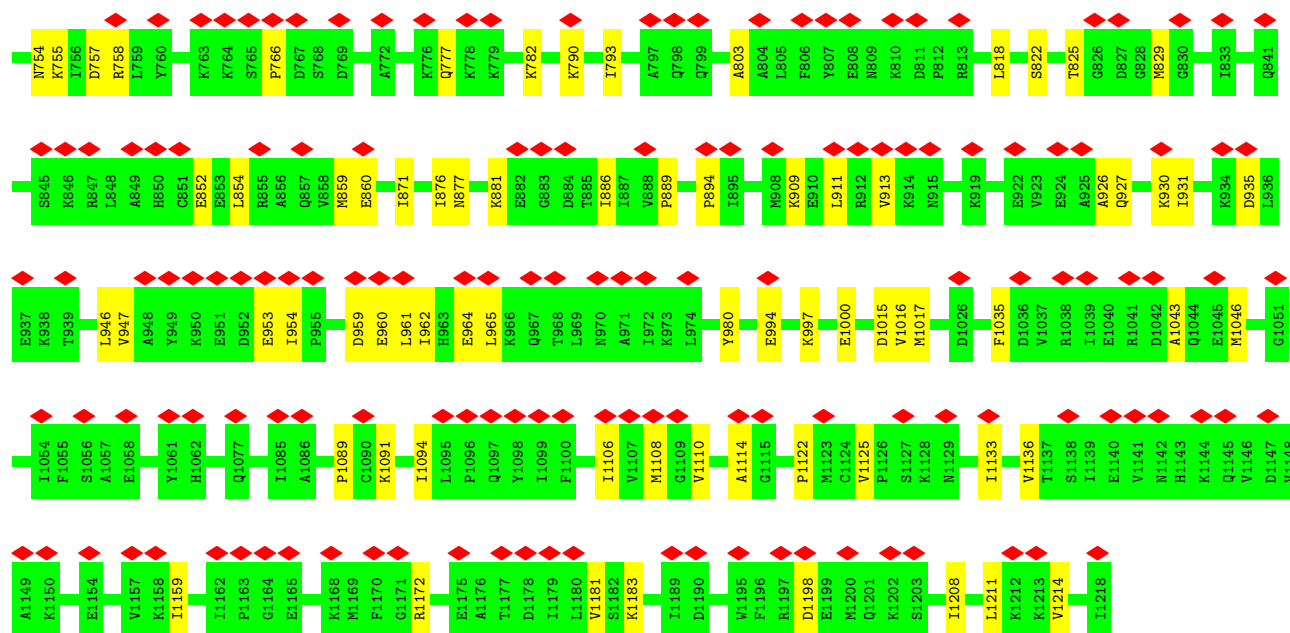


• Molecule 23: uS4

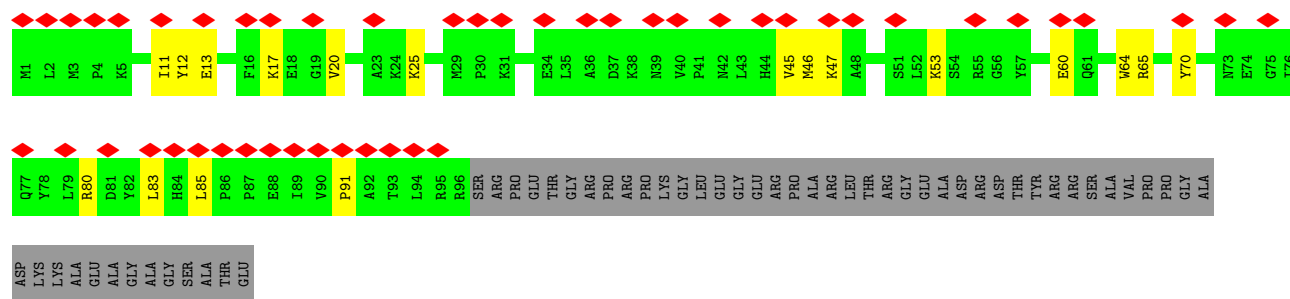


• Molecule 24: Eukaryotic translation initiation factor 5B

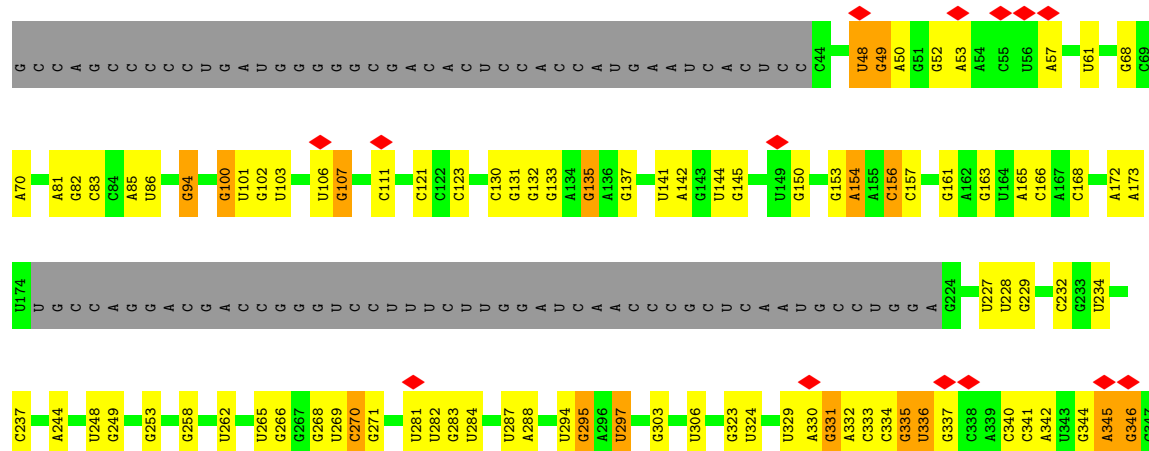




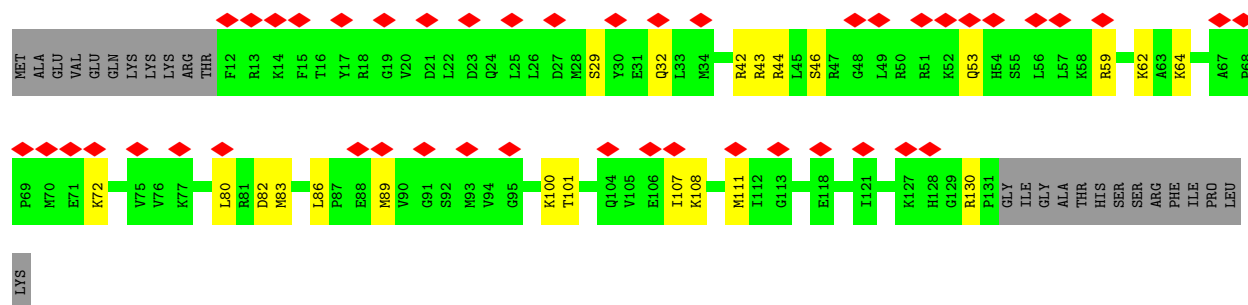
• Molecule 25: eS10



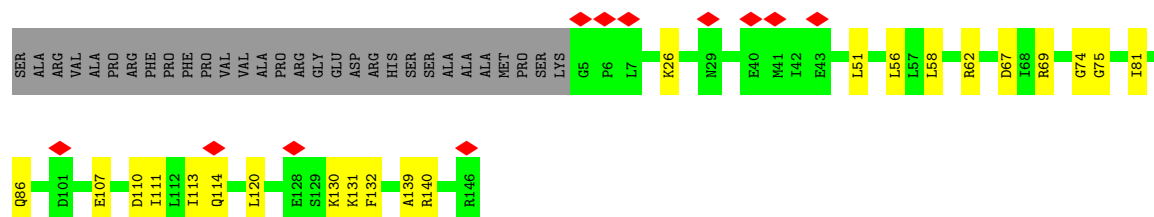
• Molecule 26: HCV IRES



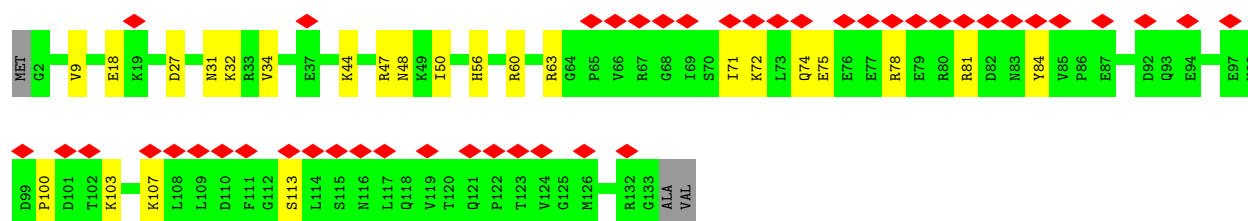
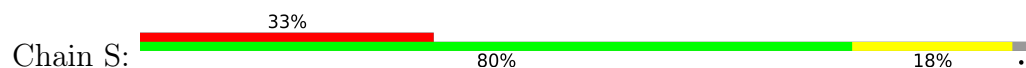




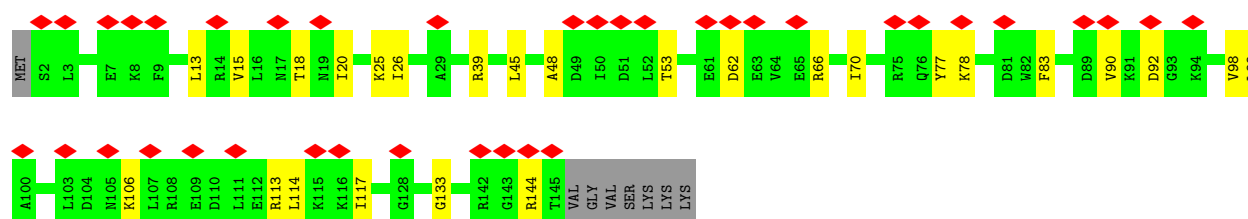
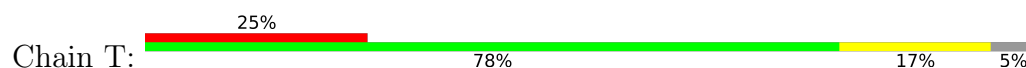
- Molecule 32: uS9



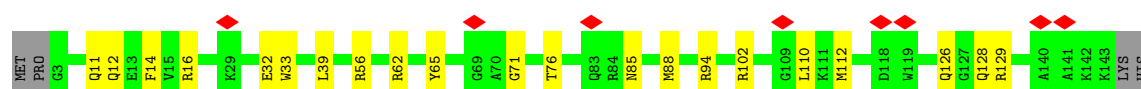
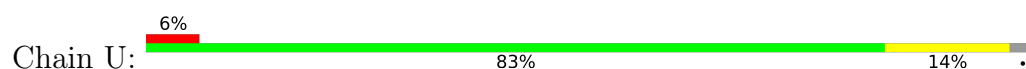
- Molecule 33: eS17



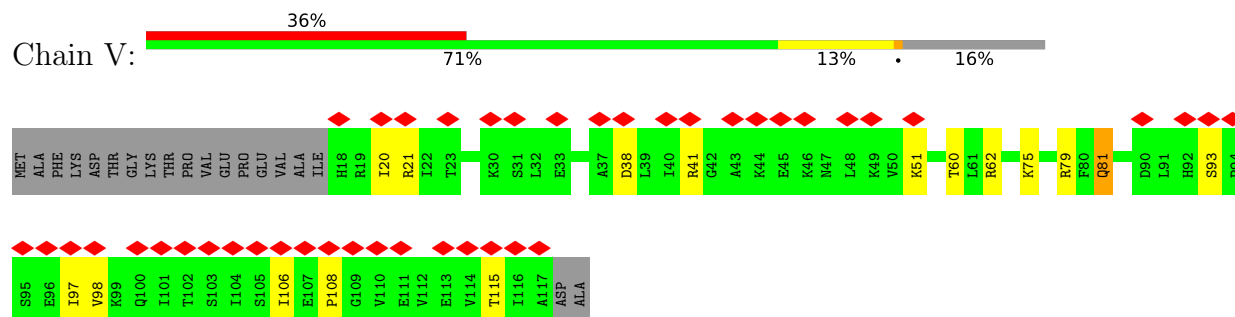
- Molecule 34: uS13



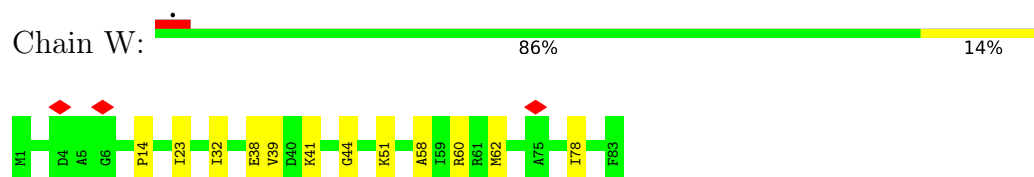
- Molecule 35: eS19



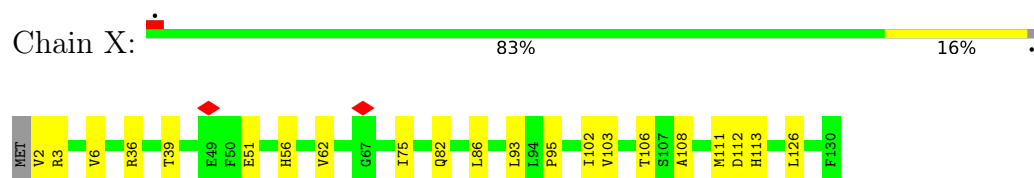
- Molecule 36: uS10



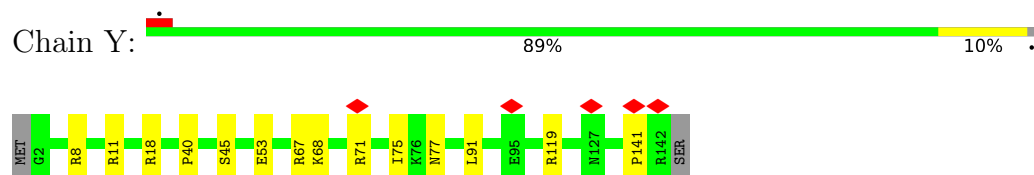
- Molecule 37: 40S ribosomal protein S21



- Molecule 38: uS8



- Molecule 39: uS12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60578	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	52000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.033	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: GTP, ZN, MG, NA

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	1/62495 (0.0%)
2	Z	0.18	0/1028	0.47	0/1366
3	A	0.20	0/833	0.54	0/1114
4	a	0.23	0/620	0.59	0/831
5	B	0.15	0/1747	0.39	0/2374
6	b	0.17	0/828	0.42	0/1109
7	C	0.14	0/1756	0.39	0/2350
8	c	0.18	0/665	0.49	0/891
9	D	0.19	0/1753	0.51	0/2369
10	d	0.23	0/532	0.52	0/712
11	E	0.16	0/1796	0.41	0/2417
12	e	0.15	0/470	0.38	0/623
13	F	0.18	0/2118	0.50	1/2849 (0.0%)
14	f	0.18	0/462	0.48	0/607
15	G	0.20	0/1531	0.53	0/2059
16	g	0.11	0/567	0.35	0/753
17	H	0.17	0/1946	0.44	1/2590 (0.0%)
18	h	0.14	0/2493	0.42	0/3394
19	I	0.20	0/1510	0.51	1/2022 (0.0%)
20	i	0.08	0/1795	0.15	0/2798
21	J	0.16	0/1715	0.41	0/2287
22	n	0.22	0/240	0.67	0/305
23	K	0.20	0/1550	0.53	1/2069 (0.0%)
24	x	0.22	0/5047	0.59	6/6803 (0.1%)
25	L	0.17	0/834	0.44	0/1125
26	z	0.25	3/6161 (0.0%)	0.32	2/9604 (0.0%)
27	M	0.17	0/1254	0.44	0/1677
28	N	0.17	0/918	0.45	0/1233
29	O	0.20	0/1226	0.48	0/1649
30	P	0.19	0/1029	0.51	1/1380 (0.1%)
31	Q	0.16	0/1017	0.53	0/1358
32	R	0.19	0/1146	0.50	1/1534 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	S	0.22	0/1082	0.61	0/1452
34	T	0.17	0/1208	0.48	0/1618
35	U	0.15	0/1115	0.41	0/1493
36	V	0.19	0/805	0.49	0/1081
37	W	0.22	0/643	0.59	1/860 (0.1%)
38	X	0.21	0/1051	0.53	0/1406
39	Y	0.17	0/1116	0.47	1/1490 (0.1%)
All	All	0.17	3/93709 (0.0%)	0.40	17/136147 (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
36	V	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	z	336	U	O3'-P	7.79	1.72	1.61
26	z	346	G	C1'-N9	-7.18	1.37	1.48
26	z	336	U	O5'-C5'	5.32	1.50	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	z	336	U	C2'-C3'-O3'	-6.34	99.99	109.50
39	Y	141	PRO	CA-N-CD	-6.34	103.12	112.00
17	H	197	GLN	N-CA-CB	5.85	119.94	110.40
26	z	336	U	C4'-C3'-O3'	5.78	118.06	109.40
24	x	964	GLU	N-CA-CB	5.70	119.69	110.40
30	P	87	GLU	N-CA-CB	5.66	119.62	110.40
24	x	766	PRO	CA-C-N	5.39	131.84	121.54
24	x	766	PRO	C-N-CA	5.39	131.84	121.54
24	x	1035	PHE	CA-C-N	5.32	131.69	121.54
24	x	1035	PHE	C-N-CA	5.32	131.69	121.54
13	F	260	GLN	N-CA-CB	5.28	119.00	110.40
19	I	15	LYS	CB-CG-CD	5.27	123.42	111.30
23	K	27	GLN	N-CA-CB	5.20	118.88	110.40
24	x	1000	GLU	CA-CB-CG	5.20	124.50	114.10
1	2	1825	A	C4'-C3'-O3'	-5.17	105.25	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	R	107	GLU	N-CA-CB	5.15	118.77	110.42
37	W	41	LYS	CB-CG-CD	5.10	123.03	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	V	81	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	284	0
2	Z	1011	0	1083	14	0
3	A	822	0	831	13	0
4	a	614	0	678	11	0
5	B	1710	0	1708	19	0
6	b	814	0	863	16	0
7	C	1729	0	1803	10	0
8	c	651	0	672	7	0
9	D	1716	0	1806	21	0
10	d	530	0	561	9	0
11	E	1768	0	1866	21	0
12	e	459	0	452	10	0
13	F	2076	0	2177	31	0
14	f	457	0	502	8	0
15	G	1509	0	1563	13	0
16	g	555	0	563	12	0
17	H	1923	0	2089	21	0
18	h	2436	0	2393	35	0
19	I	1488	0	1582	15	0
20	i	1604	0	816	7	0
21	J	1686	0	1772	17	0
22	n	239	0	289	5	0
23	K	1525	0	1640	14	0
24	x	4965	0	5124	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	L	810	0	836	13	0
26	z	5513	0	2787	32	0
27	M	1233	0	1310	16	0
28	N	908	0	939	10	0
29	O	1202	0	1289	16	0
30	P	1016	0	1039	20	0
31	Q	997	0	1045	15	0
32	R	1128	0	1195	15	0
33	S	1068	0	1121	14	0
34	T	1190	0	1249	17	0
35	U	1097	0	1130	14	0
36	V	795	0	862	11	0
37	W	636	0	637	8	0
38	X	1034	0	1080	14	0
39	Y	1098	0	1167	10	0
40	b	1	0	0	0	0
40	g	1	0	0	0	0
41	x	32	0	12	8	0
42	x	1	0	0	0	0
43	x	1	0	0	0	0
All	All	87912	0	68644	750	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 (750) 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)
24:x:639:ASP:HA	41:x:1301:GTP:H5'	1.31	1.12
1:2:1332:A:H62	1:2:1493:C:N4	1.64	0.96
1:2:1656:G:H1	1:2:1668:U:H3	1.02	0.93
1:2:1652:G:H1	1:2:1672:U:H3	1.10	0.92
1:2:1332:A:N6	1:2:1493:C:H42	1.67	0.92
1:2:16:G:H21	1:2:1195:A:H62	1.12	0.88
24:x:758:ARG:HD3	41:x:1301:GTP:N2	1.88	0.88
1:2:1722:G:H1	1:2:1812:U:H3	1.19	0.87
24:x:758:ARG:HD3	41:x:1301:GTP:HN21	1.40	0.86
24:x:726:ASP:OD1	24:x:755:LYS:HD3	1.74	0.86
1:2:934:G:H1	1:2:1008:A:H2	1.21	0.85
24:x:726:ASP:CG	24:x:755:LYS:HD3	2.02	0.83
1:2:1657:G:H1	1:2:1667:U:H3	1.25	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:z:262:U:H3	26:z:271:G:H1	1.27	0.81
1:2:1332:A:H62	1:2:1493:C:H42	0.86	0.77
30:P:27:VAL:O	30:P:92:ALA:HB3	1.84	0.76
24:x:704:HIS:ND1	24:x:705:GLU:N	2.34	0.75
1:2:16:G:N2	1:2:1195:A:H62	1.83	0.75
1:2:1472:C:H42	1:2:1476:A:H62	1.37	0.73
1:2:1748:G:H1	1:2:1786:U:H3	1.37	0.73
26:z:335:G:H5''	30:P:110:PRO:HB2	1.69	0.73
1:2:318:A:N1	1:2:333:G:C6	2.58	0.71
1:2:934:G:N1	1:2:1008:A:C2	2.57	0.67
23:K:114:VAL:HG21	23:K:130:ILE:HD11	1.78	0.66
37:W:14:PRO:HG2	37:W:23:ILE:HD11	1.79	0.64
1:2:1033:G:H1	1:2:1080:A:HO2'	1.42	0.64
18:h:27:PHE:HB2	18:h:30:MET:HB2	1.78	0.64
18:h:11:LEU:HB2	18:h:307:VAL:HB	1.80	0.64
1:2:536:A:H61	1:2:547:G:H1'	1.63	0.63
24:x:758:ARG:CD	41:x:1301:GTP:HN21	2.09	0.63
24:x:909:LYS:HD3	24:x:913:VAL:HG21	1.82	0.62
1:2:318:A:C2	1:2:333:G:N1	2.67	0.61
19:I:43:LEU:HD11	19:I:71:SER:HB2	1.82	0.61
11:E:72:VAL:HG22	25:L:20:VAL:HG21	1.82	0.60
36:V:38:ASP:OD1	36:V:41:ARG:NH2	2.34	0.60
1:2:318:A:C2	1:2:333:G:C2	2.89	0.60
1:2:1048:G:H21	1:2:1070:A:H62	1.49	0.60
9:D:196:ILE:HB	9:D:223:TYR:HB2	1.84	0.60
1:2:1719:A:N6	1:2:1814:G:O2'	2.35	0.60
1:2:934:G:N1	1:2:1008:A:H2	1.96	0.60
24:x:669:THR:HB	24:x:698:ILE:HB	1.84	0.60
1:2:677:G:H21	1:2:1028:A:H62	1.48	0.59
13:F:251:GLU:HA	13:F:254:LYS:HG2	1.84	0.59
24:x:666:ILE:HB	24:x:860:GLU:HG2	1.85	0.59
1:2:1192:U:OP2	39:Y:119:ARG:NH2	2.36	0.58
1:2:153:G:N3	17:H:13:GLN:NE2	2.50	0.58
24:x:886:ILE:HG22	24:x:947:VAL:HG22	1.85	0.58
13:F:71:LYS:HB2	13:F:91:SER:HB2	1.86	0.58
16:g:132:MET:HE2	16:g:139:HIS:HB2	1.84	0.58
11:E:40:ARG:HA	36:V:108:PRO:HB3	1.86	0.58
24:x:1122:PRO:HB2	24:x:1183:LYS:HB3	1.86	0.58
1:2:1016:U:H5''	29:O:14:SER:HB2	1.86	0.58
1:2:1475:G:OP2	1:2:1475:G:N2	2.37	0.57
18:h:174:VAL:HB	18:h:188:HIS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:g:111:ASN:HB2	16:g:113:LYS:HZ2	1.70	0.57
13:F:185:GLY:H	13:F:189:LEU:HD13	1.69	0.57
1:2:158:A:N6	1:2:466:G:N7	2.52	0.57
11:E:46:THR:HB	11:E:84:VAL:HG12	1.86	0.57
20:i:18:G:N2	20:i:55:C:N3	2.52	0.57
1:2:1091:C:HO2'	38:X:2:VAL:N	2.02	0.57
1:2:976:G:N3	30:P:50:LYS:NZ	2.53	0.56
1:2:1284:A:H5'	1:2:1285:G:H8	1.70	0.56
1:2:1405:A:H2	1:2:1443:C:H42	1.53	0.56
1:2:1563:G:H1	1:2:1572:C:H42	1.53	0.56
5:B:76:VAL:HG12	5:B:123:VAL:HB	1.88	0.56
31:Q:64:LYS:HE3	31:Q:89:MET:HB2	1.86	0.56
1:2:64:A:H2	1:2:83:A:H62	1.52	0.56
5:B:7:VAL:HG13	5:B:8:LEU:HG	1.87	0.56
33:S:27:ASP:O	33:S:31:ASN:ND2	2.38	0.56
23:K:12:THR:HG22	23:K:45:ARG:HB2	1.88	0.56
27:M:75:GLY:HA3	27:M:88:ILE:HD12	1.87	0.56
1:2:561:A:O2'	23:K:132:GLN:OE1	2.18	0.56
21:J:150:ASP:HA	21:J:153:LYS:HG2	1.87	0.56
1:2:934:G:O6	1:2:1008:A:N1	2.39	0.56
24:x:758:ARG:CD	41:x:1301:GTP:N2	2.65	0.56
1:2:16:G:H21	1:2:1195:A:N6	1.94	0.56
5:B:184:ARG:HD3	5:B:191:ARG:HG2	1.88	0.56
10:d:31:ARG:NH1	26:z:331:G:O6	2.39	0.55
24:x:704:HIS:CG	24:x:705:GLU:H	2.25	0.55
18:h:199:THR:HG21	18:h:240:CYS:HA	1.89	0.55
1:2:1126:G:OP1	5:B:41:ARG:NH1	2.39	0.55
20:i:68:U:OP2	24:x:1172:ARG:NH2	2.40	0.55
4:a:39:LYS:HD3	26:z:94:G:H5''	1.88	0.55
13:F:31:PRO:HG3	13:F:43:PRO:HG3	1.89	0.55
24:x:1091:LYS:HB3	24:x:1114:ALA:HB3	1.89	0.55
3:A:70:TRP:CZ2	26:z:345:A:H1'	2.42	0.55
35:U:110:LEU:HB3	35:U:112:MET:HE1	1.87	0.55
26:z:61:U:H3	26:z:107:G:H1	1.55	0.55
13:F:16:LYS:O	13:F:19:MET:HB3	2.06	0.55
39:Y:40:PRO:O	39:Y:77:ASN:ND2	2.40	0.55
16:g:128:ALA:HB3	28:N:44:LYS:HG2	1.89	0.54
1:2:602:G:H3'	1:2:603:C:H2'	1.89	0.54
1:2:1293:A:N6	1:2:1306:U:C2	2.75	0.54
24:x:1094:ILE:HA	24:x:1110:VAL:HG23	1.89	0.54
1:2:919:A:OP2	29:O:64:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:z:145:G:N2	26:z:248:U:O2	2.38	0.54
1:2:1679:A:H2'	15:G:60:ARG:HD3	1.90	0.54
18:h:8:ARG:HG3	18:h:311:GLN:HB3	1.90	0.54
20:i:17:G:O2'	20:i:56:G:N2	2.41	0.54
1:2:445:A:H5''	21:J:47:ARG:HH21	1.71	0.54
1:2:1203:U:O2	9:D:117:ARG:NH1	2.41	0.54
21:J:11:ARG:NH1	21:J:15:GLY:O	2.40	0.54
11:E:15:GLY:HA3	12:e:50:ILE:HG23	1.90	0.53
37:W:32:ILE:HD11	37:W:60:ARG:HD2	1.90	0.53
1:2:104:A:OP1	21:J:12:ARG:NH1	2.39	0.53
1:2:143:U:OP2	17:H:149:LYS:NZ	2.42	0.53
19:I:29:GLU:HA	19:I:32:MET:HG2	1.90	0.53
24:x:632:ILE:HG22	24:x:720:ILE:HB	1.89	0.53
31:Q:44:ARG:NH2	31:Q:82:ASP:O	2.41	0.53
39:Y:68:LYS:HB3	39:Y:91:LEU:HD22	1.91	0.53
21:J:48:VAL:HG11	21:J:54:LYS:HD3	1.89	0.53
34:T:90:VAL:HG21	34:T:113:ARG:HH12	1.71	0.53
1:2:643:A:OP1	23:K:38:ARG:NH1	2.41	0.53
1:2:1507:G:N2	16:g:87:THR:O	2.41	0.53
24:x:610:ARG:HA	24:x:613:LYS:HG2	1.89	0.53
24:x:911:LEU:HD12	24:x:930:LYS:HE3	1.91	0.53
1:2:1545:A:H4'	32:R:74:GLY:HA2	1.90	0.53
24:x:644:LYS:HG2	41:x:1301:GTP:O1A	2.08	0.53
24:x:1211:LEU:HA	24:x:1214:VAL:HG12	1.91	0.53
36:V:20:ILE:HG21	36:V:98:VAL:HG21	1.90	0.53
1:2:804:U:OP1	38:X:82:GLN:NE2	2.41	0.53
4:a:76:ARG:NH1	26:z:101:U:O2	2.42	0.53
1:2:399:C:N3	27:M:104:LYS:NZ	2.54	0.53
5:B:22:GLY:O	5:B:164:ASN:ND2	2.41	0.53
34:T:13:LEU:HB2	34:T:20:ILE:HB	1.90	0.53
1:2:1344:A:N1	1:2:1385:G:O2'	2.41	0.53
18:h:18:VAL:HA	18:h:35:SER:HA	1.91	0.53
1:2:1424:G:H2'	1:2:1425:G:H8	1.74	0.53
4:a:69:THR:HB	4:a:72:VAL:HG12	1.90	0.53
9:D:191:VAL:HG11	9:D:236:PHE:HA	1.91	0.53
15:G:71:ARG:NH2	15:G:148:ASN:OD1	2.42	0.53
6:b:23:CYS:O	30:P:142:ARG:NH1	2.41	0.52
18:h:129:ILE:HB	18:h:142:VAL:HB	1.90	0.52
1:2:1854:U:OP1	30:P:150:ARG:NH2	2.42	0.52
1:2:384:U:OP1	27:M:132:ARG:NH1	2.42	0.52
1:2:457:C:H2'	1:2:458:A:H8	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1560:U:HO2'	1:2:1583:C:HO2'	1.55	0.52
12:e:21:CYS:O	25:L:65:ARG:NH1	2.42	0.52
31:Q:29:SER:OG	31:Q:32:GLN:OE1	2.27	0.52
11:E:106:ARG:NH1	11:E:174:HIS:O	2.43	0.52
1:2:1562:C:H5''	35:U:71:GLY:HA3	1.91	0.52
1:2:1661:A:OP2	12:e:32:ARG:NH1	2.37	0.52
2:Z:21:LYS:HG3	2:Z:75:ILE:HB	1.91	0.52
5:B:36:GLN:O	5:B:53:ARG:NH1	2.42	0.52
18:h:41:ILE:HD11	18:h:55:PRO:HB3	1.91	0.52
1:2:600:G:H2'	1:2:601:G:H8	1.74	0.52
1:2:1710:C:O2	3:A:46:ARG:NH2	2.42	0.52
24:x:608:LYS:HA	24:x:611:ILE:HG12	1.91	0.52
4:a:112:ASN:O	4:a:114:LYS:NZ	2.43	0.52
9:D:114:LYS:HD3	9:D:121:ARG:HH21	1.74	0.52
21:J:101:ILE:HD12	21:J:190:LEU:HD11	1.91	0.52
36:V:93:SER:HB2	36:V:97:ILE:HD11	1.91	0.52
18:h:42:MET:HB3	18:h:57:ARG:H	1.75	0.52
33:S:44:LYS:HA	33:S:47:ARG:HD3	1.92	0.52
1:2:1300:U:OP1	31:Q:59:ARG:NH2	2.43	0.52
31:Q:108:LYS:HB2	31:Q:111:MET:HE3	1.92	0.52
33:S:18:GLU:OE1	33:S:72:LYS:NZ	2.43	0.52
1:2:1301:A:OP2	12:e:5:GLN:NE2	2.43	0.51
1:2:1711:U:H1'	3:A:46:ARG:HH12	1.76	0.51
9:D:102:LEU:HD12	9:D:130:ILE:HG13	1.91	0.51
10:d:20:ARG:NH1	10:d:25:GLY:O	2.43	0.51
11:E:141:LYS:NZ	11:E:179:GLN:O	2.43	0.51
24:x:602:ARG:NH1	24:x:605:ASP:OD2	2.42	0.51
1:2:17:C:O2'	1:2:1194:A:N1	2.39	0.51
1:2:678:U:OP2	1:2:1026:C:N4	2.44	0.51
1:2:846:G:C4	13:F:19:MET:HE1	2.45	0.51
1:2:1179:G:N2	1:2:1182:A:OP2	2.42	0.51
24:x:962:ILE:HA	24:x:965:LEU:HG	1.93	0.51
38:X:106:THR:HG22	38:X:108:ALA:H	1.75	0.51
1:2:1753:C:O2'	1:2:1754:G:O4'	2.29	0.51
11:E:28:GLU:OE2	25:L:70:TYR:OH	2.29	0.51
18:h:107:ASP:OD1	18:h:107:ASP:N	2.43	0.51
18:h:292:SER:HB3	18:h:296:GLN:H	1.76	0.51
1:2:124:U:OP1	17:H:201:LYS:NZ	2.42	0.51
1:2:126:G:OP2	17:H:198:ARG:NH1	2.43	0.51
1:2:681:U:OP1	39:Y:8:ARG:NH2	2.43	0.51
21:J:137:LEU:O	21:J:141:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1864:U:O4	6:b:34:LYS:NZ	2.42	0.51
1:2:1866:A:OP1	6:b:95:ARG:NH2	2.44	0.51
6:b:38:LYS:HB3	6:b:71:LEU:HB2	1.93	0.51
13:F:44:LEU:HD21	13:F:70:ILE:HG21	1.92	0.51
13:F:176:ASP:OD1	13:F:176:ASP:N	2.43	0.51
19:I:47:ALA:H	19:I:63:PHE:HB2	1.75	0.51
1:2:521:A:OP1	23:K:45:ARG:NH1	2.43	0.51
1:2:603:C:N4	1:2:620:G:O6	2.43	0.51
13:F:252:ARG:NH2	13:F:253:ASP:OD1	2.44	0.51
1:2:1130:G:N2	1:2:1130:G:OP2	2.44	0.51
1:2:1183:A:H2'	1:2:1184:G:H8	1.76	0.51
1:2:1841:C:OP2	22:n:2:ARG:NH1	2.44	0.51
6:b:43:ASN:HB3	6:b:66:LYS:HD2	1.93	0.51
25:L:13:GLU:OE1	25:L:17:LYS:NZ	2.43	0.51
27:M:135:SER:O	27:M:139:ARG:NH1	2.43	0.51
1:2:613:G:N2	1:2:629:A:OP2	2.42	0.51
2:Z:56:PHE:HB3	2:Z:90:ARG:HD3	1.92	0.51
1:2:1280:G:OP2	28:N:101:ARG:NH2	2.43	0.51
6:b:44:ILE:HD12	30:P:97:LEU:HD13	1.93	0.51
16:g:89:LYS:NZ	16:g:90:LYS:O	2.44	0.51
21:J:116:HIS:O	21:J:152:ARG:NH2	2.43	0.51
38:X:86:LEU:HD21	38:X:113:HIS:HB2	1.92	0.51
1:2:818:A:OP1	23:K:80:ARG:NH2	2.40	0.50
1:2:1275:G:N2	1:2:1506:A:OP2	2.39	0.50
1:2:1845:A:H2'	1:2:1846:G:H8	1.76	0.50
18:h:120:ILE:HB	18:h:132:TRP:HB2	1.93	0.50
1:2:813:A:OP1	13:F:16:LYS:NZ	2.42	0.50
1:2:887:U:H5	1:2:899:U:H3	1.58	0.50
1:2:913:A:N6	19:I:119:SER:O	2.42	0.50
1:2:1541:G:OP1	35:U:56:ARG:NH1	2.45	0.50
24:x:667:GLY:H	24:x:859:MET:HE1	1.76	0.50
1:2:156:G:N2	17:H:60:GLY:O	2.44	0.50
1:2:452:G:O2'	17:H:91:GLU:OE2	2.29	0.50
1:2:482:G:N2	1:2:485:A:OP2	2.43	0.50
11:E:75:LYS:NZ	25:L:20:VAL:O	2.44	0.50
1:2:1288:U:OP2	16:g:95:ARG:NH2	2.44	0.50
13:F:93:ASP:OD1	13:F:93:ASP:N	2.44	0.50
25:L:11:ILE:HD11	25:L:45:VAL:HG22	1.93	0.50
35:U:126:GLN:OE1	35:U:129:ARG:NH1	2.45	0.50
37:W:38:GLU:HG3	37:W:78:ILE:HD11	1.93	0.50
1:2:292:A:O2'	27:M:39:ASN:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:555:A:H61	1:2:589:G:H21	1.59	0.50
15:G:191:LYS:NZ	26:z:70:A:O3'	2.44	0.50
24:x:1136:VAL:HA	24:x:1159:ILE:HA	1.93	0.50
1:2:170:A:H5'	17:H:137:ARG:HG3	1.94	0.50
28:N:58:GLU:HB2	28:N:61:TYR:HB3	1.94	0.50
33:S:9:VAL:HG23	33:S:50:ILE:HG13	1.93	0.50
1:2:1593:C:OP2	4:a:104:ARG:NH1	2.45	0.50
5:B:94:THR:OG1	5:B:186:ARG:NH2	2.45	0.50
10:d:3:THR:OG1	10:d:4:SER:N	2.45	0.50
11:E:45:ARG:NH2	11:E:82:GLY:O	2.45	0.50
1:2:1174:U:OP1	22:n:21:ARG:NH2	2.44	0.50
2:Z:72:PHE:HE1	13:F:56:LEU:HD21	1.77	0.50
15:G:136:ARG:HB2	15:G:203:ASN:HD21	1.76	0.50
24:x:596:ASP:H	24:x:602:ARG:HG3	1.77	0.50
28:N:61:TYR:HA	28:N:64:LEU:HD12	1.92	0.50
30:P:45:THR:HA	30:P:52:THR:HA	1.94	0.50
1:2:165:G:OP2	1:2:165:G:N2	2.41	0.50
1:2:495:U:O2'	13:F:27:PHE:O	2.30	0.50
1:2:1396:A:N6	1:2:1449:G:O6	2.44	0.50
1:2:1472:C:N4	1:2:1476:A:H62	2.07	0.50
34:T:48:ALA:HA	34:T:66:ARG:HH12	1.76	0.50
1:2:28:U:H2'	1:2:29:G:H8	1.77	0.49
1:2:1549:U:OP1	12:e:34:TYR:OH	2.29	0.49
19:I:70:LYS:HA	19:I:73:GLN:HB2	1.94	0.49
25:L:80:ARG:HH22	25:L:91:PRO:HD3	1.77	0.49
1:2:598:G:O2'	1:2:605:A:N1	2.41	0.49
18:h:257:LYS:NZ	18:h:269:GLU:OE1	2.44	0.49
1:2:191:A:OP2	1:2:208:G:N2	2.45	0.49
3:A:70:TRP:CH2	26:z:345:A:H1'	2.47	0.49
9:D:210:PRO:HD3	9:D:236:PHE:HE2	1.76	0.49
30:P:74:ALA:HB1	30:P:115:ALA:HB2	1.94	0.49
1:2:1287:A:OP2	16:g:95:ARG:NH2	2.46	0.49
8:c:33:MET:N	8:c:46:VAL:O	2.44	0.49
9:D:80:GLU:HA	9:D:83:LEU:HB3	1.94	0.49
32:R:86:GLN:NE2	32:R:120:LEU:O	2.44	0.49
1:2:437:G:N2	1:2:457:C:O2	2.45	0.49
1:2:1372:U:OP1	1:2:1385:G:N2	2.44	0.49
25:L:25:LYS:HA	25:L:46:MET:HE1	1.94	0.49
35:U:65:TYR:HE1	35:U:128:GLN:HG3	1.77	0.49
1:2:77:A:H2	17:H:175:LYS:HG3	1.78	0.49
1:2:677:G:OP1	29:O:124:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1082:A:HO2'	1:2:1842:C:HO2'	1.59	0.49
5:B:192:GLU:OE2	5:B:193:HIS:ND1	2.44	0.49
1:2:359:U:OP2	39:Y:18:ARG:NH1	2.46	0.49
1:2:1528:G:O2'	1:2:1666:C:OP1	2.30	0.49
13:F:137:PRO:HB2	13:F:150:PRO:HD2	1.94	0.49
28:N:79:VAL:HG11	28:N:85:LEU:HB2	1.95	0.49
4:a:50:PHE:HZ	4:a:87:ALA:HB2	1.77	0.49
24:x:758:ARG:CG	41:x:1301:GTP:HN21	2.26	0.49
1:2:44:U:H3	1:2:482:G:H1'	1.78	0.49
25:L:83:LEU:HB3	25:L:85:LEU:HD23	1.95	0.49
1:2:67:C:H41	17:H:164:LYS:H	1.59	0.49
34:T:26:ILE:HG13	34:T:45:LEU:HD21	1.94	0.49
1:2:13:C:H5''	9:D:235:ASN:HD21	1.78	0.48
24:x:1106:ILE:HB	24:x:1159:ILE:HB	1.94	0.48
1:2:943:U:OP1	7:C:214:LYS:NZ	2.45	0.48
7:C:170:GLU:HA	7:C:173:THR:HG22	1.95	0.48
17:H:32:MET:SD	17:H:32:MET:N	2.86	0.48
24:x:617:GLU:HA	24:x:620:LYS:HG2	1.94	0.48
1:2:626:G:N2	3:A:63:GLY:O	2.47	0.48
1:2:918:U:O2'	1:2:919:A:O4'	2.32	0.48
1:2:1536:G:H2'	1:2:1537:A:H8	1.77	0.48
18:h:292:SER:OG	18:h:293:ALA:N	2.45	0.48
21:J:141:ARG:HB2	21:J:146:GLN:HG2	1.96	0.48
26:z:137:G:O6	26:z:287:U:O2	2.31	0.48
32:R:111:ILE:HA	32:R:114:GLN:HG3	1.95	0.48
1:2:318:A:C2	1:2:333:G:C6	3.01	0.48
1:2:350:C:HO2'	1:2:383:G:H1	1.62	0.48
1:2:612:U:H4'	14:f:88:GLN:HE21	1.78	0.48
7:C:191:ASP:OD1	7:C:191:ASP:N	2.46	0.48
34:T:25:LYS:HE2	34:T:53:THR:HA	1.94	0.48
1:2:400:C:OP2	39:Y:11:ARG:NH1	2.44	0.48
1:2:1012:A:OP1	29:O:3:ARG:NH1	2.46	0.48
1:2:1863:A:OP2	6:b:4:LYS:NZ	2.44	0.48
8:c:24:LEU:HD23	8:c:25:VAL:HG13	1.95	0.48
13:F:68:ARG:HE	13:F:76:VAL:HG11	1.78	0.48
15:G:68:ILE:HD11	15:G:116:ILE:HG13	1.96	0.48
23:K:75:ASN:OD1	23:K:79:ARG:NH2	2.47	0.48
24:x:1017:MET:HE1	39:Y:75:ILE:HG23	1.96	0.48
36:V:62:ARG:NH1	36:V:81:GLN:OE1	2.47	0.48
1:2:626:G:H21	3:A:64:LYS:HA	1.79	0.48
7:C:179:ASN:ND2	7:C:183:GLU:OE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:x:926:ALA:O	24:x:927:GLN:NE2	2.46	0.48
16:g:134:SER:HA	16:g:139:HIS:HD1	1.79	0.48
23:K:113:GLN:OE1	23:K:154:GLN:NE2	2.47	0.48
24:x:1016:VAL:HG21	24:x:1043:ALA:HB1	1.96	0.48
26:z:154:A:H62	26:z:227:U:H1'	1.78	0.48
32:R:51:LEU:HD13	32:R:81:ILE:HG23	1.96	0.48
1:2:960:U:O2'	1:2:963:A:N6	2.47	0.48
1:2:1121:G:O2'	7:C:204:ILE:O	2.27	0.48
15:G:32:ASP:O	15:G:36:GLN:NE2	2.46	0.48
18:h:99:ARG:HH11	18:h:100:ARG:H	1.61	0.48
24:x:715:SER:OG	24:x:745:LYS:NZ	2.47	0.48
24:x:777:GLN:O	24:x:782:LYS:NZ	2.47	0.48
1:2:433:A:OP1	21:J:25:ARG:NH2	2.46	0.48
1:2:464:A:H3'	1:2:465:A:H8	1.78	0.48
1:2:1043:G:N2	1:2:1074:C:N3	2.61	0.48
24:x:790:LYS:HA	24:x:793:ILE:HG22	1.96	0.48
24:x:1089:PRO:HG3	24:x:1208:ILE:HG13	1.95	0.48
26:z:135:G:O2'	26:z:297:U:OP1	2.29	0.48
29:O:87:ASP:OD1	29:O:87:ASP:N	2.47	0.48
29:O:129:TYR:HB3	29:O:135:LEU:HD13	1.96	0.48
30:P:31:CYS:HB2	30:P:93:LEU:HD12	1.96	0.48
35:U:12:GLN:O	35:U:16:ARG:NH1	2.46	0.48
36:V:21:ARG:HH21	36:V:115:THR:HG21	1.79	0.48
11:E:168:VAL:HG12	11:E:189:MET:HG2	1.96	0.48
19:I:12:ASN:ND2	19:I:14:GLU:OE1	2.47	0.48
23:K:130:ILE:HD13	23:K:135:ILE:HD13	1.95	0.48
24:x:871:ILE:HB	24:x:931:ILE:HB	1.96	0.48
24:x:935:ASP:OD1	24:x:935:ASP:N	2.43	0.48
26:z:156:C:N4	26:z:228:U:O4	2.46	0.48
1:2:1010:G:H2'	1:2:1011:A:H8	1.78	0.47
1:2:1617:G:N2	1:2:1620:A:OP2	2.46	0.47
2:Z:62:THR:HA	2:Z:69:THR:HG22	1.96	0.47
24:x:640:THR:HG22	24:x:726:ASP:HB2	1.95	0.47
24:x:640:THR:O	24:x:754:ASN:ND2	2.46	0.47
1:2:645:C:H2'	1:2:646:G:H8	1.80	0.47
1:2:1290:G:N2	1:2:1310:U:O2	2.47	0.47
6:b:74:CYS:SG	6:b:77:CYS:CB	2.93	0.47
18:h:231:ASP:OD1	18:h:231:ASP:N	2.45	0.47
18:h:249:CYS:SG	18:h:291:TRP:NE1	2.85	0.47
24:x:793:ILE:HG13	24:x:803:ALA:HB3	1.96	0.47
26:z:248:U:H2'	26:z:249:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:13:ARG:N	10:d:33:GLU:O	2.47	0.47
29:O:20:ARG:HH21	38:X:56:HIS:HB3	1.78	0.47
1:2:1064:C:H2'	1:2:1065:G:H8	1.80	0.47
1:2:1182:A:OP1	22:n:18:ARG:NH2	2.48	0.47
1:2:1277:C:H2'	1:2:1278:A:H8	1.79	0.47
1:2:1299:A:O2'	1:2:1301:A:OP1	2.29	0.47
24:x:650:ARG:HH11	24:x:671:VAL:HG12	1.79	0.47
1:2:183:G:O2'	1:2:184:G:O4'	2.32	0.47
1:2:1542:C:OP1	35:U:62:ARG:NH1	2.43	0.47
15:G:125:SER:OG	15:G:136:ARG:NH1	2.45	0.47
27:M:59:LYS:HD3	27:M:134:LEU:HB3	1.96	0.47
33:S:100:PRO:HA	33:S:103:LYS:HB3	1.96	0.47
1:2:223:C:H2'	1:2:224:A:H8	1.79	0.47
1:2:1595:U:OP1	4:a:102:LYS:NZ	2.47	0.47
1:2:1653:U:H3	1:2:1671:G:H1	1.62	0.47
1:2:1864:U:OP2	6:b:4:LYS:NZ	2.43	0.47
3:A:26:LEU:HD21	3:A:103:LEU:HD12	1.96	0.47
16:g:130:VAL:HA	28:N:40:LYS:HE3	1.96	0.47
18:h:8:ARG:NH1	18:h:311:GLN:OE1	2.47	0.47
19:I:158:LEU:HD11	19:I:187:PHE:HD2	1.78	0.47
21:J:87:ASN:HB3	21:J:90:LEU:HD13	1.96	0.47
24:x:822:SER:OG	24:x:825:THR:O	2.30	0.47
26:z:68:G:N7	26:z:100:G:N2	2.63	0.47
32:R:58:LEU:HB3	32:R:62:ARG:HD2	1.95	0.47
32:R:67:ASP:N	32:R:67:ASP:OD1	2.47	0.47
1:2:925:G:OP1	29:O:121:ARG:NH1	2.43	0.47
1:2:1156:U:O4	9:D:194:ARG:NH1	2.47	0.47
1:2:1480:A:H5'	32:R:131:LYS:HE2	1.97	0.47
9:D:183:LYS:HD3	38:X:95:PRO:HA	1.97	0.47
20:i:47:C:H2'	20:i:58:A:H4'	1.97	0.47
34:T:70:ILE:HG13	34:T:77:TYR:HD2	1.79	0.47
1:2:1154:U:H4'	1:2:1155:U:H3'	1.97	0.47
7:C:23:ASP:OD1	7:C:23:ASP:N	2.46	0.47
13:F:246:LEU:HD22	13:F:250:GLU:HG3	1.95	0.47
18:h:152:SER:OG	18:h:196:ASN:O	2.33	0.47
24:x:854:LEU:HD23	24:x:876:ILE:HG21	1.97	0.47
33:S:75:GLU:HG3	33:S:78:ARG:HG2	1.97	0.47
39:Y:53:GLU:HB2	39:Y:71:ARG:HB3	1.97	0.47
1:2:639:C:H2'	1:2:640:A:H8	1.80	0.47
2:Z:83:LYS:HE2	2:Z:96:LEU:HD23	1.97	0.47
18:h:217:MET:SD	18:h:219:TRP:NE1	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:S:107:LYS:NZ	33:S:113:SER:OG	2.48	0.47
6:b:53:ILE:HG23	30:P:126:ILE:HD11	1.97	0.46
28:N:26:LEU:HG	28:N:31:LEU:HD13	1.97	0.46
1:2:312:G:O2'	17:H:191:ARG:NH1	2.47	0.46
1:2:1015:U:OP2	8:c:20:LYS:NZ	2.44	0.46
1:2:615:C:OP1	3:A:62:ARG:NE	2.42	0.46
15:G:18:LYS:HA	15:G:18:LYS:HD3	1.80	0.46
17:H:142:ARG:HG3	17:H:147:LEU:HB2	1.97	0.46
24:x:757:ASP:OD1	24:x:757:ASP:N	2.49	0.46
1:2:1544:C:O2'	32:R:75:GLY:O	2.31	0.46
1:2:1209:A:H5''	6:b:82:LYS:HE3	1.96	0.46
1:2:1622:U:H4'	34:T:133:GLY:HA3	1.96	0.46
2:Z:20:ARG:NH1	2:Z:74:MET:SD	2.88	0.46
27:M:24:LEU:HG	27:M:26:GLY:H	1.80	0.46
1:2:1495:G:N2	12:e:42:CYS:SG	2.82	0.46
4:a:64:ASN:O	4:a:111:ARG:NH1	2.49	0.46
13:F:45:ILE:HG23	13:F:46:ILE:HD12	1.98	0.46
18:h:289:LEU:HD12	18:h:298:LEU:HD11	1.97	0.46
30:P:30:VAL:HG12	30:P:94:HIS:HB2	1.96	0.46
7:C:35:ALA:HB3	7:C:42:ARG:HA	1.98	0.46
10:d:36:ASP:OD1	10:d:36:ASP:N	2.46	0.46
11:E:1:MET:N	11:E:4:GLN:OE1	2.44	0.46
13:F:45:ILE:HG13	13:F:61:VAL:HG21	1.96	0.46
19:I:154:ILE:HB	19:I:185:VAL:HG22	1.98	0.46
1:2:792:C:H2'	1:2:793:G:H8	1.81	0.46
1:2:975:G:OP1	30:P:98:ARG:NH1	2.49	0.46
1:2:1522:A:O5'	34:T:144:ARG:NH2	2.45	0.46
5:B:81:ASN:HA	5:B:84:GLN:HE22	1.81	0.46
10:d:21:THR:OG1	10:d:22:GLY:N	2.49	0.46
18:h:126:ASP:OD1	18:h:126:ASP:N	2.44	0.46
24:x:656:ASP:OD1	24:x:656:ASP:N	2.43	0.46
1:2:565:G:H22	1:2:586:G:H1'	1.81	0.46
1:2:634:A:OP1	14:f:86:ARG:NH1	2.39	0.46
1:2:1226:G:N1	1:2:1639:G:OP2	2.40	0.46
1:2:1293:A:C6	1:2:1306:U:N3	2.84	0.46
1:2:1669:G:OP2	32:R:130:LYS:NZ	2.43	0.46
10:d:51:ARG:HG2	10:d:52:GLU:H	1.80	0.46
21:J:6:ASP:OD1	21:J:6:ASP:N	2.49	0.46
24:x:697:LEU:HD11	24:x:926:ALA:HB1	1.97	0.46
27:M:147:LYS:HD2	27:M:147:LYS:HA	1.80	0.46
33:S:31:ASN:HA	33:S:34:VAL:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1138:C:OP1	5:B:155:ARG:NH1	2.49	0.46
3:A:33:GLN:HB3	3:A:78:LEU:HD11	1.97	0.46
9:D:206:SER:HB3	9:D:210:PRO:HG2	1.97	0.46
14:f:103:GLY:HA2	14:f:106:LYS:HB3	1.97	0.46
15:G:155:CYS:HB3	15:G:159:ARG:HH22	1.80	0.46
18:h:99:ARG:NH1	18:h:100:ARG:O	2.49	0.46
24:x:889:PRO:HA	24:x:894:PRO:HA	1.98	0.46
38:X:103:VAL:HA	38:X:112:ASP:HA	1.99	0.45
1:2:1018:U:OP1	29:O:62:GLN:NE2	2.49	0.45
1:2:1335:G:H1	1:2:1492:U:H3	1.63	0.45
1:2:1863:A:H8	6:b:79:ILE:HG21	1.82	0.45
8:c:19:HIS:HB3	8:c:22:LYS:HG3	1.99	0.45
29:O:33:VAL:O	29:O:37:ILE:HG13	2.16	0.45
1:2:1480:A:O2'	12:e:56:ASP:O	2.35	0.45
29:O:63:VAL:HG21	29:O:71:ILE:HD11	1.99	0.45
1:2:1190:A:N3	1:2:1714:U:O2'	2.49	0.45
1:2:1781:A:O2'	1:2:1782:G:O4'	2.34	0.45
5:B:198:MET:HG3	5:B:200:ASP:H	1.81	0.45
18:h:72:SER:OG	18:h:74:ASP:OD1	2.33	0.45
24:x:953:GLU:HG3	24:x:954:ILE:HG22	1.99	0.45
1:2:982:G:H2'	1:2:983:A:H8	1.82	0.45
1:2:1464:C:OP2	33:S:63:ARG:NH1	2.50	0.45
13:F:43:PRO:HG2	13:F:46:ILE:HD13	1.98	0.45
30:P:61:LYS:HZ3	30:P:76:LEU:HB3	1.81	0.45
31:Q:59:ARG:HA	31:Q:62:LYS:HG2	1.98	0.45
1:2:855:G:O2'	27:M:71:ARG:NH1	2.31	0.45
8:c:23:ARG:NH1	8:c:27:SER:O	2.50	0.45
11:E:172:VAL:HG22	11:E:185:LYS:HG2	1.99	0.45
18:h:116:ASP:OD1	18:h:116:ASP:N	2.49	0.45
25:L:53:LYS:HE2	25:L:60:GLU:HB3	1.99	0.45
31:Q:86:LEU:HB2	31:Q:89:MET:HG3	1.98	0.45
38:X:106:THR:OG1	38:X:111:MET:SD	2.66	0.45
1:2:11:A:H5'	9:D:113:GLN:HE21	1.81	0.45
1:2:74:G:N2	1:2:77:A:OP1	2.50	0.45
1:2:346:C:O2'	13:F:30:ARG:NH2	2.49	0.45
1:2:1337:C:H2'	1:2:1338:G:H8	1.81	0.45
1:2:1808:U:H2'	1:2:1809:A:C8	2.52	0.45
7:C:170:GLU:O	7:C:174:ARG:HB2	2.16	0.45
26:z:132:G:H2'	26:z:133:G:H8	1.82	0.45
38:X:36:ARG:HA	38:X:39:THR:HG22	1.99	0.45
26:z:145:G:H1	26:z:248:U:H3	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:M:3:ASP:N	27:M:3:ASP:OD1	2.48	0.45
1:2:45:A:H4'	1:2:46:A:H5'	1.98	0.45
1:2:161:U:O4	2:Z:115:LYS:NZ	2.50	0.45
5:B:174:MET:HA	5:B:177:MET:HG2	1.99	0.45
11:E:23:GLU:HG2	25:L:64:TRP:HE1	1.81	0.45
11:E:193:ASP:OD1	11:E:193:ASP:N	2.50	0.45
14:f:111:TYR:OH	23:K:30:LYS:NZ	2.49	0.45
24:x:1043:ALA:HA	24:x:1046:MET:HE2	1.99	0.45
24:x:1198:ASP:OD1	24:x:1198:ASP:N	2.47	0.45
29:O:32:ASP:OD2	29:O:32:ASP:N	2.48	0.45
1:2:350:C:O2'	1:2:383:G:N1	2.48	0.45
1:2:981:A:H2'	1:2:982:G:C8	2.52	0.45
1:2:1252:C:OP1	36:V:75:LYS:NZ	2.42	0.45
1:2:1722:G:O6	1:2:1812:U:O4	2.34	0.45
1:2:648:A:N3	39:Y:45:SER:OG	2.48	0.44
1:2:799:U:H3	1:2:867:G:H22	1.64	0.44
1:2:1048:G:N2	1:2:1070:A:H62	2.13	0.44
4:a:96:LEU:O	4:a:112:ASN:ND2	2.51	0.44
26:z:335:G:C5'	30:P:110:PRO:HB2	2.45	0.44
30:P:33:ILE:HD13	30:P:95:ILE:HG23	1.98	0.44
34:T:39:ARG:HG3	34:T:83:PHE:HZ	1.81	0.44
38:X:103:VAL:HG23	38:X:126:LEU:HB2	1.99	0.44
23:K:136:ARG:HA	23:K:141:VAL:HA	1.98	0.44
37:W:58:ALA:O	37:W:62:MET:CB	2.65	0.44
1:2:385:G:O2'	21:J:10:LYS:NZ	2.50	0.44
1:2:1402:A:H5'	36:V:51:LYS:HD2	1.99	0.44
6:b:87:ARG:NH2	6:b:92:ARG:O	2.50	0.44
11:E:40:ARG:NH2	36:V:106:ILE:O	2.50	0.44
21:J:172:LEU:HB3	21:J:190:LEU:HD12	1.99	0.44
24:x:633:CYS:HB2	24:x:718:CYS:HB2	1.86	0.44
26:z:144:U:O2	26:z:249:G:O6	2.34	0.44
34:T:92:ASP:OD1	34:T:92:ASP:N	2.50	0.44
1:2:1593:C:OP1	4:a:103:HIS:NE2	2.44	0.44
26:z:262:U:O4	26:z:271:G:O6	2.35	0.44
27:M:85:THR:HG22	27:M:112:HIS:HA	2.00	0.44
28:N:121:LYS:HD2	28:N:121:LYS:HA	1.84	0.44
2:Z:78:SER:OG	2:Z:80:ASP:OD2	2.36	0.44
29:O:40:LEU:HB3	29:O:50:ILE:HD12	1.98	0.44
31:Q:72:LYS:HD2	31:Q:72:LYS:HA	1.80	0.44
1:2:1232:U:H3	1:2:1526:G:H1	1.65	0.44
1:2:1297:U:H2'	1:2:1298:G:H2'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1741:U:OP1	21:J:42:ARG:NH1	2.44	0.44
6:b:51:ARG:NH2	6:b:55:GLU:OE2	2.51	0.44
11:E:142:LEU:O	26:z:350:G:N2	2.50	0.44
18:h:239:LEU:HD13	18:h:250:ALA:HB2	2.00	0.44
18:h:249:CYS:HB3	18:h:258:ILE:HG22	1.99	0.44
1:2:557:U:H2'	1:2:558:G:C4	2.53	0.44
1:2:610:G:H2'	1:2:611:G:H8	1.82	0.44
1:2:1536:G:H2'	1:2:1537:A:C8	2.53	0.44
1:2:1653:U:O2	1:2:1671:G:N2	2.41	0.44
9:D:169:TYR:OH	9:D:175:GLY:O	2.34	0.44
11:E:219:PRO:HG3	18:h:189:ILE:HG22	1.99	0.44
34:T:62:ASP:OD1	34:T:62:ASP:N	2.49	0.44
1:2:805:U:N3	1:2:859:G:O6	2.51	0.44
1:2:871:U:O2'	1:2:873:G:OP1	2.36	0.44
3:A:74:SER:HB2	3:A:118:THR:HG23	2.00	0.44
15:G:14:THR:N	32:R:56:LEU:O	2.51	0.44
1:2:801:U:O4	19:I:106:ARG:NH2	2.51	0.43
1:2:809:A:OP1	13:F:187:ALA:N	2.49	0.43
1:2:1004:U:H2'	1:2:1005:G:H8	1.83	0.43
1:2:1656:G:O6	1:2:1668:U:O4	2.36	0.43
10:d:13:ARG:HE	10:d:55:VAL:HG12	1.83	0.43
1:2:829:C:O2'	1:2:845:G:N2	2.50	0.43
1:2:928:G:H2'	1:2:929:G:C8	2.53	0.43
1:2:1040:G:O6	1:2:1076:G:N1	2.51	0.43
1:2:1273:C:H1'	1:2:1274:G:H2'	2.01	0.43
8:c:67:THR:OG1	8:c:70:LYS:O	2.35	0.43
13:F:168:LYS:HA	13:F:168:LYS:HD2	1.82	0.43
16:g:137:ASP:OD1	16:g:137:ASP:N	2.50	0.43
20:i:57:A:O2'	20:i:59:A:OP2	2.35	0.43
1:2:1612:G:H2'	1:2:1613:G:H8	1.83	0.43
8:c:45:THR:OG1	8:c:82:LYS:NZ	2.50	0.43
10:d:31:ARG:NH2	26:z:329:U:O2'	2.52	0.43
11:E:39:VAL:HA	11:E:48:ILE:HG22	2.00	0.43
33:S:32:LYS:NZ	33:S:48:ASN:OD1	2.51	0.43
1:2:373:G:H2'	1:2:374:G:H8	1.84	0.43
1:2:846:G:OP2	13:F:108:ARG:NH2	2.41	0.43
1:2:953:C:N3	30:P:55:ARG:NH2	2.66	0.43
1:2:954:U:O2	30:P:55:ARG:NH2	2.51	0.43
1:2:1259:A:N6	1:2:1519:U:O5'	2.52	0.43
23:K:3:VAL:HG21	23:K:5:ARG:HH11	1.83	0.43
24:x:1125:VAL:HG23	24:x:1133:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:z:52:G:H2'	26:z:53:A:H8	1.84	0.43
27:M:35:ARG:NH2	27:M:55:TYR:O	2.40	0.43
37:W:58:ALA:O	37:W:62:MET:HB3	2.18	0.43
1:2:1599:U:OP2	4:a:46:ASN:ND2	2.50	0.43
5:B:79:SER:OG	5:B:130:ASP:OD1	2.32	0.43
12:e:43:PHE:O	12:e:47:ALA:HB2	2.18	0.43
24:x:712:ASN:OD1	24:x:712:ASN:N	2.52	0.43
24:x:1136:VAL:HG12	24:x:1159:ILE:HG12	2.00	0.43
35:U:11:GLN:HA	35:U:14:PHE:HB3	2.01	0.43
1:2:436:G:H2'	1:2:437:G:C8	2.53	0.43
1:2:467:G:O5'	17:H:72:ARG:NH2	2.52	0.43
1:2:1295:A:N6	1:2:1305:C:N3	2.67	0.43
1:2:1464:C:O5'	33:S:60:ARG:NH1	2.52	0.43
25:L:12:TYR:HB3	25:L:83:LEU:HD21	2.00	0.43
6:b:74:CYS:SG	6:b:77:CYS:HB2	2.56	0.43
7:C:88:THR:HG22	7:C:98:THR:HG22	2.00	0.43
15:G:131:ALA:O	26:z:81:A:O2'	2.36	0.43
24:x:994:GLU:HA	24:x:997:LYS:HG2	1.99	0.43
38:X:51:GLU:N	38:X:62:VAL:O	2.49	0.43
1:2:311:C:H5''	1:2:312:G:H5''	1.99	0.43
1:2:934:G:C6	1:2:1008:A:N1	2.86	0.43
1:2:1587:G:OP1	1:2:1587:G:N2	2.48	0.43
1:2:1677:U:H2'	1:2:1678:A:H8	1.82	0.43
1:2:60:A:O2'	1:2:316:G:O2'	2.37	0.43
19:I:86:LYS:HD2	19:I:87:PHE:HB2	2.00	0.43
25:L:47:LYS:HA	25:L:47:LYS:HD3	1.86	0.43
26:z:130:C:H2'	26:z:131:G:H8	1.84	0.43
1:2:1652:G:O6	1:2:1672:U:O4	2.36	0.43
5:B:78:SER:OG	5:B:125:THR:OG1	2.35	0.43
9:D:214:LEU:HD13	9:D:219:ILE:HD11	2.01	0.43
11:E:132:LYS:NZ	11:E:190:LEU:O	2.52	0.43
19:I:36:LEU:HG	19:I:40:LEU:HD13	2.01	0.43
23:K:50:LEU:HD13	23:K:105:PHE:HE2	1.83	0.43
24:x:644:LYS:HG3	41:x:1301:GTP:C8	2.53	0.43
1:2:581:U:H4'	2:Z:66:GLY:HA3	2.00	0.42
1:2:1232:U:H2'	1:2:1233:G:H8	1.84	0.42
5:B:85:ARG:NH1	5:B:203:PHE:O	2.52	0.42
9:D:68:ARG:HG2	9:D:277:HIS:HB2	2.00	0.42
24:x:703:GLY:HA2	24:x:711:ARG:HH22	1.84	0.42
27:M:125:ILE:HG23	27:M:146:THR:HB	1.99	0.42
35:U:76:THR:HB	35:U:94:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1137:U:O2'	1:2:1139:C:OP1	2.36	0.42
1:2:1660:C:H3'	12:e:32:ARG:HH22	1.82	0.42
3:A:71:ILE:HG13	3:A:94:LYS:HD3	2.00	0.42
9:D:77:SER:OG	9:D:78:LEU:N	2.52	0.42
14:f:108:ARG:O	14:f:112:ASN:ND2	2.52	0.42
16:g:89:LYS:HA	16:g:89:LYS:HD2	1.87	0.42
26:z:48:U:O2'	26:z:49:G:O4'	2.37	0.42
27:M:120:VAL:HG12	27:M:145:VAL:HG11	2.00	0.42
32:R:113:ILE:HD11	32:R:120:LEU:HD22	2.01	0.42
38:X:3:ARG:HD3	38:X:6:VAL:HG12	2.01	0.42
1:2:45:A:O2'	1:2:480:G:N2	2.51	0.42
6:b:51:ARG:HD2	6:b:51:ARG:HA	1.88	0.42
18:h:99:ARG:HA	18:h:99:ARG:HD2	1.86	0.42
19:I:119:SER:HB2	19:I:120:ARG:HH11	1.83	0.42
1:2:5:U:H2'	1:2:6:G:C8	2.55	0.42
1:2:151:C:OP1	2:Z:120:THR:OG1	2.28	0.42
5:B:31:ASP:HB3	5:B:34:MET:HG2	2.01	0.42
7:C:123:ALA:HB2	7:C:165:ARG:HG3	2.00	0.42
13:F:11:ARG:HD2	13:F:28:ALA:HB2	2.00	0.42
17:H:134:GLY:HA3	17:H:158:VAL:HG21	2.01	0.42
18:h:15:ASN:ND2	18:h:37:ASP:OD2	2.52	0.42
18:h:158:PRO:HD2	18:h:204:GLY:HA2	2.00	0.42
22:n:20:MET:HA	22:n:23:ARG:HG2	2.00	0.42
32:R:132:PHE:O	32:R:140:ARG:NH1	2.40	0.42
1:2:526:A:OP1	14:f:101:ARG:NE	2.48	0.42
1:2:1092:G:H2'	1:2:1093:A:H8	1.84	0.42
1:2:1309:C:H5''	1:2:1310:U:H5	1.83	0.42
11:E:214:LYS:HD2	11:E:214:LYS:HA	1.86	0.42
37:W:39:VAL:HB	37:W:44:GLY:HA2	2.02	0.42
1:2:149:A:H3'	1:2:150:A:H8	1.85	0.42
1:2:223:C:H2'	1:2:224:A:C8	2.54	0.42
5:B:182:VAL:O	5:B:186:ARG:HB2	2.19	0.42
13:F:47:PHE:HA	13:F:51:ARG:HD3	2.01	0.42
13:F:62:LYS:HD2	13:F:66:MET:HB3	2.00	0.42
24:x:946:LEU:HD22	24:x:961:LEU:HD11	2.02	0.42
27:M:35:ARG:HH21	27:M:63:THR:HG21	1.85	0.42
33:S:81:ARG:HA	33:S:84:TYR:HD2	1.83	0.42
37:W:32:ILE:HD11	37:W:60:ARG:HH11	1.83	0.42
1:2:453:C:O2'	17:H:92:ARG:O	2.37	0.42
1:2:889:U:N3	1:2:899:U:O2	2.51	0.42
1:2:1143:A:H5'	9:D:190:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1358:U:H5''	9:D:114:LYS:HD2	2.02	0.42
11:E:32:ASP:OD2	11:E:65:ARG:NH2	2.53	0.42
12:e:56:ASP:HB3	36:V:79:ARG:HD2	2.01	0.42
28:N:92:CYS:HB2	28:N:103:VAL:HG12	2.01	0.42
31:Q:80:LEU:HB3	31:Q:83:MET:HE3	2.02	0.42
1:2:1465:A:OP1	33:S:56:HIS:NE2	2.48	0.42
24:x:713:ARG:HE	24:x:713:ARG:HB3	1.70	0.42
24:x:980:TYR:OH	24:x:1015:ASP:OD1	2.30	0.42
34:T:78:LYS:NZ	35:U:32:GLU:OE1	2.44	0.42
24:x:1094:ILE:HG13	24:x:1108:MET:HE2	2.02	0.42
26:z:281:U:H5	26:z:283:G:H21	1.68	0.42
32:R:26:LYS:HD3	32:R:69:ARG:HH22	1.84	0.42
1:2:67:C:OP1	17:H:160:LYS:NZ	2.44	0.41
1:2:677:G:N2	1:2:1028:A:H62	2.17	0.41
1:2:980:A:H2'	1:2:981:A:C8	2.55	0.41
1:2:1616:U:OP2	31:Q:43:ARG:NH2	2.39	0.41
19:I:34:SER:O	19:I:37:LYS:NZ	2.53	0.41
26:z:137:G:O6	26:z:287:U:C2	2.73	0.41
35:U:85:ASN:HB2	35:U:88:MET:HB2	2.02	0.41
1:2:535:G:N1	1:2:550:C:O2	2.52	0.41
1:2:1550:G:H3'	1:2:1579:A:H61	1.85	0.41
18:h:124:SER:OG	18:h:125:ARG:N	2.53	0.41
18:h:127:LYS:HB3	18:h:146:SER:HB2	2.02	0.41
19:I:73:GLN:HA	19:I:76:GLN:HE22	1.85	0.41
29:O:84:LEU:HD12	29:O:84:LEU:HA	1.95	0.41
35:U:39:LEU:HD23	35:U:39:LEU:HA	1.90	0.41
34:T:15:VAL:O	34:T:18:THR:OG1	2.32	0.41
1:2:65:C:N4	17:H:134:GLY:O	2.53	0.41
1:2:317:C:OP2	17:H:183:ARG:NH2	2.54	0.41
1:2:946:U:H2'	1:2:947:G:C8	2.55	0.41
1:2:1650:A:H5''	32:R:139:ALA:HB2	2.02	0.41
21:J:139:LYS:HG3	21:J:140:LYS:HG2	2.02	0.41
24:x:829:MET:SD	24:x:829:MET:N	2.93	0.41
31:Q:100:LYS:HG2	31:Q:101:THR:HG23	2.02	0.41
35:U:110:LEU:HD23	35:U:110:LEU:HA	1.96	0.41
1:2:996:A:OP1	29:O:114:ARG:NH2	2.53	0.41
1:2:1572:C:H2'	1:2:1573:G:C8	2.55	0.41
1:2:1596:U:O3'	34:T:25:LYS:NZ	2.53	0.41
9:D:209:VAL:HA	9:D:212:LYS:HE3	2.03	0.41
24:x:959:ASP:OD1	24:x:960:GLU:N	2.54	0.41
27:M:22:ARG:HB3	27:M:25:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:O:104:ARG:HE	29:O:104:ARG:HB2	1.68	0.41
33:S:71:ILE:HD12	33:S:74:GLN:HA	2.03	0.41
35:U:33:TRP:HZ2	35:U:102:ARG:HG3	1.86	0.41
3:A:62:ARG:HB2	3:A:65:LEU:HB2	2.02	0.41
5:B:122:LEU:HD23	5:B:144:THR:HG22	2.01	0.41
13:F:181:CYS:SG	13:F:182:MET:N	2.94	0.41
18:h:155:ARG:HA	18:h:155:ARG:HD3	1.83	0.41
24:x:1091:LYS:HG3	24:x:1181:VAL:HG12	2.01	0.41
31:Q:130:ARG:HD2	31:Q:130:ARG:HA	1.93	0.41
1:2:528:A:H2'	1:2:529:A:C8	2.55	0.41
1:2:1618:C:H1'	31:Q:53:GLN:HG3	2.03	0.41
1:2:1756:C:H2'	1:2:1757:G:C5	2.56	0.41
2:Z:20:ARG:NH2	13:F:60:GLU:OE2	2.54	0.41
9:D:138:GLY:HA3	9:D:162:ILE:HG22	2.02	0.41
20:i:20:A:N6	20:i:45:G:O2'	2.53	0.41
24:x:631:VAL:HG22	24:x:697:LEU:HD12	2.03	0.41
24:x:751:VAL:O	24:x:818:LEU:HA	2.21	0.41
28:N:80:ASP:OD1	28:N:80:ASP:N	2.52	0.41
1:2:106:C:H2'	1:2:107:A:C8	2.55	0.41
2:Z:54:VAL:HB	2:Z:76:TYR:HB2	2.02	0.41
3:A:82:ARG:HH11	3:A:85:GLN:HE21	1.68	0.41
15:G:35:LEU:HD12	15:G:117:ILE:HG12	2.01	0.41
16:g:104:LYS:HA	16:g:104:LYS:HD3	1.83	0.41
19:I:105:THR:HG23	19:I:107:LYS:HG3	2.02	0.41
21:J:60:LEU:HD12	21:J:60:LEU:HA	1.93	0.41
24:x:592:ASP:OD1	24:x:592:ASP:N	2.53	0.41
30:P:66:ARG:NH1	30:P:67:ASP:OD1	2.53	0.41
32:R:110:ASP:OD1	32:R:111:ILE:N	2.54	0.41
1:2:212:C:H2'	1:2:213:G:C8	2.56	0.41
1:2:433:A:H2'	1:2:434:G:C8	2.56	0.41
1:2:1705:C:H2'	1:2:1706:G:H8	1.86	0.41
2:Z:43:LYS:HE3	2:Z:43:LYS:HB3	1.80	0.41
9:D:272:HIS:O	9:D:276:THR:OG1	2.37	0.41
13:F:139:LEU:HB2	13:F:150:PRO:HG3	2.02	0.41
14:f:100:LYS:HG2	14:f:102:THR:H	1.86	0.41
15:G:175:ASP:OD1	15:G:175:ASP:N	2.53	0.41
17:H:76:LEU:HD21	17:H:92:ARG:HD2	2.03	0.41
18:h:109:LEU:HD21	18:h:125:ARG:HE	1.86	0.41
24:x:852:GLU:H	24:x:877:ASN:HD22	1.69	0.41
34:T:98:VAL:HG11	34:T:106:LYS:HD2	2.03	0.41
1:2:615:C:O2	14:f:84:LYS:NZ	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1228:A:H2'	1:2:1229:G:C8	2.55	0.41
1:2:1856:C:H2'	1:2:1857:G:H8	1.86	0.41
31:Q:42:ARG:O	31:Q:46:SER:HB3	2.21	0.41
1:2:1213:C:H2'	1:2:1214:A:C8	2.57	0.40
1:2:1277:C:H2'	1:2:1278:A:C8	2.55	0.40
1:2:1548:G:OP1	36:V:60:THR:OG1	2.39	0.40
1:2:1658:G:OP2	1:2:1660:C:N4	2.54	0.40
2:Z:110:ARG:HG3	2:Z:113:ARG:HH22	1.86	0.40
5:B:177:MET:HA	5:B:180:ARG:HB3	2.03	0.40
23:K:60:LEU:HD23	23:K:94:LEU:HD11	2.03	0.40
24:x:704:HIS:CG	24:x:705:GLU:N	2.82	0.40
24:x:881:LYS:HB3	24:x:881:LYS:HE3	1.95	0.40
26:z:268:G:OP2	26:z:270:C:N4	2.54	0.40
31:Q:107:ILE:HG23	31:Q:111:MET:HG3	2.02	0.40
37:W:51:LYS:HD3	37:W:51:LYS:HA	1.84	0.40
1:2:5:U:H2'	1:2:6:G:H8	1.85	0.40
1:2:155:G:H4'	17:H:15:LEU:HD13	2.02	0.40
26:z:141:U:H2'	26:z:142:A:H8	1.86	0.40
30:P:139:SER:OG	30:P:140:THR:N	2.49	0.40
34:T:99:LEU:HD23	34:T:99:LEU:HA	1.89	0.40
1:2:1354:G:N2	1:2:1357:A:OP2	2.41	0.40
1:2:1497:G:H4'	1:2:1498:A:H5''	2.03	0.40
1:2:1845:A:H2'	1:2:1846:G:C8	2.55	0.40
13:F:245:ARG:HA	13:F:245:ARG:HD3	1.93	0.40
26:z:294:U:H2'	26:z:295:G:H2'	2.03	0.40
38:X:75:ILE:HD11	38:X:93:LEU:HD21	2.02	0.40
38:X:93:LEU:HD23	38:X:102:ILE:HD12	2.02	0.40
1:2:145:G:H2'	1:2:146:G:C8	2.56	0.40
1:2:618:C:H41	39:Y:67:ARG:HH22	1.69	0.40
1:2:1174:U:H5''	22:n:21:ARG:HH22	1.86	0.40
1:2:1648:G:O2'	1:2:1674:G:O6	2.36	0.40
1:2:1844:U:H2'	1:2:1845:A:C8	2.56	0.40
1:2:1050:A:OP1	1:2:1846:G:N2	2.54	0.40
1:2:1058:A:OP1	20:i:37:A:O2'	2.40	0.40
1:2:1172:U:H2'	1:2:1173:A:H8	1.87	0.40
1:2:1244:U:H2'	1:2:1245:G:H8	1.86	0.40
13:F:6:LYS:HB3	13:F:6:LYS:HE3	1.93	0.40
17:H:192:ILE:HD13	17:H:192:ILE:HA	1.94	0.40
30:P:92:ALA:HA	30:P:125:LYS:O	2.22	0.40
34:T:114:LEU:HA	34:T:117:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Z	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
3	A	100/144 (69%)	89 (89%)	11 (11%)	0	100	100
4	a	75/124 (60%)	73 (97%)	2 (3%)	0	100	100
5	B	215/295 (73%)	202 (94%)	13 (6%)	0	100	100
6	b	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	C	211/264 (80%)	203 (96%)	8 (4%)	0	100	100
8	c	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
9	D	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
10	d	65/69 (94%)	57 (88%)	8 (12%)	0	100	100
11	E	226/281 (80%)	220 (97%)	6 (3%)	0	100	100
12	e	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
13	F	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
14	f	55/133 (41%)	45 (82%)	10 (18%)	0	100	100
15	G	189/204 (93%)	180 (95%)	9 (5%)	0	100	100
16	g	66/188 (35%)	64 (97%)	2 (3%)	0	100	100
17	H	235/249 (94%)	227 (97%)	8 (3%)	0	100	100
18	h	311/317 (98%)	289 (93%)	22 (7%)	0	100	100
19	I	181/432 (42%)	174 (96%)	7 (4%)	0	100	100
21	J	204/208 (98%)	191 (94%)	13 (6%)	0	100	100
22	n	23/25 (92%)	23 (100%)	0	0	100	100
23	K	183/194 (94%)	173 (94%)	10 (6%)	0	100	100
24	x	625/627 (100%)	577 (92%)	48 (8%)	0	100	100
25	L	94/149 (63%)	86 (92%)	8 (8%)	0	100	100
27	M	149/158 (94%)	144 (97%)	5 (3%)	0	100	100
28	N	115/132 (87%)	106 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	O	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
30	P	134/168 (80%)	126 (94%)	8 (6%)	0	100	100
31	Q	118/145 (81%)	111 (94%)	7 (6%)	0	100	100
32	R	140/172 (81%)	134 (96%)	6 (4%)	0	100	100
33	S	130/135 (96%)	115 (88%)	15 (12%)	0	100	100
34	T	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
35	U	139/145 (96%)	133 (96%)	6 (4%)	0	100	100
36	V	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
37	W	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
38	X	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
39	Y	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
All	All	5551/6592 (84%)	5251 (95%)	300 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	107/113 (95%)	107 (100%)	0	100	100
3	A	87/123 (71%)	87 (100%)	0	100	100
4	a	68/102 (67%)	68 (100%)	0	100	100
5	B	180/245 (74%)	180 (100%)	0	100	100
6	b	88/88 (100%)	88 (100%)	0	100	100
7	C	194/231 (84%)	194 (100%)	0	100	100
8	c	75/76 (99%)	75 (100%)	0	100	100
9	D	187/187 (100%)	187 (100%)	0	100	100
10	d	60/62 (97%)	58 (97%)	2 (3%)	33	56
11	E	190/232 (82%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	e	48/49 (98%)	48 (100%)	0	100	100
13	F	224/225 (100%)	224 (100%)	0	100	100
14	f	47/106 (44%)	47 (100%)	0	100	100
15	G	161/170 (95%)	161 (100%)	0	100	100
16	g	61/154 (40%)	61 (100%)	0	100	100
17	H	207/218 (95%)	207 (100%)	0	100	100
18	h	272/275 (99%)	272 (100%)	0	100	100
19	I	165/360 (46%)	164 (99%)	1 (1%)	78	80
21	J	178/180 (99%)	178 (100%)	0	100	100
22	n	24/24 (100%)	24 (100%)	0	100	100
23	K	161/168 (96%)	161 (100%)	0	100	100
24	x	552/552 (100%)	552 (100%)	0	100	100
25	L	87/125 (70%)	87 (100%)	0	100	100
27	M	136/142 (96%)	136 (100%)	0	100	100
28	N	99/108 (92%)	99 (100%)	0	100	100
29	O	130/131 (99%)	130 (100%)	0	100	100
30	P	106/130 (82%)	106 (100%)	0	100	100
31	Q	109/130 (84%)	109 (100%)	0	100	100
32	R	117/140 (84%)	117 (100%)	0	100	100
33	S	119/121 (98%)	119 (100%)	0	100	100
34	T	125/132 (95%)	125 (100%)	0	100	100
35	U	111/116 (96%)	111 (100%)	0	100	100
36	V	92/107 (86%)	92 (100%)	0	100	100
37	W	67/67 (100%)	67 (100%)	0	100	100
38	X	112/113 (99%)	112 (100%)	0	100	100
39	Y	113/115 (98%)	113 (100%)	0	100	100
All	All	4859/5617 (86%)	4856 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	d	68	LEU
10	d	69	ARG

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Mol	Chain	Res	Type
19	I	39	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	Z	15	ASN
2	Z	112	ASN
5	B	50	ASN
7	C	101	HIS
7	C	202	GLN
9	D	113	GLN
9	D	235	ASN
9	D	277	HIS
11	E	56	GLN
12	e	5	GLN
13	F	138	HIS
14	f	88	GLN
14	f	112	ASN
15	G	79	HIS
15	G	110	GLN
16	g	93	HIS
17	H	110	ASN
17	H	163	ASN
19	I	114	GLN
19	I	162	GLN
19	I	193	GLN
21	J	155	ASN
24	x	655	GLN
24	x	841	GLN
24	x	877	ASN
24	x	927	GLN
25	L	7	ASN
25	L	66	HIS
29	O	58	HIS
29	O	62	GLN
29	O	105	ASN
30	P	94	HIS
33	S	31	ASN
34	T	10	GLN
34	T	72	GLN
34	T	134	GLN
35	U	63	HIS

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Mol	Chain	Res	Type
36	V	92	HIS
39	Y	61	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1669/1870 (89%)	342 (20%)	7 (0%)
20	i	74/75 (98%)	15 (20%)	0
26	z	256/400 (64%)	66 (25%)	0
All	All	1999/2345 (85%)	423 (21%)	7 (0%)

All (423) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	26	U
1	2	33	G
1	2	37	C
1	2	41	G
1	2	42	A
1	2	44	U
1	2	45	A
1	2	46	A
1	2	47	G
1	2	49	C
1	2	56	G
1	2	61	A
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	102	A
1	2	103	A
1	2	104	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	126	G

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Mol	Chain	Res	Type
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	170	A
1	2	171	A
1	2	180	G
1	2	182	C
1	2	183	G
1	2	184	G
1	2	190	G
1	2	192	C
1	2	291	G
1	2	292	A
1	2	302	A
1	2	306	C
1	2	307	G
1	2	309	G
1	2	319	C
1	2	335	G
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	371	A
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	408	A
1	2	409	C

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Mol	Chain	Res	Type
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	452	G
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	474	G
1	2	483	C
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	517	C
1	2	532	C
1	2	533	A
1	2	537	C
1	2	541	U
1	2	542	U
1	2	544	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	559	G
1	2	560	A
1	2	561	A
1	2	562	U
1	2	564	A
1	2	567	C
1	2	576	A
1	2	583	A

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Mol	Chain	Res	Type
1	2	585	C
1	2	587	A
1	2	590	A
1	2	591	U
1	2	604	A
1	2	606	G
1	2	608	C
1	2	613	G
1	2	614	C
1	2	617	G
1	2	623	G
1	2	625	G
1	2	627	U
1	2	628	A
1	2	631	U
1	2	635	G
1	2	643	A
1	2	644	G
1	2	655	A
1	2	660	C
1	2	662	G
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	684	G
1	2	688	U
1	2	752	G
1	2	754	G
1	2	756	C
1	2	790	C
1	2	794	A
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	844	U

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Mol	Chain	Res	Type
1	2	847	A
1	2	852	G
1	2	853	C
1	2	870	A
1	2	872	A
1	2	873	G
1	2	874	G
1	2	875	A
1	2	878	G
1	2	881	G
1	2	886	A
1	2	887	U
1	2	888	U
1	2	891	G
1	2	893	U
1	2	895	G
1	2	898	U
1	2	901	G
1	2	903	A
1	2	904	A
1	2	908	A
1	2	913	A
1	2	919	A
1	2	920	A
1	2	921	G
1	2	933	G
1	2	963	A
1	2	965	U
1	2	969	U
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	1017	U
1	2	1023	A
1	2	1024	A
1	2	1026	C
1	2	1027	A
1	2	1040	G
1	2	1043	G

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Mol	Chain	Res	Type
1	2	1044	G
1	2	1045	U
1	2	1060	A
1	2	1078	C
1	2	1083	A
1	2	1085	C
1	2	1088	U
1	2	1114	U
1	2	1118	C
1	2	1121	G
1	2	1138	C
1	2	1149	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1157	G
1	2	1165	G
1	2	1166	G
1	2	1168	G
1	2	1170	A
1	2	1195	A
1	2	1201	U
1	2	1203	U
1	2	1205	G
1	2	1207	G
1	2	1208	A
1	2	1210	G
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1242	U
1	2	1251	A
1	2	1256	G
1	2	1257	G
1	2	1264	C
1	2	1266	C
1	2	1274	G
1	2	1275	G
1	2	1278	A
1	2	1284	A

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Mol	Chain	Res	Type
1	2	1285	G
1	2	1286	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	1305	C
1	2	1307	U
1	2	1309	C
1	2	1310	U
1	2	1311	C
1	2	1312	G
1	2	1318	G
1	2	1332	A
1	2	1333	U
1	2	1342	U
1	2	1358	U
1	2	1360	U
1	2	1371	U
1	2	1372	U
1	2	1378	A
1	2	1380	C
1	2	1396	A
1	2	1397	U
1	2	1401	A
1	2	1404	U
1	2	1428	G
1	2	1429	G
1	2	1442	U
1	2	1452	A
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1466	G
1	2	1477	U
1	2	1489	A
1	2	1490	G
1	2	1493	C

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Mol	Chain	Res	Type
1	2	1498	A
1	2	1507	G
1	2	1521	C
1	2	1523	C
1	2	1533	A
1	2	1548	G
1	2	1551	U
1	2	1552	G
1	2	1554	C
1	2	1556	A
1	2	1557	C
1	2	1560	U
1	2	1567	G
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	1618	C
1	2	1619	A
1	2	1621	U
1	2	1622	U
1	2	1623	A
1	2	1638	G
1	2	1647	A
1	2	1648	G
1	2	1665	G
1	2	1680	G
1	2	1695	A
1	2	1699	A
1	2	1715	A
1	2	1721	U
1	2	1744	G
1	2	1751	C
1	2	1753	C
1	2	1755	C
1	2	1756	C
1	2	1758	G
1	2	1759	G

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Mol	Chain	Res	Type
1	2	1760	G
1	2	1776	G
1	2	1780	G
1	2	1781	A
1	2	1783	C
1	2	1786	U
1	2	1823	A
1	2	1824	A
1	2	1826	G
1	2	1834	A
1	2	1835	A
1	2	1836	G
1	2	1838	U
1	2	1839	U
1	2	1849	G
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
1	2	1866	A
1	2	1869	A
20	i	17	G
20	i	18	G
20	i	19	A
20	i	20	A
20	i	41	A
20	i	47	C
20	i	54	U
20	i	57	A
20	i	59	A
20	i	70	C
20	i	71	U
20	i	72	A
20	i	73	C
20	i	74	C
20	i	75	A
26	z	48	U
26	z	49	G
26	z	50	A
26	z	57	A
26	z	82	G
26	z	83	C

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Mol	Chain	Res	Type
26	z	85	A
26	z	86	U
26	z	94	G
26	z	100	G
26	z	102	G
26	z	103	U
26	z	106	U
26	z	107	G
26	z	111	C
26	z	121	C
26	z	123	C
26	z	135	G
26	z	150	G
26	z	153	G
26	z	154	A
26	z	156	C
26	z	157	C
26	z	161	G
26	z	163	G
26	z	165	A
26	z	166	C
26	z	168	C
26	z	172	A
26	z	173	A
26	z	229	G
26	z	232	C
26	z	234	U
26	z	237	C
26	z	244	A
26	z	253	G
26	z	258	G
26	z	265	U
26	z	266	G
26	z	269	U
26	z	270	C
26	z	282	U
26	z	284	U
26	z	288	A
26	z	295	G
26	z	297	U
26	z	303	G
26	z	306	U

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Mol	Chain	Res	Type
26	z	323	G
26	z	324	U
26	z	330	A
26	z	331	G
26	z	332	A
26	z	333	C
26	z	334	C
26	z	335	G
26	z	336	U
26	z	337	G
26	z	340	C
26	z	341	C
26	z	342	A
26	z	344	G
26	z	345	A
26	z	346	G
26	z	348	A
26	z	350	G

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	383	G
1	2	445	A
1	2	561	A
1	2	1204	G
1	2	1308	U
1	2	1395	C
1	2	1759	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	GTP	x	1301	42,43	33,34,34	1.12	3 (9%)	50,54,54	1.78	13 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	x	1301	42,43	-	0/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	x	1301	GTP	PA-O3A	3.68	1.63	1.59
41	x	1301	GTP	PB-O3B	2.57	1.62	1.59
41	x	1301	GTP	C8-N7	2.13	1.38	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	x	1301	GTP	C2-N3-C4	5.11	121.11	112.30
41	x	1301	GTP	C5-C4-N3	-4.00	122.02	128.39
41	x	1301	GTP	N9-C8-N7	-3.66	106.61	113.40
41	x	1301	GTP	N2-C2-N1	3.17	123.44	116.76
41	x	1301	GTP	N1-C2-N3	-2.68	118.42	123.32
41	x	1301	GTP	C5-C6-N1	2.67	120.06	113.25
41	x	1301	GTP	O3G-PG-O2G	2.61	117.59	107.80
41	x	1301	GTP	O6-C6-C5	-2.40	120.21	126.53
41	x	1301	GTP	C8-N7-C5	2.32	108.40	104.26
41	x	1301	GTP	C2-N1-C6	-2.29	120.96	125.11
41	x	1301	GTP	O3A-PB-O1B	-2.22	104.01	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	x	1301	GTP	N9-C4-N3	2.19	130.34	125.95
41	x	1301	GTP	O3G-PG-O3B	-2.04	97.80	104.64

There are no chirality outliers.

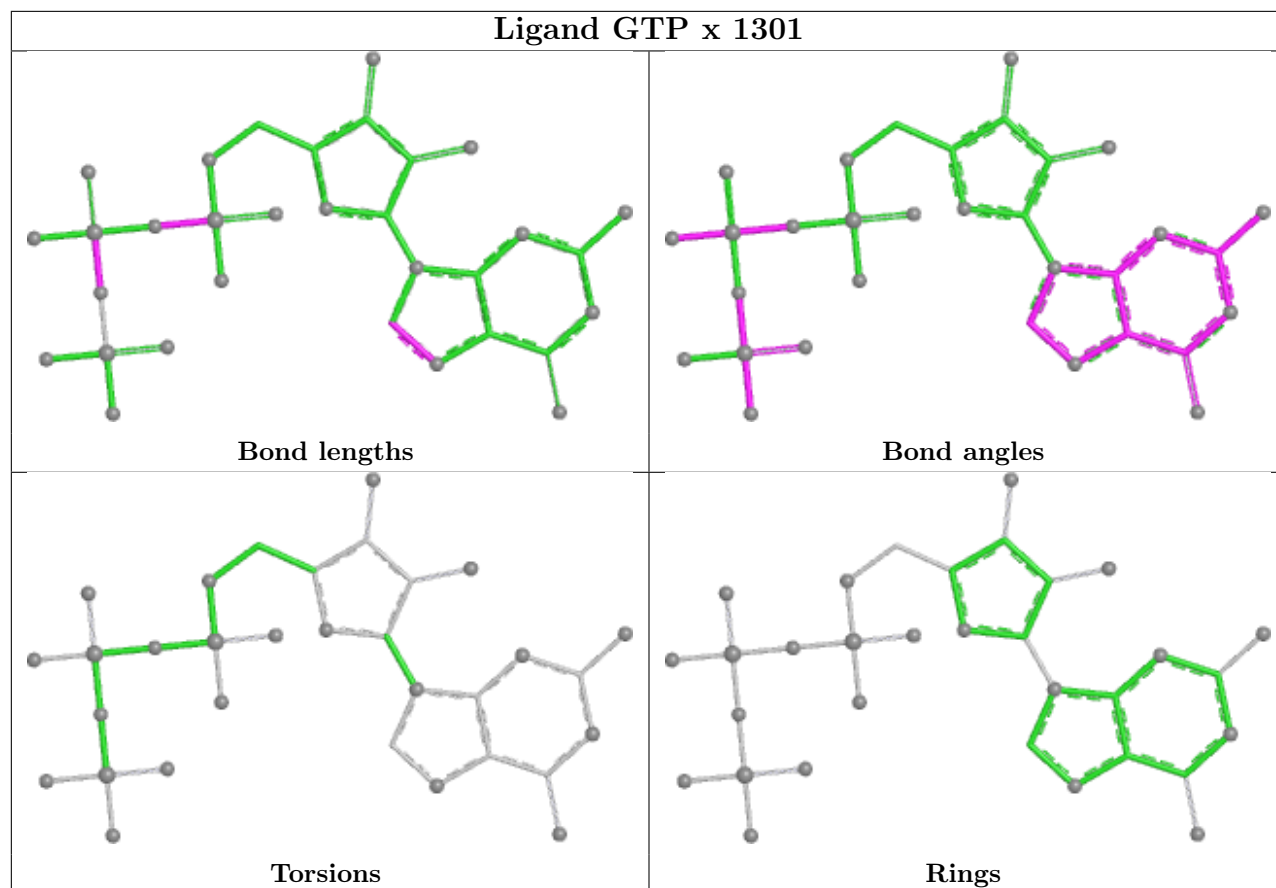
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	x	1301	GTP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

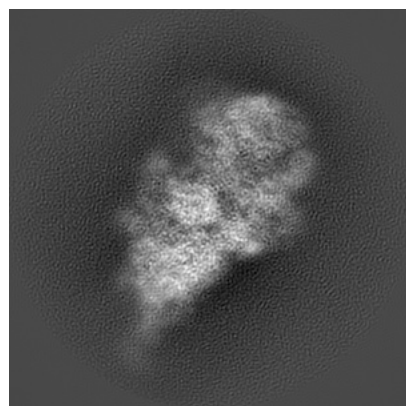
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25542. These allow visual inspection of the internal detail of the map and identification of artifacts.

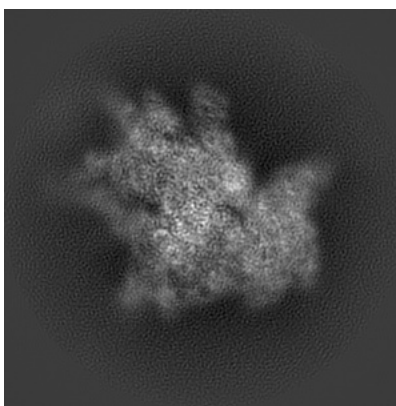
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

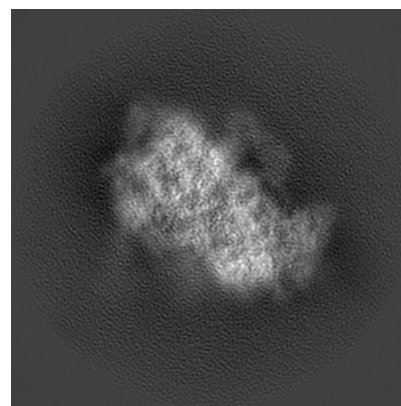
6.1.1 Primary map



X

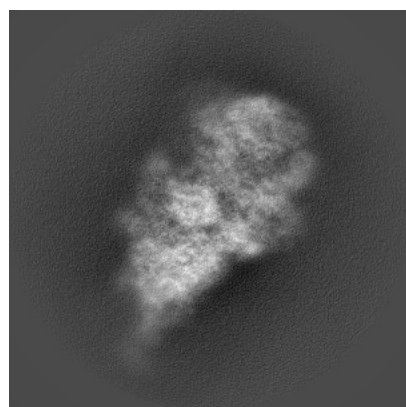


Y

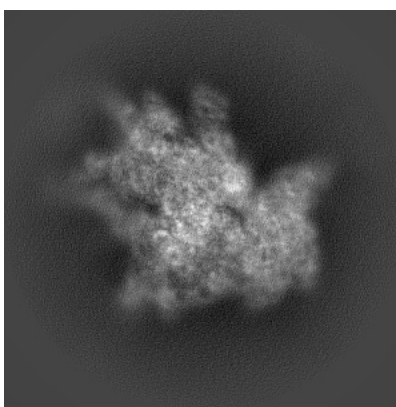


Z

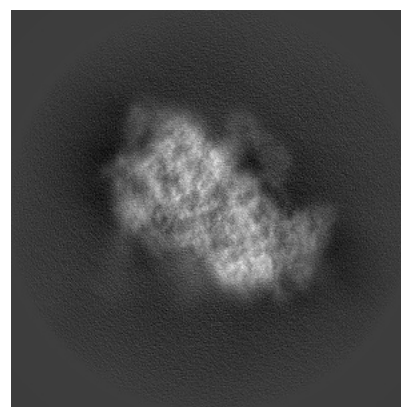
6.1.2 Raw map



X



Y

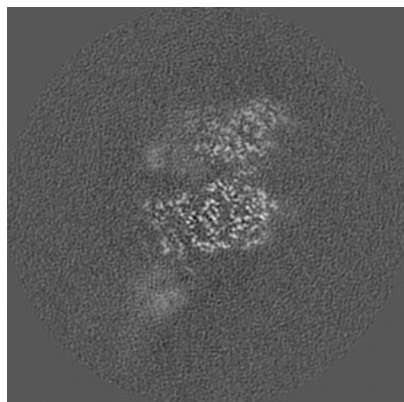


Z

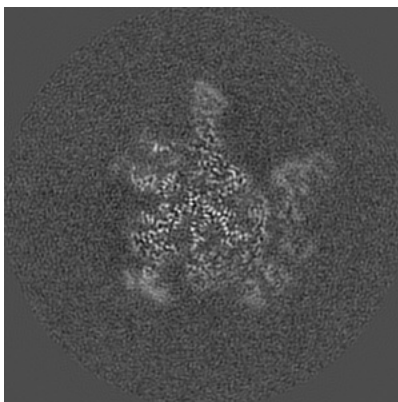
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

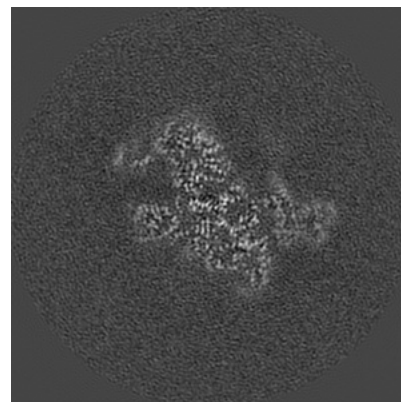
6.2.1 Primary map



X Index: 200

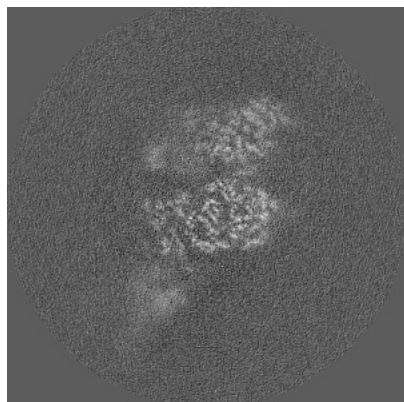


Y Index: 200

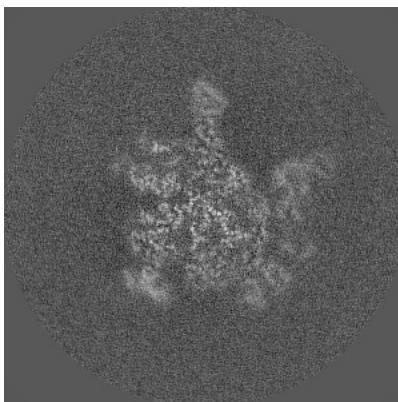


Z Index: 200

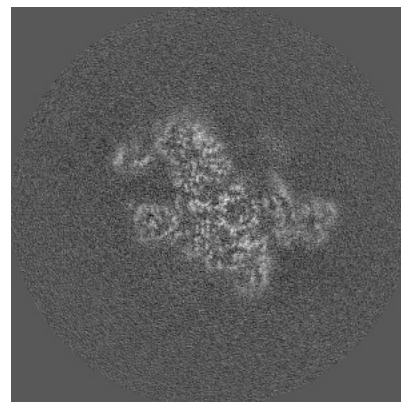
6.2.2 Raw map



X Index: 200



Y Index: 200

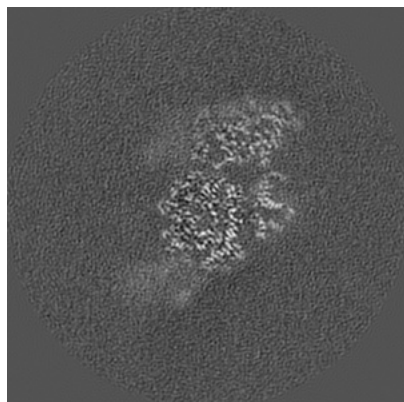


Z Index: 200

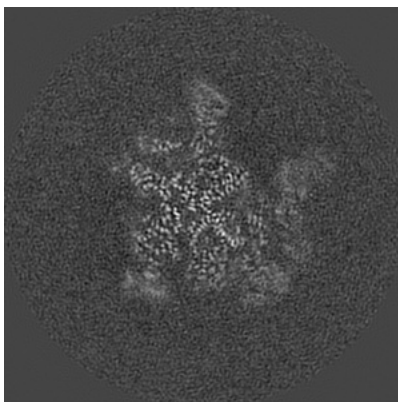
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

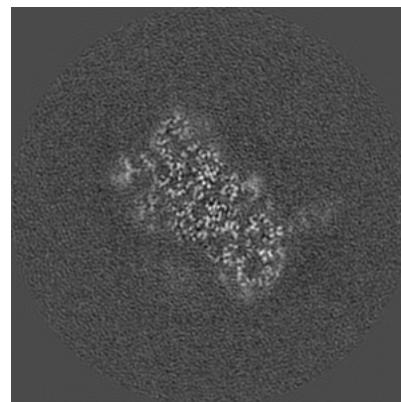
6.3.1 Primary map



X Index: 188

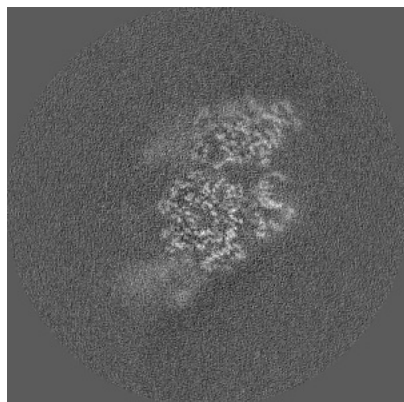


Y Index: 197

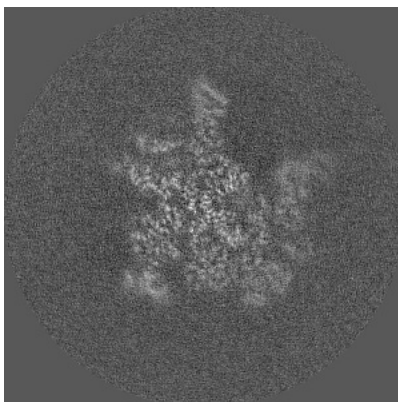


Z Index: 186

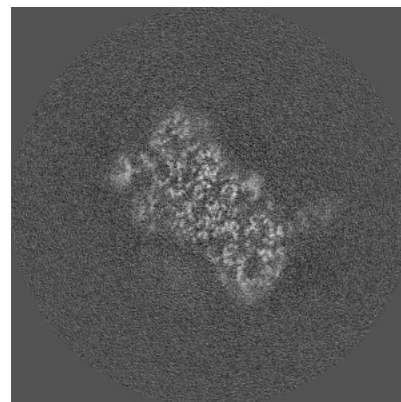
6.3.2 Raw map



X Index: 188



Y Index: 198

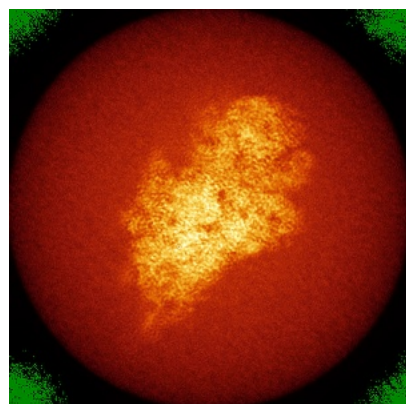


Z Index: 186

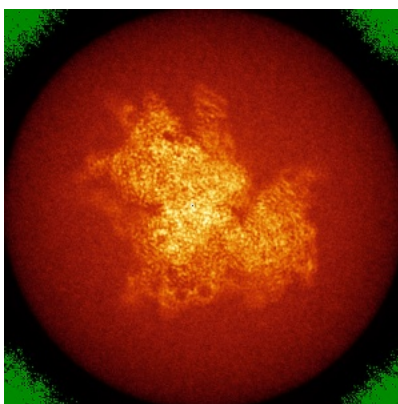
The images above show the largest variance slices of the map in three orthogonal directions.

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

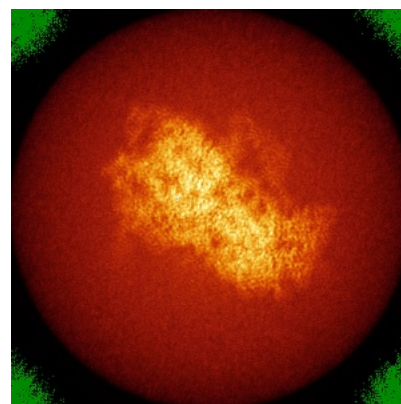
6.4.1 Primary map



X

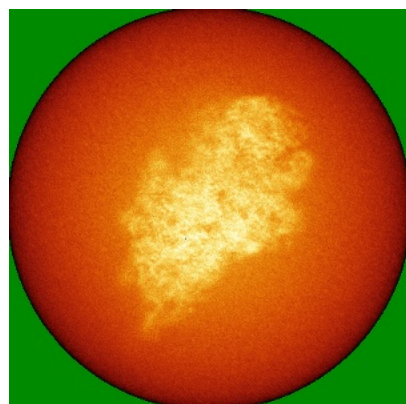


Y

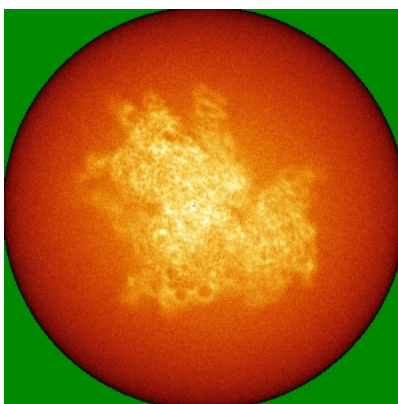


Z

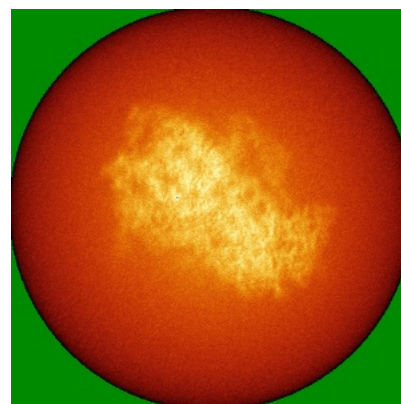
6.4.2 Raw map



X



Y

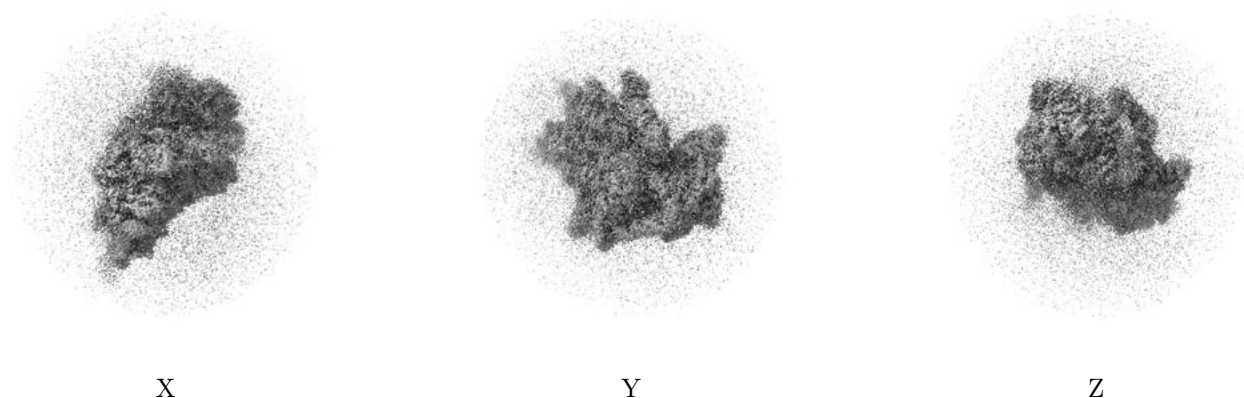


Z

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.

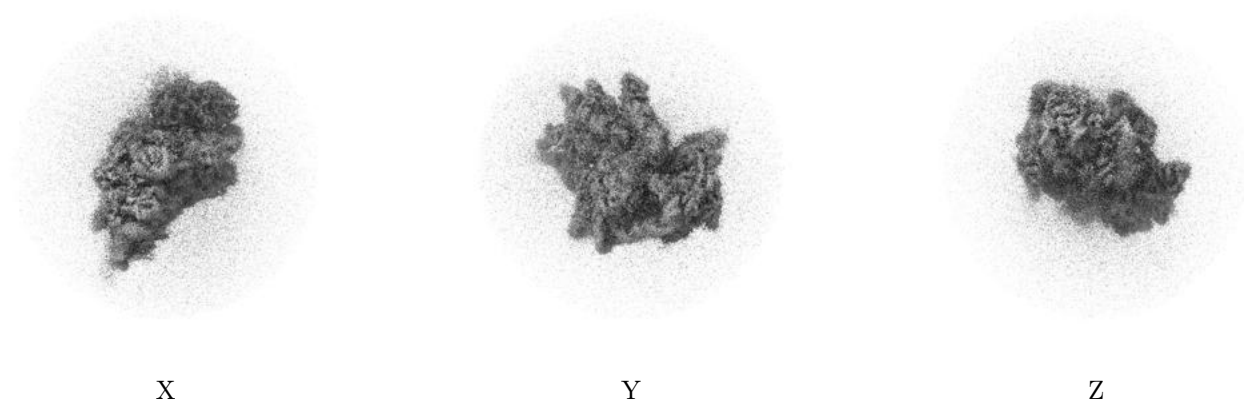
6.5 Orthogonal surface views [i](#)

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.

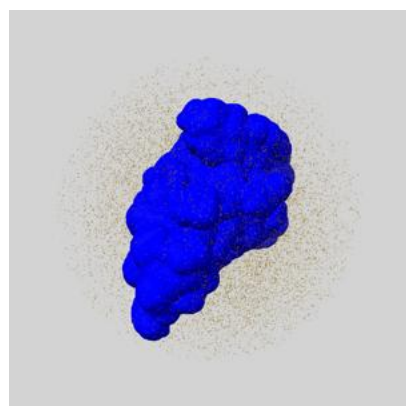
6.6 Mask visualisation [i](#)

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

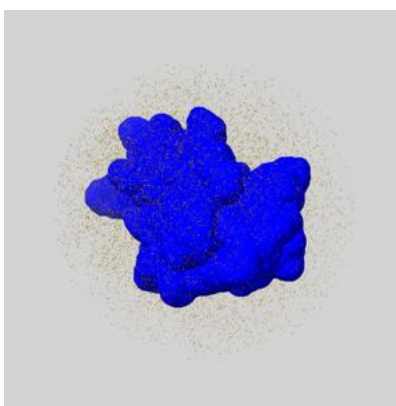
A mask typically either:

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

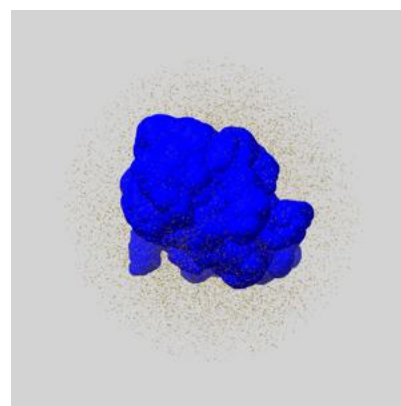
6.6.1 emd_25542_msk_1.map [i](#)



X



Y

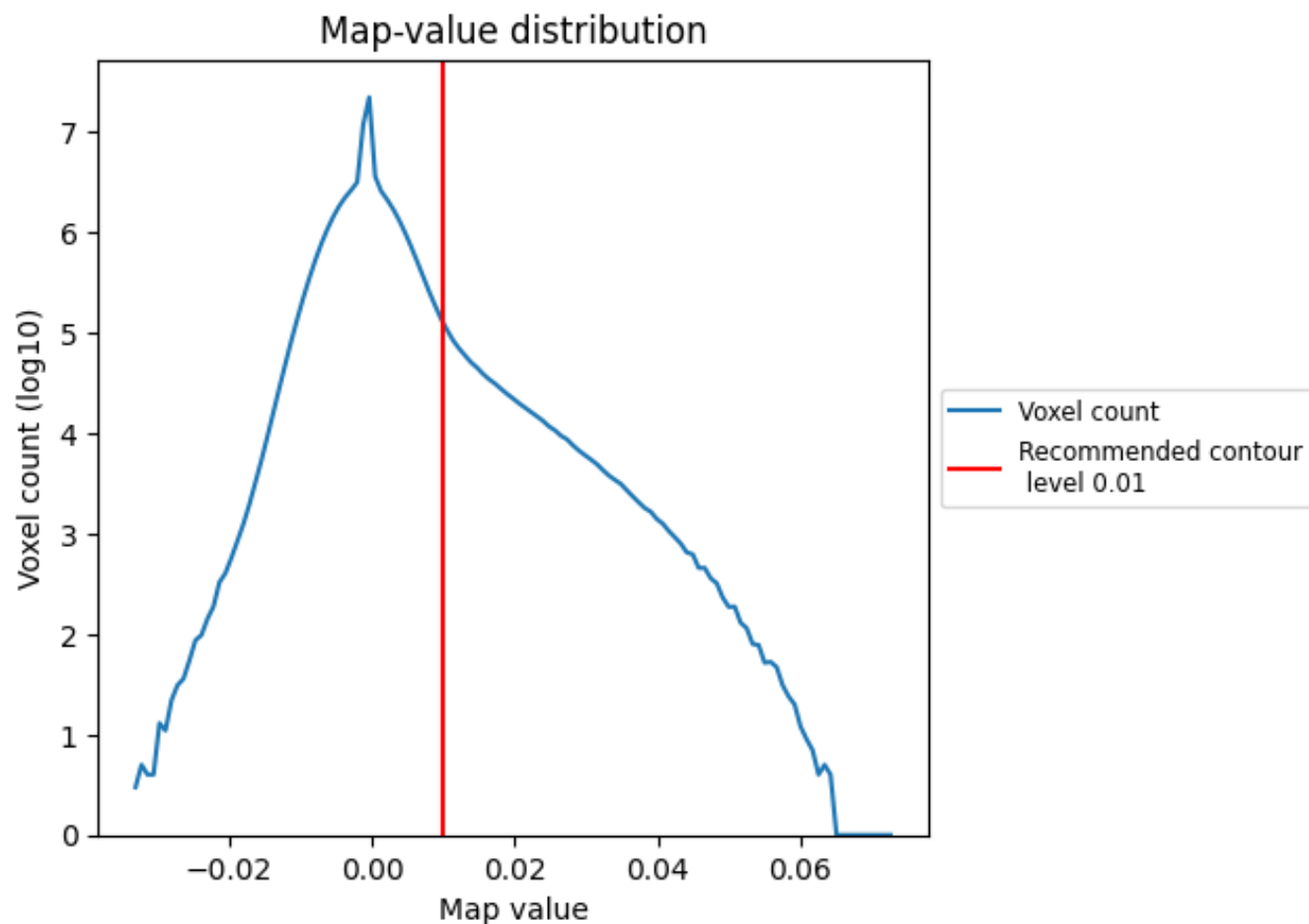


Z

7 Map analysis [i](#)

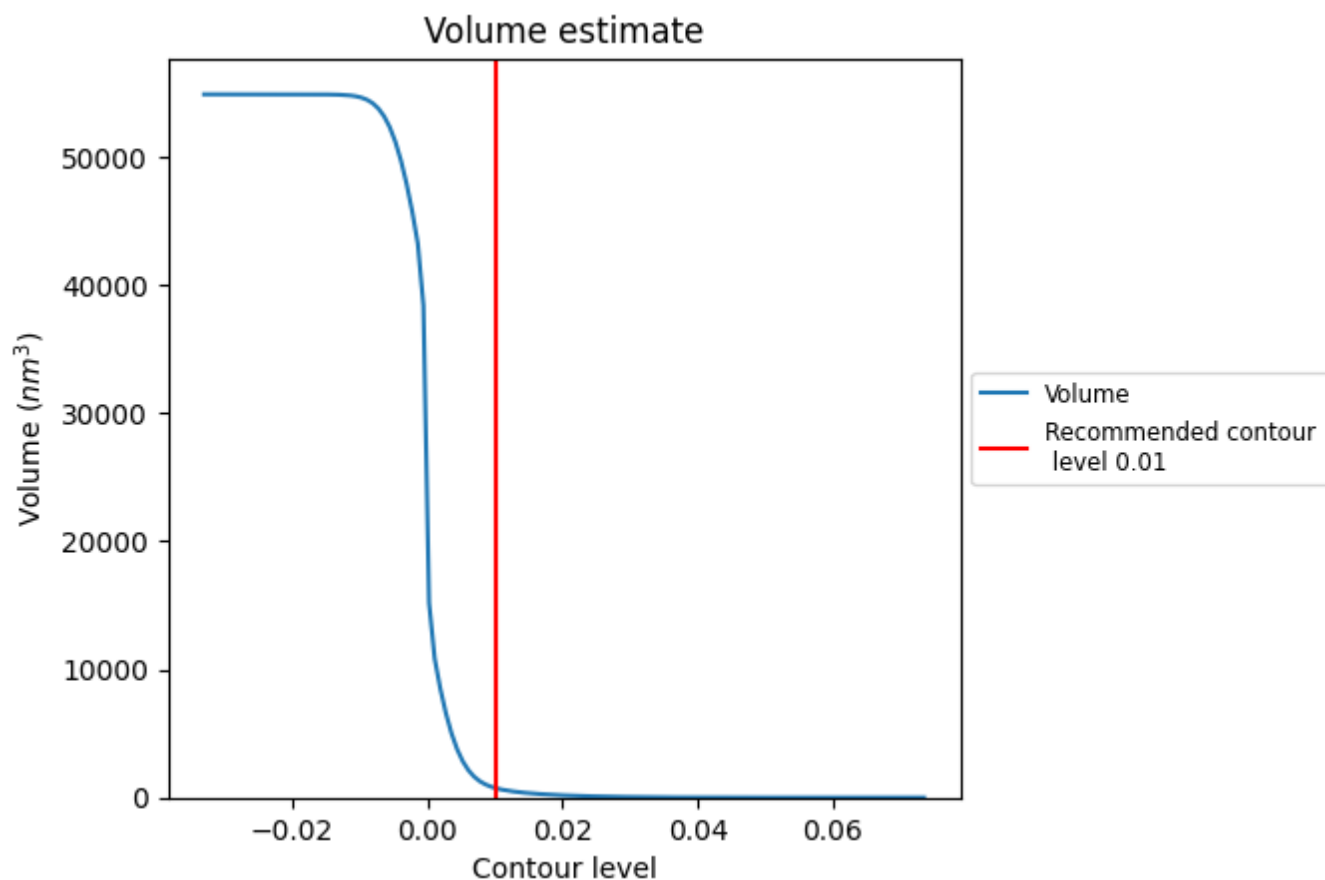
This section contains the results of statistical analysis of the map.

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.

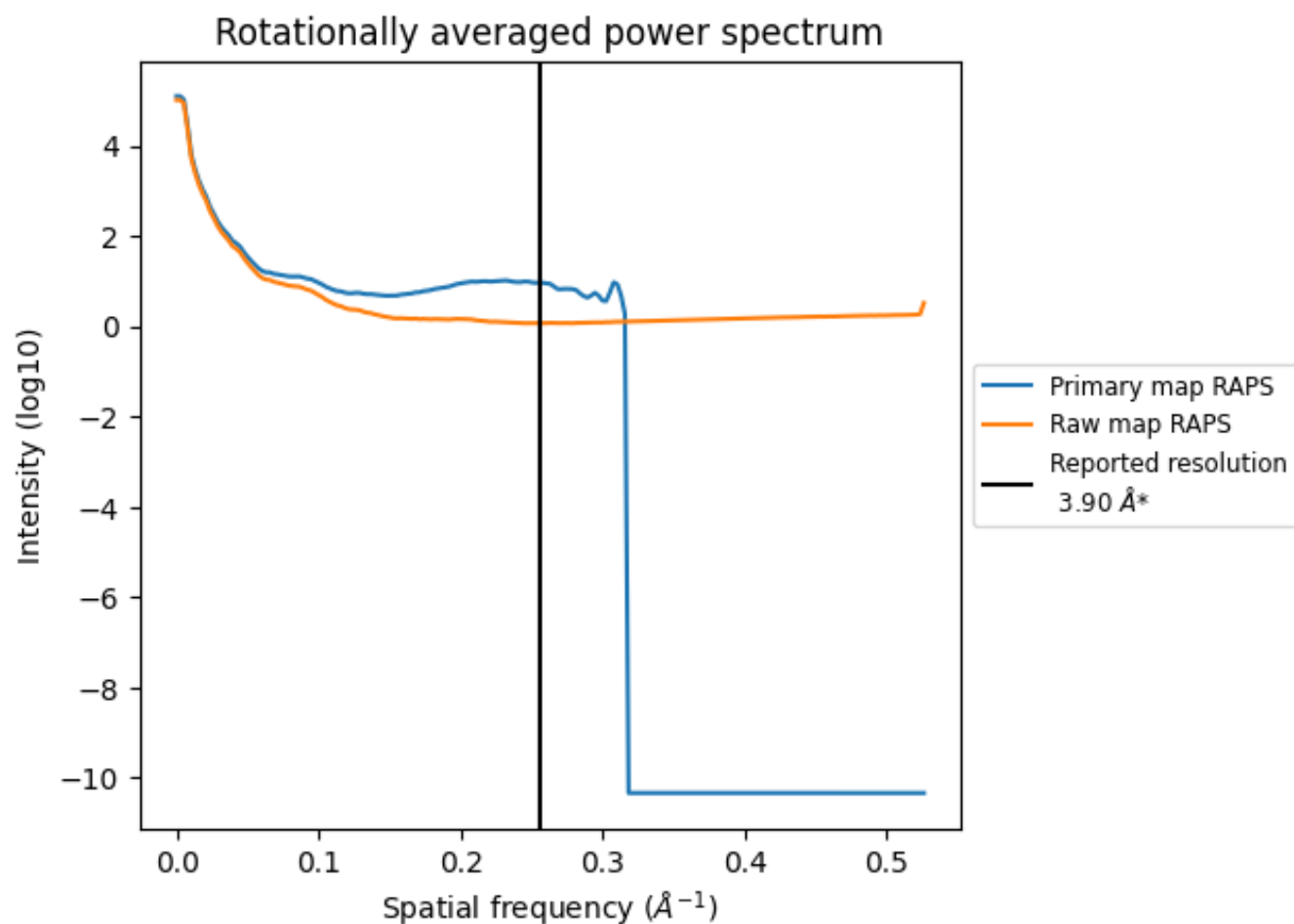
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 753 nm³; this corresponds to an approximate mass of 680 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 ⓘ

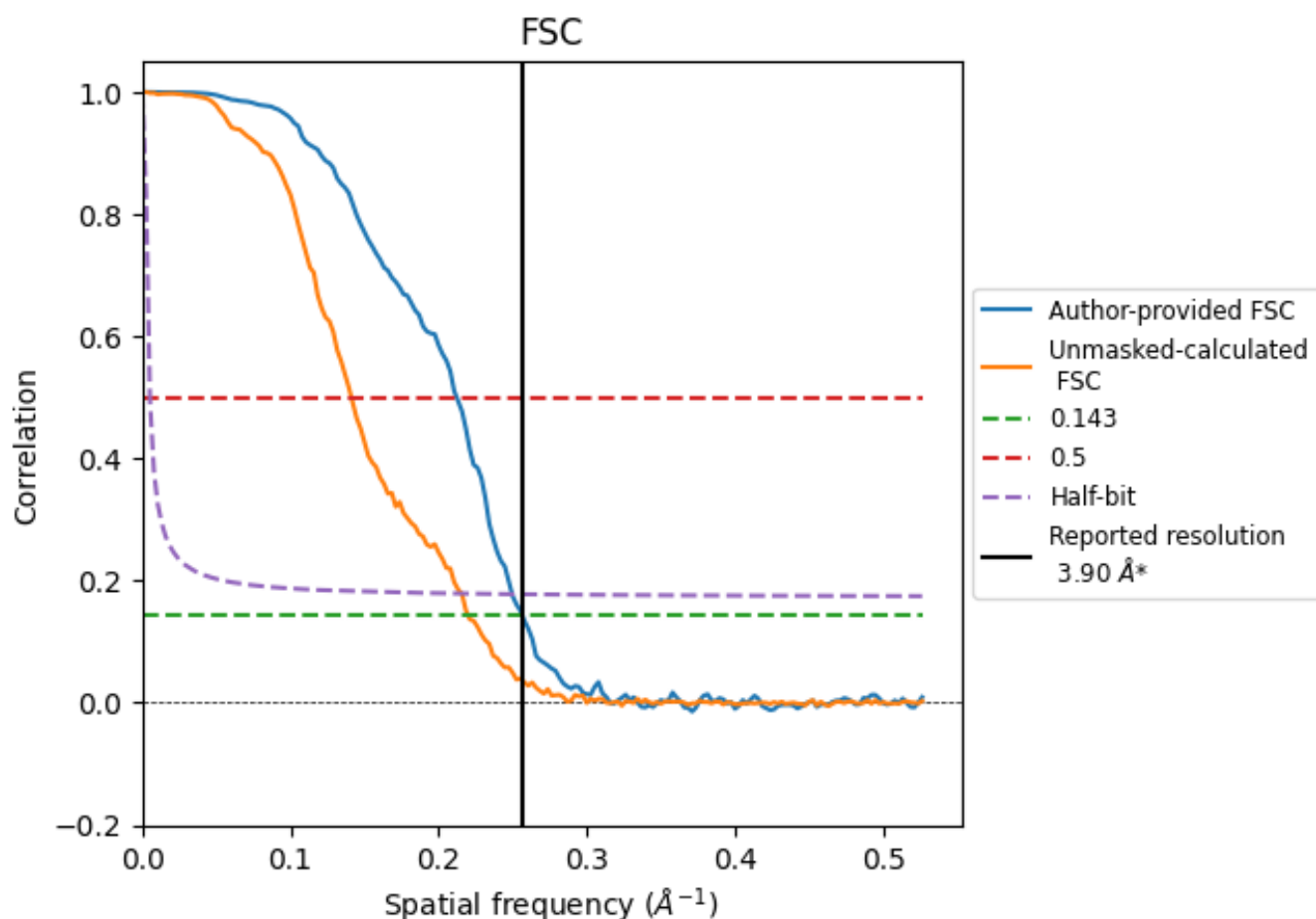


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

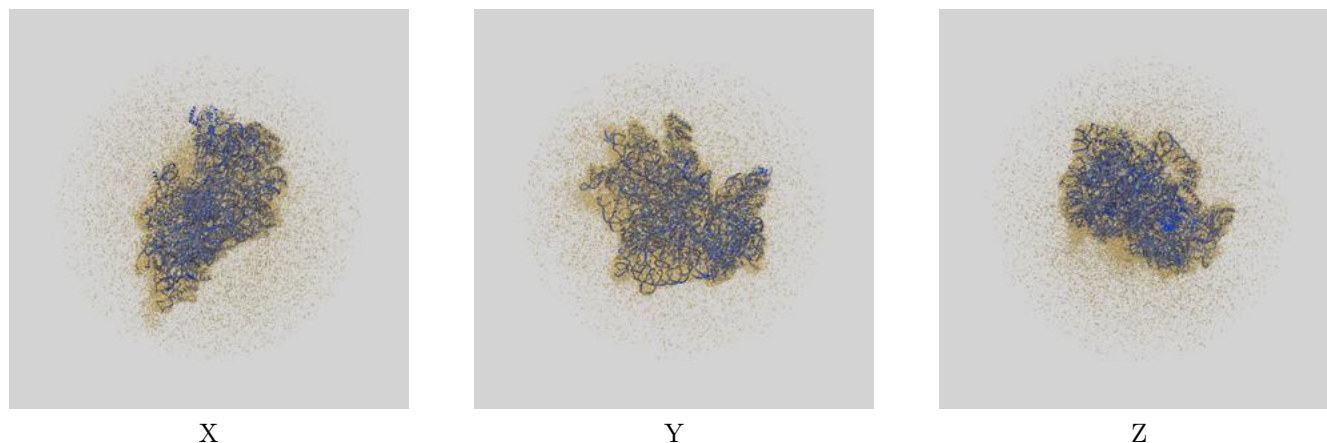
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.90	4.71	4.01
Unmasked-calculated*	4.55	7.09	4.64

*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 4.55 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

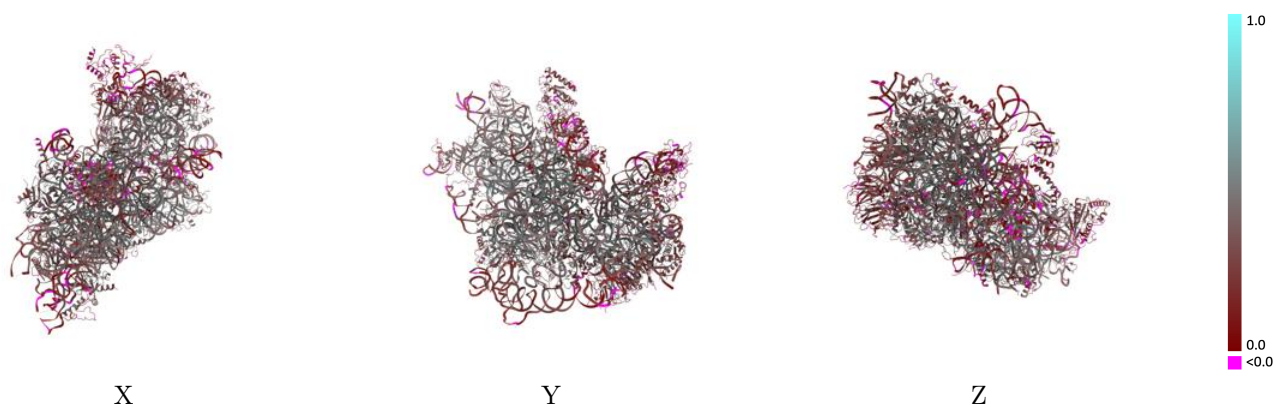
This section contains information regarding the fit between EMDB map EMD-25542 and PDB model 7SYV. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



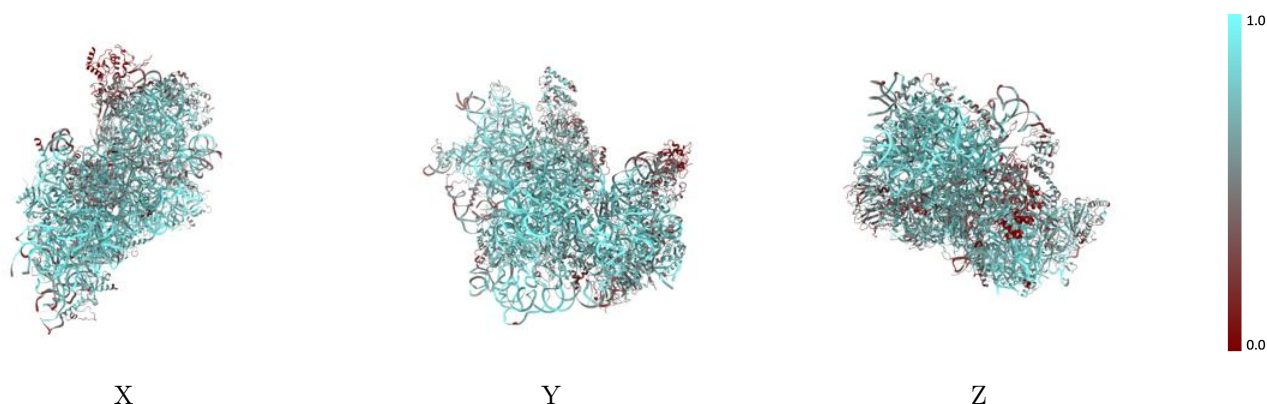
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



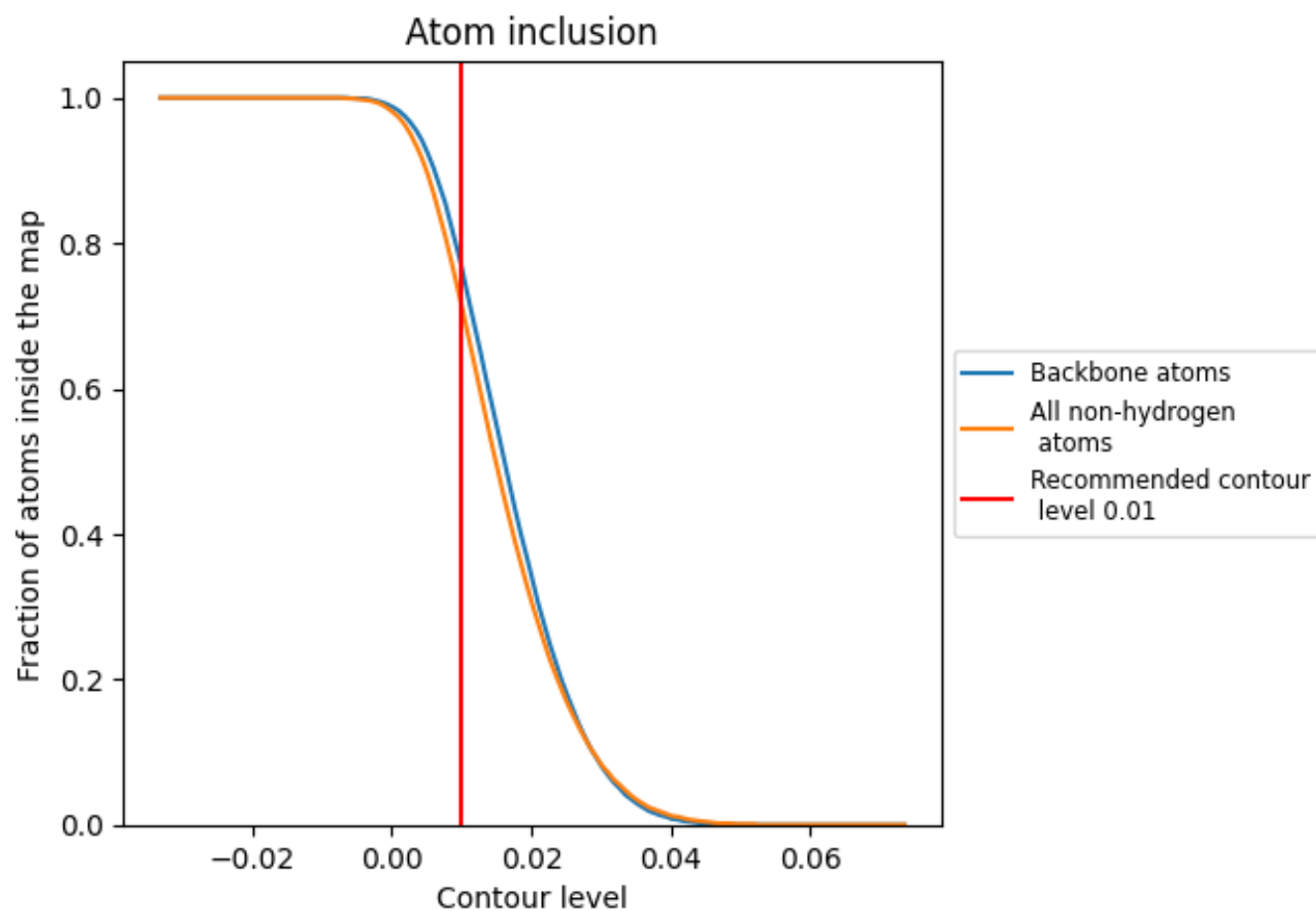
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 77% of all backbone atoms, 72% 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	 0.7170	 0.3470
2	 0.8340	 0.3850
A	 0.4780	 0.3010
B	 0.7010	 0.3830
C	 0.7520	 0.4010
D	 0.7350	 0.4140
E	 0.5390	 0.3070
F	 0.7570	 0.4050
G	 0.7130	 0.4020
H	 0.6630	 0.3060
I	 0.5280	 0.3110
J	 0.7360	 0.3800
K	 0.7500	 0.4070
L	 0.4300	 0.2220
M	 0.7250	 0.4160
N	 0.0670	 0.1230
O	 0.7530	 0.4120
P	 0.7490	 0.4060
Q	 0.5120	 0.2520
R	 0.7180	 0.3740
S	 0.4850	 0.2680
T	 0.5730	 0.3040
U	 0.7430	 0.3580
V	 0.4700	 0.2900
W	 0.7170	 0.3860
X	 0.7700	 0.4390
Y	 0.7490	 0.4370
Z	 0.7480	 0.3840
a	 0.6080	 0.3330
b	 0.7610	 0.4290
c	 0.6900	 0.3860
d	 0.6400	 0.3950
e	 0.6350	 0.3160
f	 0.4610	 0.2170
g	 0.0870	 0.1120



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Chain	Atom inclusion	Q-score
h	 0.4900	 0.2460
i	 0.6600	 0.2240
n	 0.6930	 0.3870
x	 0.5100	 0.2160
z	 0.7270	 0.2570