



Full wwPDB EM Validation Report ⓘ

Aug 11, 2026 – 09:08 am BST

PDB ID : 9TI9 / pdb_00009ti9
EMDB ID : EMD-55948
Title : Staphylococcus aureus 70S ribosome in complex with RRF, EF-G and fusidic acid (70S-RRF-EF-G-FA)
Authors : Gonzalez-Lopez, A.; Selmer, M.
Deposited on : 2025-12-05
Resolution : 3.06 Å (reported)
Based on initial models : ., 9GHG, 8P2G

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:

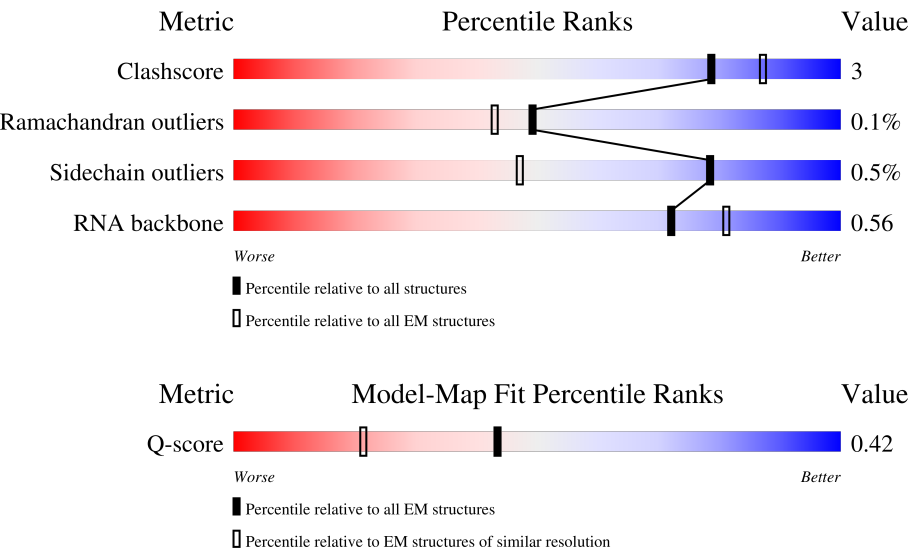
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.06 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	13976 (2.56 - 3.56)

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	1	62	
2	2	69	
3	3	59	

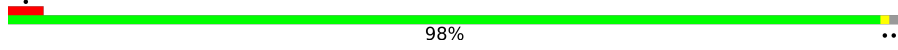
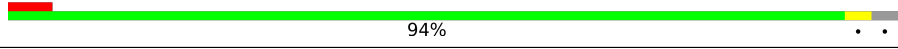
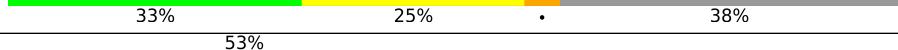
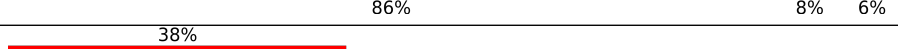
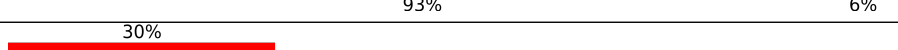
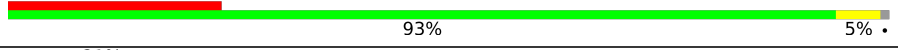
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Mol	Chain	Length	Quality of chain
4	4	84	
5	5	57	
6	6	49	
7	7	45	
8	8	66	
9	9	37	
10	A	2923	
11	B	115	
12	C	186	
13	D	93	
14	E	693	
15	G	277	
16	H	220	
17	I	207	
18	J	179	
19	K	178	
20	M	145	
21	N	122	
22	O	146	
23	P	144	
24	Q	122	
25	R	119	
26	S	116	
27	T	118	
28	U	102	

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Mol	Chain	Length	Quality of chain
29	V	117	
30	W	91	
31	X	105	
32	Y	217	
33	Z	94	
34	a	1555	
35	b	24	
36	c	255	
37	d	217	
38	e	200	
39	f	166	
40	g	98	
41	h	156	
42	i	132	
43	j	132	
44	k	102	
45	l	129	
46	m	137	
47	n	121	
48	o	61	
49	p	89	
50	q	91	
51	r	87	
52	s	80	
53	t	92	

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Mol	Chain	Length	Quality of chain
54	u	83	7% 93% 5%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147288 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	61	Total	C	N	O	S	0	0
			482	298	104	79	1		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	65	Total	C	N	O	S	0	0
			535	329	100	105	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	57	Total	C	N	O	0	0
			446	277	84	85		

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	59	Total	C	N	O	S	0	0
			485	310	76	96	3		

- Molecule 5 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	53	Total	C	N	O	S	0	0
			422	256	86	75	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	?	-	ARG	deletion	UNP Q2FZF1

- Molecule 6 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	48	Total	C	N	O	S	0	0
			402	245	79	73	5		

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	65	Total	C	N	O	S	0	0
			531	330	115	84	2		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2808	Total	C	N	O	P	0	0
			60220	26892	11024	19496	2808		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 12 is a protein called Ribosome-recycling factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	185	Total	C	N	O	S	0	0
			1433	874	257	297	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q2FZ21
C	-1	HIS	-	expression tag	UNP Q2FZ21

- Molecule 13 is a RNA chain called tRNA(Ser3).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	D	93	Total	C	N	O	P	S	0	0
			2000	893	365	648	92	2		

- Molecule 14 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	E	661	Total	C	N	O	S		0	0
			5114	3207	854	1025	28			

- Molecule 15 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	G	273	Total	C	N	O	S		0	0
			2085	1297	413	370	5			

- Molecule 16 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	H	215	Total	C	N	O	S		0	0
			1628	1018	299	306	5			

- Molecule 17 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	I	205	Total	C	N	O	S		0	0
			1569	983	287	297	2			

- Molecule 18 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	J	177	Total	C	N	O	S		0	0
			1403	891	242	263	7			

- Molecule 19 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	177	Total	C	N	O	S	0	0
			1382	858	253	268	3		

- Molecule 20 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	145	Total	C	N	O	S	0	0
			1151	717	211	220	3		

- Molecule 21 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 22 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	146	Total	C	N	O	S	0	0
			1099	680	215	203	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

- Molecule 25 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	119	Total	C	N	O	S	0	0
			922	574	174	173	1		

- Molecule 26 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	S	114	Total	C	N	O		
			922	580	185	157	0	0

- Molecule 27 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	T	117	Total	C	N	O	S	
			953	599	191	159	4	0

- Molecule 28 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	102	Total	C	N	O	S	
			799	506	142	150	1	0

- Molecule 29 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	V	111	Total	C	N	O	S	
			853	532	163	155	3	0

- Molecule 30 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	W	90	Total	C	N	O	S	
			734	461	132	137	4	0

- Molecule 31 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	X	102	Total	C	N	O	S	
			787	497	144	144	2	0

- Molecule 32 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	94	Total	C	N	O	S	
			738	471	131	134	2	0

- Molecule 33 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Z	76	Total	C	N	O	0	0
			585	361	114	110		

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1534	Total	C	N	O	P	0	0
			32869	14681	5998	10656	1534		

- Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	15	Total	C	N	O	P	0	0
			331	148	69	99	15		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	204	Total	C	N	O	S	0	0
			1609	1012	302	293	2		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	157	Total	C	N	O	S	0	0
			1169	735	214	218	2		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	94	Total	C	N	O	S	0	0
			781	494	137	147	3		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	146	Total	C	N	O	S	0	0
			1165	727	222	212	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	128	Total	C	N	O	S	0	0
			1017	629	203	184	1		

- Molecule 44 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	98	Total	C	N	O	S	0	0
			783	494	143	145	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	118	Total	C	N	O	S	0	0
			876	542	166	165	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	114	Total	C	N	O	S	0	0
			909	559	180	169	1		

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	60	Total	C	N	O	S	0	0
			502	317	100	80	5		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	86	Total	C	N	O	S	0	0
			721	445	148	127	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	81	Total	C	N	O	S	0	0
			671	424	121	125	1		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	64	Total	C	N	O	S	0	0
			525	335	97	90	3		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	83	Total	C	N	O	S	0	0
			672	432	122	116	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	81	Total	C	N	O	S	0	0
			611	370	120	119	2		

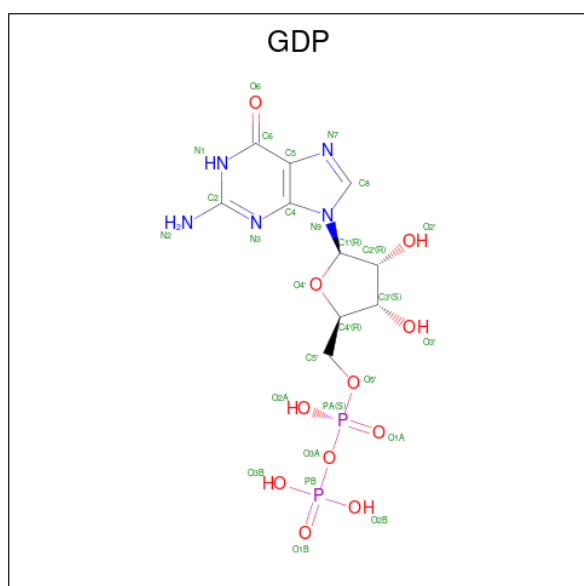
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	5	1	Total	Zn	0
			1	1	
55	9	1	Total	Zn	0
			1	1	
55	o	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

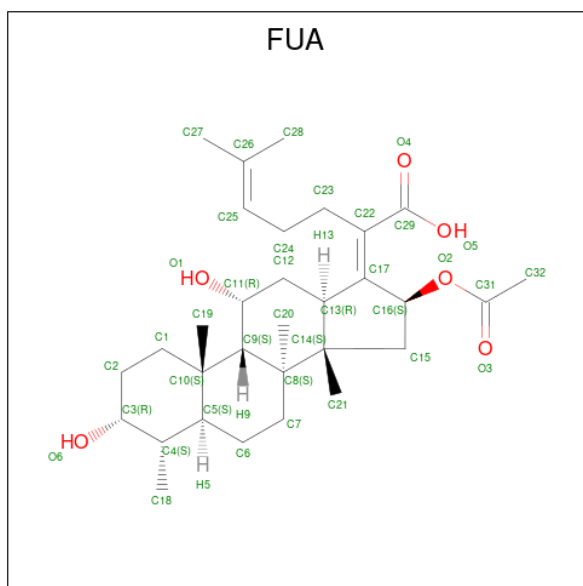
Mol	Chain	Residues	Atoms		AltConf
56	A	87	Total	Mg	0
			87	87	
56	E	1	Total	Mg	0
			1	1	
56	G	1	Total	Mg	0
			1	1	
56	H	1	Total	Mg	0
			1	1	

- Molecule 57 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
57	E	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 58 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by depositor).

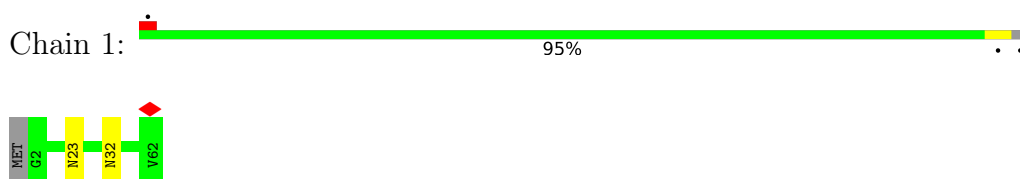


Mol	Chain	Residues	Atoms			AltConf
58	E	1	Total	C	O	0
			37	31	6	

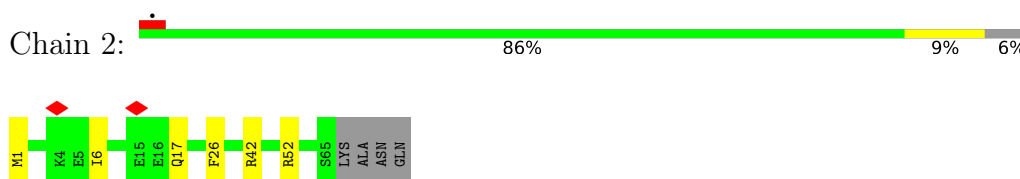
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

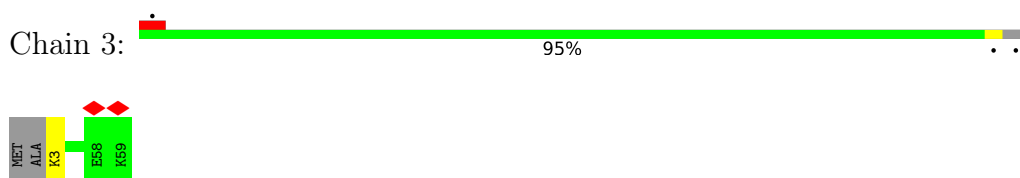
- Molecule 1: 50S ribosomal protein L28



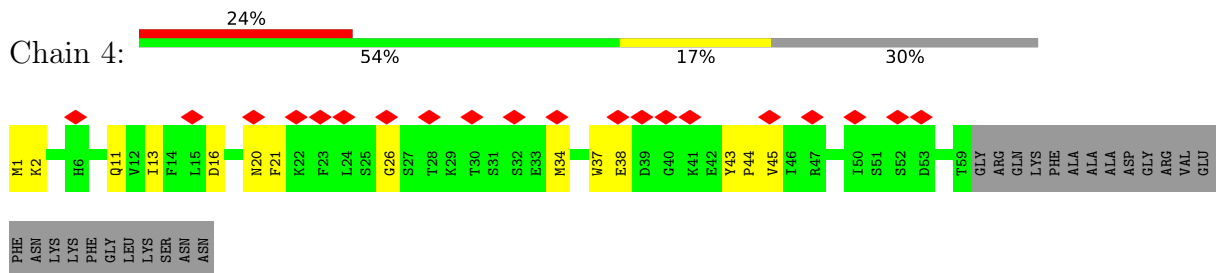
- Molecule 2: 50S ribosomal protein L29



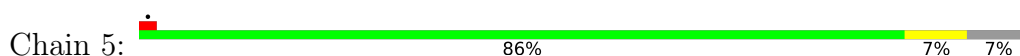
- Molecule 3: 50S ribosomal protein L30



- Molecule 4: 50S ribosomal protein L31 type B

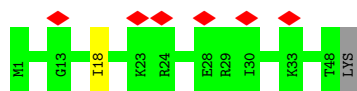


- Molecule 5: Large ribosomal subunit protein bL32





- Molecule 6: Large ribosomal subunit protein bL33A



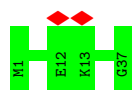
- Molecule 7: 50S ribosomal protein L34



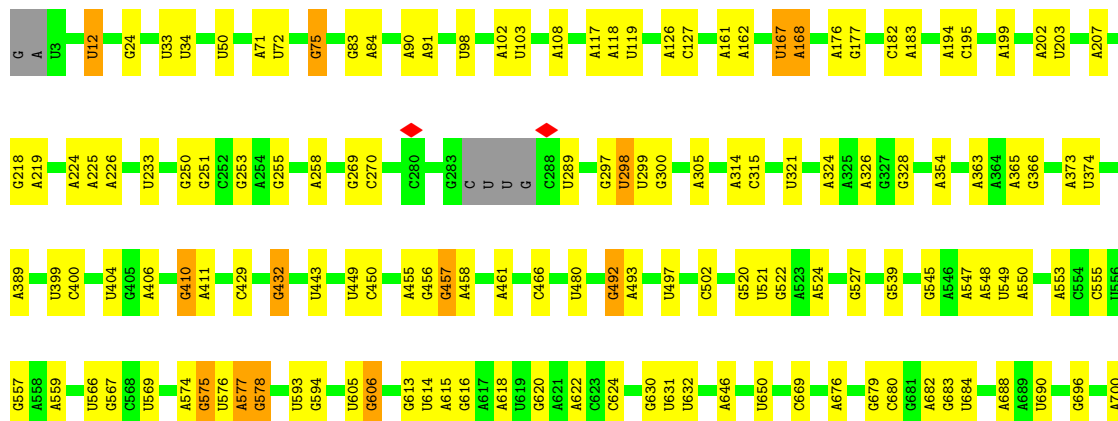
- Molecule 8: 50S ribosomal protein L35



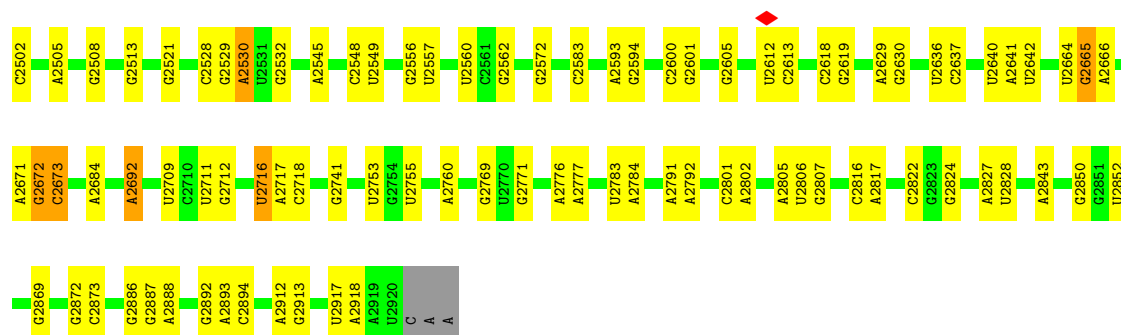
- Molecule 9: 50S ribosomal protein L36



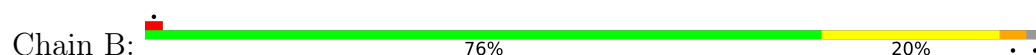
- Molecule 10: 23S rRNA



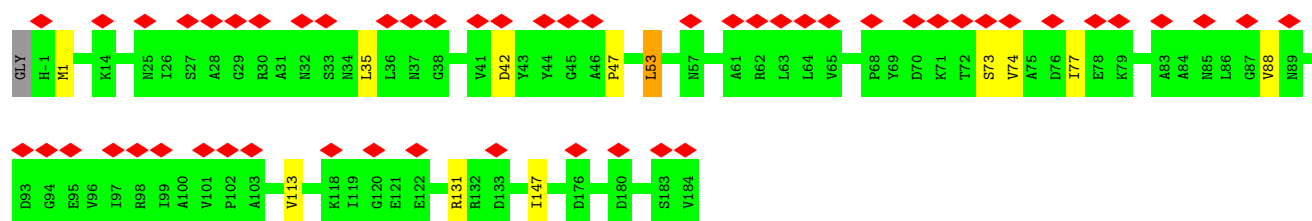




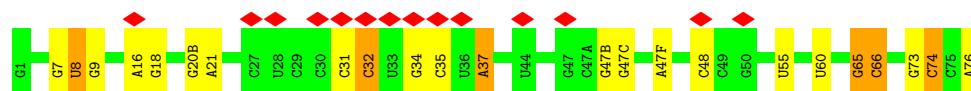
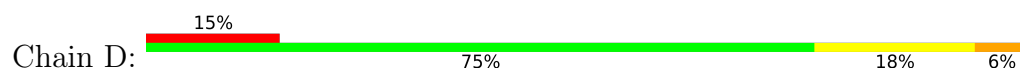
• Molecule 11: 5S rRNA



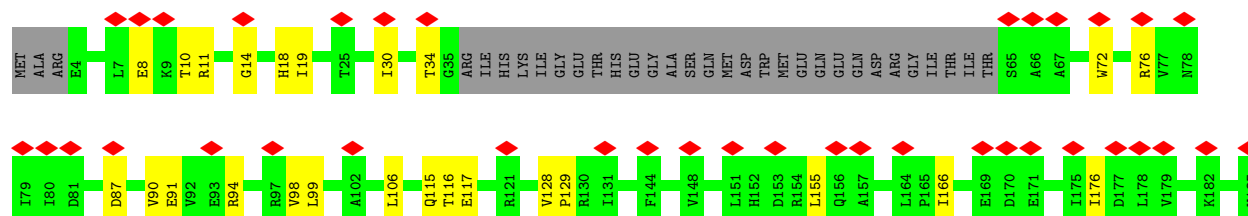
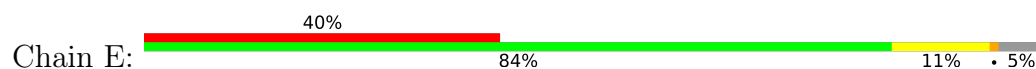
• Molecule 12: Ribosome-recycling factor

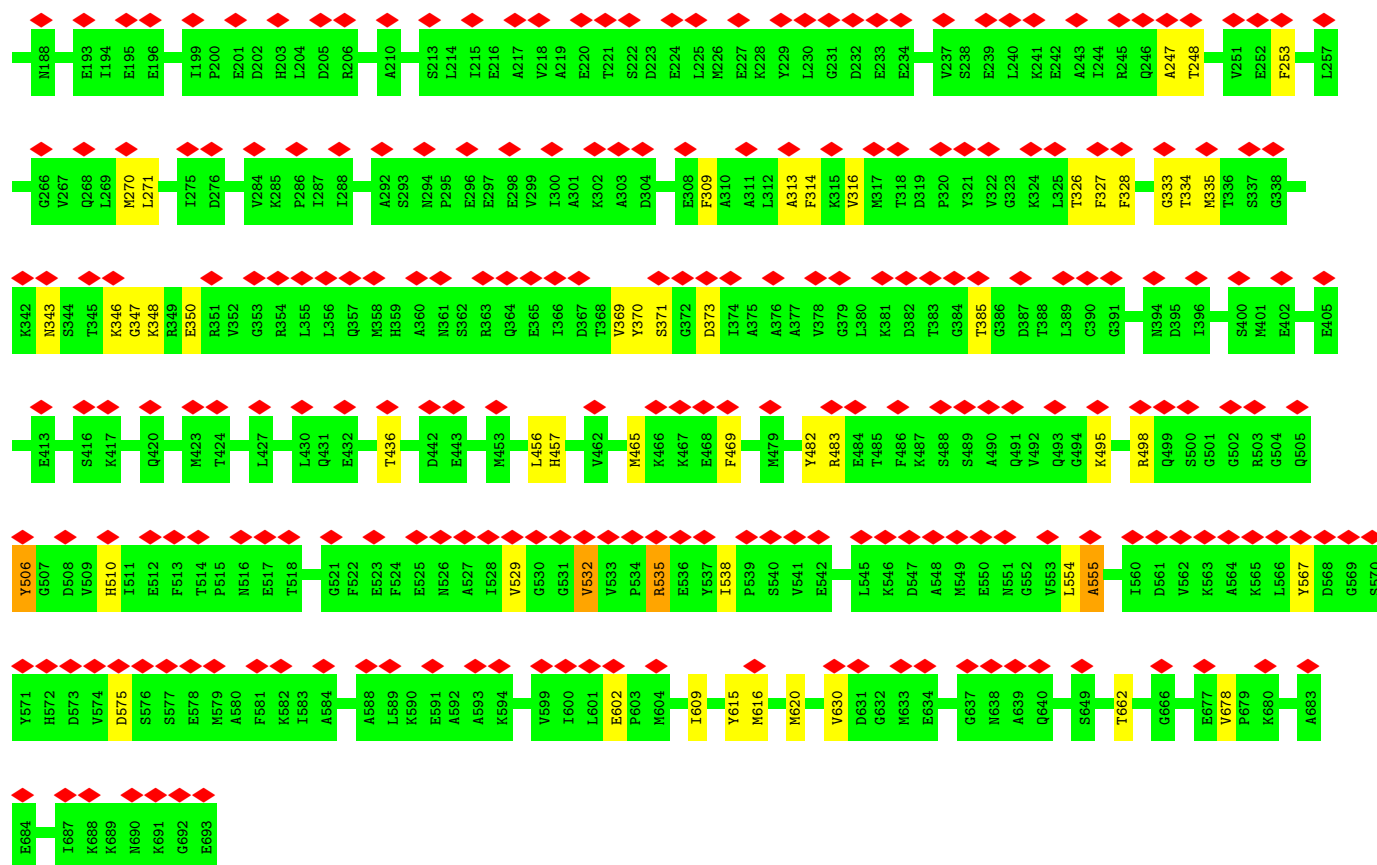


• Molecule 13: tRNA(Ser3)



• Molecule 14: Elongation factor G





- Molecule 15: 50S ribosomal protein L2

Chain G: 97%



- Molecule 16: 50S ribosomal protein L3

Chain H: 96%

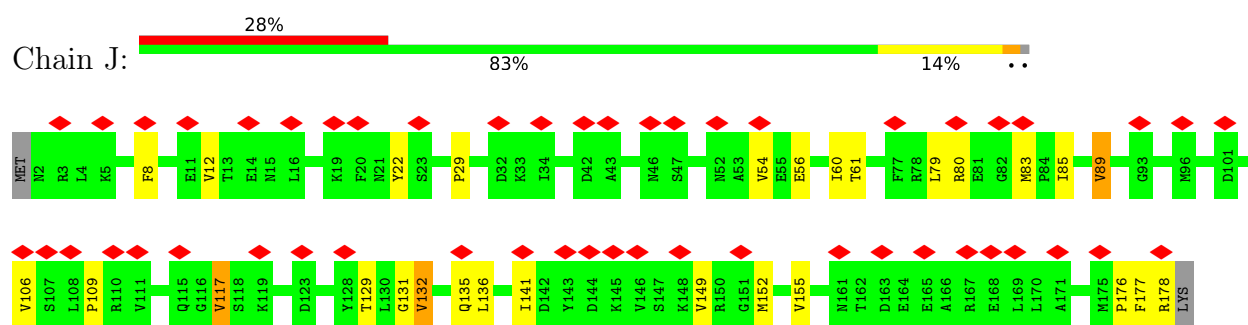


- Molecule 17: 50S ribosomal protein L4

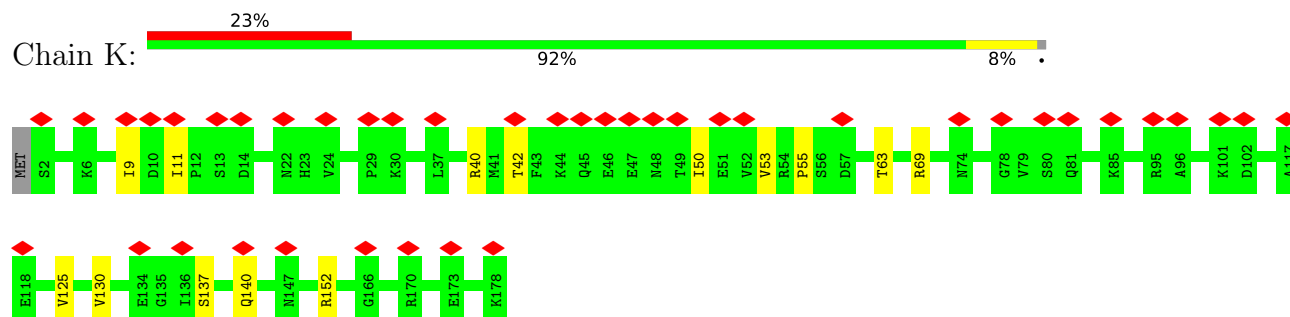
Chain I: 97%



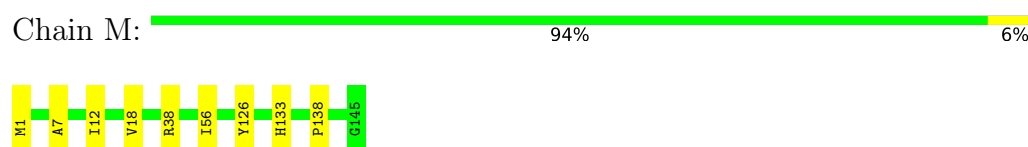
- Molecule 18: 50S ribosomal protein L5



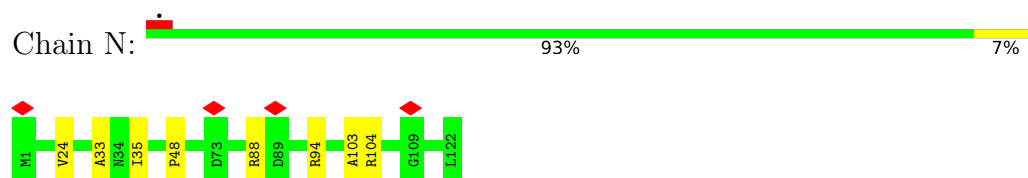
- Molecule 19: Large ribosomal subunit protein uL6



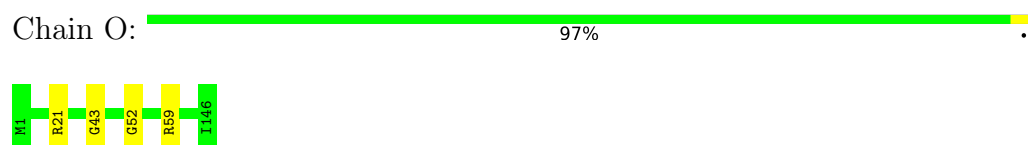
- Molecule 20: 50S ribosomal protein L13



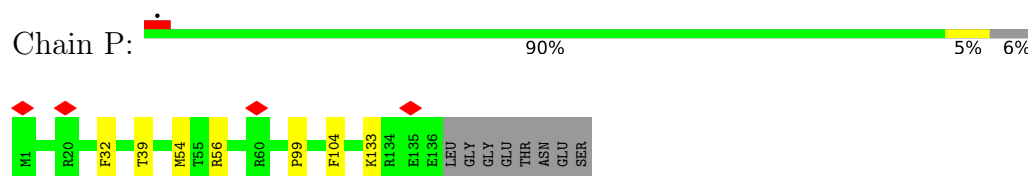
- Molecule 21: 50S ribosomal protein L14



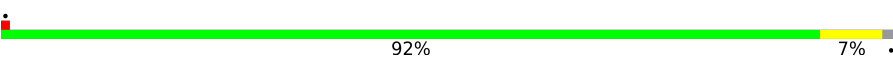
- Molecule 22: 50S ribosomal protein L15



- Molecule 23: 50S ribosomal protein L16

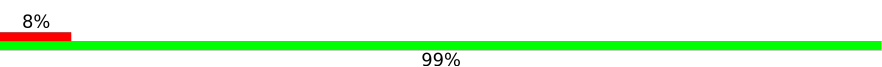


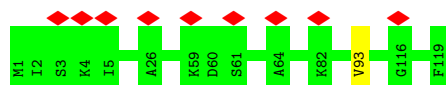
- Molecule 24: 50S ribosomal protein L17

Chain Q:  92% 7%

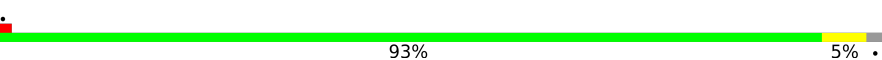


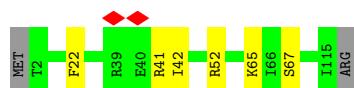
- Molecule 25: 50S ribosomal protein L18

Chain R:  8% 99%

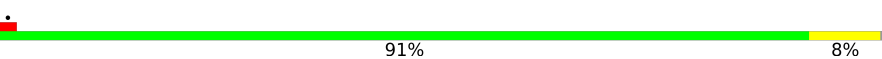


- Molecule 26: 50S ribosomal protein L19

Chain S:  93% 5%

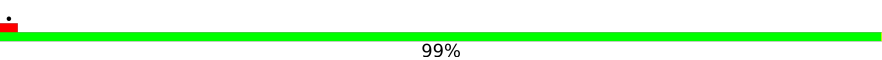


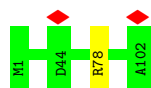
- Molecule 27: 50S ribosomal protein L20

Chain T:  91% 8%



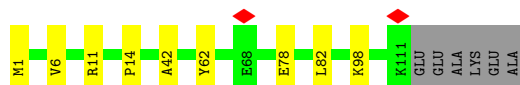
- Molecule 28: 50S ribosomal protein L21

Chain U:  99%

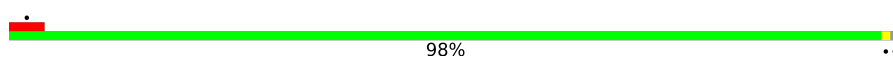


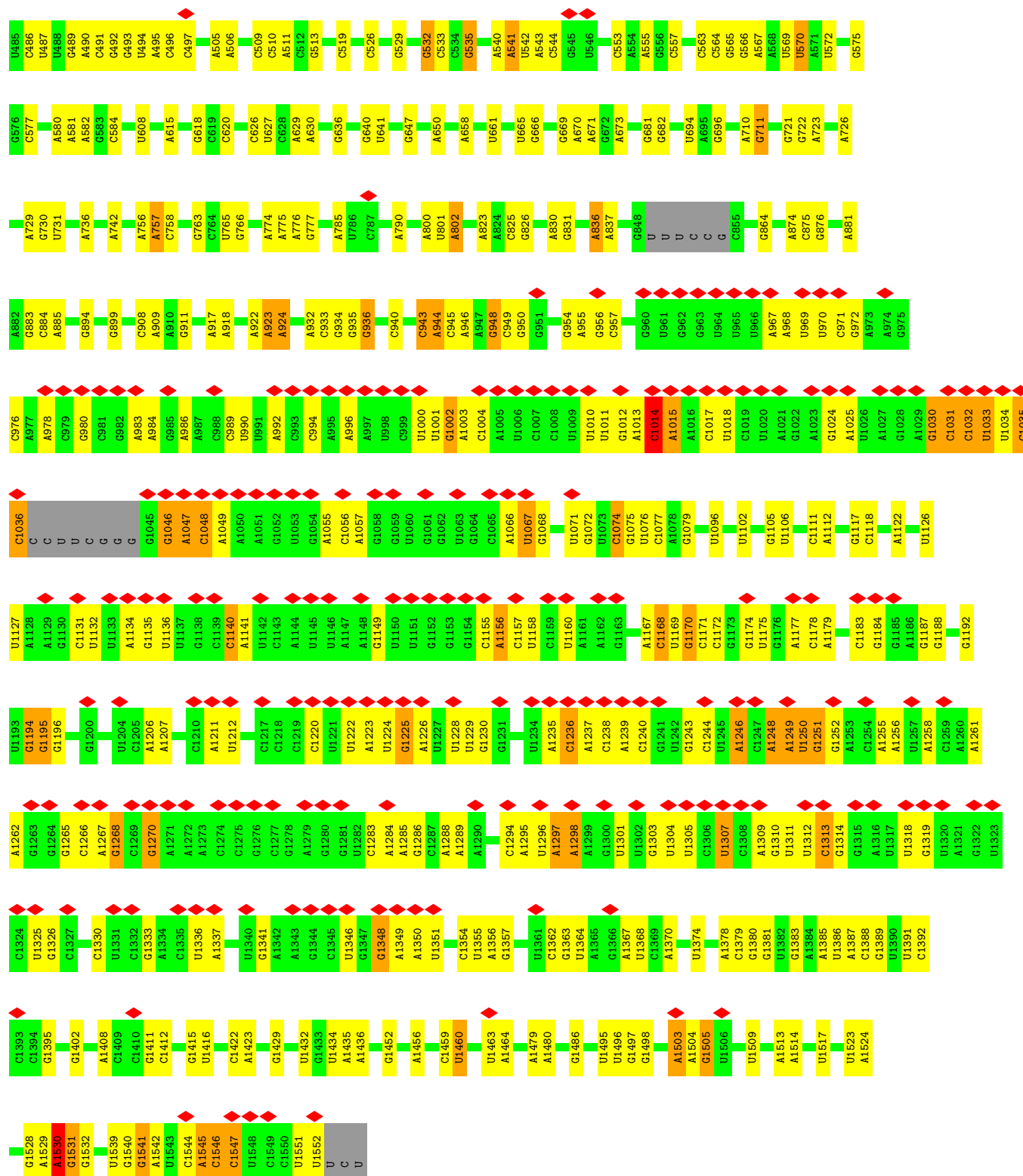
- Molecule 29: 50S ribosomal protein L22

Chain V:  87% 8% 5%

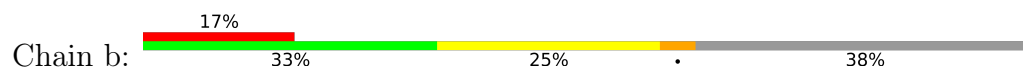


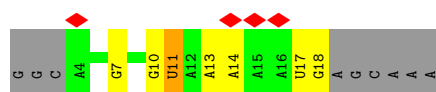
- Molecule 30: 50S ribosomal protein L23

Chain W:  98%

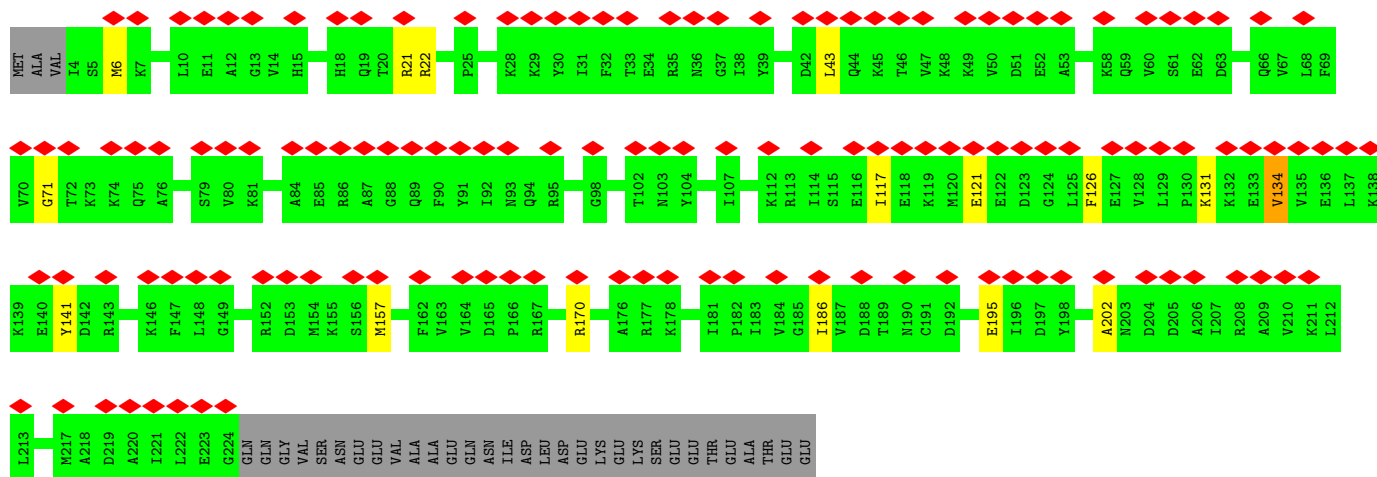
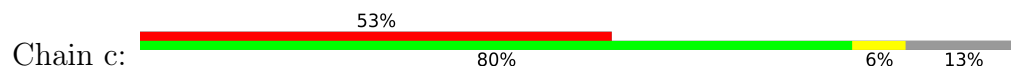


• Molecule 35: mRNA

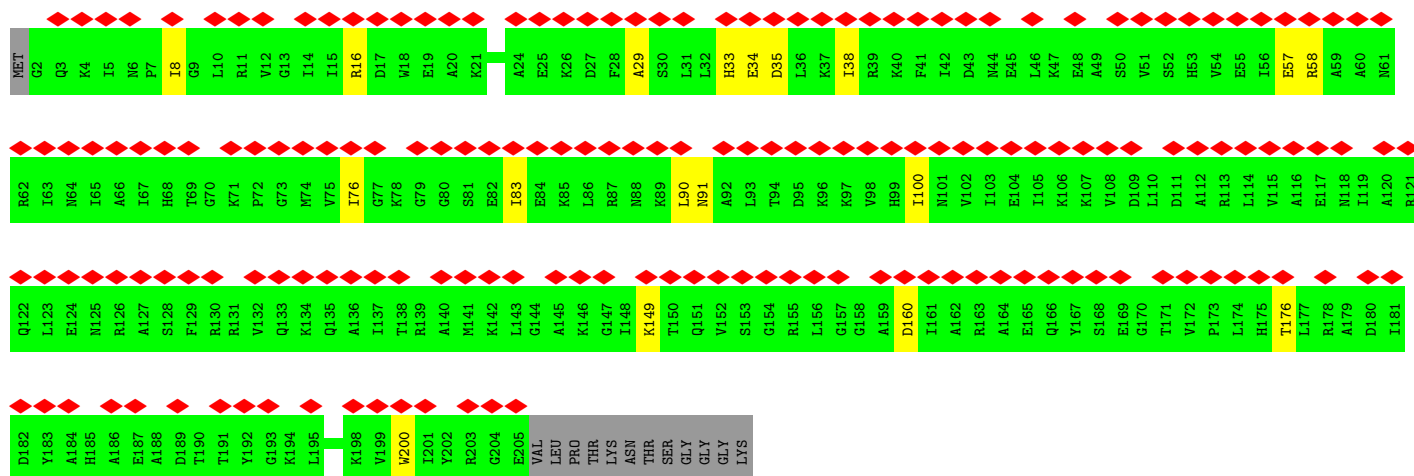
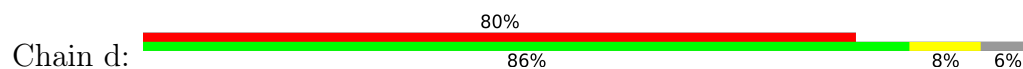




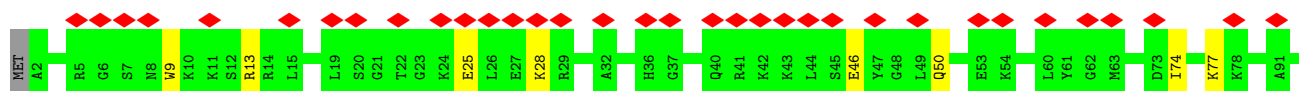
• Molecule 36: 30S ribosomal protein S2



• Molecule 37: 30S ribosomal protein S3

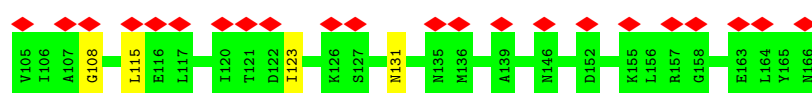
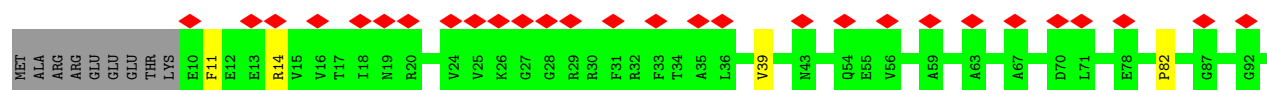
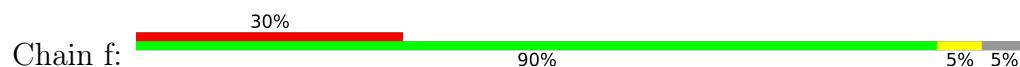


• Molecule 38: 30S ribosomal protein S4

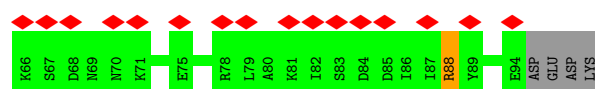
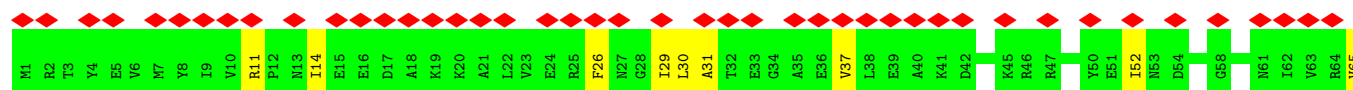
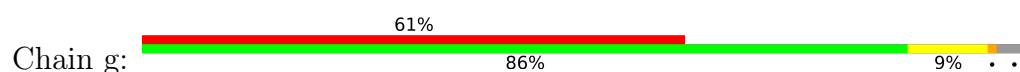




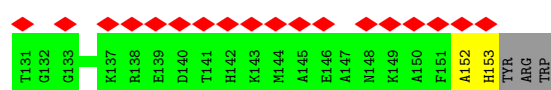
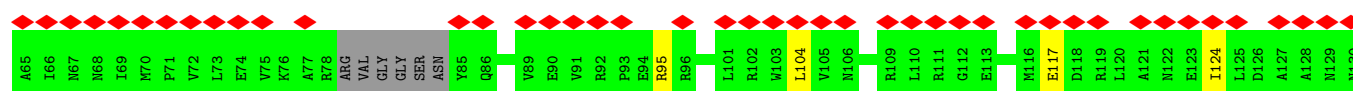
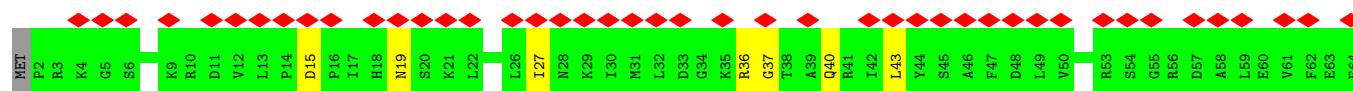
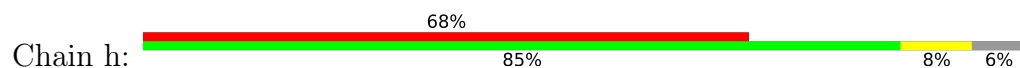
• Molecule 39: 30S ribosomal protein S5



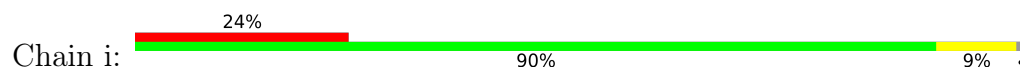
• Molecule 40: 30S ribosomal protein S6

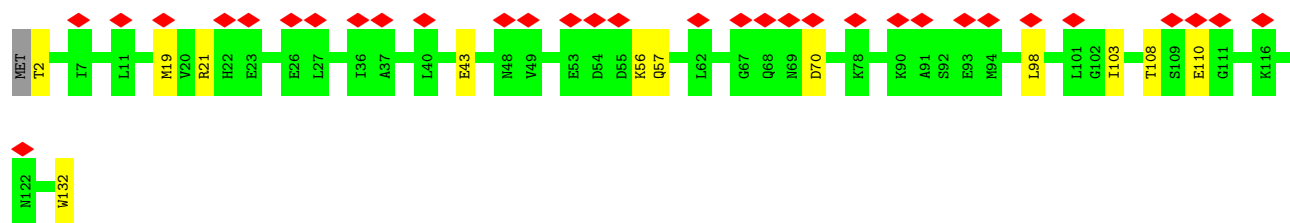


• Molecule 41: 30S ribosomal protein S7

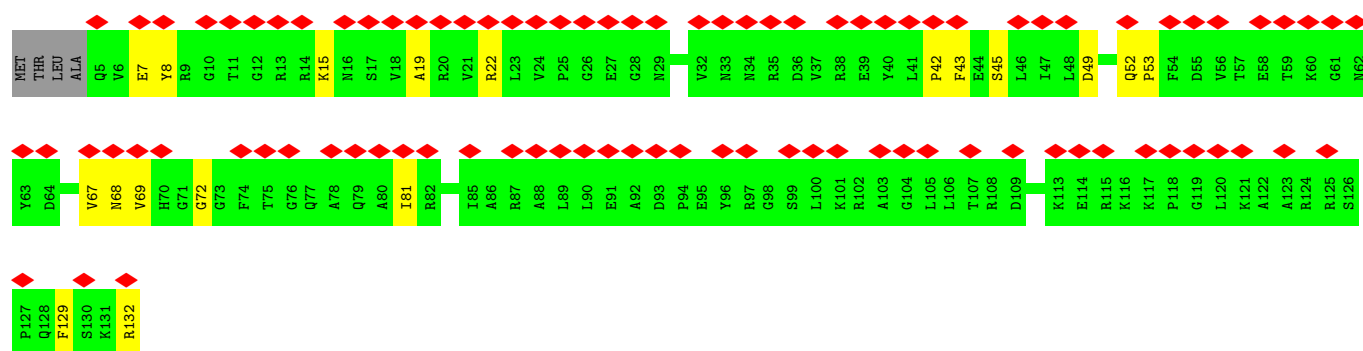
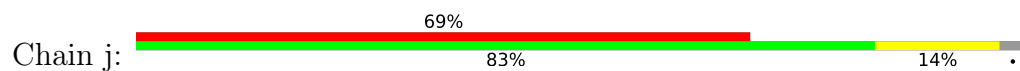


• Molecule 42: 30S ribosomal protein S8

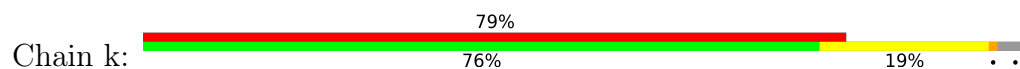




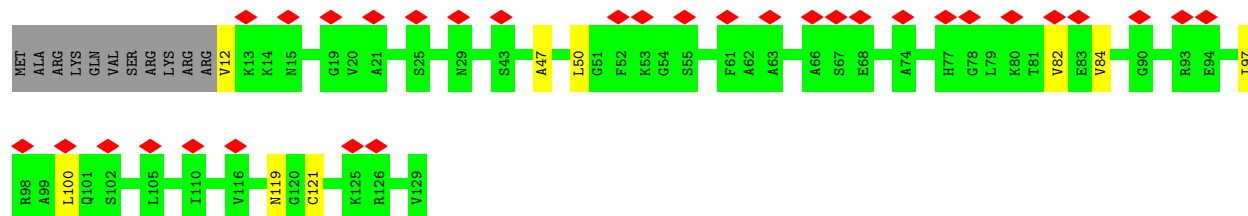
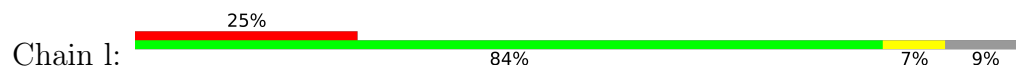
- Molecule 43: 30S ribosomal protein S9



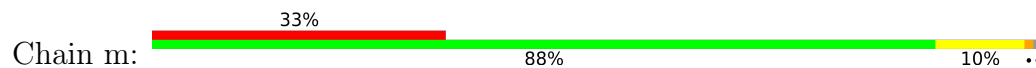
- Molecule 44: Small ribosomal subunit protein uS10

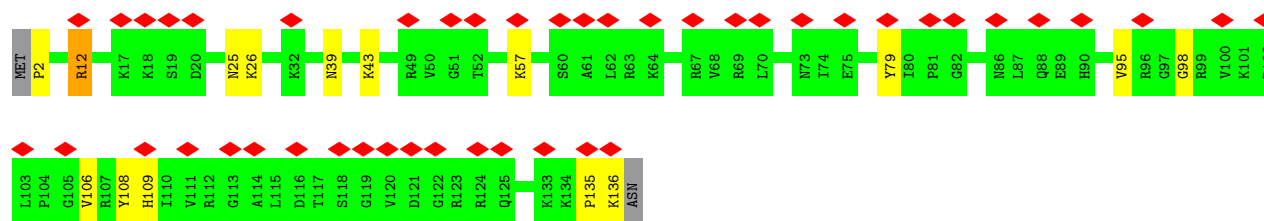


- Molecule 45: 30S ribosomal protein S11

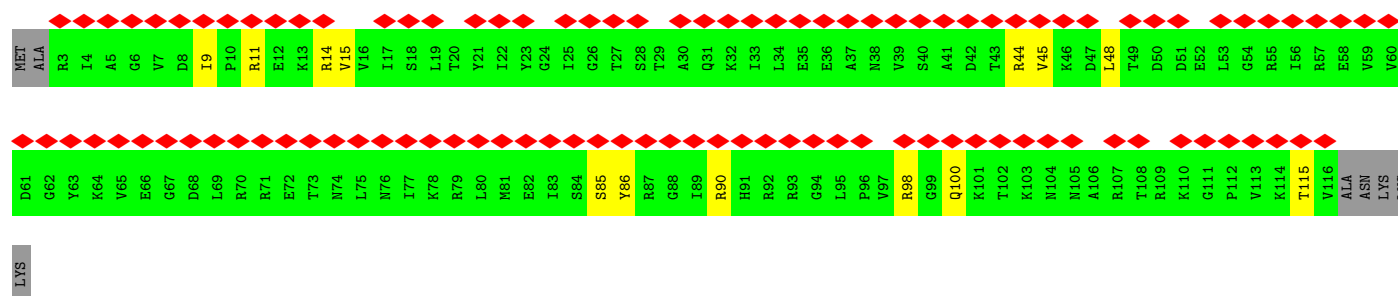
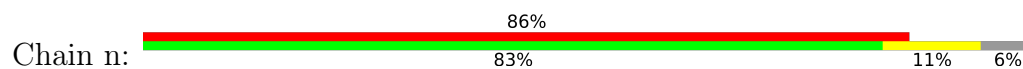


- Molecule 46: 30S ribosomal protein S12

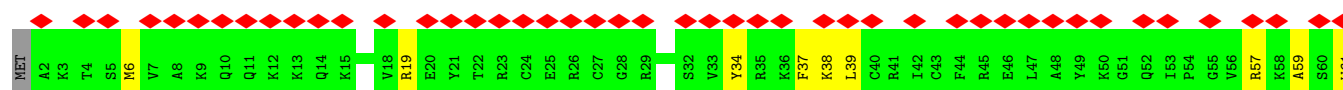
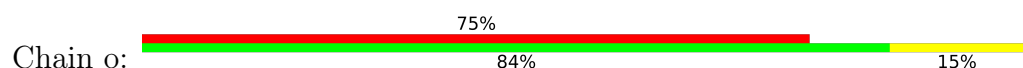




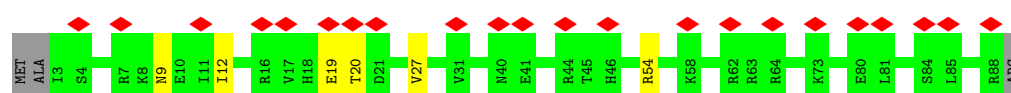
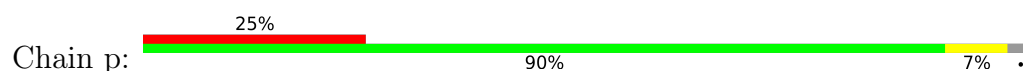
• Molecule 47: 30S ribosomal protein S13



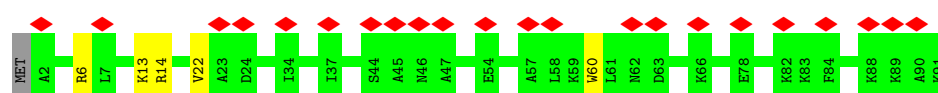
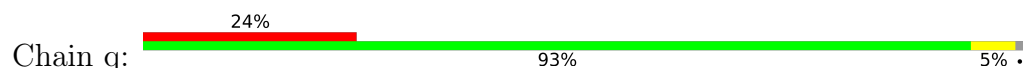
• Molecule 48: 30S ribosomal protein S14 type Z



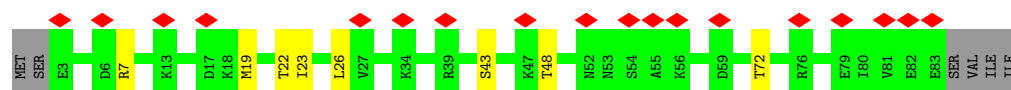
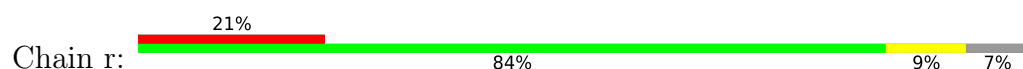
• Molecule 49: 30S ribosomal protein S15



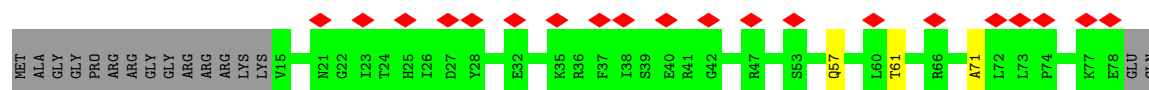
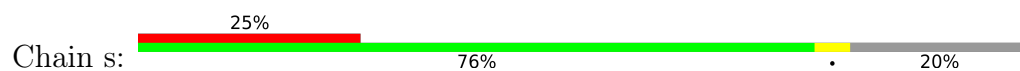
• Molecule 50: 30S ribosomal protein S16



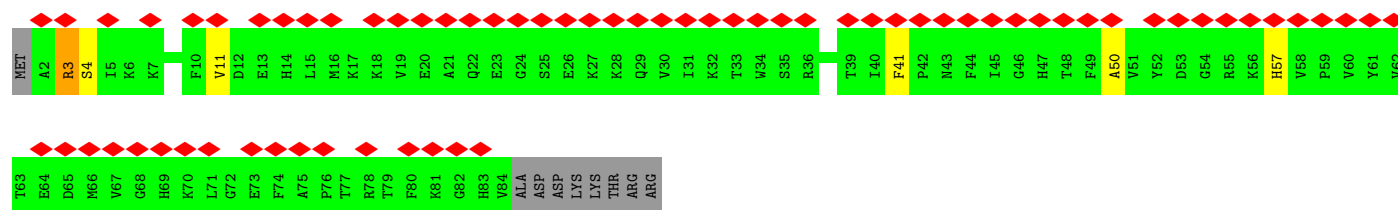
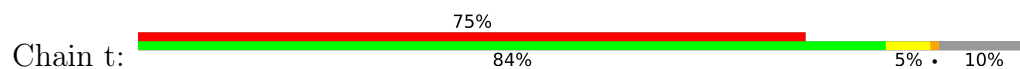
• Molecule 51: 30S ribosomal protein S17



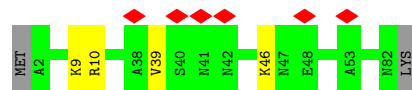
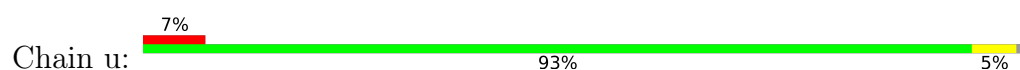
• Molecule 52: 30S ribosomal protein S18



• Molecule 53: 30S ribosomal protein S19



• Molecule 54: 30S ribosomal protein S20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9322	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	22.579	Depositor
Minimum map value	-13.091	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.970	Depositor
Recommended contour level	2.5	Depositor
Map size ($\text{\AA}$)	403.19998, 403.19998, 403.19998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.672, 0.672, 0.672	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, 5MC, UR3, RSP, FUA, PSU, OMG, 2MA, MG, T6A, GDP, 4SU, 4OC, MA6, 5MU, 3TD, 2MG, G7M, 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	1	0.48	0/488	0.84	0/649
2	2	0.44	0/536	1.06	0/713
3	3	0.48	0/448	0.94	0/601
4	4	0.51	0/499	0.93	0/674
5	5	0.51	0/429	0.87	0/571
6	6	0.47	0/407	0.86	0/545
7	7	0.50	0/377	0.97	0/491
8	8	0.49	0/536	0.91	0/701
9	9	0.52	0/300	0.85	0/393
10	A	0.53	1/67216 (0.0%)	0.80	10/104821 (0.0%)
11	B	0.56	0/2692	0.75	0/4193
12	C	0.49	0/1442	1.05	0/1940
13	D	0.58	1/2088 (0.0%)	0.79	0/3255
14	E	0.49	0/5204	0.96	1/7037 (0.0%)
15	G	0.51	0/2120	0.88	0/2847
16	H	0.49	0/1652	0.89	0/2216
17	I	0.49	0/1592	0.94	0/2148
18	J	0.47	0/1421	0.97	0/1907
19	K	0.50	0/1400	0.93	0/1881
20	M	0.48	0/1173	0.89	0/1578
21	N	0.48	0/927	0.91	0/1243
22	O	0.50	0/1113	0.90	0/1482
23	P	0.49	0/1113	0.89	0/1493
24	Q	0.46	0/956	0.94	0/1277
25	R	0.49	0/931	0.97	0/1244
26	S	0.50	0/934	0.88	0/1249
27	T	0.46	0/965	1.01	0/1276
28	U	0.48	0/809	0.82	0/1080
29	V	0.50	0/861	0.91	0/1159
30	W	0.47	0/742	0.91	0/989
31	X	0.50	0/796	0.90	0/1063

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.48	0/746	0.90	0/1000
33	Z	0.49	0/591	0.90	0/785
34	a	0.56	2/36619 (0.0%)	0.78	1/57097 (0.0%)
35	b	0.57	0/373	0.79	0/581
36	c	0.48	0/1808	1.01	0/2426
37	d	0.49	0/1631	0.95	0/2190
38	e	0.48	0/1647	0.96	0/2211
39	f	0.51	0/1183	0.94	0/1595
40	g	0.46	0/792	0.94	0/1062
41	h	0.51	0/1181	1.03	0/1587
42	i	0.49	0/1044	0.93	0/1401
43	j	0.52	0/1033	0.95	0/1386
44	k	0.53	0/795	0.97	0/1071
45	l	0.54	0/891	0.93	0/1203
46	m	0.52	0/1075	0.89	0/1439
47	n	0.49	0/916	1.07	0/1228
48	o	0.48	0/512	0.94	0/678
49	p	0.47	0/730	1.06	0/975
50	q	0.51	0/723	0.95	0/971
51	r	0.48	0/679	0.91	0/907
52	s	0.48	0/534	0.96	0/716
53	t	0.51	0/690	0.94	0/926
54	u	0.47	0/611	1.10	0/817
All	All	0.53	4/158971 (0.0%)	0.84	12/236968 (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
2	2	0	1
5	5	0	1
14	E	0	1
15	G	0	1
19	K	0	1
21	N	0	1
31	X	0	1
38	e	0	1
39	f	0	1
40	g	0	1
43	j	0	1

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
44	k	0	2
46	m	0	2
51	r	0	1
All	All	0	16

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	37	T6A	O3'-P	5.08	1.61	1.56
34	a	535	G7M	O3'-P	5.05	1.61	1.56
34	a	1509	UR3	O3'-P	5.03	1.61	1.56
10	A	2601	G7M	O3'-P	5.02	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1812	A	O3'-P-O5'	-6.39	94.41	104.00
10	A	863	G	O3'-P-O5'	-6.37	94.45	104.00
10	A	207	A	O3'-P-O5'	-6.16	94.76	104.00
10	A	2087	A	O3'-P-O5'	-5.69	95.47	104.00
10	A	2673	C	O3'-P-O5'	-5.67	95.50	104.00
34	a	1014	C	C2'-C3'-O3'	5.38	117.57	109.50
10	A	1962	G	O3'-P-O5'	-5.34	96.00	104.00
10	A	1017	A	O3'-P-O5'	-5.32	96.03	104.00
10	A	1224	U	O3'-P-O5'	-5.29	96.06	104.00
14	E	128	VAL	N-CA-CB	5.17	114.89	110.08
10	A	806	A	O3'-P-O5'	-5.09	96.36	104.00
10	A	826	A	O3'-P-O5'	-5.06	96.42	104.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	52	ARG	Sidechain
5	5	6	ARG	Sidechain
14	E	535	ARG	Sidechain
15	G	177	ARG	Sidechain
19	K	152	ARG	Sidechain
21	N	104	ARG	Sidechain
31	X	92	ARG	Sidechain
38	e	105	ARG	Sidechain

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Mol	Chain	Res	Type	Group
39	f	14	ARG	Sidechain
40	g	88	ARG	Sidechain
43	j	132	ARG	Sidechain
44	k	62	ARG	Sidechain
44	k	7	ARG	Sidechain
46	m	12	ARG	Sidechain
46	m	57	LYS	Peptide
51	r	7	ARG	Sidechain

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	1	482	0	523	2	0
2	2	535	0	566	3	0
3	3	446	0	486	0	0
4	4	485	0	458	8	0
5	5	422	0	426	2	0
6	6	402	0	413	1	0
7	7	373	0	420	0	0
8	8	531	0	599	2	0
9	9	297	0	339	0	0
10	A	60220	0	30287	212	0
11	B	2408	0	1218	10	0
12	C	1433	0	1464	7	0
13	D	2000	0	1020	10	0
14	E	5114	0	5010	46	0
15	G	2085	0	2192	3	0
16	H	1628	0	1667	3	0
17	I	1569	0	1614	2	0
18	J	1403	0	1457	16	0
19	K	1382	0	1415	7	0
20	M	1151	0	1145	6	0
21	N	920	0	981	4	0
22	O	1099	0	1142	4	0
23	P	1089	0	1155	4	0
24	Q	952	0	999	5	0
25	R	922	0	968	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	S	922	0	994	2	0
27	T	953	0	1027	6	0
28	U	799	0	836	1	0
29	V	853	0	914	6	0
30	W	734	0	767	1	0
31	X	787	0	853	1	0
32	Y	738	0	787	5	0
33	Z	585	0	597	1	0
34	a	32869	0	16564	232	0
35	b	331	0	164	2	0
36	c	1781	0	1844	8	0
37	d	1609	0	1668	12	0
38	e	1617	0	1646	10	0
39	f	1169	0	1229	4	0
40	g	781	0	784	6	0
41	h	1165	0	1204	7	0
42	i	1032	0	1082	7	0
43	j	1017	0	1039	13	0
44	k	783	0	825	15	0
45	l	876	0	895	5	0
46	m	1058	0	1130	8	0
47	n	909	0	959	9	0
48	o	502	0	523	11	0
49	p	721	0	751	3	0
50	q	712	0	744	5	0
51	r	671	0	708	4	0
52	s	525	0	554	2	0
53	t	672	0	677	3	0
54	u	611	0	655	3	0
55	5	1	0	0	0	0
55	9	1	0	0	0	0
55	o	1	0	0	0	0
56	A	87	0	0	0	0
56	E	1	0	0	0	0
56	G	1	0	0	0	0
56	H	1	0	0	0	0
57	E	28	0	12	0	0
58	E	37	0	47	4	0
All	All	147288	0	100443	657	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (657) 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)
34:a:26:C:H5'	34:a:532:G:H1'	1.62	0.82
32:Y:7:ILE:HD11	32:Y:65:VAL:HA	1.68	0.76
10:A:1968:C:O2	12:C:131:ARG:NH2	2.20	0.75
34:a:1246:A:H4'	34:a:1314:G:H4'	1.70	0.73
18:J:61:THR:HG21	18:J:89:VAL:HG21	1.72	0.72
34:a:777:G:H4'	34:a:1524:A:H4'	1.71	0.70
14:E:106:LEU:HD21	14:E:116:THR:HG21	1.75	0.69
10:A:1111:A:H1'	14:E:630:VAL:O	1.92	0.68
43:j:8:TYR:O	43:j:22:ARG:HA	1.94	0.67
10:A:1953:U:H4'	10:A:1954:A:OP1	1.95	0.66
10:A:2332:U:H5''	18:J:131:GLY:HA3	1.78	0.66
44:k:34:ALA:HB2	44:k:83:THR:HG21	1.80	0.64
40:g:30:LEU:HB3	40:g:65:VAL:HG11	1.80	0.63
11:B:31:G:N2	11:B:33:U:O4	2.30	0.63
4:4:16:ASP:HB3	4:4:21:PHE:HB3	1.80	0.63
21:N:48:PRO:HB3	34:a:1432:U:H5'	1.80	0.63
18:J:135:GLN:HG2	18:J:141:ILE:HG21	1.81	0.62
34:a:831:G:HO2'	42:i:2:THR:N	1.97	0.62
43:j:67:VAL:HG11	43:j:81:ILE:HG12	1.82	0.62
34:a:1261:A:H1'	34:a:1379:C:O2'	2.00	0.61
37:d:57:GLU:HB3	44:k:94:SER:HB2	1.81	0.61
21:N:88:ARG:HG2	21:N:94:ARG:HD2	1.83	0.61
12:C:42:ASP:HA	12:C:47:PRO:HA	1.83	0.61
10:A:195:C:O2'	10:A:847:A:N3	2.33	0.60
34:a:411:C:H5''	38:e:129:PRO:HD2	1.83	0.60
34:a:1378:A:OP1	44:k:64:GLN:NE2	2.34	0.60
37:d:57:GLU:HB3	44:k:94:SER:CB	2.32	0.59
10:A:923:A:H1'	10:A:924:G:O5'	2.03	0.59
14:E:34:THR:HG22	14:E:72:TRP:HB2	1.84	0.59
34:a:1318:U:H2'	34:a:1319:G:C8	2.38	0.59
34:a:1298:A:N1	34:a:1381:G:H1'	2.18	0.59
14:E:620:MET:HG2	14:E:630:VAL:HG21	1.85	0.58
34:a:151:A:H3'	34:a:152:A:H8	1.67	0.58
10:A:2041:A:H2'	10:A:2042:A:C8	2.39	0.58
12:C:1:MET:HE2	12:C:1:MET:HA	1.86	0.58
34:a:240:A:O2'	34:a:270:A:N6	2.37	0.57
10:A:1238:U:H1'	27:T:4:VAL:HG22	1.87	0.57
10:A:963:A:H5''	11:B:94:C:O2'	2.04	0.57
10:A:1996:A:O2'	10:A:1999:G:N3	2.36	0.57
10:A:2405:A:H1'	25:R:93:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:955:A:H2'	10:A:956:A:C8	2.40	0.57
10:A:877:G:N3	22:O:52:GLY:HA3	2.20	0.57
34:a:1530:MA6:H3'	34:a:1531:G:O4'	2.05	0.57
10:A:33:U:O4	10:A:492:G:O2'	2.22	0.56
34:a:1014:C:O2'	34:a:1015:A:N3	2.38	0.56
46:m:135:PRO:O	46:m:136:LYS:C	2.48	0.56
10:A:1675:G:H1'	10:A:1679:A:N6	2.20	0.56
10:A:1571:G:H22	10:A:1593:G:H1	1.53	0.56
10:A:1764:A:H2'	10:A:1765:A:O4'	2.05	0.56
37:d:34:GLU:O	37:d:38:ILE:HG12	2.05	0.56
24:Q:26:ILE:HD11	24:Q:69:VAL:HG21	1.88	0.56
34:a:955:A:H2'	34:a:956:G:C8	2.40	0.56
34:a:1025:A:H4'	34:a:1228:U:H4'	1.86	0.56
34:a:1071:U:H2'	34:a:1072:G:H8	1.70	0.56
46:m:26:LYS:O	46:m:43:LYS:NZ	2.37	0.56
52:s:57:GLN:O	52:s:61:THR:HG23	2.06	0.56
10:A:2717:A:C6	24:Q:3:TYR:HB2	2.41	0.56
34:a:665:U:H3	34:a:757:A:H62	1.54	0.55
10:A:1880:A:H2'	10:A:1881:A:C8	2.41	0.55
10:A:1941:C:H2'	10:A:1942:3TD:H6	1.89	0.55
14:E:117:GLU:HA	14:E:155:LEU:HD21	1.87	0.55
34:a:1074:C:H2'	34:a:1075:G:C8	2.41	0.55
34:a:1415:G:H4'	34:a:1530:MA6:H4'	1.87	0.55
34:a:491:C:O2'	50:q:14:ARG:NH2	2.39	0.55
44:k:10:LEU:HB3	44:k:18:ILE:HD11	1.88	0.55
10:A:688:A:N1	10:A:2396:A:O2'	2.34	0.55
20:M:7:ALA:HB1	20:M:12:ILE:HD11	1.87	0.55
44:k:46:LYS:HD2	44:k:66:GLU:HB2	1.88	0.55
34:a:944:A:H2'	34:a:945:C:O4'	2.07	0.55
34:a:1031:C:H3'	34:a:1032:C:H2'	1.88	0.55
34:a:1251:G:H2'	34:a:1252:G:C8	2.42	0.55
47:n:86:TYR:CZ	47:n:90:ARG:HD2	2.42	0.55
10:A:2548:C:C2	10:A:2572:G:N2	2.75	0.55
34:a:765:U:H2'	34:a:766:G:O4'	2.07	0.54
32:Y:7:ILE:HG22	32:Y:43:VAL:HB	1.88	0.54
34:a:1297:A:H2'	34:a:1298:A:C8	2.43	0.54
53:t:50:ALA:HB1	53:t:57:HIS:HB3	1.88	0.54
10:A:622:A:O2'	10:A:2046:U:OP1	2.24	0.54
34:a:563:C:H2'	34:a:564:C:C6	2.43	0.54
34:a:1318:U:H2'	34:a:1319:G:H8	1.73	0.54
34:a:757:A:H2'	34:a:758:C:O4'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:954:G:H2'	34:a:954:G:N3	2.22	0.54
10:A:852:U:O2'	10:A:2087:A:N1	2.40	0.54
20:M:18:VAL:HG23	20:M:138:PRO:HB2	1.90	0.54
14:E:14:GLY:HA3	14:E:99:LEU:HD13	1.90	0.54
34:a:57:U:H2'	34:a:58:G:C8	2.43	0.54
34:a:681:G:O3'	40:g:88:ARG:NH2	2.41	0.53
10:A:945:A:H2'	10:A:946:A:O4'	2.08	0.53
42:i:108:THR:HG22	42:i:110:GLU:H	1.73	0.53
32:Y:73:MET:HB2	32:Y:94:ILE:HD11	1.90	0.53
34:a:756:A:H1'	34:a:757:A:H2	1.73	0.53
34:a:756:A:H1'	34:a:757:A:C2	2.44	0.53
34:a:1357:G:N7	43:j:15:LYS:HE2	2.23	0.53
41:h:152:ALA:O	41:h:153:HIS:C	2.51	0.53
34:a:775:A:H2'	34:a:776:A:O4'	2.08	0.53
10:A:522:G:H4'	10:A:547:A:N1	2.23	0.53
18:J:8:PHE:HA	18:J:12:VAL:HB	1.89	0.53
19:K:11:ILE:HD11	19:K:50:ILE:HG13	1.91	0.53
34:a:989:C:H1'	48:o:19:ARG:HG3	1.91	0.53
34:a:1229:U:OP1	48:o:19:ARG:NH1	2.42	0.53
34:a:160:A:H2'	34:a:161:A:O4'	2.09	0.53
34:a:1194:G:H2'	34:a:1194:G:N3	2.23	0.53
44:k:18:ILE:HD12	44:k:96:VAL:HG23	1.90	0.53
10:A:1493:U:HO2'	10:A:1574:G:HO2'	1.54	0.53
17:I:81:PRO:HB3	17:I:89:VAL:HG23	1.91	0.53
34:a:694:U:H3	34:a:711:G:H1'	1.73	0.53
37:d:35:ASP:OD1	37:d:58:ARG:NH2	2.42	0.53
14:E:8:GLU:O	14:E:11:ARG:NH1	2.41	0.52
34:a:1002:G:H2'	34:a:1004:C:H41	1.74	0.52
10:A:12:U:H2'	10:A:12:U:O2	2.08	0.52
10:A:1757:U:H2'	10:A:1758:A:H5''	1.91	0.52
34:a:1229:U:H2'	34:a:1230:G:C8	2.44	0.52
10:A:620:G:O2'	10:A:1292:A:OP1	2.26	0.52
10:A:2092:C:H4'	10:A:2278:OMG:HM22	1.92	0.52
14:E:313:ALA:HA	14:E:328:PHE:HA	1.91	0.52
34:a:949:C:H2'	34:a:950:G:C8	2.45	0.52
34:a:75:A:H2'	34:a:75:A:N3	2.25	0.52
34:a:565:G:H2'	34:a:566:G:C8	2.45	0.52
34:a:956:G:H2'	34:a:957:C:O4'	2.10	0.52
34:a:1541:G:H2'	34:a:1542:A:C8	2.44	0.52
14:E:98:VAL:HG11	14:E:314:PHE:HB3	1.92	0.52
34:a:722:G:H2'	34:a:723:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:n:11:ARG:HA	47:n:45:VAL:HB	1.91	0.52
10:A:2227:C:O2'	10:A:2254:A:N1	2.39	0.52
34:a:620:C:N3	34:a:636:G:O6	2.43	0.52
44:k:66:GLU:HB3	48:o:59:ALA:HB2	1.92	0.52
10:A:1131:G:H1'	10:A:1133:G:O4'	2.10	0.52
37:d:33:HIS:CE1	48:o:38:LYS:HB2	2.44	0.52
34:a:922:A:H1'	34:a:923:A:H1'	1.92	0.52
34:a:6:U:H4'	34:a:7:G:O5'	2.10	0.51
10:A:1108:C:H2'	10:A:1109:U:O4'	2.10	0.51
34:a:409:C:H1'	34:a:630:A:H1'	1.91	0.51
34:a:1479:A:H2'	34:a:1480:A:O4'	2.09	0.51
10:A:669:C:O2'	10:A:702:U:OP1	2.28	0.51
10:A:788:A:O2'	10:A:1703:U:OP1	2.28	0.51
10:A:788:A:OP1	16:H:144:GLY:HA2	2.10	0.51
34:a:489:G:O2'	34:a:491:C:N4	2.39	0.51
34:a:726:A:H5'	45:l:119:ASN:HB2	1.92	0.51
10:A:161:A:H2'	10:A:162:A:C8	2.45	0.51
10:A:756:A:H2'	10:A:757:G:O4'	2.11	0.51
34:a:946:A:N6	34:a:1355:U:O4	2.43	0.51
10:A:539:G:H4'	29:V:6:VAL:HB	1.92	0.51
34:a:495:A:H2'	34:a:496:C:O4'	2.10	0.51
42:i:21:ARG:NH1	42:i:70:ASP:O	2.43	0.51
10:A:250:G:H4'	10:A:432:G:C5	2.45	0.51
46:m:25:ASN:HA	46:m:39:ASN:HA	1.91	0.51
4:4:16:ASP:O	4:4:20:ASN:N	2.44	0.51
34:a:1000:U:H1'	34:a:1002:G:H1'	1.93	0.51
27:T:31:LEU:HB2	27:T:34:VAL:HG12	1.93	0.51
41:h:27:ILE:HG13	41:h:43:LEU:HD23	1.93	0.51
1:1:32:ASN:HB2	10:A:443:U:H5''	1.93	0.51
14:E:98:VAL:HG21	14:E:314:PHE:CG	2.46	0.51
34:a:10:G:H4'	39:f:108:GLY:HA3	1.91	0.51
34:a:384:G:H5''	50:q:6:ARG:HB2	1.93	0.51
34:a:317:G:O2'	34:a:615:A:N1	2.40	0.50
34:a:736:A:OP1	49:p:54:ARG:NH2	2.43	0.50
10:A:194:A:H2'	10:A:195:C:C6	2.45	0.50
10:A:1680:U:H2'	10:A:1681:U:C6	2.47	0.50
10:A:2037:G:H5''	29:V:42:ALA:HB2	1.92	0.50
24:Q:52:LYS:NZ	24:Q:96:ARG:O	2.45	0.50
10:A:24:G:O2'	29:V:78:GLU:O	2.28	0.50
2:2:1:MET:HE1	2:2:17:GLN:HG2	1.92	0.50
10:A:729:G:C2	10:A:839:A:C2	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1818:A:N6	10:A:1855:G:O2'	2.42	0.50
39:f:115:LEU:HD13	39:f:123:ILE:HG21	1.93	0.50
10:A:1630:A:H1'	10:A:1631:G:H1'	1.94	0.50
11:B:38:U:H1'	11:B:43:A:H61	1.75	0.50
45:l:84:VAL:HG11	45:l:97:ILE:HG12	1.94	0.50
10:A:83:G:H21	10:A:102:A:H2	1.59	0.50
10:A:1424:A:C2	10:A:1438:G:C2	3.00	0.50
10:A:2709:U:O4	10:A:2755:U:H1'	2.12	0.50
14:E:554:LEU:O	14:E:555:ALA:HB3	2.11	0.50
5:5:13:LYS:NZ	10:A:1301:U:OP1	2.37	0.50
34:a:1122:A:N1	37:d:176:THR:HA	2.27	0.50
34:a:1386:U:H2'	34:a:1387:A:C8	2.46	0.50
14:E:90:VAL:HG21	14:E:436:THR:OG1	2.13	0.49
14:E:334:THR:HG22	14:E:370:TYR:HA	1.93	0.49
34:a:1411:G:H2'	34:a:1412:4OC:O4'	2.12	0.49
34:a:134:A:H2'	34:a:135:C:O4'	2.12	0.49
34:a:1326:G:H5'	34:a:1370:A:H1'	1.94	0.49
34:a:1036:C:H3'	34:a:1046:G:C4	2.46	0.49
34:a:1252:G:H1	34:a:1305:U:H3	1.60	0.49
12:C:53:LEU:HD11	12:C:77:ILE:HD11	1.93	0.49
34:a:923:A:H2'	34:a:924:A:H5'	1.95	0.49
4:4:11:GLN:HA	4:4:26:GLY:HA2	1.93	0.49
10:A:1730:C:H2'	10:A:1731:G:O4'	2.13	0.49
34:a:1155:C:H4'	34:a:1156:A:H5'	1.94	0.49
34:a:1265:G:O2'	34:a:1268:G:N3	2.45	0.49
18:J:60:ILE:HD11	18:J:135:GLN:HB2	1.94	0.49
34:a:106:G:N7	54:u:10:ARG:NH2	2.56	0.49
34:a:435:C:OP1	38:e:13:ARG:NH2	2.46	0.49
10:A:2496:A:H4'	23:P:56:ARG:NE	2.28	0.49
34:a:51:A:N1	34:a:368:G:O2'	2.45	0.49
34:a:971:C:H2'	34:a:972:G:H8	1.78	0.49
10:A:2253:C:H2'	10:A:2254:A:O4'	2.12	0.49
14:E:554:LEU:O	14:E:555:ALA:CB	2.61	0.48
34:a:1301:U:H4'	43:j:42:PRO:HB2	1.94	0.48
34:a:943:C:C5	34:a:1354:C:H2'	2.48	0.48
37:d:29:ALA:O	37:d:33:HIS:ND1	2.45	0.48
10:A:631:U:H2'	10:A:632:U:C6	2.48	0.48
10:A:2018:U:H2'	10:A:2019:G:H5''	1.95	0.48
10:A:2776:A:H1'	19:K:63:THR:HG22	1.95	0.48
14:E:343:ASN:HB2	14:E:350:GLU:HG3	1.94	0.48
34:a:9:A:C5	38:e:200:ARG:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:765:U:OP1	34:a:830:A:O2'	2.30	0.48
13:D:31:C:H4'	34:a:1348:G:H21	1.77	0.48
34:a:41:C:H2'	34:a:42:G:C8	2.49	0.48
34:a:1261:A:H2'	34:a:1262:A:C8	2.48	0.48
10:A:84:A:N1	10:A:98:U:O2'	2.44	0.48
10:A:830:U:H2'	10:A:831:C:C6	2.48	0.48
14:E:91:GLU:HA	14:E:94:ARG:HD2	1.95	0.48
34:a:108:A:C6	34:a:334:G:C6	3.01	0.48
10:A:2711:U:C4	10:A:2712:G:N7	2.82	0.48
12:C:1:MET:HE3	12:C:147:ILE:HG21	1.95	0.48
34:a:577:C:H1'	34:a:582:A:H2'	1.96	0.48
36:c:186:ILE:HG23	36:c:202:ALA:HB3	1.96	0.48
10:A:774:G:C5	15:G:207:LYS:HB2	2.49	0.48
10:A:1829:A:H2'	10:A:1830:A:C8	2.48	0.48
14:E:30:ILE:HG23	14:E:271:LEU:HD21	1.96	0.48
34:a:68:C:H2'	34:a:69:G:C8	2.49	0.48
34:a:1544:C:H2'	34:a:1545:A:C4	2.49	0.48
10:A:126:A:H5''	10:A:127:C:O4'	2.14	0.48
10:A:1146:C:H2'	10:A:1147:A:C8	2.49	0.48
41:h:104:LEU:HD11	41:h:124:ILE:HG22	1.95	0.48
49:p:19:GLU:O	49:p:20:THR:OG1	2.28	0.48
10:A:1766:C:H2'	10:A:1767:G:O4'	2.14	0.48
10:A:2354:A:H2'	10:A:2355:A:C8	2.49	0.48
14:E:309:PHE:CD1	14:E:335:MET:HB2	2.49	0.48
46:m:79:TYR:HB2	46:m:106:VAL:HG11	1.94	0.48
10:A:12:U:O2	10:A:12:U:C2'	2.62	0.47
34:a:421:G:H1'	34:a:436:G:H21	1.79	0.47
34:a:1187:G:H2'	34:a:1188:G:O4'	2.14	0.47
34:a:1285:A:H2'	34:a:1286:G:O4'	2.13	0.47
10:A:2618:C:H2'	10:A:2619:G:C8	2.49	0.47
34:a:1055:A:C6	34:a:1056:C:H1'	2.48	0.47
34:a:1325:U:O2'	34:a:1370:A:N3	2.47	0.47
10:A:789:C:OP2	16:H:146:HIS:NE2	2.47	0.47
54:u:39:VAL:HA	54:u:46:LYS:HD3	1.96	0.47
10:A:297:G:C2	10:A:298:U:O4	2.67	0.47
14:E:76:ARG:NH1	14:E:373:ASP:OD2	2.47	0.47
14:E:510:HIS:HB3	14:E:567:TYR:CE2	2.50	0.47
34:a:1024:G:H2'	34:a:1025:A:O4'	2.14	0.47
34:a:1225:G:H2'	34:a:1225:G:N3	2.30	0.47
13:D:74:C:O2	13:D:74:C:O4'	2.29	0.47
58:E:703:FUA:H5	58:E:703:FUA:H202	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:310:G:O2'	34:a:564:C:H5''	2.14	0.47
39:f:11:PHE:HB3	39:f:39:VAL:HG13	1.96	0.47
41:h:15:ASP:O	41:h:19:ASN:N	2.48	0.47
10:A:774:G:C6	15:G:207:LYS:HB2	2.49	0.47
10:A:856:U:H2'	22:O:21:ARG:HA	1.96	0.47
10:A:2495:A:O2'	10:A:2508:G:N2	2.47	0.47
34:a:1288:A:N3	34:a:1288:A:H5'	2.29	0.47
40:g:11:ARG:HG3	40:g:14:ILE:HB	1.96	0.47
34:a:51:A:O2'	34:a:368:G:N2	2.48	0.47
34:a:1030:G:H2'	34:a:1031:C:H4'	1.96	0.47
34:a:1283:C:H2'	34:a:1284:A:O4'	2.14	0.47
51:r:26:LEU:HD11	51:r:43:SER:HB3	1.96	0.47
10:A:363:A:H4'	10:A:365:A:C8	2.50	0.47
10:A:1959:A:H2'	10:A:1960:G:O4'	2.15	0.47
34:a:262:G:OP1	51:r:72:THR:HG22	2.15	0.47
34:a:802:A:H4'	34:a:1532:G:O2'	2.14	0.47
10:A:1263:A:H2'	10:A:1264:A:C8	2.50	0.47
34:a:627:U:H2'	38:e:128:ILE:HD11	1.97	0.47
10:A:991:A:H2'	10:A:992:A:C8	2.50	0.46
34:a:990:U:H5''	48:o:6:MET:HE1	1.96	0.46
10:A:253:G:H4'	22:O:59:ARG:HD2	1.95	0.46
18:J:136:LEU:HD13	18:J:149:VAL:HG12	1.97	0.46
34:a:1047:A:H3'	34:a:1048:C:C6	2.51	0.46
34:a:1048:C:H2'	34:a:1049:A:C8	2.50	0.46
34:a:1066:A:O2'	37:d:160:ASP:O	2.33	0.46
10:A:745:G:O2'	10:A:1676:A:N3	2.46	0.46
10:A:1806:U:H5	10:A:1811:A:N7	2.14	0.46
14:E:535:ARG:HA	14:E:538:ILE:HD12	1.97	0.46
34:a:1035:C:O2	34:a:1047:A:N6	2.34	0.46
38:e:74:ILE:HA	38:e:77:LYS:HD3	1.98	0.46
40:g:31:ALA:HB2	40:g:37:VAL:HG23	1.97	0.46
34:a:417:U:H2'	34:a:418:G:O4'	2.15	0.46
34:a:1011:U:H2'	34:a:1012:G:C8	2.51	0.46
34:a:1336:U:H2'	34:a:1337:A:C8	2.50	0.46
34:a:81:A:H4'	34:a:82:G:OP1	2.16	0.46
34:a:476:C:O4'	34:a:476:C:O2	2.33	0.46
34:a:1003:A:C4	34:a:1226:A:H4'	2.51	0.46
4:4:13:ILE:HG13	4:4:43:TYR:HB2	1.98	0.46
8:8:15:LYS:HE3	10:A:676:A:H5''	1.98	0.46
34:a:401:A:OP2	50:q:13:LYS:HD2	2.16	0.46
10:A:922:G:N1	10:A:943:C:H2'	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:k:57:LYS:HE3	44:k:58:TYR:CZ	2.51	0.46
10:A:455:A:H2'	10:A:456:G:C8	2.51	0.46
10:A:575:G:O2'	10:A:577:A:N7	2.39	0.46
10:A:1008:C:O2'	10:A:2300:A:N3	2.42	0.46
14:E:19:ILE:HD12	14:E:19:ILE:H	1.80	0.46
18:J:22:TYR:CE2	18:J:29:PRO:HD3	2.51	0.46
34:a:302:C:P	34:a:618:G:H21	2.39	0.46
34:a:400:G:H4'	50:q:14:ARG:HE	1.81	0.46
4:4:1:MET:HG2	11:B:41:C:H5''	1.98	0.45
10:A:566:U:H2'	10:A:567:G:C8	2.52	0.45
4:4:2:LYS:HE3	11:B:38:U:H2'	1.97	0.45
11:B:11:A:N1	11:B:67:G:O2'	2.48	0.45
13:D:37:T6A:N1	13:D:37:T6A:N11	2.63	0.45
34:a:722:G:N2	45:l:121:CYS:SG	2.89	0.45
10:A:1121:A:C2	10:A:1132:A:H2'	2.51	0.45
10:A:1944:U:H2'	10:A:1945:A:C8	2.52	0.45
34:a:1350:A:H2'	34:a:1351:U:O4'	2.16	0.45
10:A:902:A:N6	10:A:903:G:C6	2.85	0.45
10:A:1455:U:O4	10:A:1630:A:H5''	2.17	0.45
14:E:87:ASP:HB3	14:E:457:HIS:HB2	1.98	0.45
34:a:80:A:N6	34:a:88:U:O2	2.42	0.45
34:a:976:5MC:H4'	43:j:129:PHE:HZ	1.81	0.45
34:a:1495:U:H2'	34:a:1496:U:O4'	2.16	0.45
42:i:56:LYS:O	42:i:57:GLN:HB3	2.16	0.45
10:A:1618:A:H2'	10:A:1619:A:C8	2.51	0.45
34:a:509:C:H2'	34:a:510:C:C6	2.51	0.45
34:a:541:A:O2'	34:a:543:A:OP1	2.35	0.45
41:h:37:GLY:HA3	43:j:43:PHE:CZ	2.51	0.45
47:n:45:VAL:HA	47:n:48:LEU:HG	1.99	0.45
10:A:577:A:H4'	10:A:578:G:C8	2.51	0.45
10:A:1177:A:N6	10:A:2052:C:O2'	2.49	0.45
21:N:24:VAL:HG13	21:N:33:ALA:HB2	1.98	0.45
44:k:46:LYS:HD3	44:k:68:ARG:HB3	1.98	0.45
10:A:794:A:H4'	10:A:1309:G:N3	2.30	0.45
11:B:35:C:H2'	11:B:36:C:O4'	2.17	0.45
14:E:10:THR:HA	14:E:76:ARG:HB3	1.99	0.45
34:a:420:U:O2	34:a:420:U:O4'	2.31	0.45
34:a:1383:G:N7	43:j:15:LYS:NZ	2.53	0.45
8:8:42:ARG:O	8:8:45:ARG:HG2	2.15	0.45
10:A:461:A:C2	10:A:2436:G:C2	3.05	0.45
10:A:1712:A:O2'	10:A:1718:G:N7	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1255:A:H2'	34:a:1256:A:C8	2.52	0.45
51:r:19:MET:HB2	51:r:22:THR:HB	1.98	0.45
10:A:1806:U:OP2	10:A:1811:A:N6	2.45	0.45
19:K:125:VAL:HA	19:K:130:VAL:O	2.17	0.45
34:a:509:C:H1'	34:a:557:C:H1'	1.98	0.45
34:a:954:G:C2	34:a:955:A:C8	3.05	0.45
14:E:482:TYR:O	14:E:483:ARG:NH1	2.50	0.45
19:K:9:ILE:HD11	19:K:69:ARG:HG2	1.98	0.45
20:M:126:TYR:OH	20:M:133:HIS:NE2	2.47	0.45
29:V:82:LEU:HB2	29:V:98:LYS:HB2	1.99	0.45
34:a:1497:G:H2'	34:a:1498:G:C8	2.51	0.45
47:n:85:SER:O	47:n:86:TYR:C	2.60	0.44
14:E:535:ARG:HH12	34:a:1220:C:H5''	1.82	0.44
34:a:932:A:N6	34:a:1402:G:O6	2.51	0.44
10:A:749:G:N3	10:A:771:G:C2	2.86	0.44
14:E:346:LYS:HB3	14:E:348:LYS:HG2	2.00	0.44
18:J:129:THR:HG23	18:J:155:VAL:HG22	2.00	0.44
10:A:1125:U:H2'	10:A:1126:U:C6	2.52	0.44
10:A:1304:G:O2'	10:A:2039:G:O6	2.35	0.44
10:A:1053:A:H2'	10:A:1054:A:C8	2.53	0.44
10:A:1138:U:H1'	10:A:1141:U:H5	1.81	0.44
10:A:2869:G:O2'	10:A:2886:G:N2	2.51	0.44
11:B:93:G:O6	32:Y:15:ARG:NH2	2.51	0.44
34:a:409:C:H2'	34:a:410:G:C8	2.52	0.44
34:a:933:C:H2'	34:a:934:G:C8	2.53	0.44
34:a:968:A:H1'	34:a:994:C:H1'	2.00	0.44
48:o:34:TYR:O	48:o:38:LYS:N	2.50	0.44
10:A:167:U:H2'	10:A:168:A:O4'	2.18	0.44
10:A:559:A:N3	10:A:624:C:O2'	2.50	0.44
10:A:1875:A:H2'	10:A:1876:G:O4'	2.17	0.44
34:a:1168:C:C6	34:a:1170:G:H1'	2.52	0.44
34:a:1434:U:H2'	34:a:1435:A:C8	2.53	0.44
44:k:80:THR:HB	44:k:83:THR:HG23	1.99	0.44
53:t:3:ARG:O	53:t:4:SER:C	2.61	0.44
19:K:42:THR:HB	19:K:53:VAL:HB	2.00	0.44
34:a:437:U:H3'	38:e:9:TRP:CD1	2.53	0.44
34:a:666:G:H1'	34:a:757:A:C8	2.53	0.44
34:a:1422:C:H2'	34:a:1423:A:C8	2.53	0.44
34:a:1459:C:H2'	34:a:1460:U:C6	2.53	0.44
4:4:37:TRP:CG	4:4:38:GLU:H	2.35	0.44
10:A:715:A:OP1	22:O:43:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1477:U:H2'	10:A:1478:A:C8	2.52	0.44
10:A:1885:G:H1'	10:A:1911:A:N6	2.32	0.44
10:A:2335:G:N3	10:A:2335:G:H2'	2.33	0.44
12:C:73:SER:O	12:C:74:VAL:C	2.61	0.44
18:J:177:PHE:O	18:J:178:ARG:C	2.60	0.44
19:K:137:SER:HB2	19:K:140:GLN:HB2	1.99	0.44
10:A:1092:A:H2'	10:A:1092:A:N3	2.33	0.44
10:A:2548:C:C4	10:A:2549:U:C4	3.06	0.44
10:A:2671:A:H2'	10:A:2672:G:O4'	2.18	0.44
13:D:34:G:H2'	13:D:35:C:C6	2.53	0.44
14:E:602:GLU:HB3	14:E:678:VAL:HG22	1.99	0.44
40:g:52:ILE:HD11	52:s:71:ALA:HB2	1.99	0.44
10:A:1312:A:N3	10:A:1313:G:H1'	2.33	0.43
10:A:1874:A:H4'	10:A:1875:A:OP1	2.18	0.43
10:A:2801:C:H2'	10:A:2802:A:O4'	2.18	0.43
31:X:10:LYS:HB2	31:X:71:LEU:HD21	1.98	0.43
36:c:157:MET:HE2	36:c:157:MET:HA	1.99	0.43
10:A:748:U:H2'	10:A:749:G:O4'	2.18	0.43
10:A:1024:A:H2'	10:A:1025:A:C8	2.53	0.43
18:J:117:VAL:HG22	18:J:176:PRO:O	2.18	0.43
27:T:108:GLN:O	27:T:112:LYS:HD3	2.18	0.43
34:a:6:U:O2'	34:a:7:G:OP2	2.33	0.43
34:a:345:G:H2'	34:a:346:A:C8	2.52	0.43
34:a:1250:U:C6	34:a:1250:U:H5''	2.53	0.43
34:a:1503:A:H62	34:a:1505:G:H1'	1.82	0.43
40:g:26:PHE:HA	40:g:29:ILE:HD12	1.99	0.43
44:k:66:GLU:N	48:o:57:ARG:O	2.47	0.43
45:l:47:ALA:HA	45:l:50:LEU:HD12	2.00	0.43
10:A:1711:G:O2'	10:A:2018:U:O4	2.37	0.43
10:A:1949:G:N3	10:A:1949:G:H2'	2.33	0.43
10:A:1952:C:H2'	10:A:1954:A:OP1	2.19	0.43
14:E:535:ARG:HH22	34:a:1220:C:H5'	1.82	0.43
18:J:79:LEU:CD1	18:J:85:ILE:HG21	2.49	0.43
46:m:95:VAL:HG13	46:m:108:TYR:HB3	1.98	0.43
10:A:524:A:N1	10:A:545:G:H4'	2.33	0.43
10:A:1675:G:H1'	10:A:1679:A:H61	1.82	0.43
10:A:1696:C:H2'	10:A:1697:G:O4'	2.18	0.43
10:A:2053:U:H2'	10:A:2054:G:O4'	2.18	0.43
14:E:456:LEU:HD21	58:E:703:FUA:H273	2.00	0.43
14:E:616:MET:HG2	14:E:620:MET:HE2	2.00	0.43
23:P:54:MET:HE1	23:P:104:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:670:A:H2'	34:a:671:A:C8	2.53	0.43
34:a:967:A:N3	34:a:994:C:O2'	2.51	0.43
34:a:1126:U:H1'	48:o:61:TRP:HA	2.00	0.43
34:a:1381:G:H5''	43:j:72:GLY:HA2	2.01	0.43
10:A:102:A:H2'	10:A:103:U:O4'	2.18	0.43
10:A:1053:A:N3	10:A:1197:C:O2'	2.51	0.43
10:A:1378:U:OP2	10:A:1431:U:O2'	2.29	0.43
20:M:18:VAL:HG22	20:M:56:ILE:HB	2.00	0.43
10:A:72:U:O2'	10:A:75:G:N2	2.52	0.43
10:A:226:A:O2'	10:A:466:C:O2	2.36	0.43
10:A:1800:A:N7	10:A:1856:A:H1'	2.34	0.43
10:A:2418:G:C6	10:A:2454:C:H1'	2.53	0.43
14:E:316:VAL:HG22	14:E:326:THR:HG23	2.00	0.43
34:a:418:G:H2'	34:a:437:U:C4	2.54	0.43
34:a:948:G:OP2	41:h:95:ARG:NH1	2.51	0.43
34:a:1362:C:H2'	34:a:1363:G:O4'	2.18	0.43
43:j:52:GLN:N	43:j:53:PRO:HD2	2.34	0.43
6:6:18:ILE:HD13	10:A:2446:U:H5''	2.00	0.43
11:B:29:C:O2'	11:B:51:A:N1	2.47	0.43
34:a:884:C:H4'	42:i:19:MET:HE1	2.00	0.43
34:a:1379:C:H2'	34:a:1380:G:C8	2.53	0.43
14:E:30:ILE:HD11	14:E:270:MET:HE1	2.00	0.43
14:E:91:GLU:HG3	58:E:703:FUA:H212	2.00	0.43
14:E:333:GLY:N	14:E:371:SER:OG	2.52	0.43
19:K:40:ARG:HB3	19:K:55:PRO:HG3	2.01	0.43
29:V:14:PRO:HG2	29:V:78:GLU:HG2	2.00	0.43
34:a:227:C:H2'	34:a:228:A:O4'	2.18	0.43
36:c:170:ARG:NH1	36:c:195:GLU:OE1	2.51	0.43
1:1:23:ASN:OD1	10:A:2106:U:O2'	2.34	0.43
10:A:786:U:C2	10:A:802:G:N2	2.87	0.43
10:A:1251:A:N3	10:A:1276:G:O2'	2.50	0.43
10:A:1320:G:N2	10:A:1322:G:H3'	2.33	0.43
10:A:1891:U:OP1	10:A:2437:G:O2'	2.32	0.43
10:A:2548:C:C2	10:A:2572:G:C2	3.07	0.43
34:a:59:C:H2'	34:a:60:A:H8	1.84	0.43
48:o:37:PHE:O	48:o:39:LEU:HG	2.19	0.43
10:A:1149:U:H2'	10:A:1150:A:C8	2.53	0.43
10:A:1400:C:O2'	10:A:1836:A:N3	2.45	0.43
10:A:1462:G:O2'	10:A:1463:A:O4'	2.34	0.43
14:E:18:HIS:ND1	14:E:115:GLN:HB2	2.34	0.43
26:S:65:LYS:HE3	26:S:67:SER:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:825:G:H2'	10:A:827:A:N7	2.34	0.42
10:A:1072:A:N3	10:A:2513:G:O2'	2.48	0.42
10:A:1447:A:H2'	10:A:1448:U:C6	2.53	0.42
10:A:1874:A:O2'	10:A:1875:A:H8	2.02	0.42
34:a:18:U:H2'	34:a:19:C:C6	2.54	0.42
34:a:681:G:H2'	34:a:682:G:C8	2.54	0.42
34:a:1131:C:H2'	34:a:1132:U:O4'	2.19	0.42
34:a:1301:U:H5''	43:j:43:PHE:CE1	2.54	0.42
10:A:363:A:H4'	10:A:365:A:N7	2.35	0.42
10:A:2298:G:OP1	33:Z:26:SER:HB3	2.18	0.42
10:A:2341:A:H2'	10:A:2342:U:C6	2.55	0.42
10:A:2917:U:H2'	10:A:2918:A:C8	2.55	0.42
18:J:56:GLU:CD	18:J:135:GLN:HE21	2.27	0.42
34:a:9:A:N6	38:e:196:GLU:O	2.52	0.42
34:a:462:A:N6	34:a:487:U:O2	2.52	0.42
34:a:1270:G:H4'	34:a:1294:C:H5'	2.00	0.42
34:a:1367:A:H2'	34:a:1368:U:C6	2.53	0.42
42:i:43:GLU:HG3	42:i:103:ILE:HD13	2.00	0.42
42:i:98:LEU:HD22	42:i:132:TRP:HB2	2.00	0.42
44:k:42:LEU:HB3	44:k:43:PRO:HD2	2.01	0.42
4:4:34:MET:HA	4:4:44:PRO:HA	2.00	0.42
10:A:1806:U:O2	10:A:1810:A:N6	2.52	0.42
10:A:1916:A:H2'	10:A:1917:A:C8	2.54	0.42
14:E:529:VAL:O	14:E:532:VAL:HG13	2.19	0.42
34:a:532:G:H2'	34:a:533:C:C6	2.54	0.42
34:a:836:A:H2'	34:a:837:A:O4'	2.20	0.42
10:A:1013:U:H2'	10:A:1014:U:C6	2.55	0.42
10:A:2372:G:N3	10:A:2408:C:H2'	2.33	0.42
10:A:2684:A:H1'	10:A:2692:A:N6	2.33	0.42
18:J:106:VAL:C	18:J:109:PRO:HD2	2.44	0.42
34:a:210:A:H2'	34:a:211:A:C8	2.55	0.42
34:a:908:C:H2'	34:a:909:A:C8	2.54	0.42
37:d:8:ILE:HG23	37:d:16:ARG:HD2	2.01	0.42
10:A:1354:G:C6	10:A:1355:A:C5	3.08	0.42
10:A:1697:G:C6	24:Q:5:LYS:HB2	2.55	0.42
13:D:9:G:O4'	13:D:21:A:N6	2.51	0.42
14:E:314:PHE:CZ	14:E:327:PHE:HB3	2.54	0.42
32:Y:7:ILE:C	32:Y:7:ILE:HD12	2.44	0.42
34:a:462:A:H2'	34:a:463:U:O4'	2.20	0.42
34:a:774:A:H2'	34:a:775:A:O4'	2.19	0.42
34:a:1117:G:H2'	34:a:1118:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1304:U:H2'	34:a:1305:U:C6	2.54	0.42
43:j:19:ALA:HB2	43:j:69:VAL:HG23	2.01	0.42
10:A:2872:G:H2'	10:A:2873:C:O4'	2.20	0.42
34:a:72:C:H2'	34:a:73:G:C8	2.54	0.42
34:a:390:A:H2'	34:a:391:A:C8	2.55	0.42
34:a:1194:G:C8	34:a:1194:G:H5'	2.55	0.42
14:E:506:TYR:HB3	14:E:575:ASP:HB3	2.02	0.42
24:Q:105:LYS:HA	24:Q:117:VAL:HG12	2.02	0.42
27:T:58:ARG:HA	27:T:61:TRP:CE3	2.54	0.42
34:a:1140:C:OP1	43:j:68:ASN:ND2	2.52	0.42
34:a:1551:U:H2'	34:a:1552:U:C6	2.54	0.42
36:c:117:ILE:HG21	36:c:141:TYR:HB2	2.01	0.42
44:k:15:HIS:HA	44:k:18:ILE:HG22	2.02	0.42
53:t:11:VAL:HB	53:t:41:PHE:HE2	1.85	0.42
10:A:680:C:O2'	10:A:684:U:OP1	2.38	0.42
10:A:1450:A:N1	10:A:1633:A:H8	2.18	0.42
10:A:1802:U:O4	10:A:1816:A:H2	2.02	0.42
10:A:2393:A:H2'	10:A:2394:G:O4'	2.20	0.42
58:E:703:FUA:H121	58:E:703:FUA:H232	2.01	0.42
26:S:22:PHE:O	26:S:52:ARG:NH1	2.50	0.42
27:T:76:TYR:CZ	27:T:80:MET:HG3	2.55	0.42
34:a:629:A:H2'	34:a:630:A:O4'	2.20	0.42
10:A:575:G:N3	10:A:575:G:H2'	2.35	0.42
10:A:605:U:O4'	10:A:2063:C:H5'	2.20	0.42
10:A:1943:A:H2'	10:A:1944:U:O4'	2.18	0.42
10:A:2437:G:H2'	10:A:2438:A:O4'	2.19	0.42
10:A:2664:U:H2'	10:A:2665:G:O4'	2.19	0.42
34:a:224:U:H2'	34:a:225:G:C8	2.55	0.42
34:a:970:U:C2	34:a:992:A:C5	3.08	0.42
34:a:1055:A:C5	34:a:1056:C:H1'	2.54	0.42
34:a:1243:G:C2	34:a:1244:C:C2	3.08	0.42
2:2:1:MET:HE3	2:2:6:ILE:HG12	2.01	0.42
5:5:10:LYS:O	5:5:14:ASN:ND2	2.53	0.42
34:a:7:G:O2'	34:a:8:G:H5'	2.20	0.42
34:a:1126:U:H2'	34:a:1127:U:C6	2.55	0.42
10:A:1081:G:C2	10:A:1163:U:O2	2.73	0.41
10:A:1841:G:C6	10:A:1842:A:C6	3.07	0.41
10:A:2282:G:H2'	10:A:2283:G:O4'	2.20	0.41
10:A:2560:U:OP1	10:A:2692:A:O2'	2.30	0.41
13:D:65:G:O2'	13:D:66:C:OP1	2.35	0.41
13:D:74:C:H4'	13:D:74:C:OP1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:166:ILE:HD11	14:E:176:ILE:HD11	2.02	0.41
20:M:1:MET:O	27:T:93:LYS:NZ	2.44	0.41
34:a:421:G:N7	38:e:28:LYS:NZ	2.64	0.41
34:a:1235:A:H2'	34:a:1236:C:C6	2.55	0.41
34:a:1318:U:P	47:n:100:GLN:HE22	2.43	0.41
45:l:82:VAL:HG11	45:l:100:LEU:HD12	2.01	0.41
10:A:613:G:H2'	10:A:2057:A:N7	2.35	0.41
10:A:1480:G:O2'	10:A:1521:A:H1'	2.19	0.41
10:A:2251:G:H4'	10:A:2253:C:C2	2.55	0.41
10:A:2358:G:O2'	10:A:2363:A:N1	2.51	0.41
34:a:8:G:H5''	34:a:306:A:O4'	2.20	0.41
34:a:1010:U:H2'	34:a:1011:U:C6	2.55	0.41
34:a:1530:MA6:C5	34:a:1531:G:H1'	2.50	0.41
34:a:1546:C:H2'	34:a:1547:C:C6	2.55	0.41
37:d:90:LEU:HD12	37:d:100:ILE:HD11	2.02	0.41
38:e:9:TRP:HA	38:e:25:GLU:HG2	2.02	0.41
38:e:46:GLU:OE2	38:e:50:GLN:NE2	2.53	0.41
10:A:1674:U:H2'	10:A:1675:G:O4'	2.21	0.41
10:A:2007:G:O2'	10:A:2009:U:OP2	2.36	0.41
13:D:32:RSP:H4'	34:a:1349:A:O2'	2.20	0.41
13:D:73:G:H3'	13:D:74:C:H5''	2.01	0.41
14:E:343:ASN:O	14:E:347:GLY:N	2.53	0.41
34:a:74:G:H1	34:a:94:G:H3'	1.84	0.41
34:a:103:G:N7	54:u:9:LYS:NZ	2.60	0.41
34:a:328:A:H2'	34:a:329:A:O4'	2.20	0.41
34:a:477:U:H2'	34:a:478:G:O4'	2.20	0.41
34:a:1238:C:H4'	47:n:115:THR:HA	2.01	0.41
36:c:131:LYS:O	36:c:134:VAL:HG22	2.19	0.41
2:2:26:PHE:CG	30:W:4:ARG:HD2	2.55	0.41
10:A:2457:A:H2'	10:A:2457:A:N3	2.35	0.41
10:A:2709:U:O2	16:H:24:PRO:HB3	2.20	0.41
34:a:874:A:H2'	34:a:875:C:O4'	2.19	0.41
44:k:48:VAL:HG11	48:o:61:TRP:CZ3	2.56	0.41
10:A:2439:A:H2'	10:A:2440:G:O4'	2.20	0.41
15:G:114:GLN:HE22	15:G:126:VAL:HG23	1.85	0.41
34:a:358:G:H2'	34:a:359:G:C8	2.56	0.41
34:a:413:U:H1'	34:a:506:A:H2'	2.01	0.41
10:A:305:A:N6	10:A:410:G:H22	2.18	0.41
10:A:606:G:OP2	28:U:78:ARG:NH1	2.53	0.41
10:A:1449:A:H8	10:A:1634:A:H62	1.68	0.41
10:A:1592:A:H2'	10:A:1593:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2285:C:O2'	10:A:2454:C:OP2	2.38	0.41
10:A:2716:U:O2	10:A:2716:U:H2'	2.21	0.41
12:C:35:LEU:HD21	12:C:88:VAL:HG11	2.02	0.41
34:a:923:A:H2'	34:a:923:A:N3	2.36	0.41
34:a:1067:U:H2'	34:a:1068:G:H8	1.86	0.41
34:a:1183:C:H2'	34:a:1184:G:C8	2.55	0.41
36:c:121:GLU:HA	36:c:126:PHE:HB2	2.02	0.41
41:h:36:ARG:O	41:h:40:GLN:HG3	2.21	0.41
10:A:328:G:N2	10:A:399:U:H1'	2.35	0.41
18:J:132:VAL:HG22	18:J:152:MET:HG2	2.02	0.41
23:P:32:PHE:HD1	23:P:133:LYS:HG2	1.86	0.41
34:a:226:U:H2'	34:a:227:C:O4'	2.21	0.41
34:a:1251:G:H2'	34:a:1252:G:H8	1.86	0.41
36:c:6:MET:HE3	36:c:43:LEU:HB2	2.01	0.41
10:A:2109:A:H2'	10:A:2110:G:O4'	2.21	0.41
34:a:1195:G:H2'	34:a:1196:G:C8	2.56	0.41
34:a:1319:G:N7	47:n:98:ARG:NH2	2.67	0.41
10:A:457:G:OP2	10:A:2433:C:O2'	2.38	0.41
10:A:1110:U:O2'	10:A:1113:A:N7	2.53	0.41
10:A:1642:C:H2'	10:A:1643:C:C6	2.56	0.41
10:A:1812:A:OP2	10:A:2009:U:H5''	2.21	0.41
10:A:2338:A:H1'	18:J:85:ILE:HD12	2.02	0.41
14:E:94:ARG:NH2	14:E:385:THR:HG21	2.36	0.41
14:E:129:PRO:HB3	14:E:248:THR:O	2.20	0.41
14:E:615:TYR:CG	14:E:662:THR:HA	2.56	0.41
23:P:39:THR:OG1	23:P:99:PRO:HD3	2.21	0.41
34:a:11:A:OP2	39:f:131:ASN:HB2	2.21	0.41
34:a:575:G:O6	46:m:2:PRO:HD3	2.21	0.41
34:a:776:A:N3	34:a:1523:U:O2'	2.51	0.41
34:a:1075:G:OP2	34:a:1395:G:O2'	2.38	0.41
35:b:10:G:H3'	35:b:11:U:H5''	2.03	0.41
43:j:45:SER:O	43:j:49:ASP:N	2.51	0.41
47:n:14:ARG:O	47:n:15:VAL:C	2.64	0.41
50:q:22:VAL:HG21	50:q:60:TRP:CD1	2.56	0.41
10:A:326:A:N1	10:A:400:C:O2'	2.51	0.41
10:A:923:A:H2'	10:A:923:A:N3	2.36	0.41
10:A:1115:G:H1'	10:A:1133:G:C8	2.56	0.41
10:A:1423:C:H2'	10:A:1424:A:C8	2.55	0.41
10:A:2113:U:O2	10:A:2261:G:C2	2.74	0.41
14:E:465:MET:HA	14:E:469:PHE:HD2	1.86	0.41
18:J:80:ARG:HB2	18:J:83:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:1:MET:SD	29:V:62:TYR:HB3	2.61	0.41
34:a:936:G:O2'	34:a:1514:A:N7	2.47	0.41
34:a:1157:C:H2'	34:a:1158:U:C6	2.56	0.41
34:a:1261:A:N1	34:a:1364:U:O2'	2.52	0.41
34:a:1379:C:OP1	48:o:61:TRP:NE1	2.52	0.41
34:a:1391:U:H2'	34:a:1392:C:O4'	2.20	0.41
46:m:98:GLY:O	46:m:109:HIS:ND1	2.54	0.41
10:A:1051:C:OP1	20:M:38:ARG:NH1	2.54	0.40
10:A:2355:A:H2'	10:A:2356:A:C8	2.56	0.40
11:B:37:A:H2'	11:B:38:U:C6	2.56	0.40
36:c:21:ARG:HG3	36:c:22:ARG:HG3	2.03	0.40
37:d:76:ILE:HA	37:d:83:ILE:HB	2.03	0.40
10:A:813:G:N2	10:A:1416:U:O2'	2.53	0.40
10:A:1809:C:H1'	10:A:2636:U:H5''	2.03	0.40
34:a:454:G:N2	34:a:497:C:C2	2.90	0.40
34:a:510:C:H2'	34:a:511:A:C8	2.57	0.40
34:a:1032:C:H1'	34:a:1033:U:O4'	2.22	0.40
34:a:1239:A:H2'	34:a:1240:C:O4'	2.21	0.40
34:a:1307:U:OP2	47:n:44:ARG:NH2	2.54	0.40
10:A:2358:G:C2	10:A:2412:C:C2	3.09	0.40
34:a:570:U:H1'	46:m:12:ARG:HB3	2.04	0.40
34:a:608:U:C2	34:a:647:G:C2	3.09	0.40
34:a:1249:A:H4'	34:a:1250:U:O5'	2.22	0.40
51:r:23:ILE:HG13	51:r:48:THR:HB	2.02	0.40
10:A:852:U:O2	17:I:74:ARG:NH2	2.54	0.40
10:A:991:A:N3	10:A:1028:G:H8	2.20	0.40
10:A:1153:C:H2'	10:A:1154:G:O4'	2.22	0.40
10:A:1247:G:O2'	10:A:1275:A:N1	2.46	0.40
10:A:1364:C:H2'	10:A:1365:G:C8	2.56	0.40
34:a:490:A:H2'	34:a:491:C:O4'	2.21	0.40
34:a:721:G:H2'	34:a:722:G:C8	2.56	0.40
34:a:1171:C:H2'	34:a:1172:C:C6	2.57	0.40
34:a:1248:A:C6	34:a:1313:C:H5'	2.56	0.40
10:A:2120:G:N7	10:A:2252:A:H2'	2.37	0.40
10:A:2474:G:C8	10:A:2528:C:C6	3.10	0.40
13:D:31:C:H4'	34:a:1348:G:N2	2.36	0.40
14:E:247:ALA:HB1	14:E:253:PHE:HB3	2.03	0.40
21:N:35:ILE:HG21	21:N:103:ALA:HB3	2.04	0.40
34:a:641:U:O2	34:a:641:U:H2'	2.21	0.40
34:a:917:A:H2'	34:a:918:A:C8	2.56	0.40
35:b:13:A:H2'	35:b:14:A:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:d:149:LYS:HB3	37:d:200:TRP:HB2	2.02	0.40
49:p:9:ASN:HA	49:p:12:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
2	2	63/69 (91%)	63 (100%)	0	0	100	100
3	3	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
4	4	57/84 (68%)	57 (100%)	0	0	100	100
5	5	51/57 (90%)	49 (96%)	2 (4%)	0	100	100
6	6	46/49 (94%)	46 (100%)	0	0	100	100
7	7	42/45 (93%)	42 (100%)	0	0	100	100
8	8	63/66 (96%)	63 (100%)	0	0	100	100
9	9	35/37 (95%)	35 (100%)	0	0	100	100
12	C	183/186 (98%)	180 (98%)	3 (2%)	0	100	100
14	E	657/693 (95%)	645 (98%)	11 (2%)	1 (0%)	43	70
15	G	271/277 (98%)	266 (98%)	5 (2%)	0	100	100
16	H	213/220 (97%)	205 (96%)	8 (4%)	0	100	100
17	I	203/207 (98%)	198 (98%)	5 (2%)	0	100	100
18	J	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
19	K	175/178 (98%)	172 (98%)	3 (2%)	0	100	100
20	M	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
21	N	120/122 (98%)	112 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	O	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
23	P	134/144 (93%)	129 (96%)	5 (4%)	0	100	100
24	Q	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
25	R	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
26	S	112/116 (97%)	108 (96%)	4 (4%)	0	100	100
27	T	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
28	U	100/102 (98%)	100 (100%)	0	0	100	100
29	V	109/117 (93%)	108 (99%)	1 (1%)	0	100	100
30	W	88/91 (97%)	88 (100%)	0	0	100	100
31	X	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
32	Y	92/217 (42%)	91 (99%)	1 (1%)	0	100	100
33	Z	74/94 (79%)	71 (96%)	3 (4%)	0	100	100
36	c	219/255 (86%)	213 (97%)	5 (2%)	1 (0%)	24	52
37	d	202/217 (93%)	197 (98%)	5 (2%)	0	100	100
38	e	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
39	f	155/166 (93%)	149 (96%)	5 (3%)	1 (1%)	21	48
40	g	92/98 (94%)	90 (98%)	2 (2%)	0	100	100
41	h	142/156 (91%)	140 (99%)	2 (1%)	0	100	100
42	i	129/132 (98%)	124 (96%)	5 (4%)	0	100	100
43	j	126/132 (96%)	120 (95%)	6 (5%)	0	100	100
44	k	96/102 (94%)	95 (99%)	0	1 (1%)	12	37
45	l	116/129 (90%)	108 (93%)	8 (7%)	0	100	100
46	m	133/137 (97%)	131 (98%)	2 (2%)	0	100	100
47	n	112/121 (93%)	106 (95%)	6 (5%)	0	100	100
48	o	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
49	p	84/89 (94%)	83 (99%)	1 (1%)	0	100	100
50	q	88/91 (97%)	86 (98%)	2 (2%)	0	100	100
51	r	79/87 (91%)	76 (96%)	3 (4%)	0	100	100
52	s	62/80 (78%)	62 (100%)	0	0	100	100
53	t	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
54	u	79/83 (95%)	77 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6164/6654 (93%)	6017 (98%)	143 (2%)	4 (0%)	49 75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	E	555	ALA
39	f	82	PRO
44	k	57	LYS
36	c	71	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	51/52 (98%)	51 (100%)	0	100 100
2	2	59/62 (95%)	58 (98%)	1 (2%)	53 71
3	3	52/53 (98%)	51 (98%)	1 (2%)	50 69
4	4	56/75 (75%)	55 (98%)	1 (2%)	51 70
5	5	48/50 (96%)	48 (100%)	0	100 100
6	6	46/47 (98%)	46 (100%)	0	100 100
7	7	39/40 (98%)	39 (100%)	0	100 100
8	8	56/57 (98%)	56 (100%)	0	100 100
9	9	35/35 (100%)	35 (100%)	0	100 100
12	C	162/162 (100%)	160 (99%)	2 (1%)	63 75
14	E	552/579 (95%)	546 (99%)	6 (1%)	65 76
15	G	220/224 (98%)	220 (100%)	0	100 100
16	H	173/177 (98%)	173 (100%)	0	100 100
17	I	168/169 (99%)	167 (99%)	1 (1%)	78 81
18	J	156/158 (99%)	152 (97%)	4 (3%)	40 65
19	K	154/155 (99%)	154 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	M	123/123 (100%)	123 (100%)	0	100	100
21	N	100/100 (100%)	100 (100%)	0	100	100
22	O	112/112 (100%)	112 (100%)	0	100	100
23	P	113/119 (95%)	113 (100%)	0	100	100
24	Q	101/102 (99%)	101 (100%)	0	100	100
25	R	95/95 (100%)	95 (100%)	0	100	100
26	S	100/102 (98%)	98 (98%)	2 (2%)	48	69
27	T	97/98 (99%)	97 (100%)	0	100	100
28	U	86/86 (100%)	86 (100%)	0	100	100
29	V	90/94 (96%)	89 (99%)	1 (1%)	65	76
30	W	81/82 (99%)	81 (100%)	0	100	100
31	X	87/90 (97%)	87 (100%)	0	100	100
32	Y	83/190 (44%)	82 (99%)	1 (1%)	63	75
33	Z	59/75 (79%)	59 (100%)	0	100	100
36	c	192/221 (87%)	191 (100%)	1 (0%)	81	82
37	d	165/175 (94%)	164 (99%)	1 (1%)	78	81
38	e	174/175 (99%)	174 (100%)	0	100	100
39	f	123/131 (94%)	123 (100%)	0	100	100
40	g	82/86 (95%)	82 (100%)	0	100	100
41	h	124/132 (94%)	123 (99%)	1 (1%)	73	79
42	i	112/113 (99%)	112 (100%)	0	100	100
43	j	106/109 (97%)	105 (99%)	1 (1%)	70	78
44	k	88/91 (97%)	87 (99%)	1 (1%)	65	76
45	l	94/104 (90%)	93 (99%)	1 (1%)	65	76
46	m	117/119 (98%)	117 (100%)	0	100	100
47	n	99/104 (95%)	98 (99%)	1 (1%)	68	77
48	o	52/53 (98%)	52 (100%)	0	100	100
49	p	79/81 (98%)	78 (99%)	1 (1%)	61	74
50	q	76/77 (99%)	76 (100%)	0	100	100
51	r	76/82 (93%)	76 (100%)	0	100	100
52	s	57/68 (84%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	t	72/80 (90%)	71 (99%)	1 (1%)	59	73
54	u	67/69 (97%)	67 (100%)	0	100	100
All	All	5309/5633 (94%)	5280 (100%)	29 (0%)	78	82

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	42	ARG
3	3	3	LYS
4	4	45	VAL
12	C	53	LEU
12	C	113	VAL
14	E	369	VAL
14	E	495	LYS
14	E	498	ARG
14	E	506	TYR
14	E	532	VAL
14	E	609	ILE
17	I	49	HIS
18	J	54	VAL
18	J	89	VAL
18	J	117	VAL
18	J	132	VAL
26	S	41	ARG
26	S	42	ILE
29	V	11	ARG
32	Y	4	LEU
36	c	134	VAL
37	d	91	ASN
41	h	117	GLU
43	j	7	GLU
44	k	72	ARG
45	l	12	VAL
47	n	9	ILE
49	p	27	VAL
53	t	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	17	GLN
4	4	10	HIS
4	4	55	HIS
5	5	14	ASN
12	C	32	ASN
14	E	294	ASN
14	E	661	ASN
15	G	114	GLN
15	G	134	ASN
15	G	153	GLN
15	G	199	GLN
16	H	14	GLN
16	H	136	GLN
16	H	181	GLN
16	H	200	ASN
17	I	38	ASN
17	I	119	GLN
17	I	188	ASN
18	J	45	GLN
18	J	161	ASN
19	K	99	GLN
20	M	119	GLN
20	M	137	GLN
23	P	13	HIS
24	Q	106	GLN
28	U	81	ASN
29	V	40	ASN
31	X	76	ASN
32	Y	38	ASN
36	c	93	ASN
37	d	61	ASN
37	d	91	ASN
37	d	118	ASN
37	d	122	GLN
37	d	151	GLN
39	f	145	GLN
40	g	77	GLN
41	h	67	ASN
41	h	153	HIS
42	i	18	ASN
43	j	77	GLN
44	k	56	HIS
45	l	77	HIS

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Mol	Chain	Res	Type
47	n	76	ASN
53	t	43	ASN
54	u	82	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2803/2923 (95%)	405 (14%)	94 (3%)
11	B	112/115 (97%)	14 (12%)	4 (3%)
13	D	92/93 (98%)	13 (14%)	2 (2%)
34	a	1531/1555 (98%)	274 (17%)	0
35	b	14/24 (58%)	4 (28%)	0
All	All	4552/4710 (96%)	710 (15%)	100 (2%)

All (710) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	12	U
10	A	34	U
10	A	71	A
10	A	75	G
10	A	90	A
10	A	91	A
10	A	117	A
10	A	118	A
10	A	119	U
10	A	167	U
10	A	168	A
10	A	176	A
10	A	177	G
10	A	183	A
10	A	199	A
10	A	202	A
10	A	203	U
10	A	218	G
10	A	219	A
10	A	224	A
10	A	225	A
10	A	233	U
10	A	251	G
10	A	255	G

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Mol	Chain	Res	Type
10	A	269	G
10	A	270	C
10	A	289	U
10	A	299	U
10	A	300	G
10	A	314	A
10	A	315	C
10	A	321	U
10	A	324	A
10	A	354	A
10	A	373	A
10	A	374	U
10	A	388	A
10	A	389	A
10	A	404	U
10	A	406	A
10	A	410	G
10	A	411	A
10	A	429	C
10	A	432	G
10	A	449	U
10	A	450	C
10	A	457	G
10	A	458	A
10	A	492	G
10	A	493	A
10	A	497	U
10	A	502	C
10	A	520	G
10	A	521	U
10	A	527	G
10	A	548	A
10	A	549	U
10	A	550	A
10	A	553	A
10	A	555	C
10	A	574	A
10	A	575	G
10	A	576	U
10	A	577	A
10	A	578	G
10	A	593	U

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Mol	Chain	Res	Type
10	A	594	G
10	A	606	G
10	A	614	U
10	A	615	A
10	A	616	G
10	A	618	A
10	A	630	G
10	A	646	A
10	A	650	U
10	A	679	G
10	A	682	A
10	A	683	G
10	A	690	U
10	A	696	G
10	A	700	A
10	A	701	G
10	A	713	A
10	A	731	U
10	A	760	A
10	A	761	A
10	A	771	G
10	A	774	G
10	A	775	A
10	A	792	5MU
10	A	807	U
10	A	808	G
10	A	820	G
10	A	827	A
10	A	829	U
10	A	835	U
10	A	838	A
10	A	847	A
10	A	850	G
10	A	857	C
10	A	872	U
10	A	873	U
10	A	891	A
10	A	903	G
10	A	904	G
10	A	910	C
10	A	911	A
10	A	912	C

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Mol	Chain	Res	Type
10	A	920	A
10	A	923	A
10	A	924	G
10	A	943	C
10	A	944	G
10	A	945	A
10	A	955	A
10	A	960	C
10	A	969	A
10	A	970	U
10	A	971	U
10	A	985	A
10	A	988	C
10	A	989	A
10	A	990	G
10	A	1005	G
10	A	1018	A
10	A	1027	A
10	A	1040	A
10	A	1053	A
10	A	1056	U
10	A	1057	A
10	A	1066	G
10	A	1070	A
10	A	1077	U
10	A	1090	A
10	A	1091	G
10	A	1111	A
10	A	1112	G
10	A	1113	A
10	A	1114	A
10	A	1117	A
10	A	1119	C
10	A	1124	A
10	A	1126	U
10	A	1129	A
10	A	1132	A
10	A	1133	G
10	A	1134	U
10	A	1141	U
10	A	1142	A
10	A	1149	U

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Mol	Chain	Res	Type
10	A	1155	A
10	A	1156	G
10	A	1174	U
10	A	1176	U
10	A	1177	A
10	A	1178	C
10	A	1179	C
10	A	1186	A
10	A	1215	U
10	A	1216	U
10	A	1217	U
10	A	1265	G
10	A	1276	G
10	A	1291	A
10	A	1292	A
10	A	1294	G
10	A	1309	G
10	A	1310	A
10	A	1318	G
10	A	1326	C
10	A	1337	A
10	A	1345	A
10	A	1351	C
10	A	1357	G
10	A	1358	A
10	A	1381	U
10	A	1382	C
10	A	1402	A
10	A	1405	G
10	A	1415	A
10	A	1416	U
10	A	1417	G
10	A	1421	A
10	A	1433	U
10	A	1434	U
10	A	1440	A
10	A	1449	A
10	A	1451	U
10	A	1455	U
10	A	1456	U
10	A	1457	U
10	A	1458	A

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Mol	Chain	Res	Type
10	A	1459	A
10	A	1463	A
10	A	1471	A
10	A	1472	C
10	A	1481	A
10	A	1490	G
10	A	1497	A
10	A	1504	U
10	A	1505	G
10	A	1511	C
10	A	1526	G
10	A	1533	A
10	A	1536	C
10	A	1537	A
10	A	1552	U
10	A	1553	A
10	A	1560	A
10	A	1569	G
10	A	1574	G
10	A	1578	A
10	A	1586	U
10	A	1606	C
10	A	1614	A
10	A	1616	A
10	A	1625	U
10	A	1631	G
10	A	1635	A
10	A	1651	C
10	A	1652	A
10	A	1658	A
10	A	1690	A
10	A	1691	G
10	A	1692	C
10	A	1718	G
10	A	1740	G
10	A	1742	A
10	A	1747	G
10	A	1758	A
10	A	1759	G
10	A	1772	G
10	A	1783	G
10	A	1789	A

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Mol	Chain	Res	Type
10	A	1790	G
10	A	1791	G
10	A	1800	A
10	A	1809	C
10	A	1813	A
10	A	1814	A
10	A	1818	A
10	A	1827	C
10	A	1828	U
10	A	1829	A
10	A	1843	U
10	A	1856	A
10	A	1874	A
10	A	1875	A
10	A	1885	G
10	A	1896	U
10	A	1899	U
10	A	1907	U
10	A	1927	A
10	A	1928	A
10	A	1933	G
10	A	1934	G
10	A	1939	A
10	A	1940	A
10	A	1941	C
10	A	1949	G
10	A	1950	U
10	A	1951	C
10	A	1952	C
10	A	1953	U
10	A	1954	A
10	A	1955	A
10	A	1957	G
10	A	1958	U
10	A	1963	A
10	A	1964	A
10	A	1965	A
10	A	1982	U
10	A	1994	C
10	A	1997	A
10	A	1998	A
10	A	1999	G

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Mol	Chain	Res	Type
10	A	2009	U
10	A	2019	G
10	A	2020	U
10	A	2040	A
10	A	2047	A
10	A	2050	A
10	A	2057	A
10	A	2058	A
10	A	2059	G
10	A	2060	A
10	A	2062	G
10	A	2063	C
10	A	2070	C
10	A	2082	C
10	A	2083	G
10	A	2087	A
10	A	2088	G
10	A	2089	A
10	A	2096	G
10	A	2120	G
10	A	2215	U
10	A	2217	G
10	A	2226	A
10	A	2237	U
10	A	2238	U
10	A	2239	A
10	A	2252	A
10	A	2265	G
10	A	2295	A
10	A	2305	A
10	A	2306	G
10	A	2309	G
10	A	2310	C
10	A	2313	A
10	A	2314	A
10	A	2315	A
10	A	2316	G
10	A	2333	U
10	A	2334	G
10	A	2335	G
10	A	2339	U
10	A	2347	A

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Mol	Chain	Res	Type
10	A	2348	G
10	A	2349	A
10	A	2352	G
10	A	2358	G
10	A	2361	U
10	A	2362	A
10	A	2374	C
10	A	2377	C
10	A	2406	G
10	A	2410	G
10	A	2412	C
10	A	2416	G
10	A	2418	G
10	A	2429	U
10	A	2433	C
10	A	2437	G
10	A	2449	C
10	A	2450	U
10	A	2451	C
10	A	2452	A
10	A	2455	G
10	A	2456	G
10	A	2457	A
10	A	2458	U
10	A	2468	C
10	A	2474	G
10	A	2475	A
10	A	2486	A
10	A	2495	A
10	A	2496	A
10	A	2502	C
10	A	2505	A
10	A	2521	G
10	A	2529	G
10	A	2530	2MA
10	A	2532	G
10	A	2545	A
10	A	2556	G
10	A	2557	U
10	A	2562	G
10	A	2583	C
10	A	2593	A

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Mol	Chain	Res	Type
10	A	2594	G
10	A	2600	C
10	A	2605	G
10	A	2612	U
10	A	2613	C
10	A	2629	A
10	A	2630	G
10	A	2637	C
10	A	2640	U
10	A	2641	A
10	A	2642	U
10	A	2665	G
10	A	2666	A
10	A	2672	G
10	A	2673	C
10	A	2692	A
10	A	2716	U
10	A	2718	C
10	A	2741	G
10	A	2753	U
10	A	2760	A
10	A	2769	G
10	A	2771	G
10	A	2777	A
10	A	2784	A
10	A	2791	A
10	A	2792	A
10	A	2805	A
10	A	2806	U
10	A	2807	G
10	A	2816	C
10	A	2817	A
10	A	2824	G
10	A	2827	A
10	A	2828	U
10	A	2843	A
10	A	2850	G
10	A	2852	U
10	A	2887	G
10	A	2888	A
10	A	2892	G
10	A	2893	A

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Mol	Chain	Res	Type
10	A	2894	C
10	A	2912	A
10	A	2913	G
11	B	10	U
11	B	27	A
11	B	33	U
11	B	42	G
11	B	43	A
11	B	51	A
11	B	54	U
11	B	55	A
11	B	64	A
11	B	65	G
11	B	87	C
11	B	88	G
11	B	105	C
11	B	106	G
13	D	7	G
13	D	8	4SU
13	D	16	A
13	D	18	G
13	D	20(B)	G
13	D	47(B)	G
13	D	47(C)	G
13	D	47(F)	A
13	D	48	C
13	D	65	G
13	D	66	C
13	D	74	C
13	D	76	A
34	a	6	U
34	a	7	G
34	a	8	G
34	a	9	A
34	a	10	G
34	a	32	G
34	a	33	A
34	a	40	G
34	a	48	C
34	a	49	C
34	a	50	U
34	a	51	A

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Mol	Chain	Res	Type
34	a	52	A
34	a	74	G
34	a	75	A
34	a	79	G
34	a	82	G
34	a	83	C
34	a	84	U
34	a	85	U
34	a	86	G
34	a	91	U
34	a	94	G
34	a	95	A
34	a	97	G
34	a	100	A
34	a	115	A
34	a	118	A
34	a	119	A
34	a	120	C
34	a	129	A
34	a	131	C
34	a	146	G
34	a	159	G
34	a	173	U
34	a	183	U
34	a	190	A
34	a	212	A
34	a	213	G
34	a	220	U
34	a	221	U
34	a	222	G
34	a	248	U
34	a	249	G
34	a	255	G
34	a	258	A
34	a	259	G
34	a	261	U
34	a	274	G
34	a	275	C
34	a	284	G
34	a	285	C
34	a	297	G
34	a	313	G

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Mol	Chain	Res	Type
34	a	314	A
34	a	324	C
34	a	329	A
34	a	335	A
34	a	336	C
34	a	338	C
34	a	340	G
34	a	355	G
34	a	360	C
34	a	362	G
34	a	364	A
34	a	375	U
34	a	380	C
34	a	392	G
34	a	400	G
34	a	405	A
34	a	413	U
34	a	414	G
34	a	419	A
34	a	420	U
34	a	421	G
34	a	422	A
34	a	429	U
34	a	430	C
34	a	431	G
34	a	432	G
34	a	437	U
34	a	447	U
34	a	456	A
34	a	461	C
34	a	478	G
34	a	483	C
34	a	484	A
34	a	486	C
34	a	492	G
34	a	493	G
34	a	494	U
34	a	505	A
34	a	513	G
34	a	519	C
34	a	526	C
34	a	529	G

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Mol	Chain	Res	Type
34	a	532	G
34	a	535	G7M
34	a	540	A
34	a	541	A
34	a	542	U
34	a	544	C
34	a	553	C
34	a	555	A
34	a	567	A
34	a	569	U
34	a	570	U
34	a	572	U
34	a	580	A
34	a	581	A
34	a	584	C
34	a	626	C
34	a	640	G
34	a	650	A
34	a	658	A
34	a	661	U
34	a	669	G
34	a	673	A
34	a	696	G
34	a	710	A
34	a	711	G
34	a	729	A
34	a	730	G
34	a	731	U
34	a	742	A
34	a	757	A
34	a	763	G
34	a	785	A
34	a	790	A
34	a	800	A
34	a	801	U
34	a	802	A
34	a	823	A
34	a	825	C
34	a	826	G
34	a	836	A
34	a	864	G
34	a	876	G

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Mol	Chain	Res	Type
34	a	881	A
34	a	883	G
34	a	885	A
34	a	894	G
34	a	899	G
34	a	911	G
34	a	923	A
34	a	924	A
34	a	935	G
34	a	936	G
34	a	940	C
34	a	943	C
34	a	944	A
34	a	948	G
34	a	969	U
34	a	978	A
34	a	980	G
34	a	983	A
34	a	984	A
34	a	986	A
34	a	996	A
34	a	1001	U
34	a	1002	G
34	a	1013	A
34	a	1014	C
34	a	1015	A
34	a	1017	C
34	a	1018	U
34	a	1030	G
34	a	1031	C
34	a	1032	C
34	a	1033	U
34	a	1034	U
34	a	1035	C
34	a	1036	C
34	a	1046	G
34	a	1047	A
34	a	1048	C
34	a	1057	A
34	a	1067	U
34	a	1074	C
34	a	1076	U

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Mol	Chain	Res	Type
34	a	1077	C
34	a	1079	G
34	a	1096	U
34	a	1102	U
34	a	1105	G
34	a	1106	U
34	a	1111	C
34	a	1112	A
34	a	1134	A
34	a	1135	G
34	a	1136	U
34	a	1140	C
34	a	1141	A
34	a	1149	G
34	a	1156	A
34	a	1160	U
34	a	1167	A
34	a	1168	C
34	a	1169	U
34	a	1170	G
34	a	1174	G
34	a	1175	U
34	a	1177	A
34	a	1178	C
34	a	1179	A
34	a	1192	G
34	a	1194	G
34	a	1195	G
34	a	1206	A
34	a	1207	A
34	a	1211	A
34	a	1212	U
34	a	1222	U
34	a	1223	A
34	a	1224	U
34	a	1225	G
34	a	1236	C
34	a	1237	A
34	a	1246	A
34	a	1248	A
34	a	1249	A
34	a	1250	U

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Mol	Chain	Res	Type
34	a	1251	G
34	a	1258	A
34	a	1266	C
34	a	1267	A
34	a	1268	G
34	a	1270	G
34	a	1289	A
34	a	1295	A
34	a	1296	U
34	a	1297	A
34	a	1298	A
34	a	1303	G
34	a	1307	U
34	a	1309	A
34	a	1310	G
34	a	1311	U
34	a	1312	U
34	a	1313	C
34	a	1330	C
34	a	1333	G
34	a	1341	G
34	a	1346	U
34	a	1348	G
34	a	1356	A
34	a	1374	U
34	a	1385	A
34	a	1388	C
34	a	1389	G
34	a	1408	A
34	a	1416	U
34	a	1429	G
34	a	1436	A
34	a	1452	G
34	a	1456	A
34	a	1460	U
34	a	1463	U
34	a	1464	A
34	a	1486	G
34	a	1503	A
34	a	1504	A
34	a	1505	G
34	a	1513	A

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Mol	Chain	Res	Type
34	a	1517	U
34	a	1528	G
34	a	1530	MA6
34	a	1531	G
34	a	1539	U
34	a	1540	G
34	a	1541	G
34	a	1545	A
34	a	1546	C
34	a	1547	C
35	b	7	G
35	b	11	U
35	b	17	U
35	b	18	G

All (100) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	50	U
10	A	90	A
10	A	108	A
10	A	118	A
10	A	176	A
10	A	182	C
10	A	202	A
10	A	258	A
10	A	298	U
10	A	366	G
10	A	374	U
10	A	388	A
10	A	449	U
10	A	480	U
10	A	492	G
10	A	493	A
10	A	520	G
10	A	548	A
10	A	557	G
10	A	569	U
10	A	574	A
10	A	614	U
10	A	807	U
10	A	809	A

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Mol	Chain	Res	Type
10	A	891	A
10	A	903	G
10	A	910	C
10	A	911	A
10	A	923	A
10	A	969	A
10	A	988	C
10	A	1028	G
10	A	1112	G
10	A	1133	G
10	A	1135	G
10	A	1176	U
10	A	1177	A
10	A	1178	C
10	A	1185	U
10	A	1186	A
10	A	1224	U
10	A	1291	A
10	A	1348	U
10	A	1357	G
10	A	1381	U
10	A	1433	U
10	A	1434	U
10	A	1504	U
10	A	1646	U
10	A	1651	C
10	A	1691	G
10	A	1750	U
10	A	1789	A
10	A	1813	A
10	A	1826	G
10	A	1874	A
10	A	1927	A
10	A	1933	G
10	A	1940	A
10	A	1950	U
10	A	1951	C
10	A	1953	U
10	A	1954	A
10	A	2049	U
10	A	2062	G
10	A	2094	G

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Mol	Chain	Res	Type
10	A	2237	U
10	A	2309	G
10	A	2313	A
10	A	2315	A
10	A	2334	G
10	A	2338	A
10	A	2347	A
10	A	2373	A
10	A	2418	G
10	A	2429	U
10	A	2449	C
10	A	2450	U
10	A	2457	A
10	A	2485	U
10	A	2495	A
10	A	2612	U
10	A	2641	A
10	A	2665	G
10	A	2672	G
10	A	2783	U
10	A	2791	A
10	A	2805	A
10	A	2807	G
10	A	2816	C
10	A	2822	C
10	A	2887	G
10	A	2893	A
10	A	2912	A
11	B	32	U
11	B	42	G
11	B	64	A
11	B	105	C
13	D	60	U
13	D	65	G

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

22 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
13	5MU	D	54	13	19,22,23	0.27	0	28,32,35	0.27	0
34	2MG	a	975	34	23,26,27	0.39	0	32,38,41	0.37	0
34	4OC	a	1412	34	20,23,24	0.39	0	26,32,35	0.59	0
34	MA6	a	1529	34	23,26,27	0.26	0	34,38,41	0.72	1 (2%)
10	G7M	A	2601	56,10	23,26,27	0.68	1 (4%)	35,39,42	0.55	0
13	PSU	D	55	13	18,21,22	0.92	1 (5%)	22,30,33	0.57	0
10	H2U	A	2476	10	18,21,22	0.60	0	21,30,33	0.83	1 (4%)
13	RSP	D	32	13	17,21,22	0.38	0	22,30,33	0.84	1 (4%)
13	4SU	D	8	13	18,21,22	0.39	0	26,30,33	1.20	3 (11%)
34	5MC	a	976	34	18,22,23	0.32	0	26,32,35	0.49	0
10	OMG	A	2278	10	23,26,27	0.31	0	33,38,41	0.56	1 (3%)
10	5MU	A	792	10	19,22,23	0.25	0	28,32,35	0.35	0
10	2MA	A	2530	56,10	22,25,26	0.23	0	33,37,40	0.69	2 (6%)
10	5MU	A	1966	10	19,22,23	0.31	0	28,32,35	0.35	0
34	UR3	a	1509	34	19,22,23	0.29	0	26,32,35	0.75	1 (3%)
10	3TD	A	1942	10	18,22,23	0.93	1 (5%)	22,32,35	0.76	0
34	MA6	a	1530	34	23,26,27	0.28	0	34,38,41	0.69	1 (2%)
10	2MG	A	2472	10	23,26,27	0.40	0	32,38,41	0.36	0
10	OMG	A	2580	10	23,26,27	0.34	0	33,38,41	0.38	0
13	H2U	D	20(A)	13	18,21,22	0.66	0	21,30,33	0.85	0
34	G7M	a	535	34	23,26,27	0.70	1 (4%)	35,39,42	0.61	0
13	T6A	D	37	13	31,34,35	0.49	0	44,49,52	0.60	0

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
13	5MU	D	54	13	-	0/7/25/26	0/2/2/2
34	2MG	a	975	34	-	0/9/27/28	0/3/3/3
34	4OC	a	1412	34	-	0/9/29/30	0/2/2/2
34	MA6	a	1529	34	-	0/11/29/30	0/3/3/3
10	G7M	A	2601	56,10	-	0/7/25/26	0/3/3/3
13	PSU	D	55	13	-	0/7/25/26	0/2/2/2
10	H2U	A	2476	10	-	0/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	RSP	D	32	13	-	0/7/25/26	0/2/2/2
13	4SU	D	8	13	-	0/7/25/26	0/2/2/2
34	5MC	a	976	34	-	0/7/25/26	0/2/2/2
10	OMG	A	2278	10	-	3/9/27/28	0/3/3/3
10	5MU	A	792	10	-	0/7/25/26	0/2/2/2
10	2MA	A	2530	56,10	-	1/7/25/26	0/3/3/3
10	5MU	A	1966	10	-	0/7/25/26	0/2/2/2
34	UR3	a	1509	34	-	2/7/25/26	0/2/2/2
10	3TD	A	1942	10	-	0/7/25/26	0/2/2/2
34	MA6	a	1530	34	-	3/11/29/30	0/3/3/3
10	2MG	A	2472	10	-	0/9/27/28	0/3/3/3
10	OMG	A	2580	10	-	2/9/27/28	0/3/3/3
13	H2U	D	20(A)	13	-	5/7/38/39	0/2/2/2
34	G7M	a	535	34	-	2/7/25/26	0/3/3/3
13	T6A	D	37	13	-	0/23/41/42	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	55	PSU	C6-C5	3.60	1.39	1.35
10	A	1942	3TD	C6-C5	3.49	1.39	1.35
34	a	535	G7M	C8-N7	2.40	1.37	1.33
10	A	2601	G7M	C8-N7	2.24	1.37	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	8	4SU	C4-N3-C2	-4.27	123.19	127.34
34	a	1529	MA6	C2-N1-C6	2.92	118.66	111.75
34	a	1530	MA6	C2-N1-C6	2.91	118.62	111.75
13	D	32	RSP	C3'-C2'-C1'	2.70	106.55	101.43
10	A	2278	OMG	O2'-C2'-C1'	2.66	114.27	109.08
13	D	8	4SU	C5-C4-N3	2.64	117.14	114.69
10	A	2530	2MA	C5-C4-N3	-2.45	124.44	127.19
13	D	8	4SU	N3-C2-N1	2.31	117.95	114.89
10	A	2530	2MA	N3-C4-N9	2.16	129.99	126.99
34	a	1509	UR3	C6-N1-C2	-2.13	119.88	121.79
10	A	2476	H2U	O2-C2-N1	-2.05	120.53	123.11

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	535	G7M	C3'-C4'-C5'-O5'
10	A	2278	OMG	C1'-C2'-O2'-CM2
13	D	20(A)	H2U	O4'-C4'-C5'-O5'
13	D	20(A)	H2U	C3'-C4'-C5'-O5'
13	D	20(A)	H2U	C2'-C1'-N1-C6
34	a	535	G7M	O4'-C4'-C5'-O5'
34	a	1530	MA6	C3'-C4'-C5'-O5'
10	A	2278	OMG	O4'-C4'-C5'-O5'
34	a	1530	MA6	O4'-C4'-C5'-O5'
10	A	2278	OMG	C3'-C4'-C5'-O5'
34	a	1509	UR3	O4'-C4'-C5'-O5'
13	D	20(A)	H2U	C2'-C1'-N1-C2
13	D	20(A)	H2U	O4'-C1'-N1-C2
34	a	1530	MA6	C4'-C5'-O5'-P
34	a	1509	UR3	C3'-C4'-C5'-O5'
10	A	2580	OMG	O4'-C4'-C5'-O5'
10	A	2530	2MA	O4'-C4'-C5'-O5'
10	A	2580	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	1412	4OC	1	0
13	D	32	RSP	1	0
34	a	976	5MC	1	0
10	A	2278	OMG	1	0
10	A	1942	3TD	1	0
34	a	1530	MA6	3	0
13	D	37	T6A	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 93 are monoatomic - leaving 2 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$
57	GDP	E	701	-	28,30,30	0.46	0	44,47,47	0.44	0
58	FUA	E	703	-	39,40,40	1.46	3 (7%)	49,64,64	1.10	3 (6%)

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
57	GDP	E	701	-	-	1/16/32/32	0/3/3/3
58	FUA	E	703	-	-	5/15/92/92	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	E	703	FUA	C29-C22	-7.68	1.36	1.47
58	E	703	FUA	C9-C11	2.61	1.58	1.54
58	E	703	FUA	O5-C29	-2.45	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	E	703	FUA	C16-O2-C31	2.43	120.75	117.06
58	E	703	FUA	C6-C7-C8	2.19	116.61	112.84
58	E	703	FUA	C18-C4-C5	2.14	116.06	113.04

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	E	703	FUA	C13-C17-C22-C29
58	E	703	FUA	C17-C22-C29-O5
58	E	703	FUA	C32-C31-O2-C16
58	E	703	FUA	O3-C31-O2-C16

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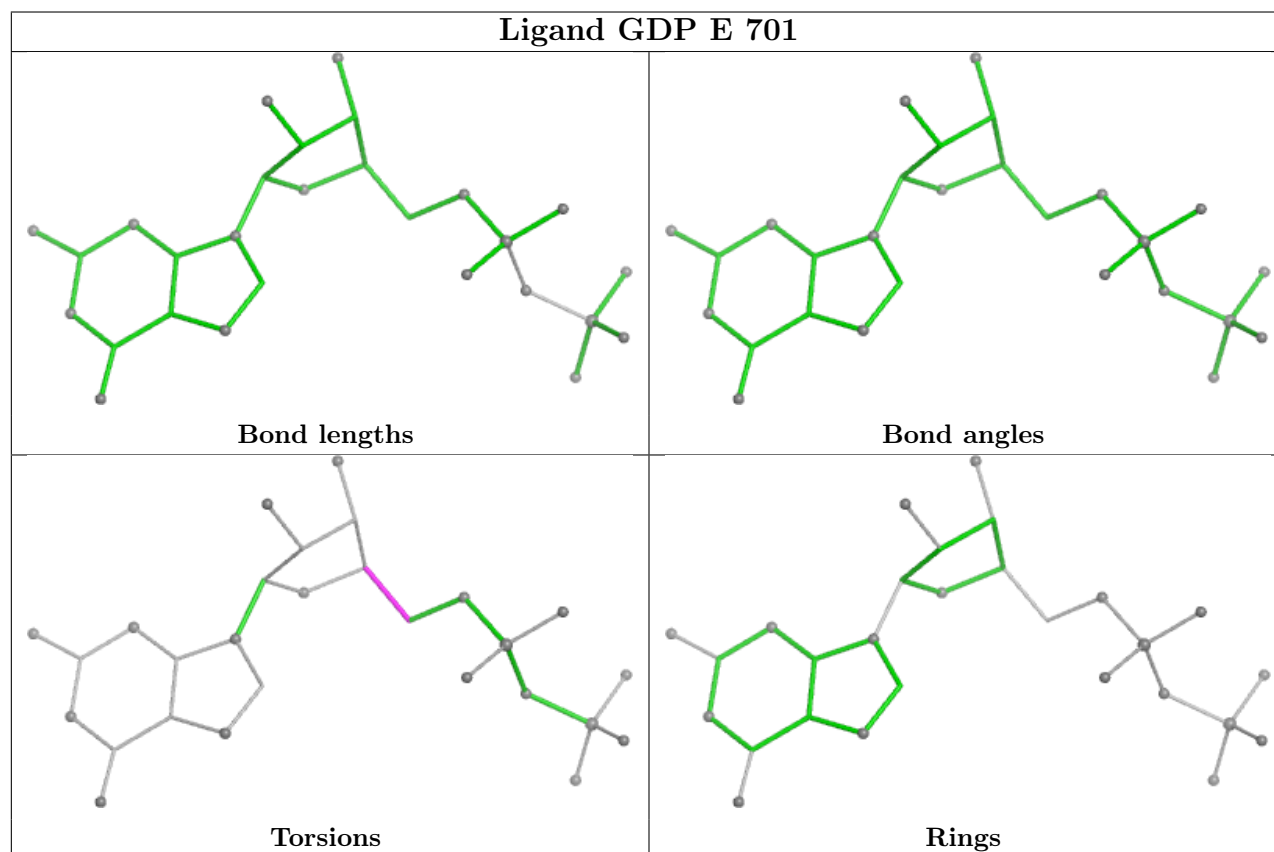
Mol	Chain	Res	Type	Atoms
57	E	701	GDP	O4'-C4'-C5'-O5'
58	E	703	FUA	C17-C22-C29-O4

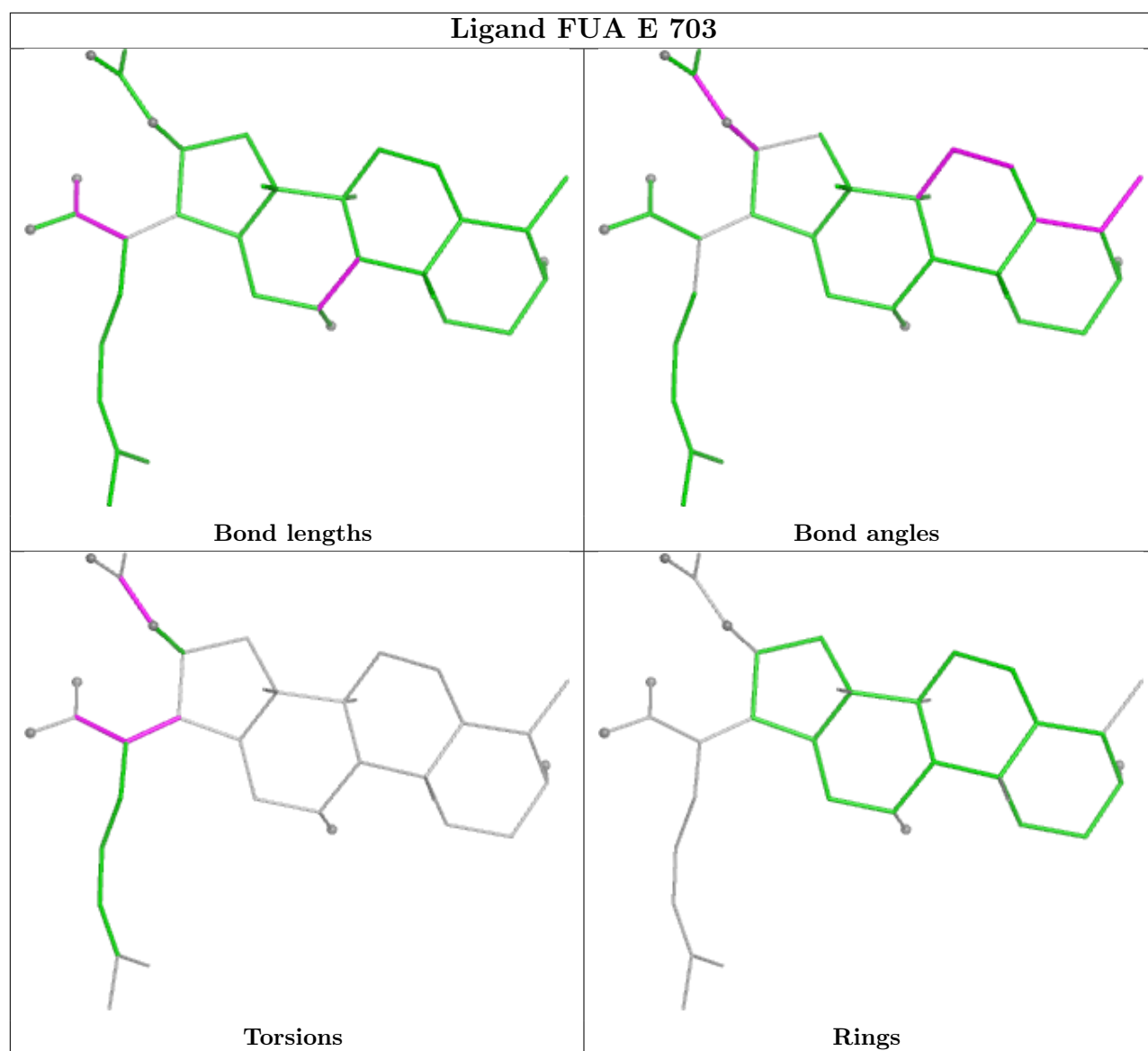
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	E	703	FUA	4	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.

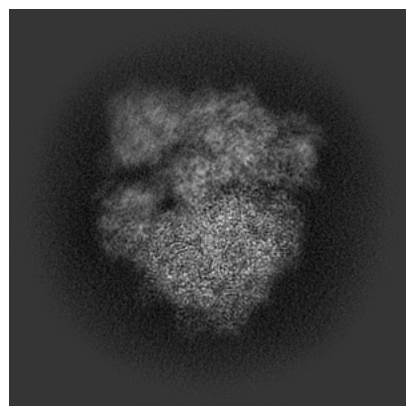
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55948. These allow visual inspection of the internal detail of the map and identification of artifacts.

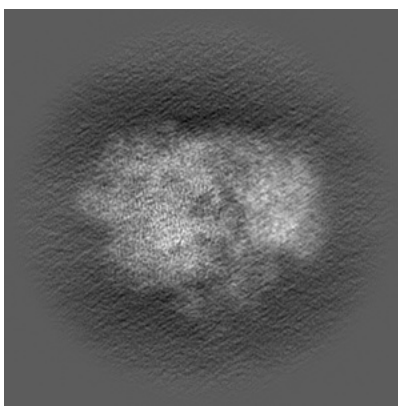
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

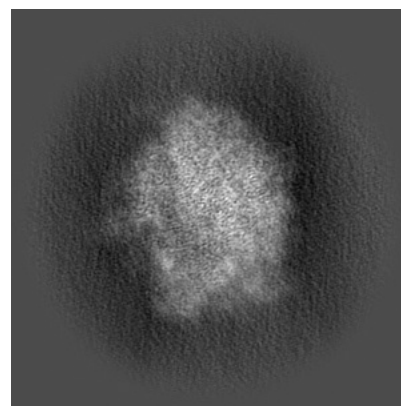
6.1.1 Primary map



X

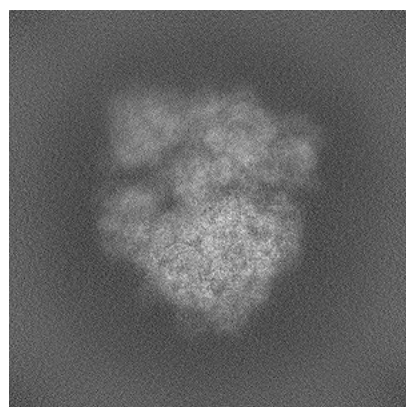


Y

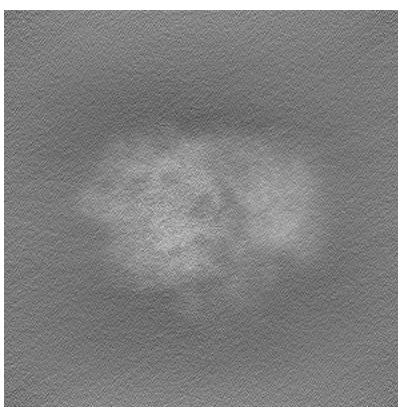


Z

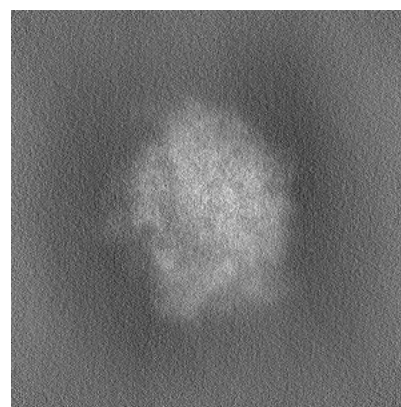
6.1.2 Raw map



X



Y

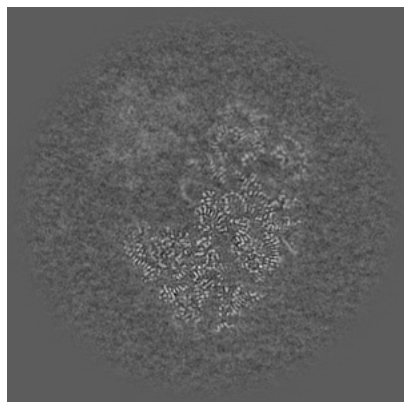


Z

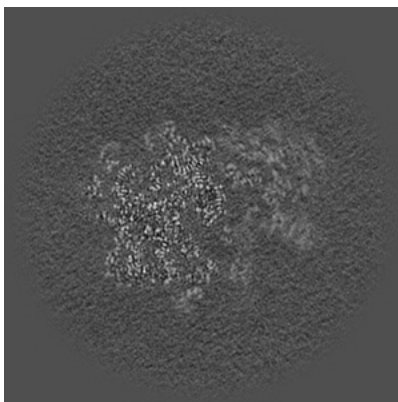
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

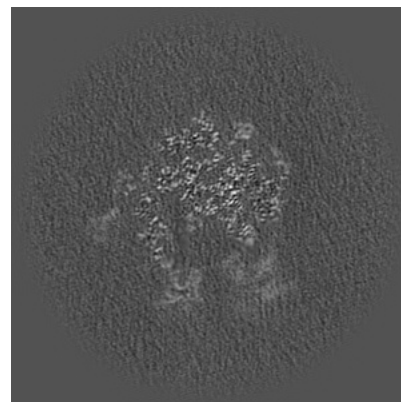
6.2.1 Primary map



X Index: 300

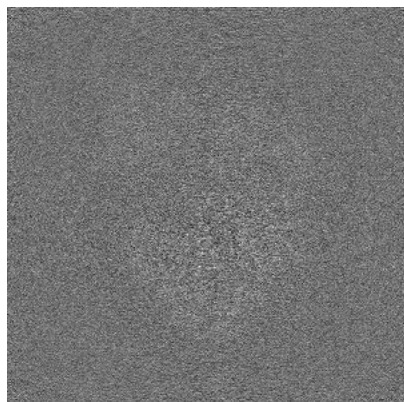


Y Index: 300

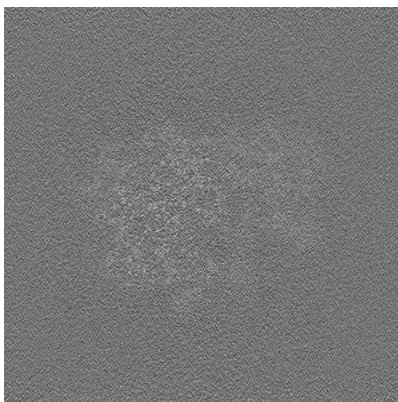


Z Index: 300

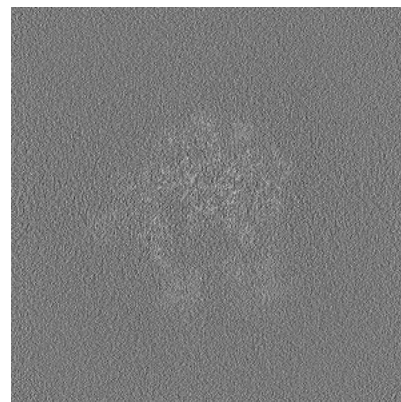
6.2.2 Raw map



X Index: 300



Y Index: 300

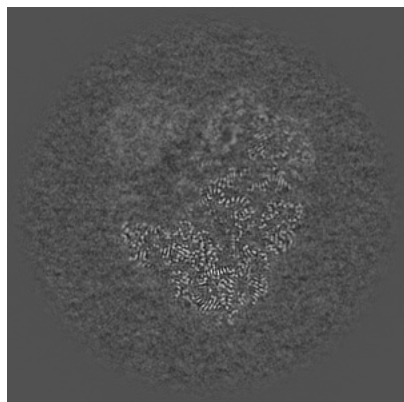


Z Index: 300

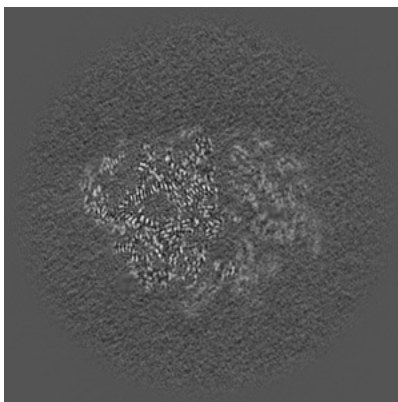
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

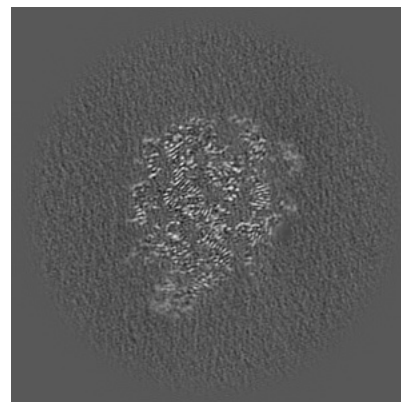
6.3.1 Primary map



X Index: 287

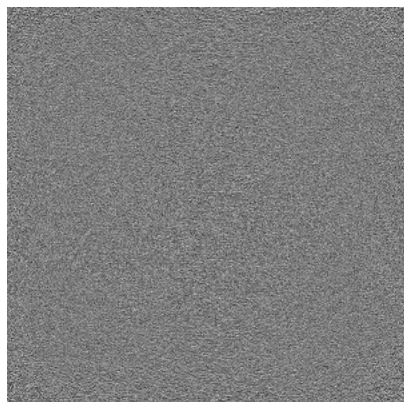


Y Index: 329

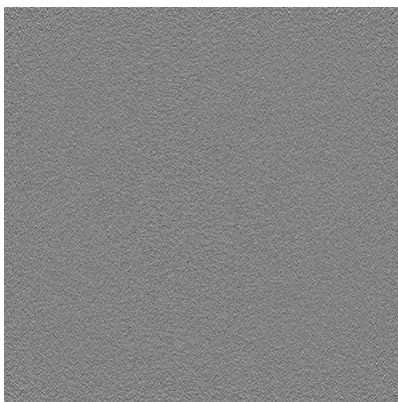


Z Index: 243

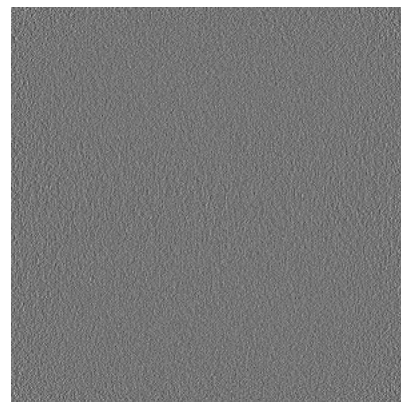
6.3.2 Raw map



X Index: 0



Y Index: 0

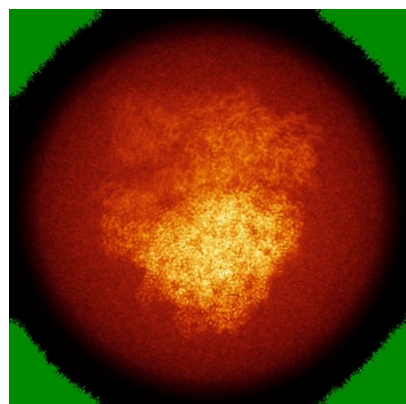


Z Index: 0

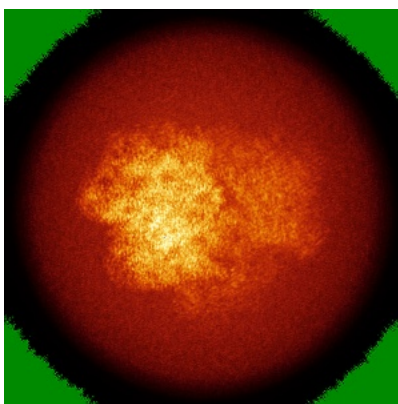
The images above show the largest variance slices of the map in three orthogonal directions.

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

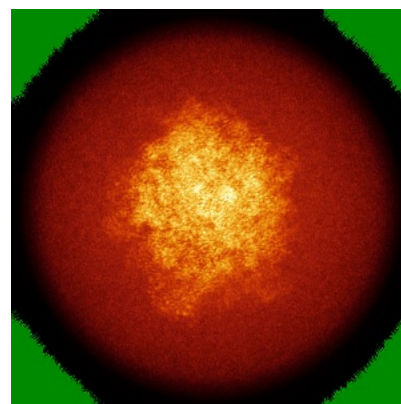
6.4.1 Primary map



X

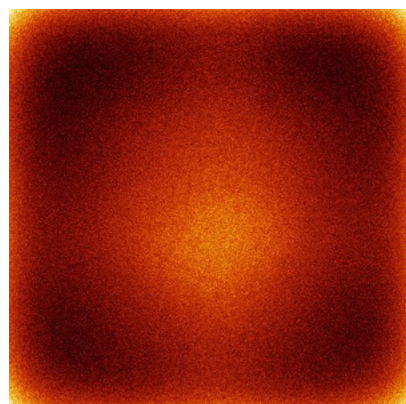


Y

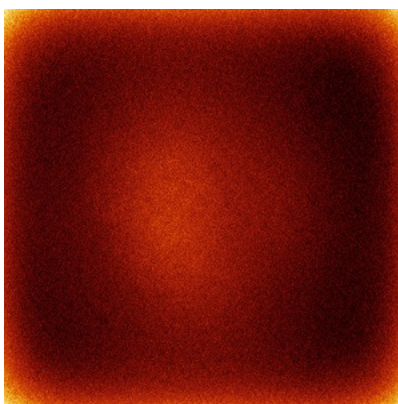


Z

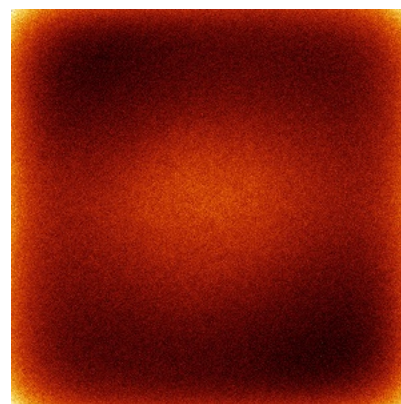
6.4.2 Raw map



X



Y

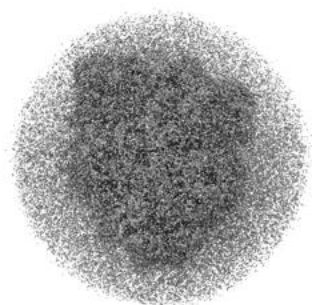


Z

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

6.5 Orthogonal surface views [i](#)

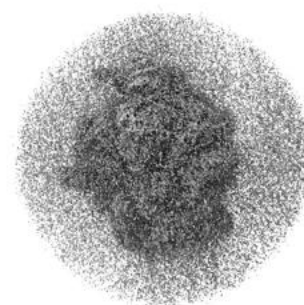
6.5.1 Primary map



X



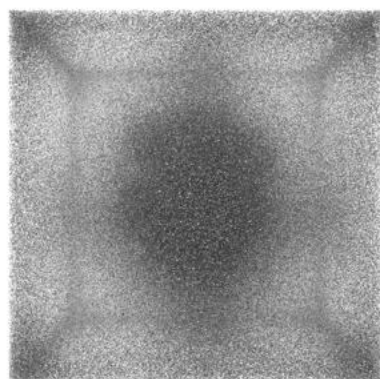
Y



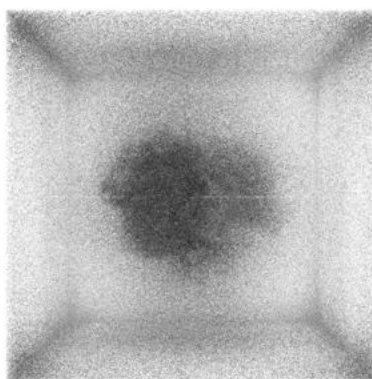
Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

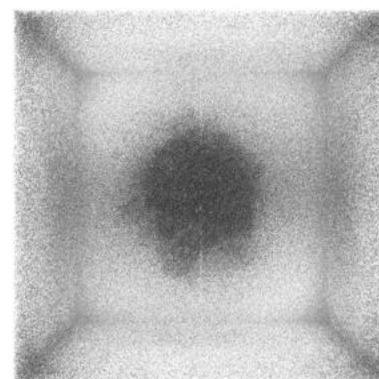
6.5.2 Raw map



X



Y



Z

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

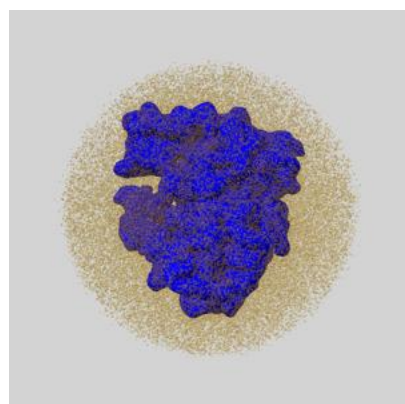
6.6 Mask visualisation [i](#)

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

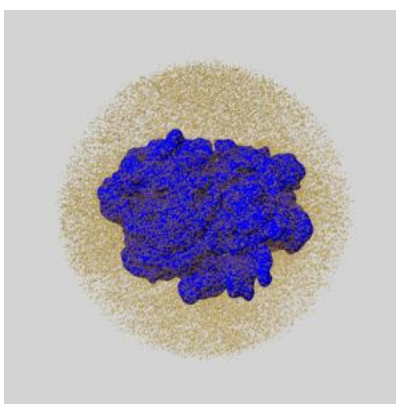
A mask typically either:

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

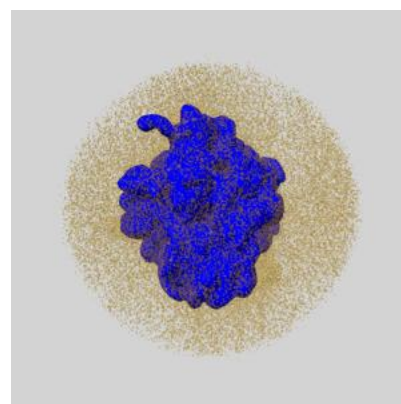
6.6.1 emd_55948_msk_1.map [i](#)



X

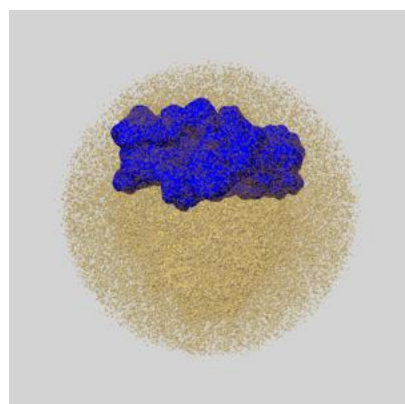


Y

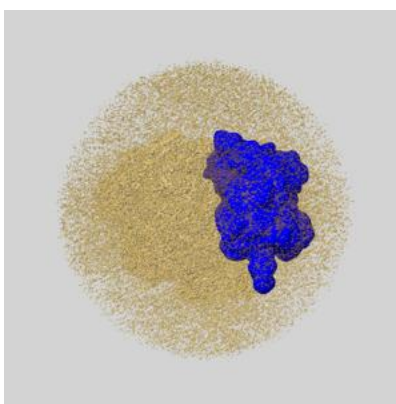


Z

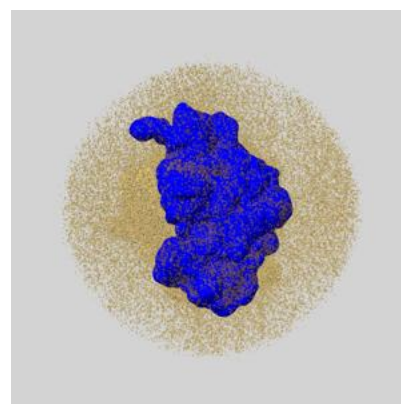
6.6.2 emd_55948_msk_2.map [i](#)



X

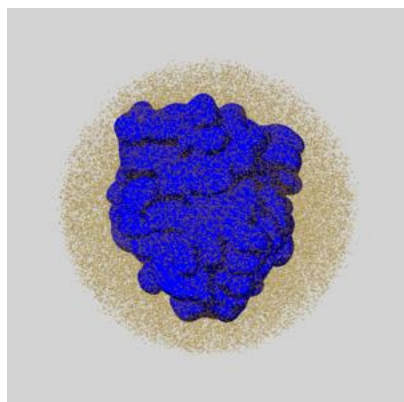


Y

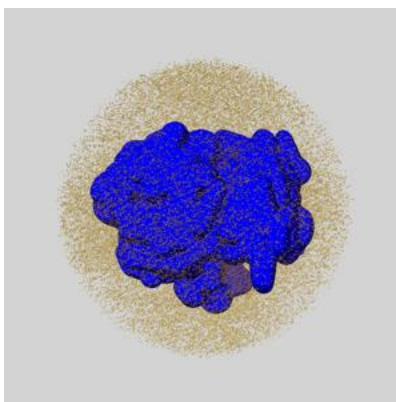


Z

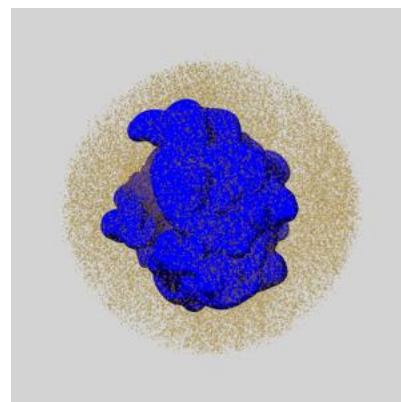
6.6.3 emd_55948_msk_3.map [i](#)



X

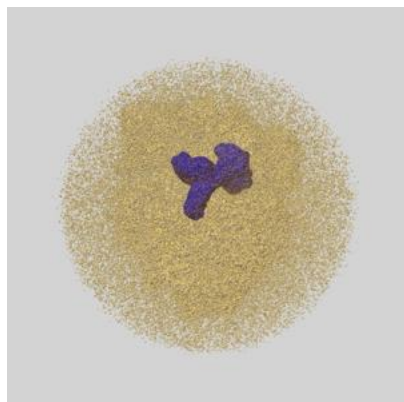


Y

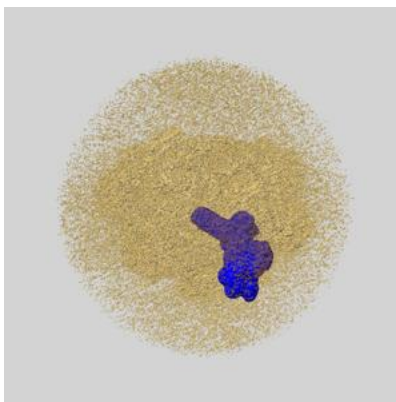


Z

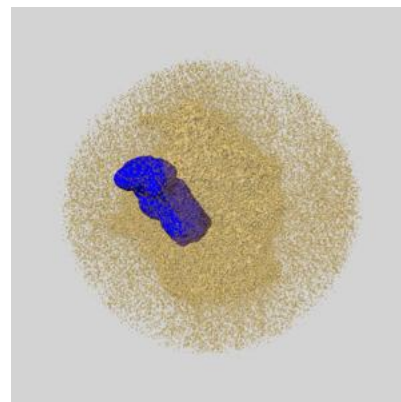
6.6.4 emd_55948_msk_4.map [i](#)



X



Y

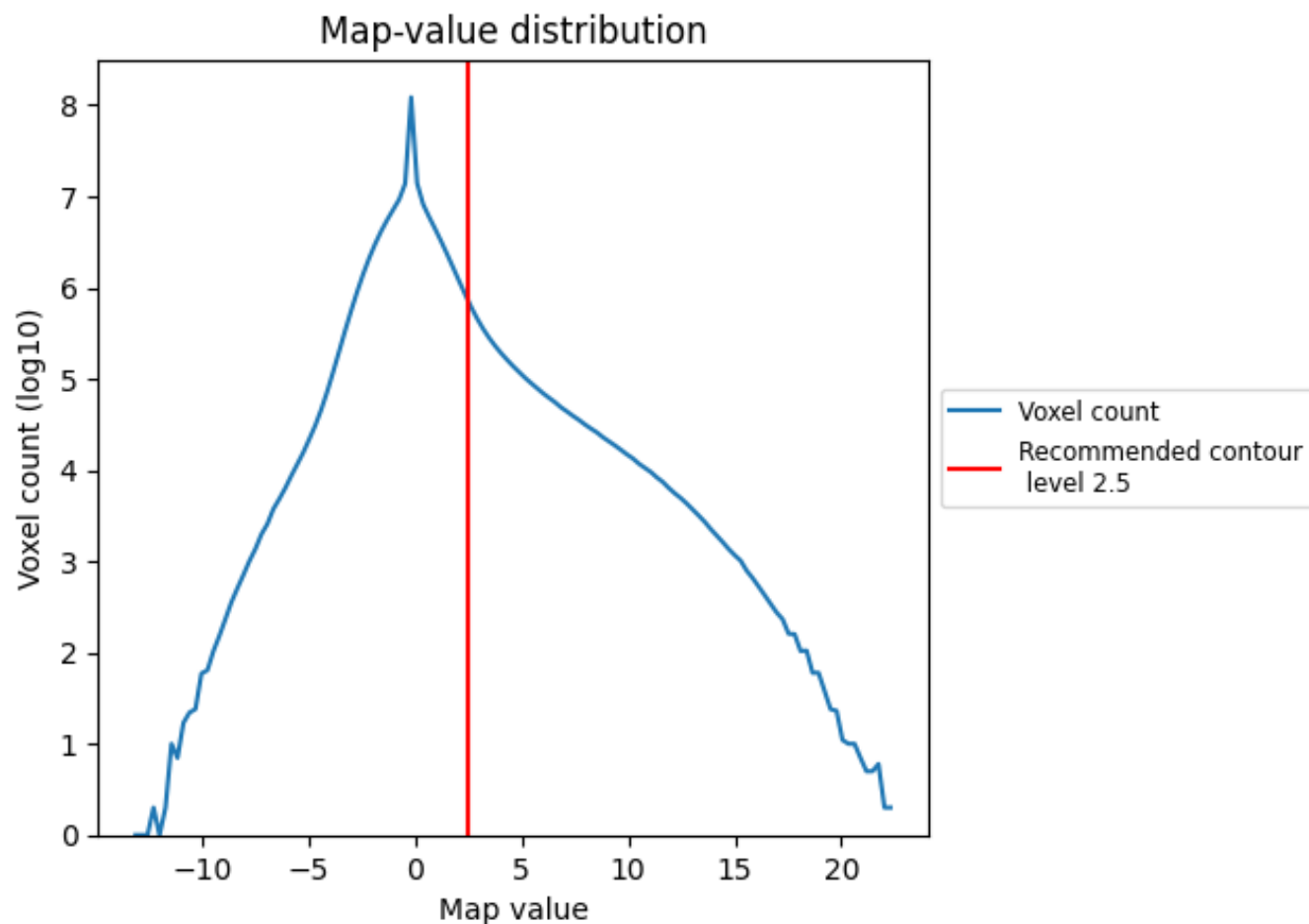


Z

7 Map analysis [i](#)

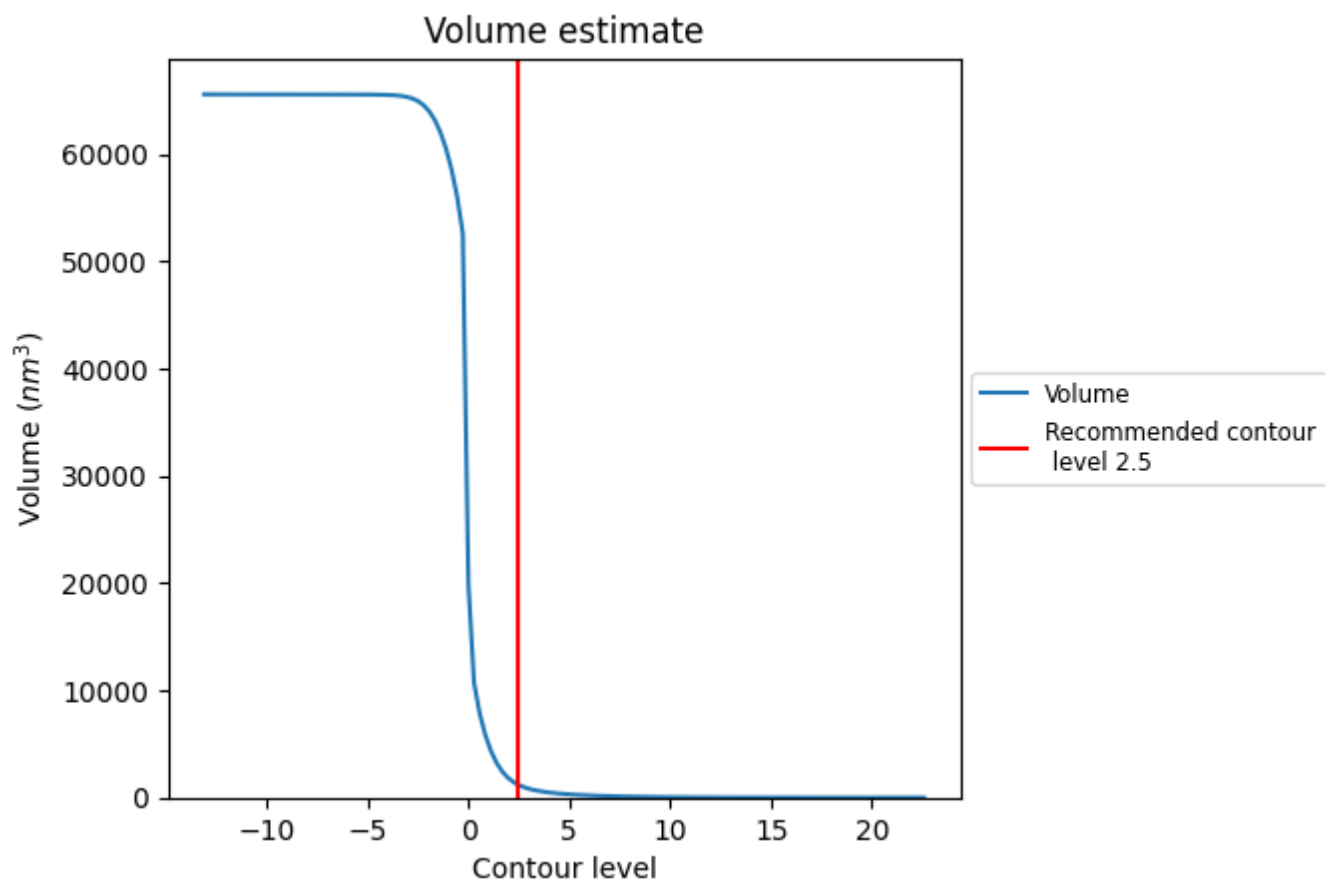
This section contains the results of statistical analysis of the map.

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.

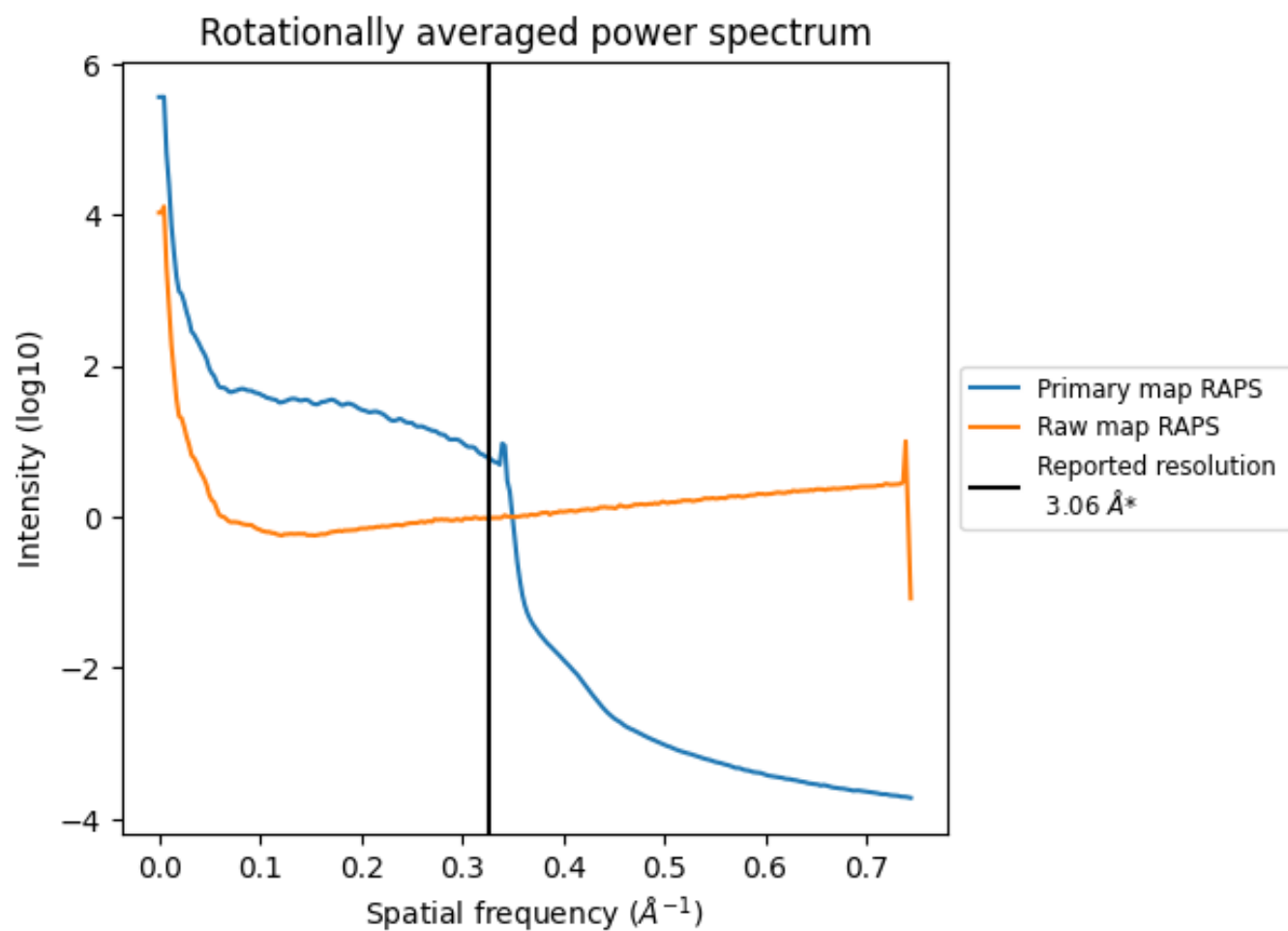
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1169 nm^3 ; this corresponds to an approximate mass of 1056 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

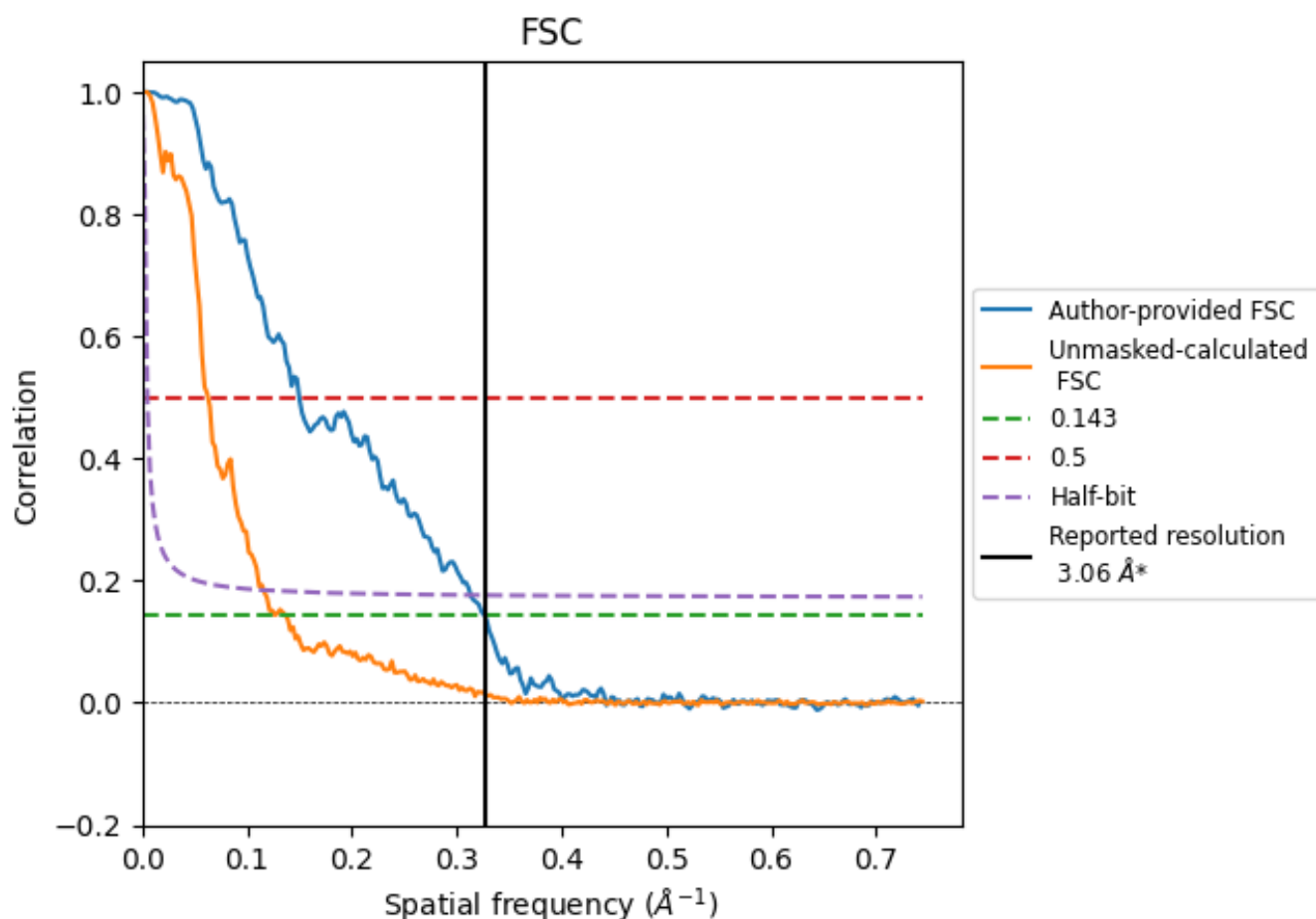


*Reported resolution corresponds to spatial frequency of 0.327 $\text{\AA}^{-1}$

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 0.327 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

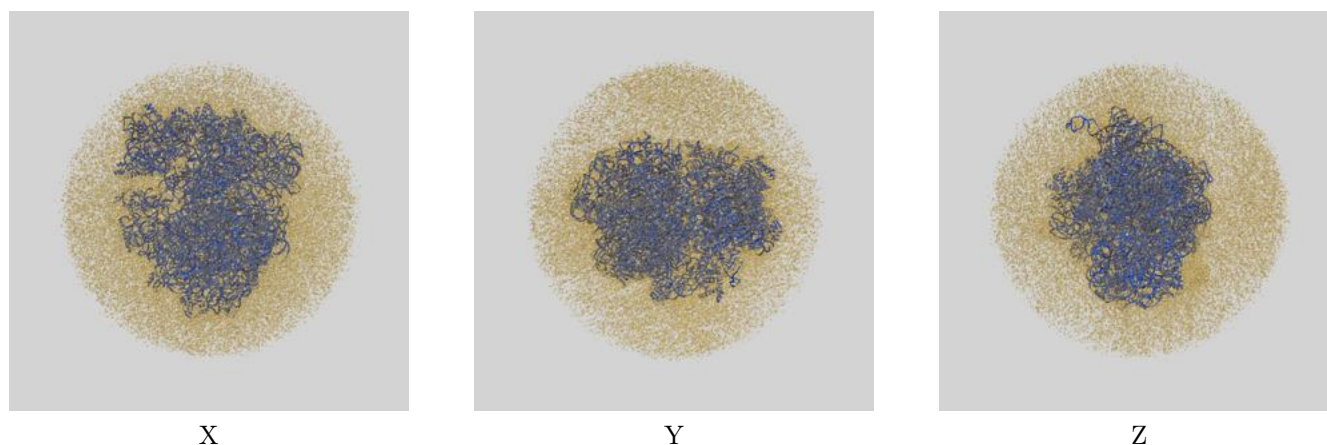
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	6.68	3.19
Unmasked-calculated*	7.31	15.95	8.64

*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 7.31 differs from the reported value 3.06 by more than 10 %

9 Map-model fit [i](#)

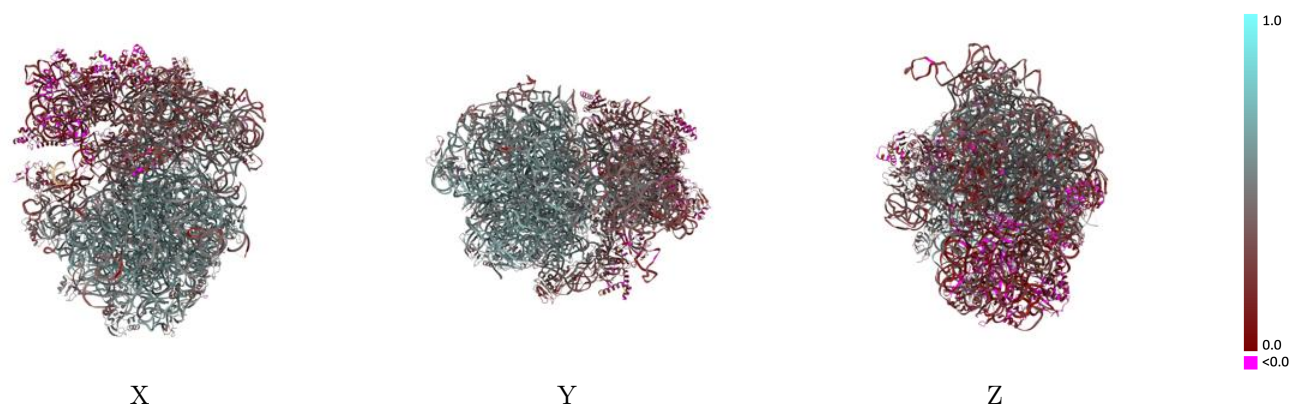
This section contains information regarding the fit between EMDB map EMD-55948 and PDB model 9TI9. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



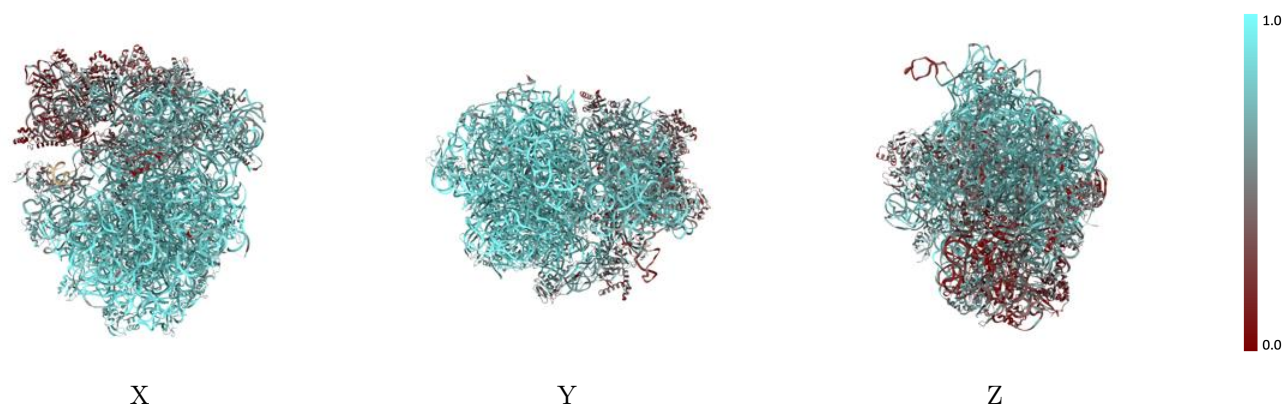
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



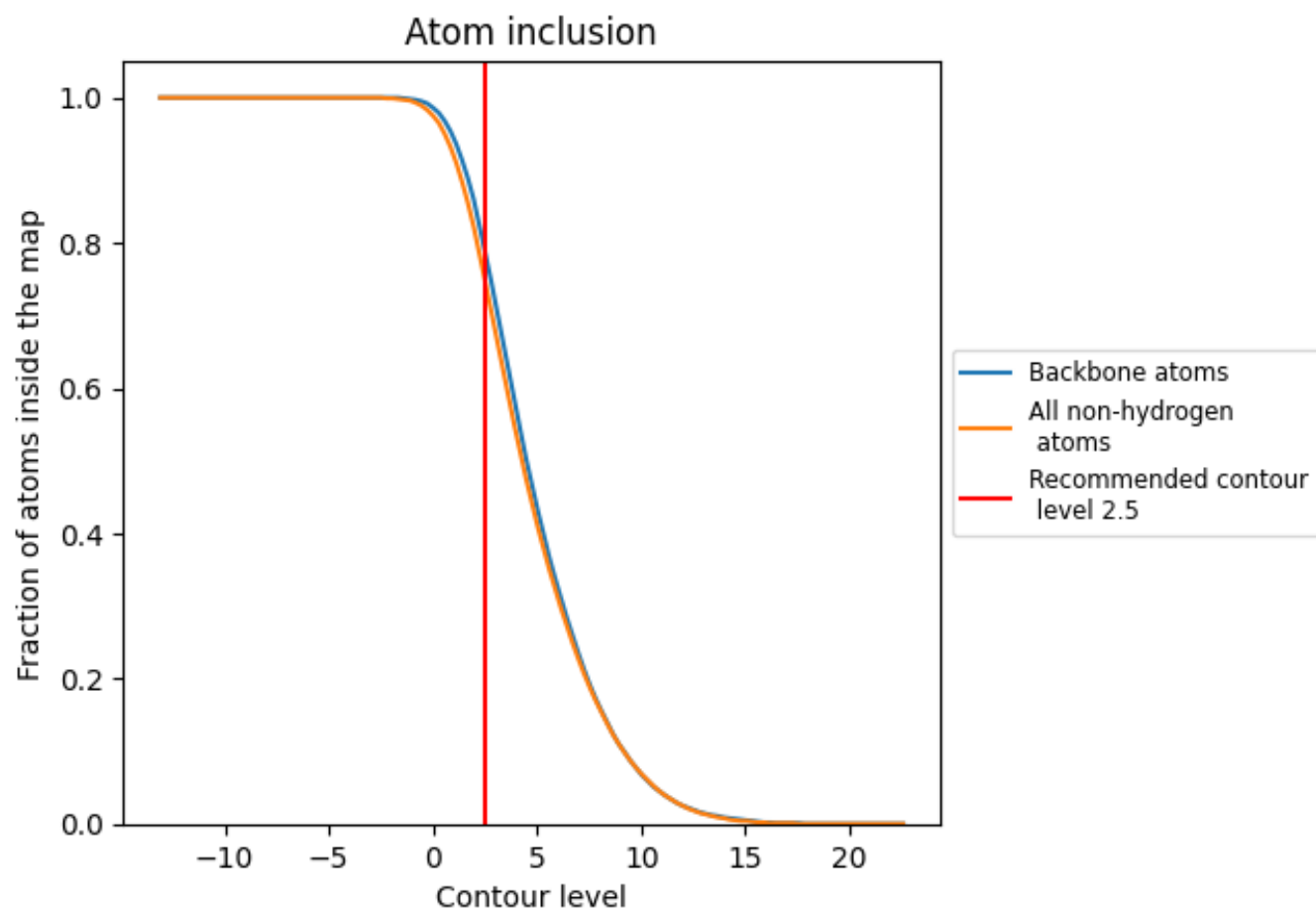
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.4200
1	 0.8020	 0.4960
2	 0.6920	 0.4110
3	 0.8010	 0.4950
4	 0.4840	 0.2020
5	 0.8730	 0.5300
6	 0.6670	 0.4290
7	 0.8980	 0.5770
8	 0.8850	 0.5470
9	 0.8050	 0.5170
A	 0.9160	 0.5420
B	 0.8120	 0.4130
C	 0.5230	 0.3440
D	 0.5220	 0.2100
E	 0.4710	 0.2380
G	 0.8620	 0.5430
H	 0.8640	 0.5440
I	 0.8320	 0.5140
J	 0.5160	 0.2310
K	 0.5730	 0.3500
M	 0.8300	 0.5340
N	 0.7930	 0.5020
O	 0.8310	 0.5200
P	 0.8100	 0.5010
Q	 0.8300	 0.5130
R	 0.6620	 0.3560
S	 0.8060	 0.5100
T	 0.8480	 0.5520
U	 0.8070	 0.5160
V	 0.8470	 0.5320
W	 0.8000	 0.4840
X	 0.7140	 0.4340
Y	 0.6060	 0.3990
Z	 0.8130	 0.5060
a	 0.6820	 0.3310



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.4680	 0.2200
c	 0.3440	 0.1320
d	 0.2090	 0.0770
e	 0.4860	 0.2120
f	 0.5120	 0.2670
g	 0.3500	 0.1910
h	 0.2560	 0.0980
i	 0.5400	 0.2880
j	 0.2630	 0.0850
k	 0.2200	 0.0980
l	 0.5490	 0.2590
m	 0.4860	 0.2850
n	 0.1390	 0.0940
o	 0.2780	 0.0710
p	 0.5680	 0.2890
q	 0.5760	 0.3120
r	 0.5750	 0.2960
s	 0.5030	 0.2360
t	 0.1990	 0.0940
u	 0.6630	 0.3620