



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 03:18 pm BST

PDB ID : 7QGR
EMDB ID : EMD-13958
Title : Structure of the SmrB-bound E. coli disome - collided 70S ribosome
Authors : Kratzat, H.; Buschauer, R.; Berninghausen, O.; Beckmann, R.
Deposited on : 2021-12-09
Resolution : 5.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

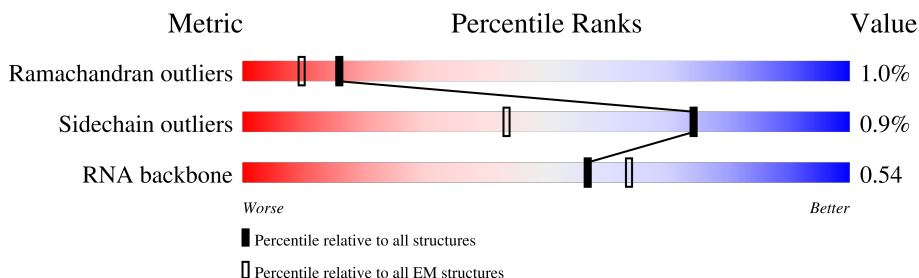
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	O	120	
2	P	273	
3	Q	209	
4	R	201	
5	S	179	
6	T	177	
7	V	142	
8	W	142	

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Mol	Chain	Length	Quality of chain
9	X	123	<div>80%</div> <div>95%</div> <div>..</div>
10	Y	144	<div>65%</div> <div>89%</div> <div>8%</div> <div>..</div>
11	Z	136	<div>60%</div> <div>90%</div> <div>9%</div> <div>.</div>
12	a	127	<div>59%</div> <div>83%</div> <div>10%</div> <div>6%</div>
13	b	117	<div>72%</div> <div>94%</div> <div>5%</div> <div>.</div>
14	c	115	<div>76%</div> <div>92%</div> <div>5%</div> <div>..</div>
15	d	118	<div>51%</div> <div>88%</div> <div>10%</div> <div>..</div>
16	e	103	<div>73%</div> <div>95%</div> <div>..</div> <div>..</div>
17	f	110	<div>71%</div> <div>97%</div> <div>.</div>
18	g	100	<div>70%</div> <div>90%</div> <div>.</div> <div>7%</div>
19	h	104	<div>56%</div> <div>94%</div> <div>...</div>
20	i	94	<div>45%</div> <div>100%</div>
21	j	85	<div>18%</div> <div>82%</div> <div>5%</div> <div>12%</div>
22	k	78	<div>59%</div> <div>92%</div> <div>6%</div> <div>.</div>
23	l	63	<div>70%</div> <div>94%</div> <div>6%</div>
24	m	59	<div>46%</div> <div>95%</div> <div>..</div>
25	n	57	<div>42%</div> <div>82%</div> <div>16%</div> <div>.</div>
26	o	55	<div>69%</div> <div>85%</div> <div>5%</div> <div>9%</div>
27	p	46	<div>57%</div> <div>87%</div> <div>13%</div>
28	q	65	<div>46%</div> <div>88%</div> <div>9%</div> <div>..</div>
29	r	55	<div>49%</div> <div>60%</div> <div>9%</div> <div>31%</div>
30	N	2903	<div>15%</div> <div>66%</div> <div>29%</div> <div>5%</div>
31	L	70	<div>77%</div> <div>76%</div> <div>.</div> <div>23%</div>
32	C	223	<div>60%</div> <div>60%</div> <div>40%</div>
33	U	149	<div>99%</div> <div>98%</div> <div>.</div>

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Mol	Chain	Length	Quality of chain
34	M	75	
35	x	692	
36	0	1539	
37	1	239	
38	2	218	
39	3	206	
40	4	162	
41	5	131	
42	6	152	
43	7	130	
44	8	130	
45	9	103	
46	A	129	
47	B	124	
48	D	118	
49	E	101	
50	F	89	
51	G	82	
52	H	84	
53	I	75	
54	J	92	
55	K	87	
56	s	71	
57	t	557	
58	u	73	

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Mol	Chain	Length	Quality of chain
59	v	182	<div><div></div><div>74%</div><div></div><div>92%</div><div></div><div>...</div></div>

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 149850 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	209	Total	C	N	O	S	0	0
			1564	979	288	293	4		

- Molecule 4 is a protein called 50S ribosomal protein L4.

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

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	177	Total	C	N	O	S	0	0
			1397	891	249	251	6		

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	176	Total	C	N	O	S	0	0
			1322	832	243	245	2		

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	141	Total	C	N	O	S	0	0
			1031	651	179	195	6		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	W	142	Total	C	N	O	S	0	0
			1128	714	212	198	4		

- Molecule 9 is a protein called 50S ribosomal protein L14.

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

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	143	Total	C	N	O	S	0	0
			1044	649	206	188	1		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	136	Total	C	N	O	S	0	0
			1073	686	205	176	6		

- Molecule 12 is a protein called 50S ribosomal protein L17.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	123	ALA	GLU	conflict	UNP A0A829CNM8

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	b	116	Total	C	N	O	0	0
			891	552	178	161		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	114	Total	C	N	O	S	0	0
			915	573	179	162	1		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	d	117	Total	C	N	O	0	0
			946	604	192	150		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	e	103	Total	C	N	O	S	0	0
			815	516	153	144	2		

- Molecule 17 is a protein called 50S ribosomal protein L22.

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

- Molecule 18 is a protein called 50S ribosomal protein L23.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	98	SER	GLY	conflict	UNP A0A829CFV1

- Molecule 19 is a protein called 50S ribosomal protein L24.

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

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	i	94	Total	C	N	O	S	0
			752	479	137	133	3	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	j	75	Total	C	N	O	S	0
			568	353	113	101	1	0

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	k	77	Total	C	N	O	S	0
			624	388	129	105	2	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	l	63	Total	C	N	O	S	0
			508	313	99	94	2	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	m	58	Total	C	N	O	S	0
			448	281	87	78	2	0

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	n	56	Total	C	N	O	S	0
			443	269	94	79	1	0

- Molecule 26 is a protein called 50S ribosomal protein L33.

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

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	p	46	Total	C	N	O	S	0	0
			376	228	90	56	2		

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	q	64	Total	C	N	O	S	0	0
			503	323	105	73	2		

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	r	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	2897	Total	C	N	O	P	1	0
			62215	27754	11448	20115	2898		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	54	Total	C	N	O	S	0	0
			415	256	75	78	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	68	SER	GLY	conflict	UNP A0A1X3HZV8

- Molecule 32 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	C	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	75	Total	C	N	O	P	0	0
			1594	711	281	527	75		

- Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	x	44	Total	C	N	O	P	0	0
			928	416	160	308	44		

- Molecule 36 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	0	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1	218	Total	C	N	O	S	0	0
			1699	1078	303	311	7		

- Molecule 38 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 39 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3	205	Total	C	N	O	S	0	0
			1642	1026	315	297	4		

- Molecule 40 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	4	MET	ILE	conflict	UNP A0A377C6M5

- Molecule 41 is a protein called 30S ribosomal protein S6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	101	SER	PRO	conflict	UNP P02358

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	6	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 43 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	7	129	Total	C	N	O	S	0	0
			978	616	173	183	6		

- Molecule 44 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	8	127	Total	C	N	O	S	0	0
			1021	634	206	178	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	3	ASP	GLU	conflict	UNP A0A1Z3UZ18

- Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	9	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 46 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	A	117	Total	C	N	O	S	0	0
			876	540	174	159	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	PRO	conflict	UNP A0A829AF87

- Molecule 47 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	B	123	Total	C	N	O	S	0	0
			954	590	196	164	4		

- Molecule 48 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	D	114	Total	C	N	O	S	0	0
			877	543	175	156	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	MET	conflict	UNP A0A7U9IV78

- Molecule 49 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	E	96	Total	C	N	O	S	0	0
			773	483	160	127	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	40	ALA	GLU	conflict	UNP A0A090BZT4

- Molecule 50 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	F	88	Total	C	N	O	S	0	0
			709	437	143	128	1		

- Molecule 51 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	G	82	Total	C	N	O	S	0	0
			648	406	128	113	1		

- Molecule 52 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	H	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	2	ALA	THR	conflict	UNP A0A829A8C6

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	I	55	Total	C	N	O	0	0
			455	288	86	81		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	15	THR	ALA	conflict	UNP A0A376I7P4
I	58	ALA	CYS	conflict	UNP A0A376I7P4

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	J	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	82	TYR	GLY	conflict	UNP S1EA57
J	83	TYR	HIS	conflict	UNP S1EA57

- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	K	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	LEU	MET	conflict	UNP P0A7U7

- Molecule 56 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	s	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 57 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	t	143	Total	C	N	O		0	0
			704	418	143	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	241	VAL	ILE	conflict	UNP A0A829CYC5

- Molecule 58 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	u	73	Total	C	N	O	P	0	0
			1561	695	279	514	73		

- Molecule 59 is a protein called UPF0115 protein YfcN.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	v	175	Total	C	N	O	S	0	0
			1256	796	226	229	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	99	ALA	ASP	conflict	UNP Q6KCY1
v	101	ALA	HIS	conflict	UNP Q6KCY1

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	u	2	Total	Mg	0
			2	2	

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
61	u	1	Total	K	0
			1	1	

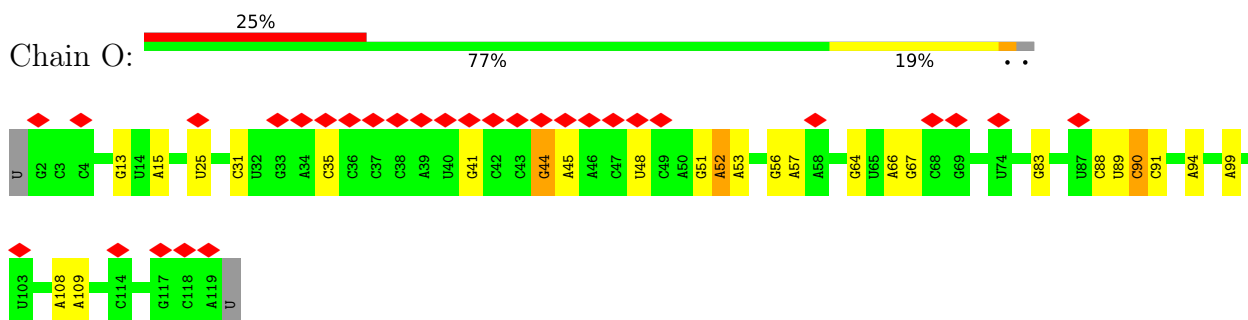
- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
62	u	9	Total	O	0
			9	9	

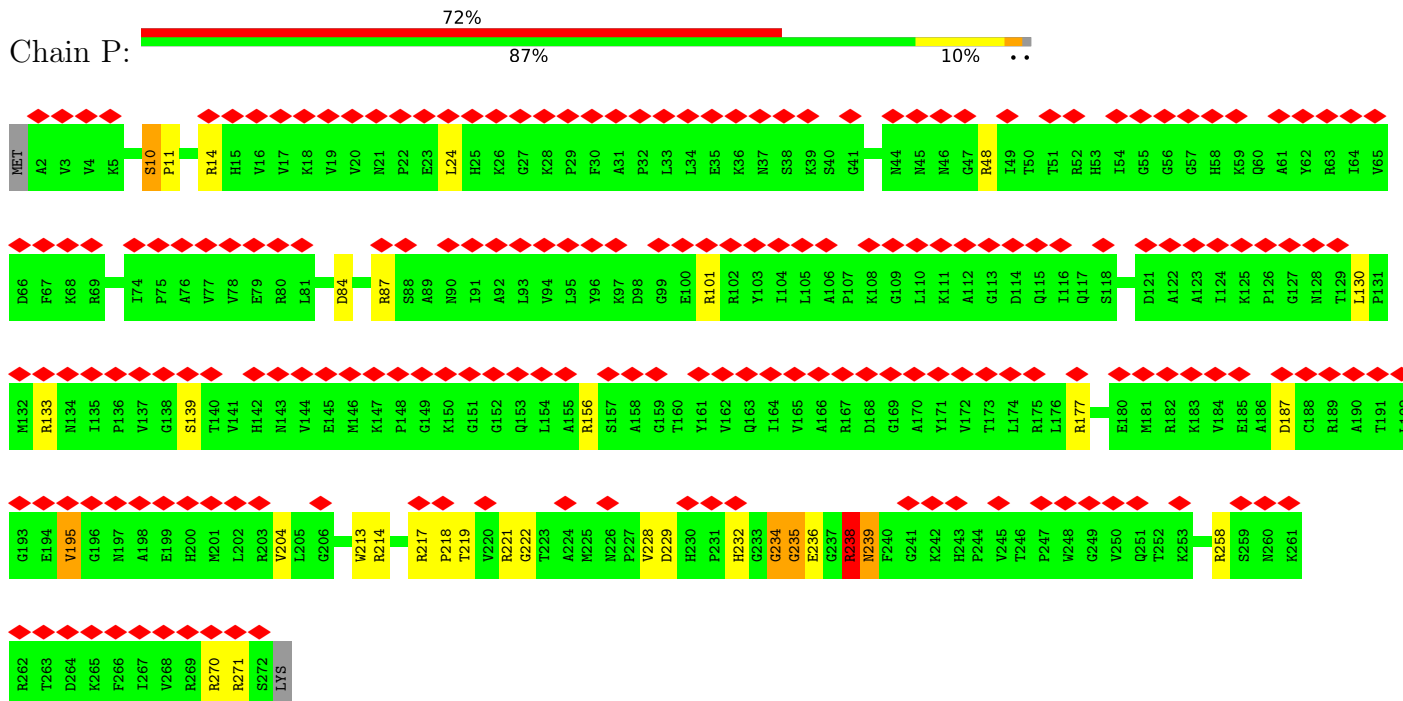
3 Residue-property plots [i](#)

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.

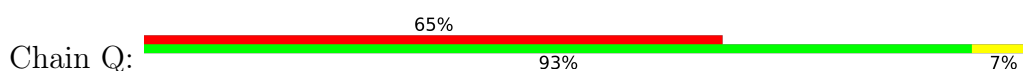
• Molecule 1: 5S rRNA

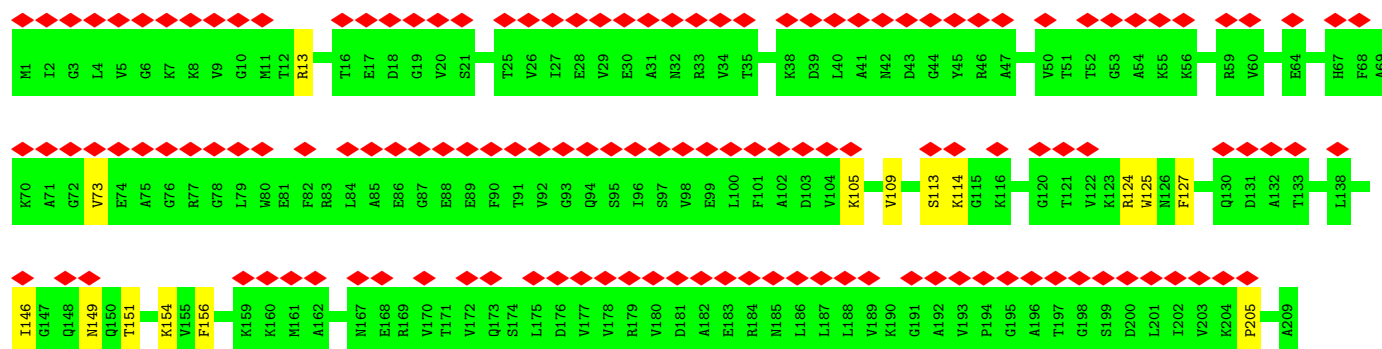


• Molecule 2: 50S ribosomal protein L2

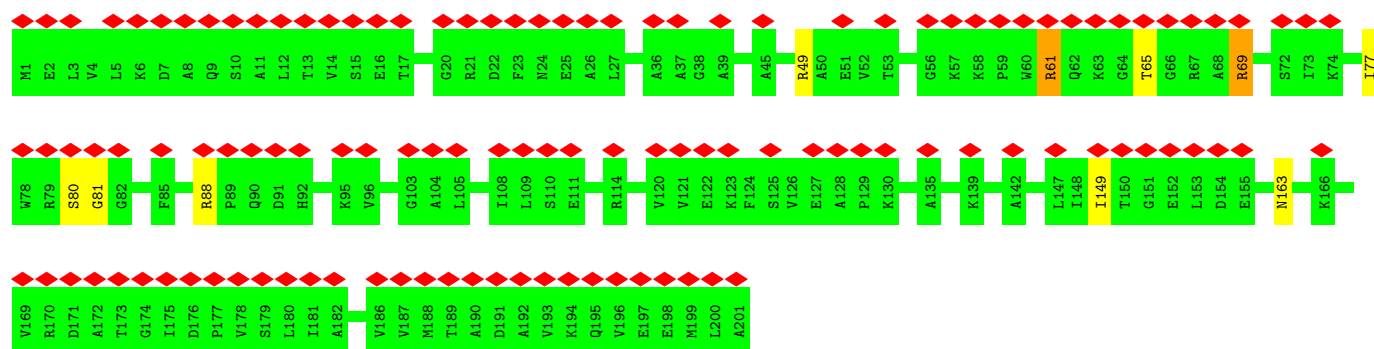


• Molecule 3: 50S ribosomal protein L3

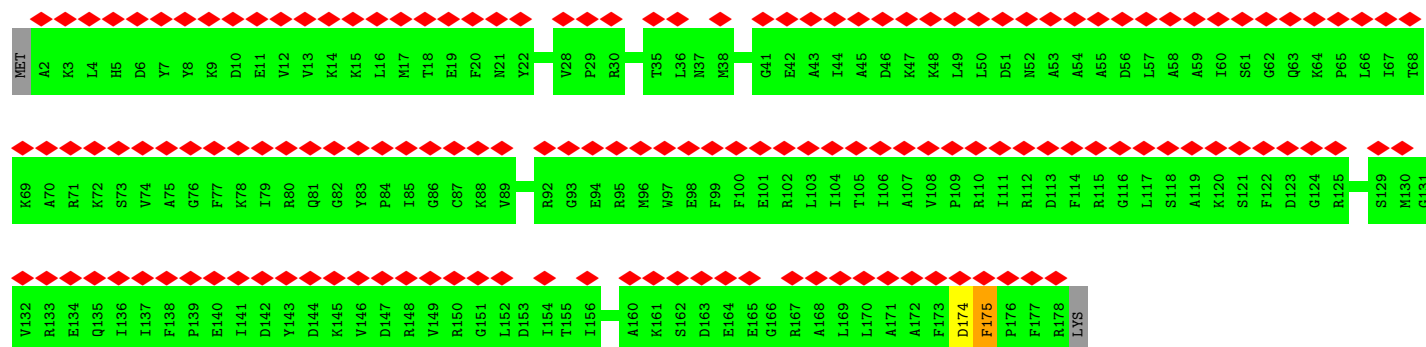
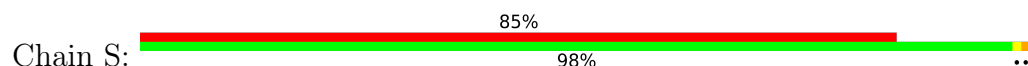




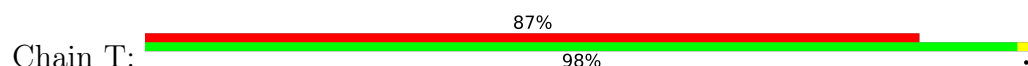
• Molecule 4: 50S ribosomal protein L4

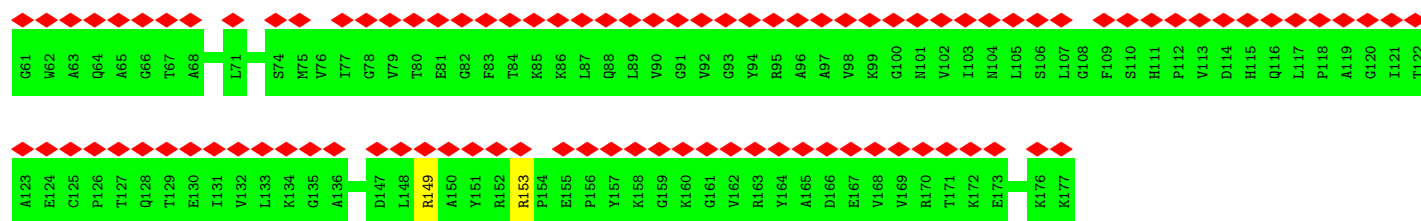


• Molecule 5: 50S ribosomal protein L5



• Molecule 6: 50S ribosomal protein L6

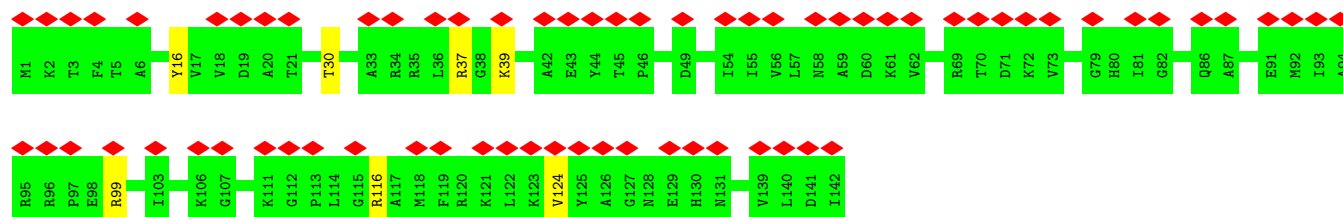




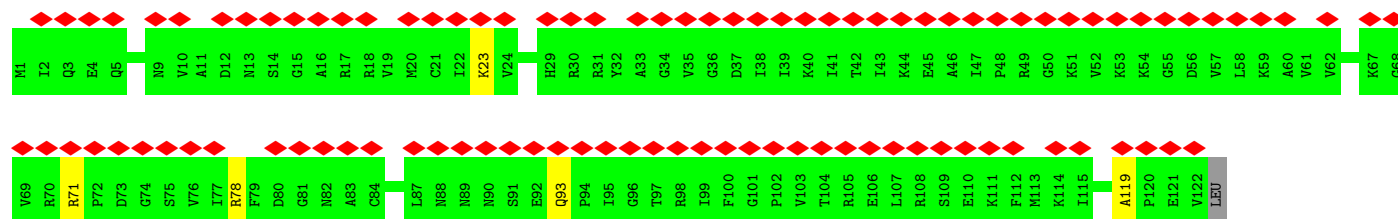
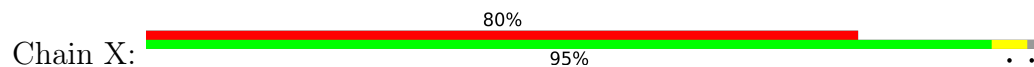
• Molecule 7: 50S ribosomal protein L11



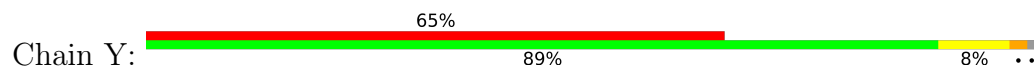
• Molecule 8: 50S ribosomal protein L13

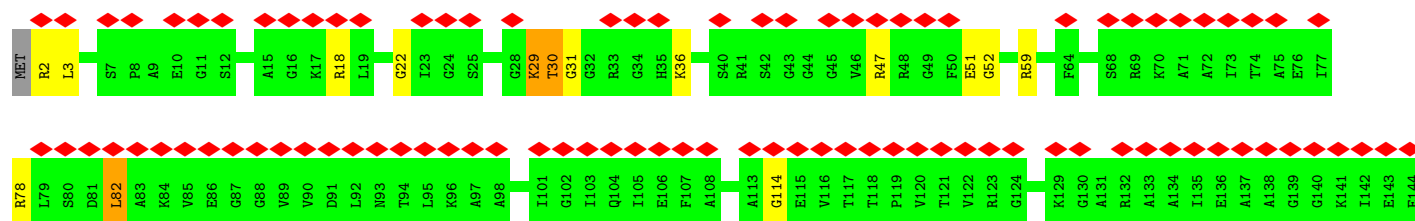


• Molecule 9: 50S ribosomal protein L14

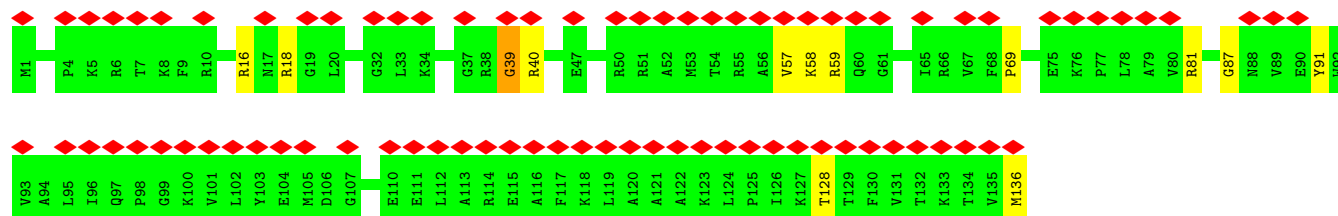
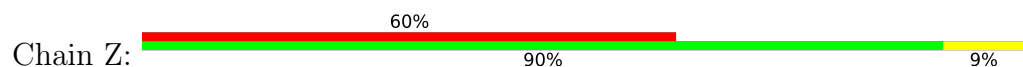


• Molecule 10: 50S ribosomal protein L15

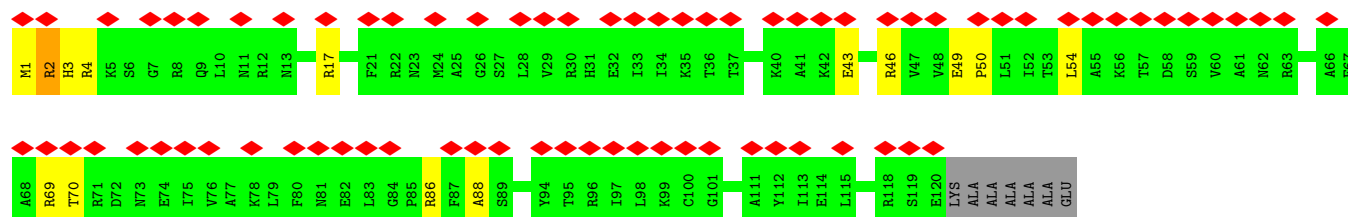
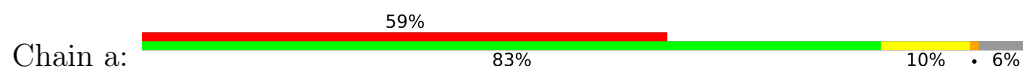




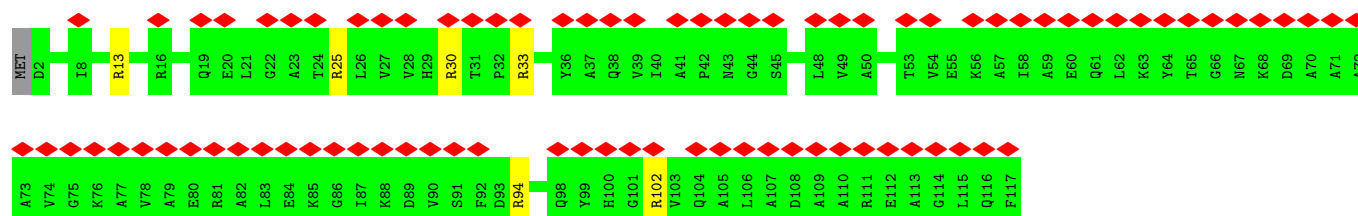
• Molecule 11: 50S ribosomal protein L16



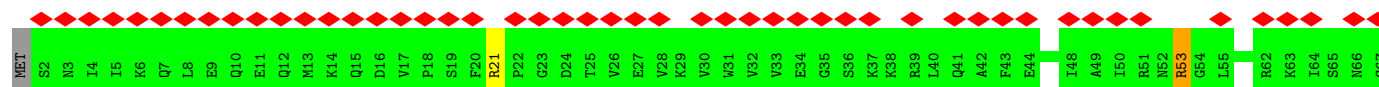
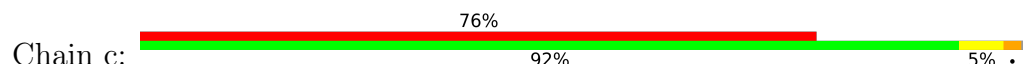
• Molecule 12: 50S ribosomal protein L17

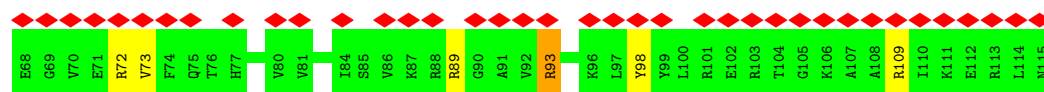


• Molecule 13: 50S ribosomal protein L18

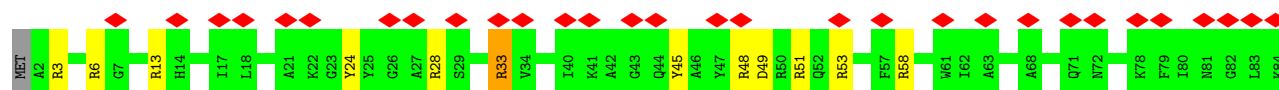
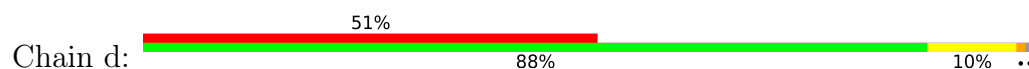


• Molecule 14: 50S ribosomal protein L19

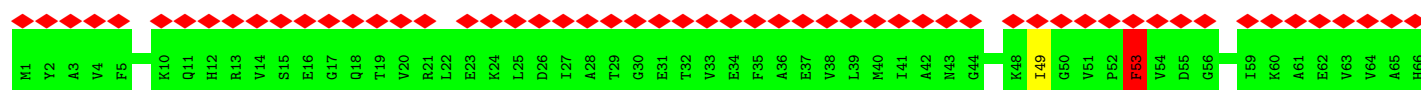
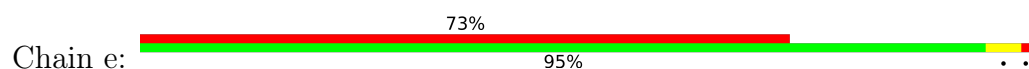




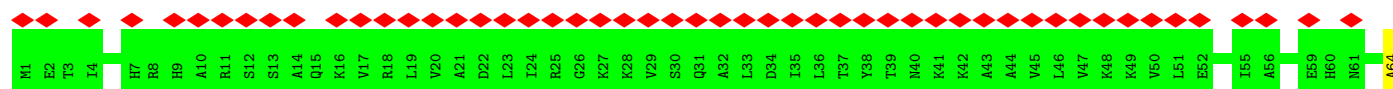
- Molecule 15: 50S ribosomal protein L20



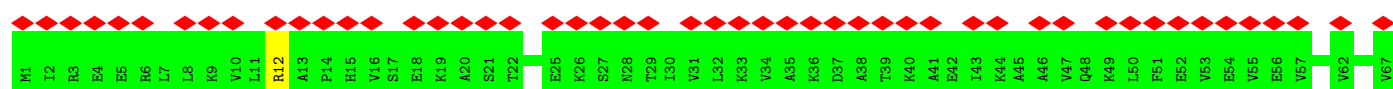
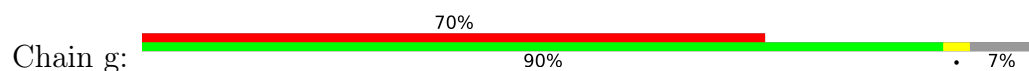
- Molecule 16: 50S ribosomal protein L21



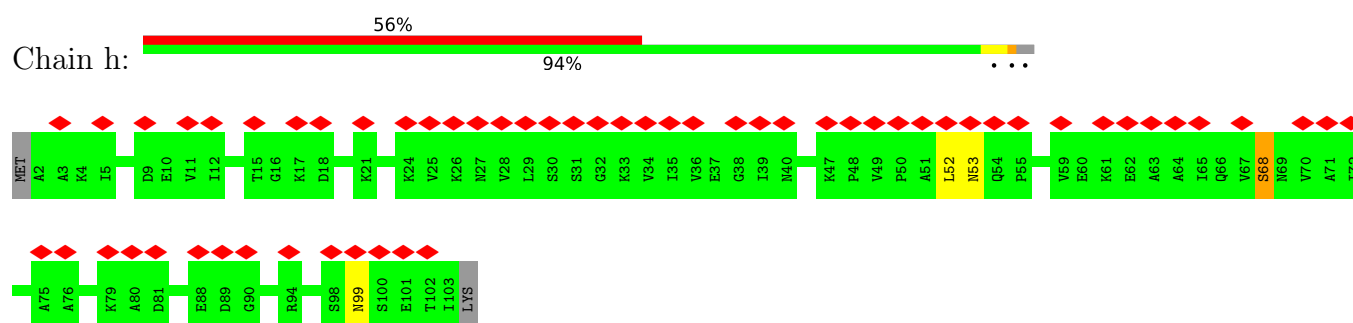
- Molecule 17: 50S ribosomal protein L22



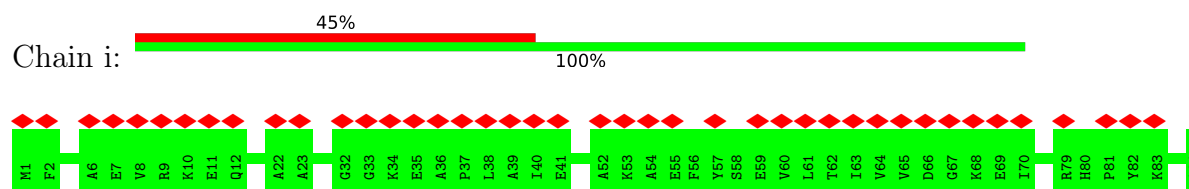
- Molecule 18: 50S ribosomal protein L23



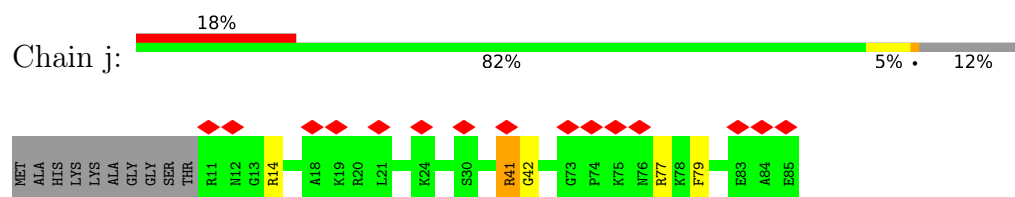
- Molecule 19: 50S ribosomal protein L24



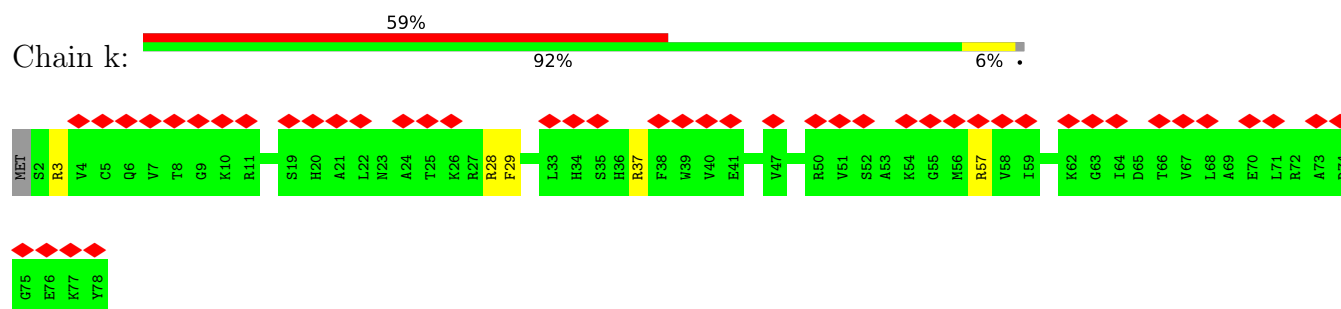
- Molecule 20: 50S ribosomal protein L25



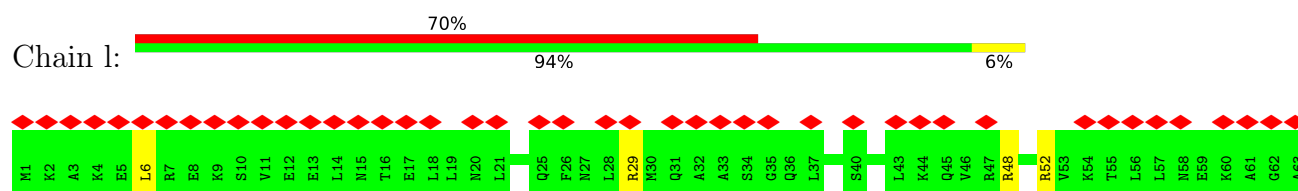
- Molecule 21: 50S ribosomal protein L27



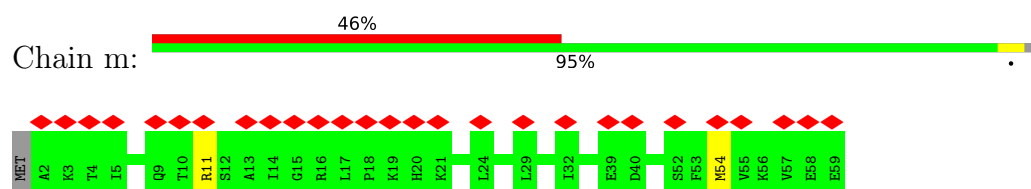
- Molecule 22: 50S ribosomal protein L28



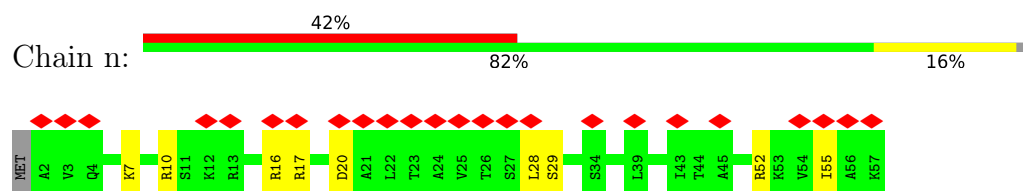
- Molecule 23: 50S ribosomal protein L29



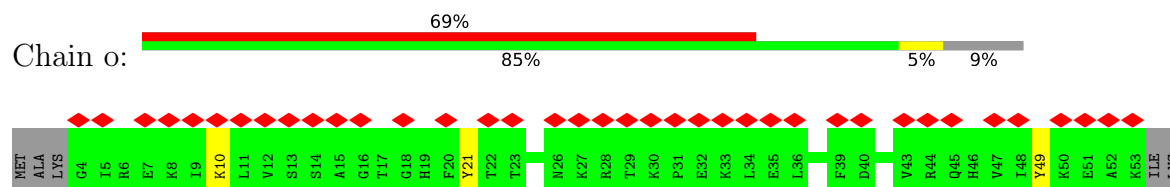
- Molecule 24: 50S ribosomal protein L30



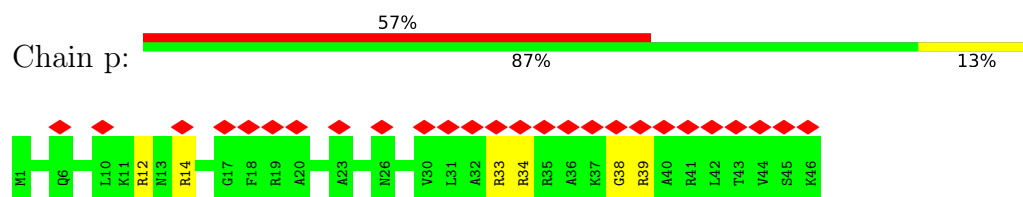
- Molecule 25: 50S ribosomal protein L32



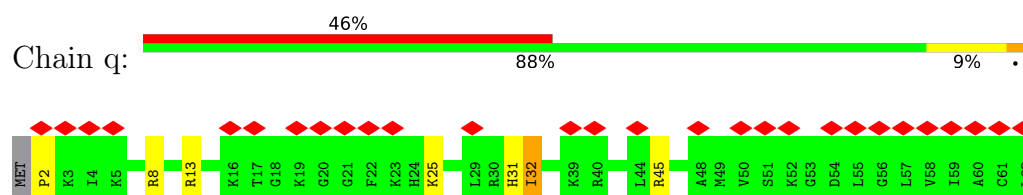
- Molecule 26: 50S ribosomal protein L33



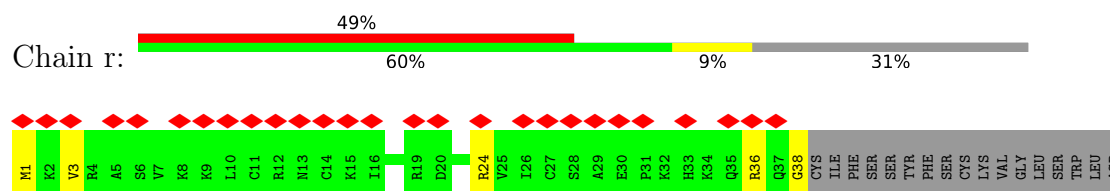
- Molecule 27: 50S ribosomal protein L34



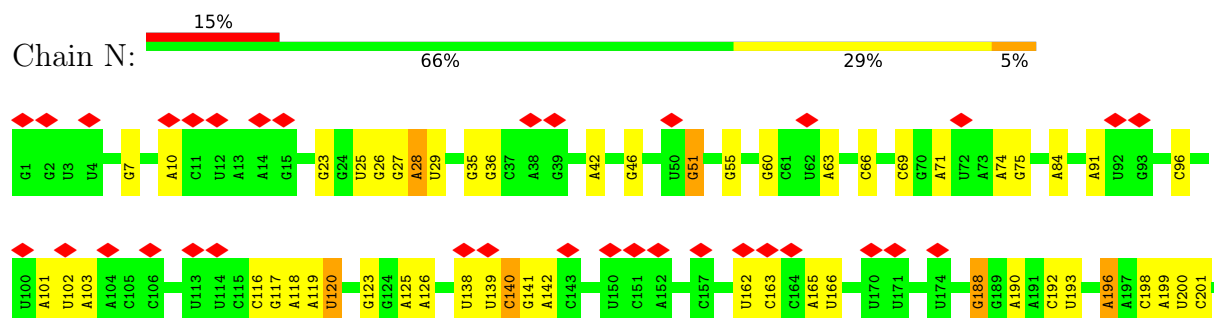
- Molecule 28: 50S ribosomal protein L35

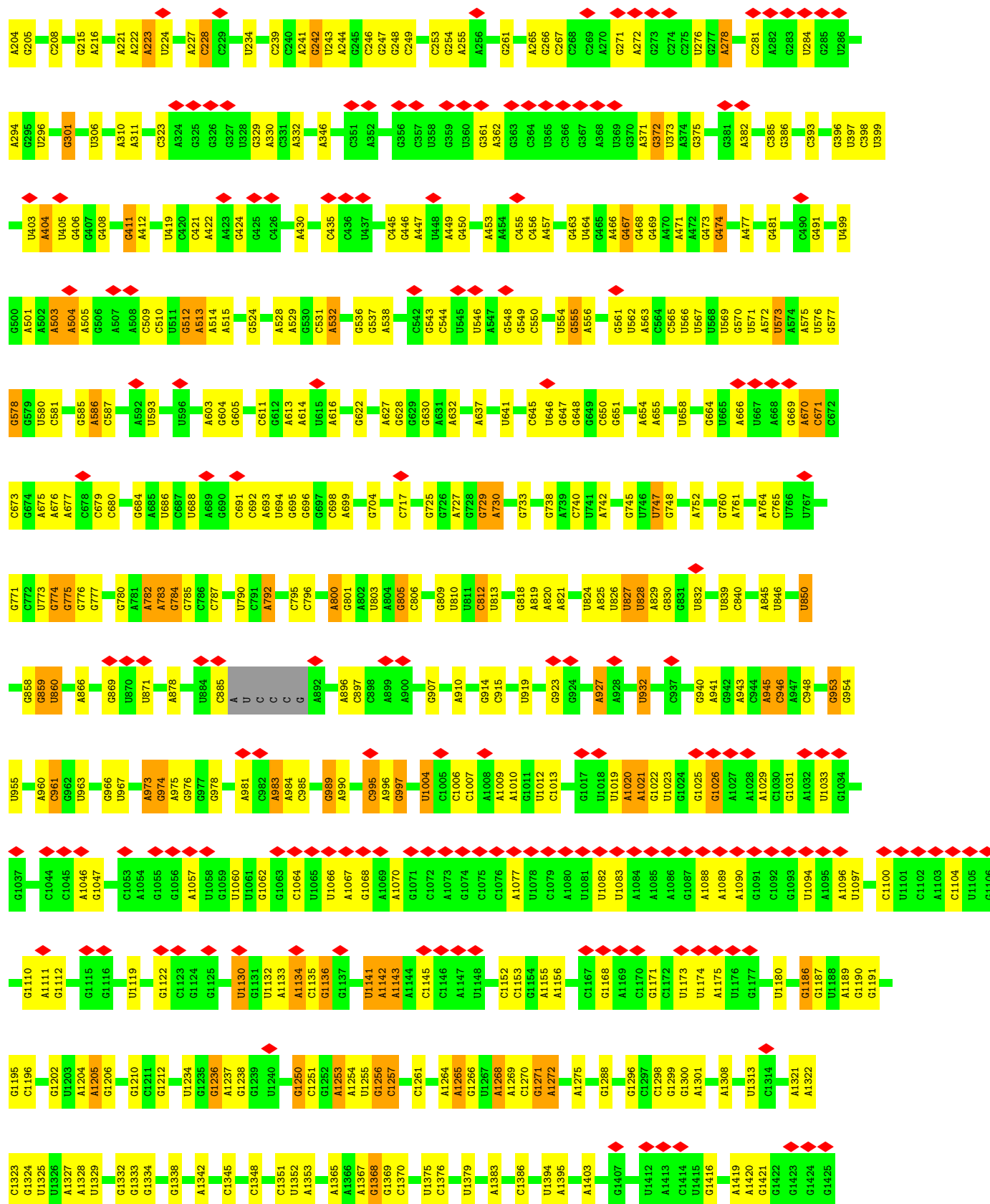


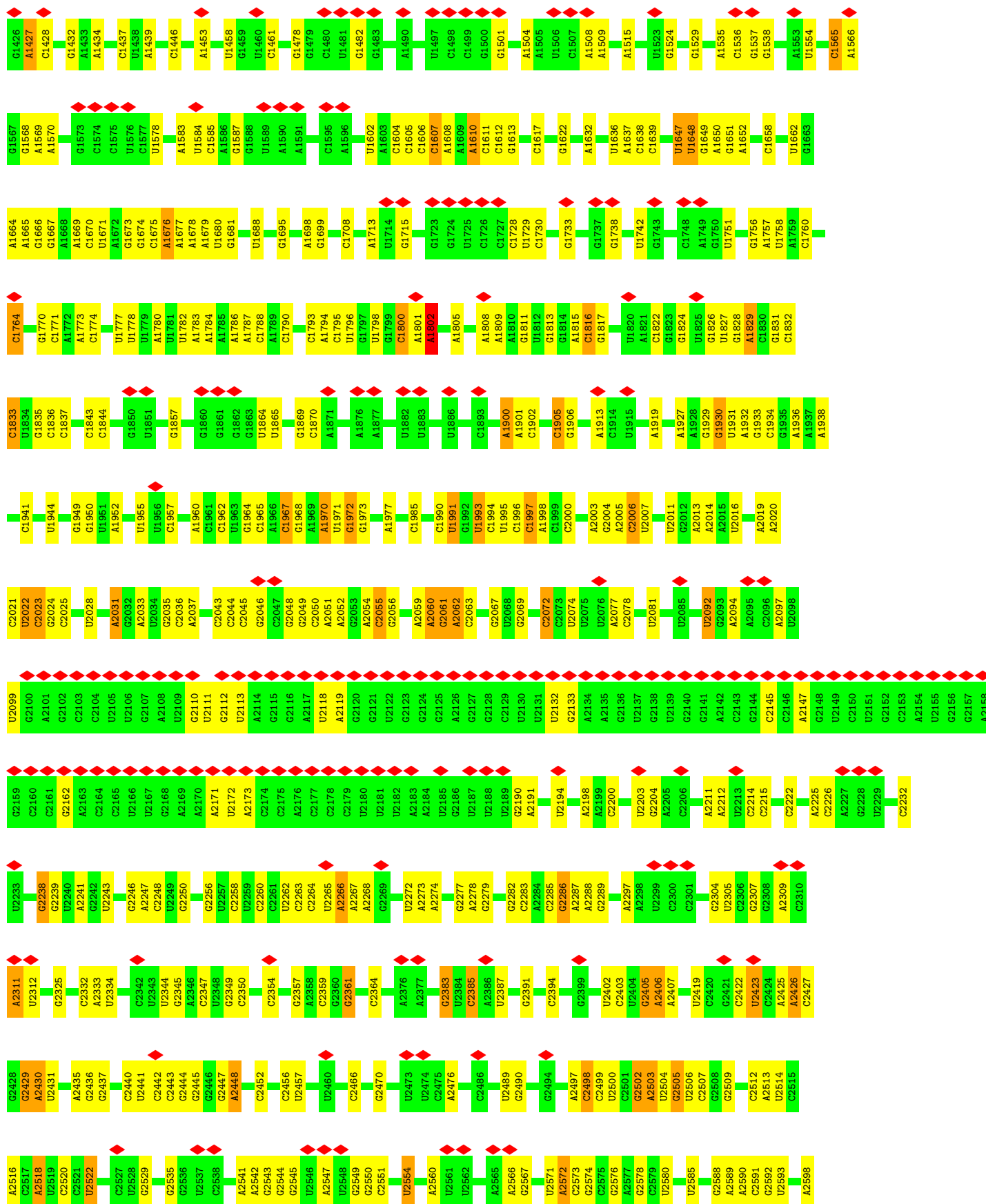
- Molecule 29: 50S ribosomal protein L36

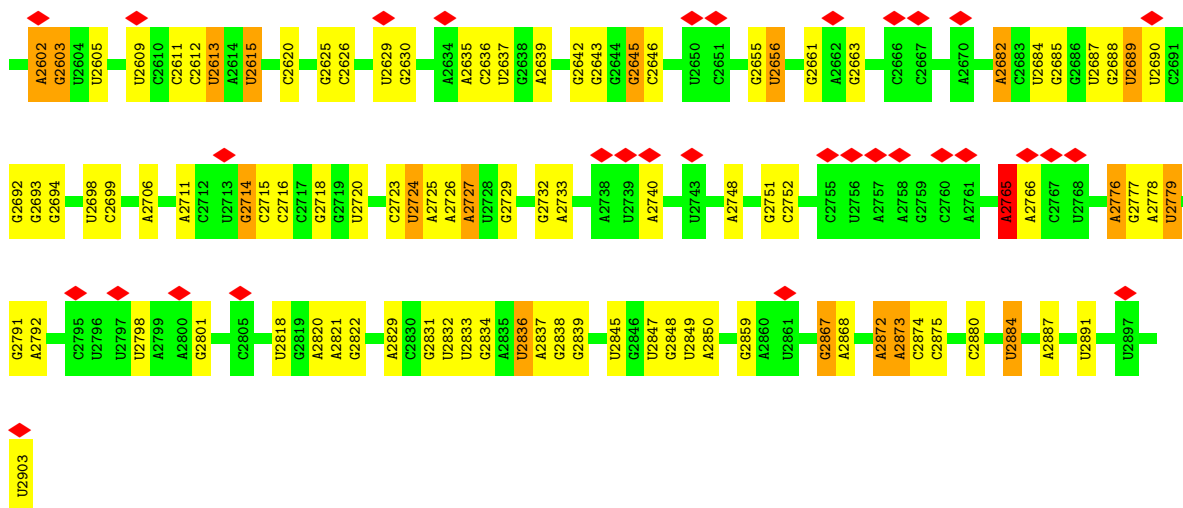


- Molecule 30: 23S rRNA

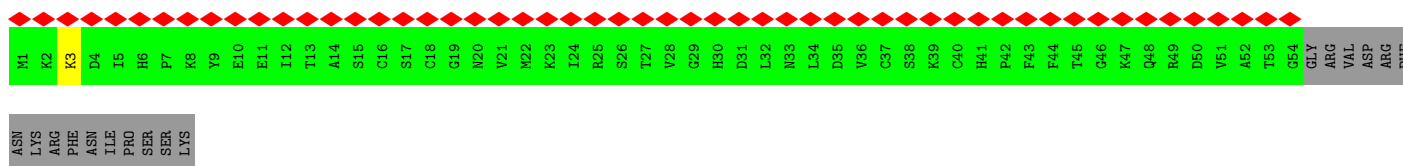
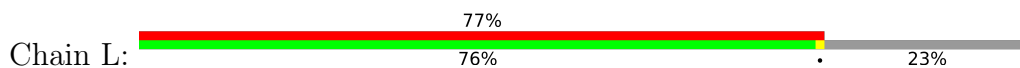




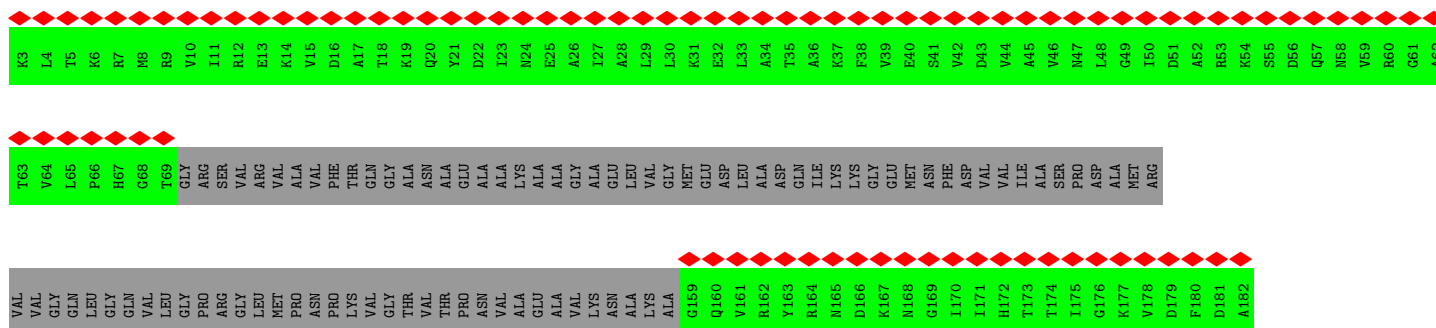




- Molecule 31: 50S ribosomal protein L31

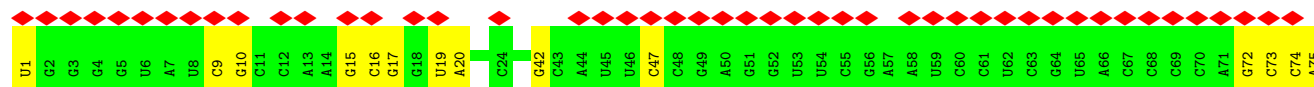
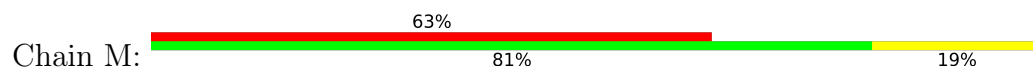


- Molecule 32: 50S ribosomal protein L1

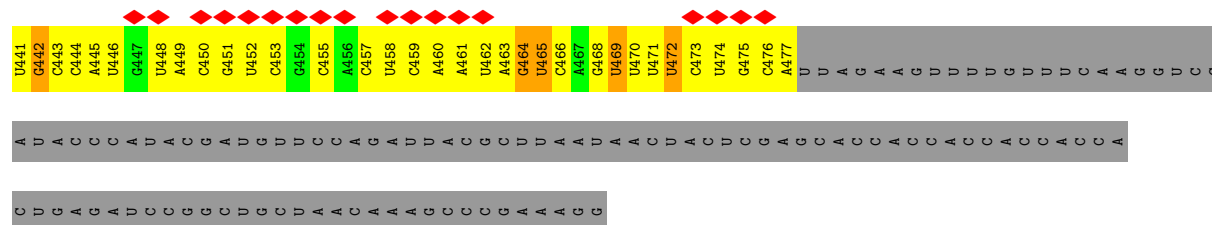
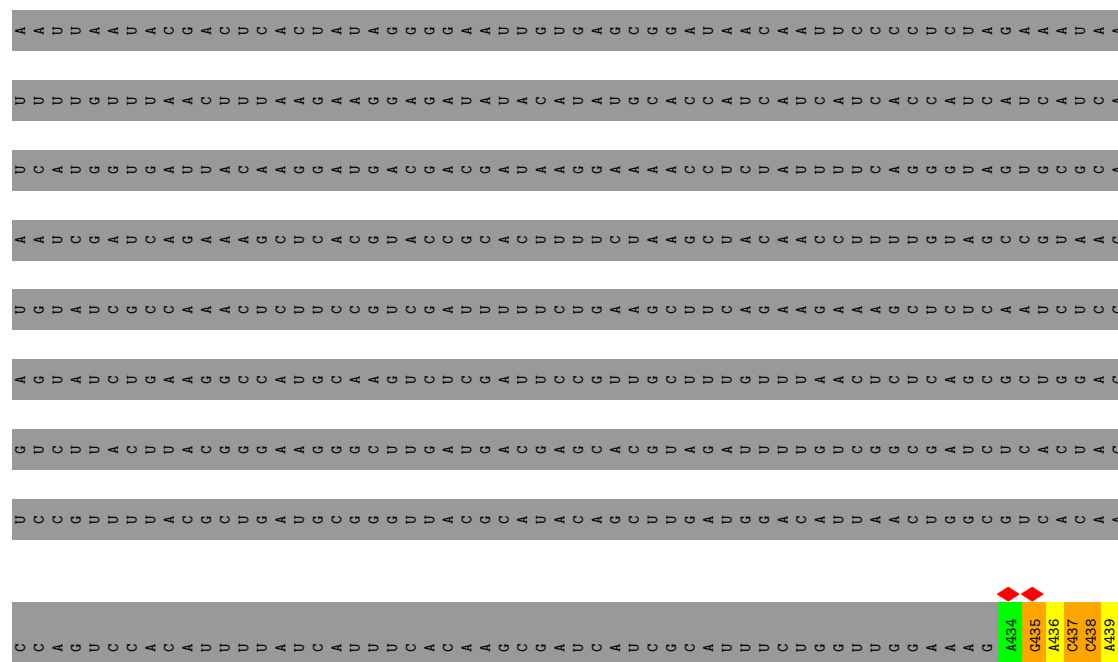




- Molecule 34: P-site tRNA

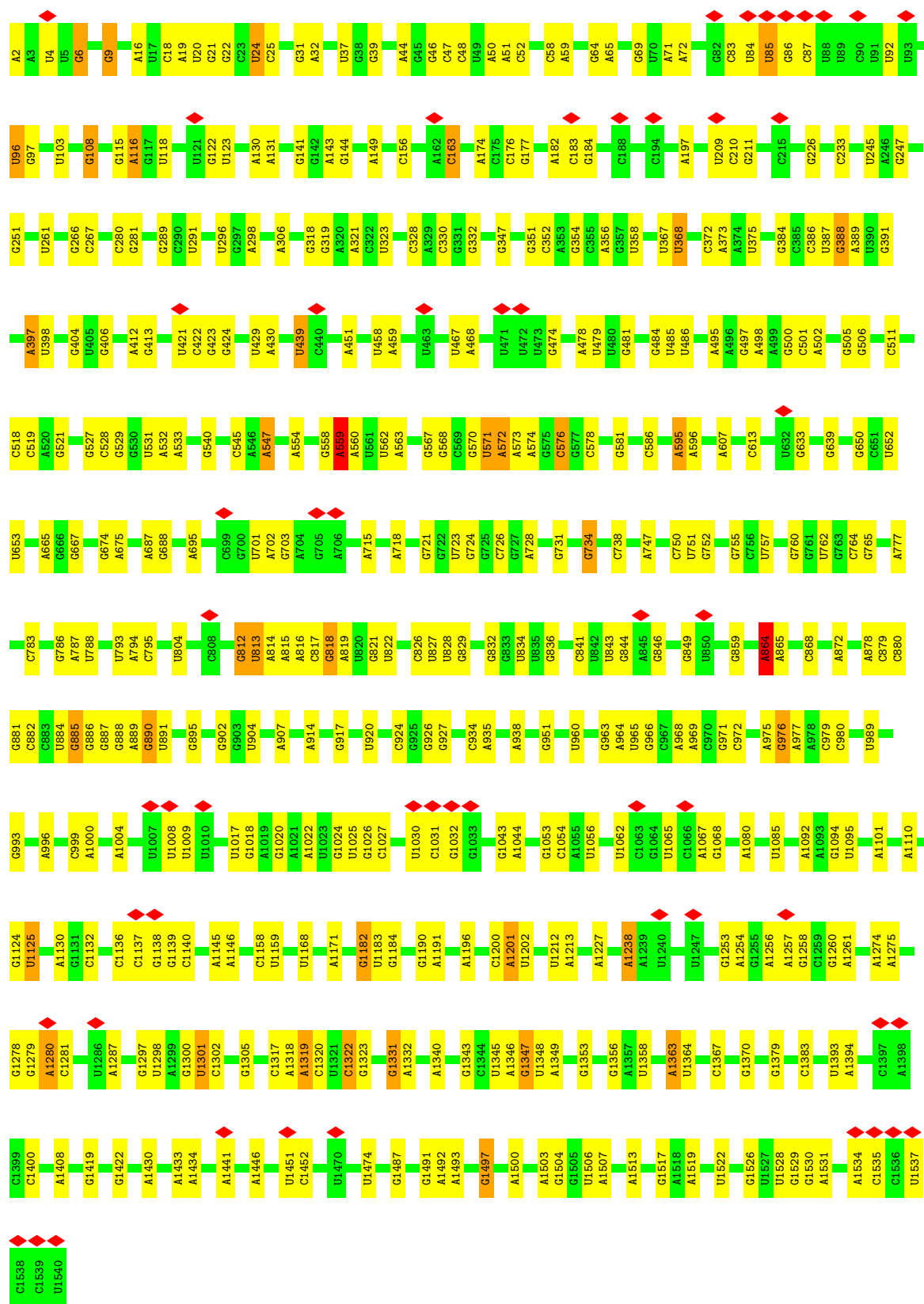


- Molecule 35: mRNA




- Molecule 36: 16S rRNA



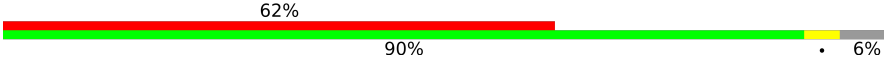


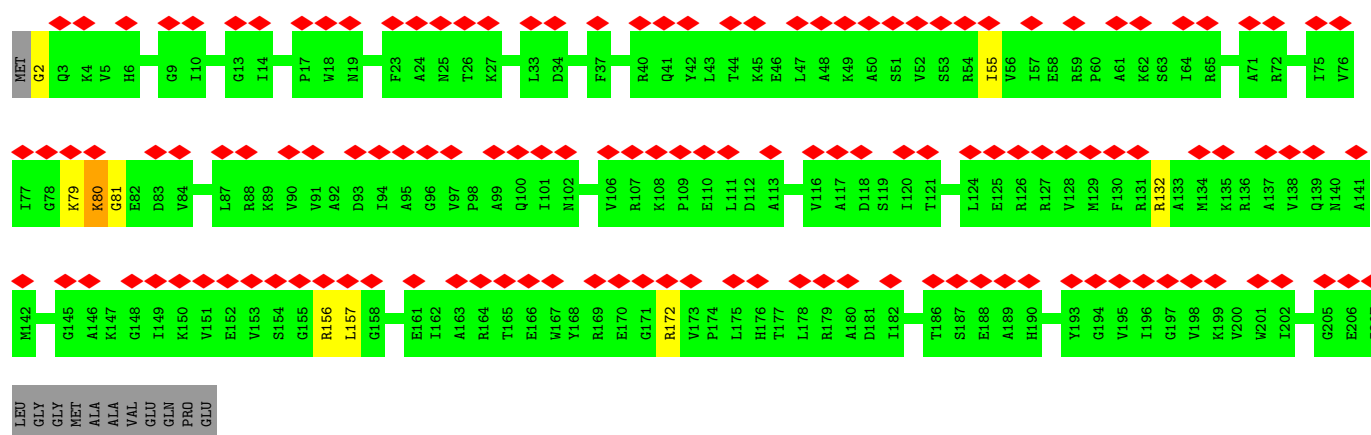
• Molecule 37: 30S ribosomal protein S2

Chain 1: 



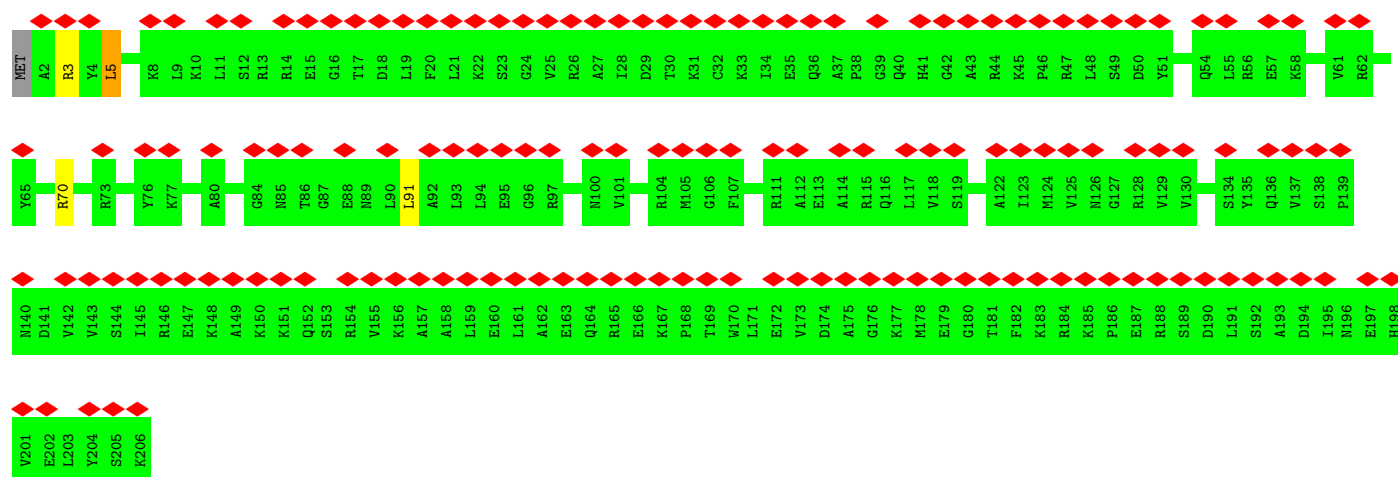
• Molecule 38: 30S ribosomal protein S3

Chain 2: 



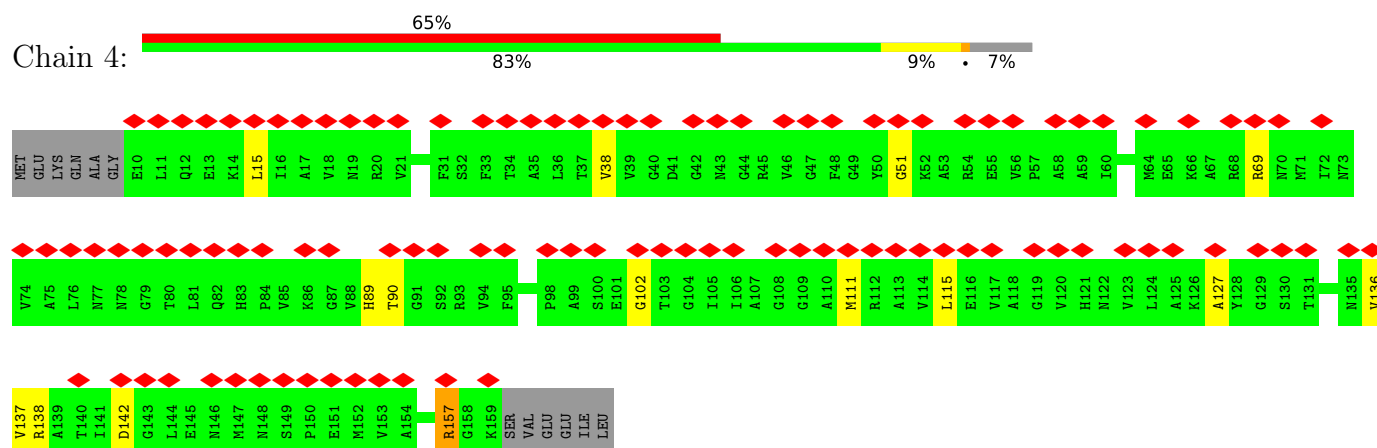
• Molecule 39: 30S ribosomal protein S4

Chain 3: 



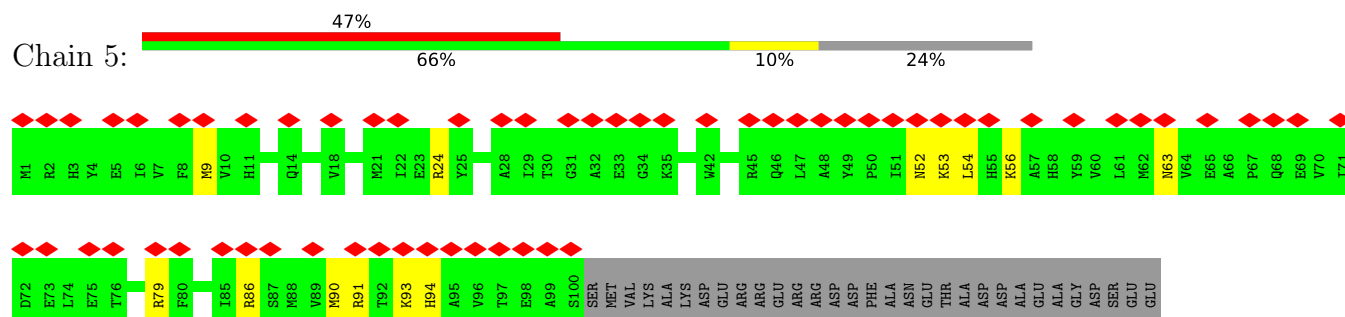
- Molecule 40: 30S ribosomal protein S5

Chain 4:



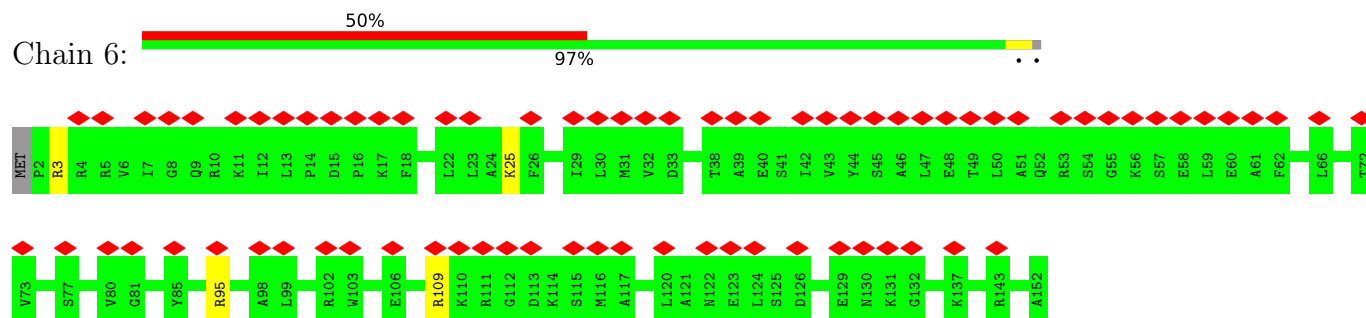
- Molecule 41: 30S ribosomal protein S6, non-modified isoform

Chain 5:



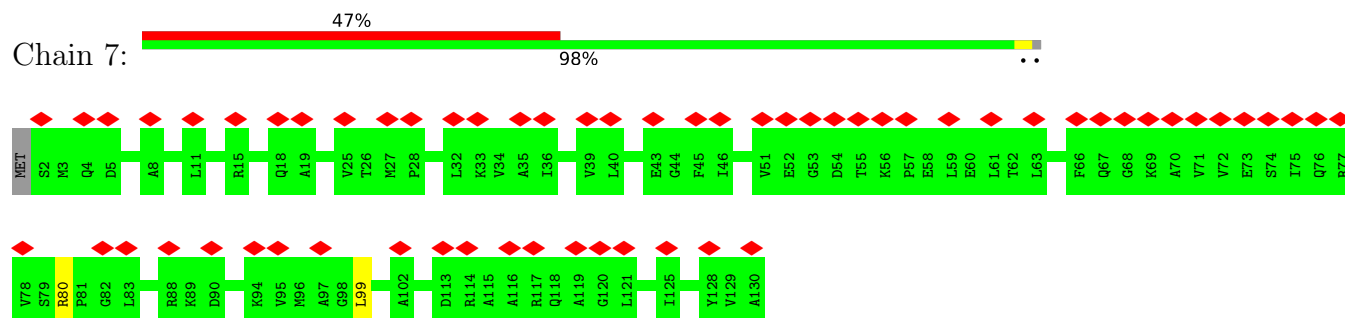
- Molecule 42: 30S ribosomal protein S7

Chain 6:

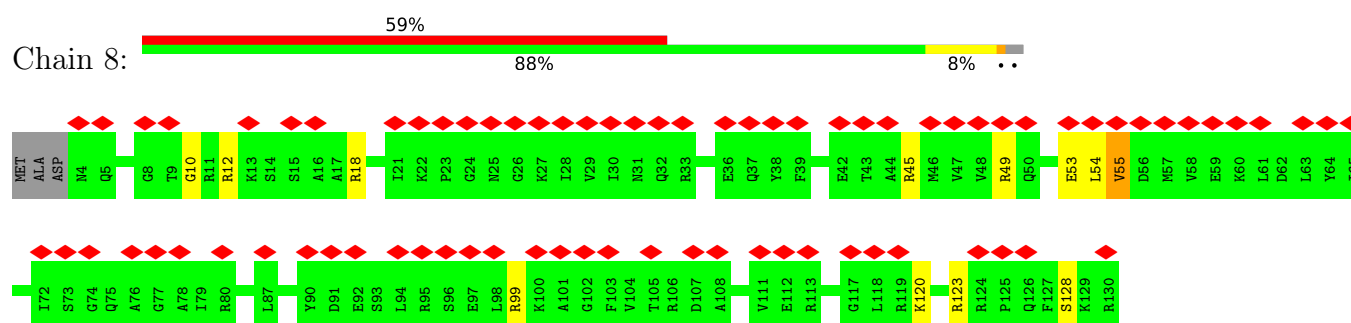


- Molecule 43: 30S ribosomal protein S8

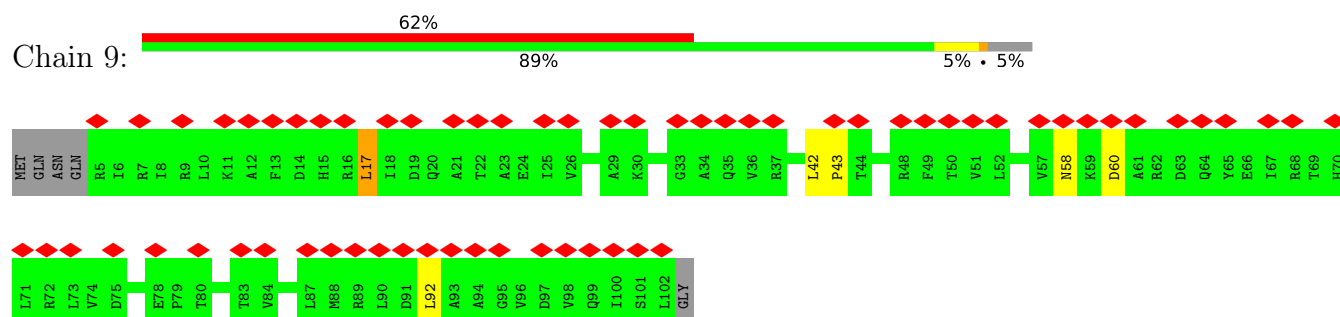
Chain 7:



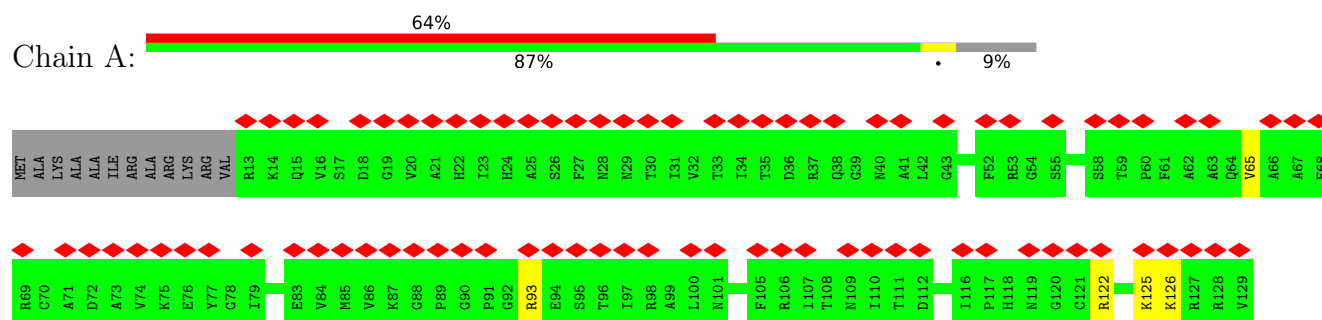
- Molecule 44: 30S ribosomal protein S9



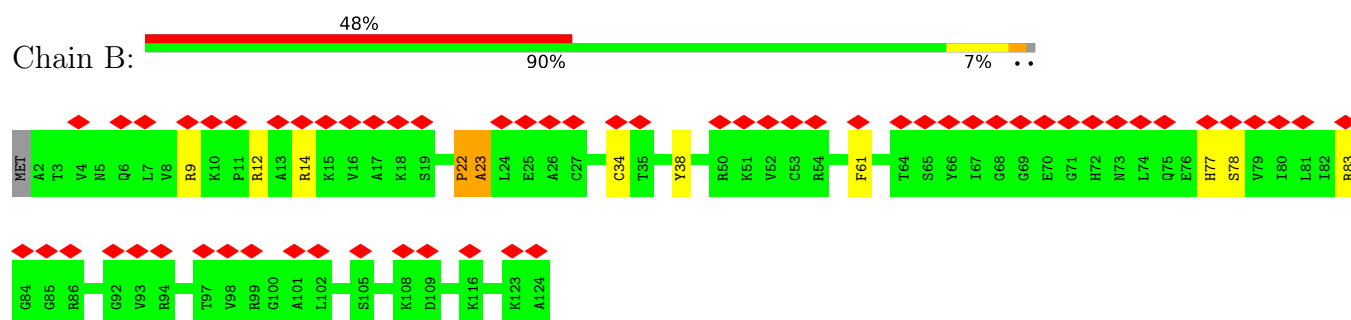
• Molecule 45: 30S ribosomal protein S10



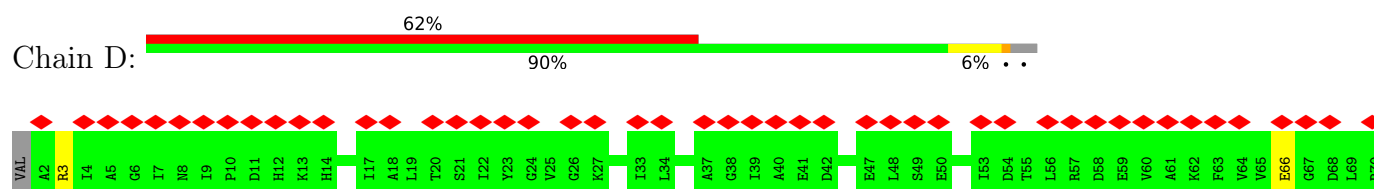
• Molecule 46: 30S ribosomal protein S11

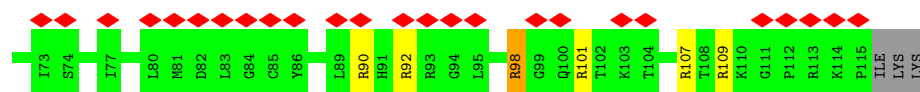


• Molecule 47: 30S ribosomal protein S12

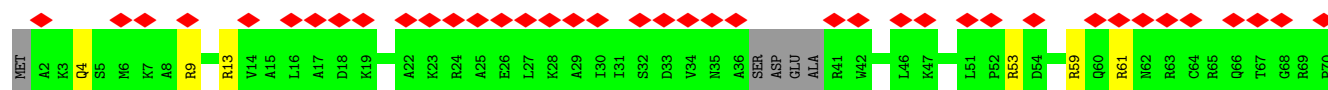
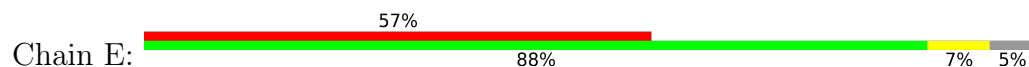


• Molecule 48: 30S ribosomal protein S13

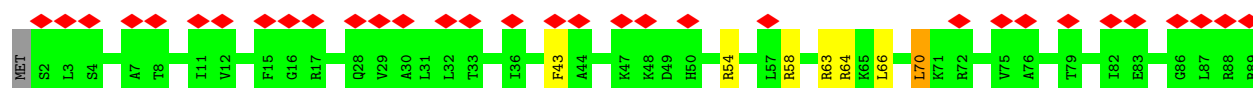




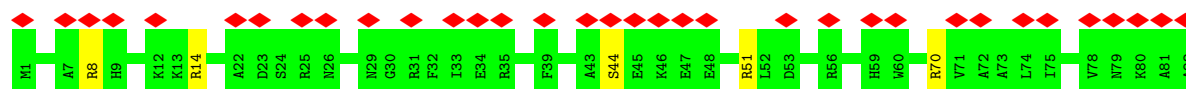
- Molecule 49: 30S ribosomal protein S14



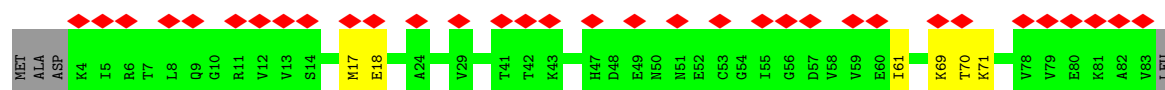
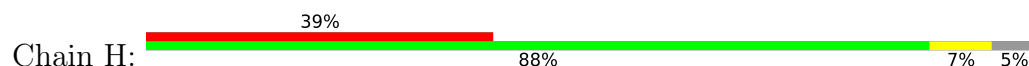
- Molecule 50: 30S ribosomal protein S15



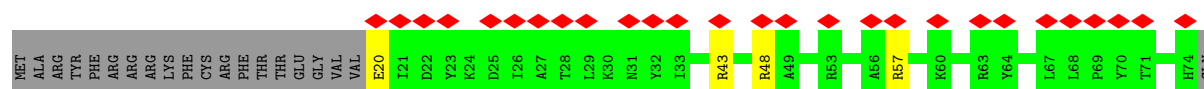
- Molecule 51: 30S ribosomal protein S16



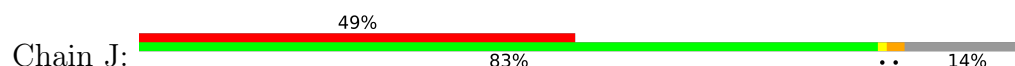
- Molecule 52: 30S ribosomal protein S17

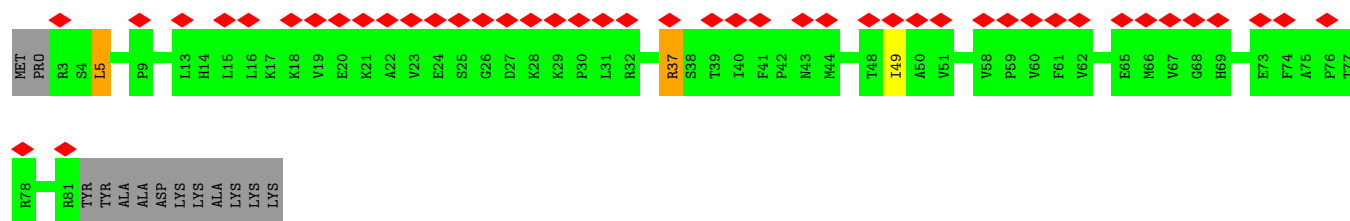


- Molecule 53: 30S ribosomal protein S18

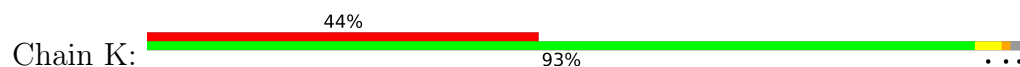


- Molecule 54: 30S ribosomal protein S19

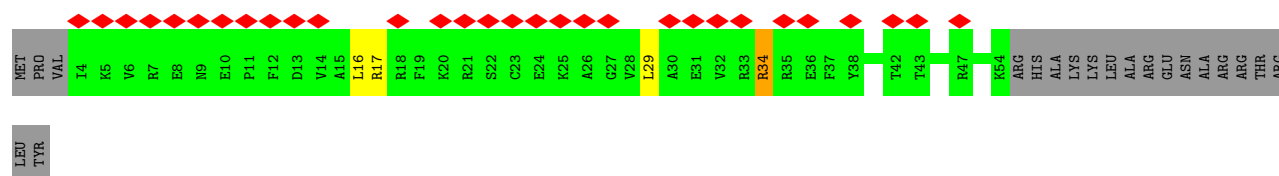
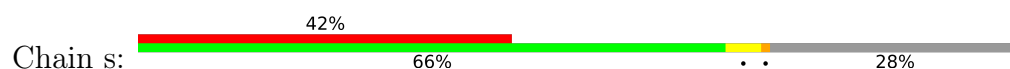




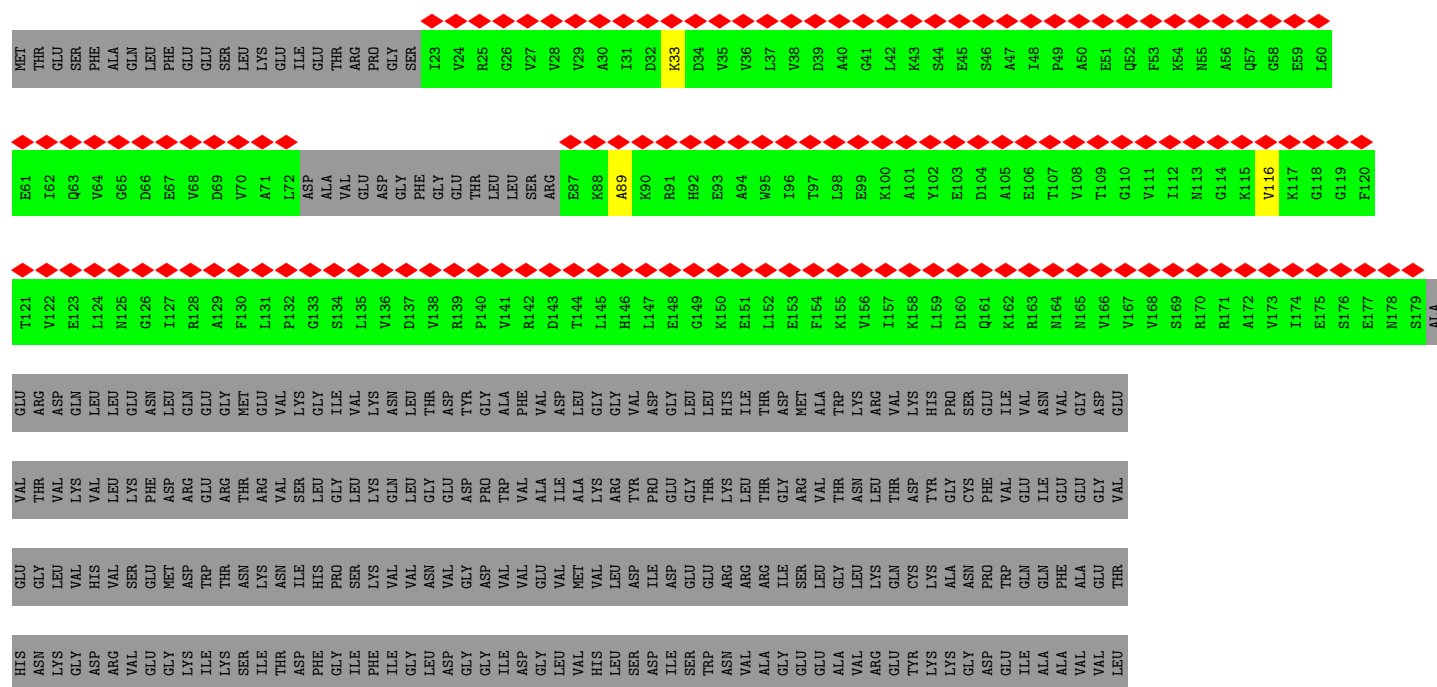
- Molecule 55: 30S ribosomal protein S20



- Molecule 56: 30S ribosomal protein S21

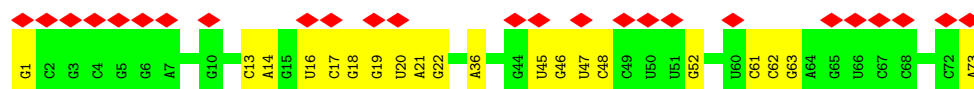
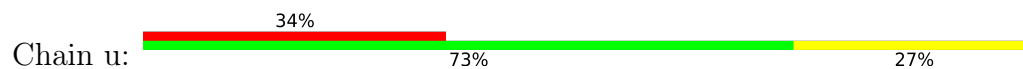


- Molecule 57: 30S ribosomal protein S1

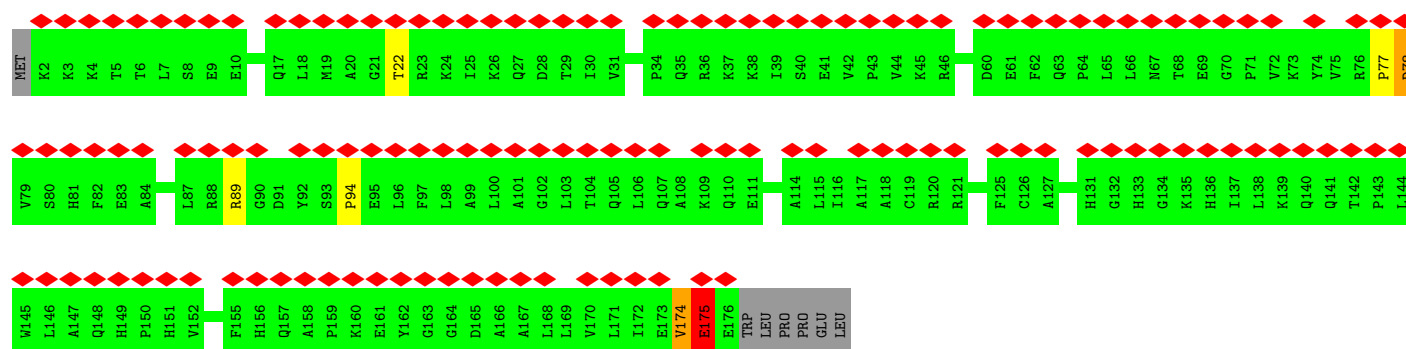
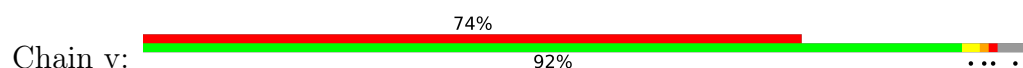


GLN	SER
VAL	VAL
ASP	ASP
ALA	ALA
GLU	GLU
ARG	ARG
GLU	GLU
ARG	ARG
ILE	ILE
GLU	GLU
SER	SER
ALA	ALA
LEU	LEU
GLY	GLY
VAL	VAL
LYS	LYS
GLN	GLN
LEU	LEU
VAL	VAL
ALA	ALA
GLY	GLY
ASP	ASP
GLU	GLU
ASP	ASP
PRO	PRO
PHE	PHE
GLU	GLU
ASN	ASN
ALA	ALA
ASN	ASN
TRP	TRP
VAL	VAL
ALA	ALA
LEU	LEU
ASN	ASN
LYS	LYS
GLY	GLY
ASP	ASP
LYS	LYS
GLY	GLY
ILE	ILE
THR	THR
THR	THR
GLY	GLY
LYS	LYS
VAL	VAL
THR	THR
VAL	VAL
ARG	ARG
ALA	ALA
LYS	LYS
ASP	ASP
ALA	ALA
LYS	LYS
GLY	GLY
ALA	ALA
GLY	GLY
ALA	ALA
ASP	ASP
GLU	GLU
VAL	VAL
LEU	LEU
ALA	ALA
ALA	ALA
ASP	ASP
ALA	ALA
ASP	ASP
GLU	GLU
TYR	TYR
LEU	LEU
ASP	ASP
ALA	ALA

• Molecule 58: A-site tRNA



• Molecule 59: UPF0115 protein YfcN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32412	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.070	Depositor
Minimum map value	-0.867	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	847.19995, 847.19995, 847.19995	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.412, 1.412, 1.412	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG

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	O	0.80	1/2828 (0.0%)	0.88	6/4410 (0.1%)
2	P	1.41	22/2121 (1.0%)	1.32	27/2852 (0.9%)
3	Q	1.18	3/1585 (0.2%)	1.13	8/2134 (0.4%)
4	R	0.97	3/1571 (0.2%)	1.02	9/2113 (0.4%)
5	S	0.67	0/1420	0.85	0/1907
6	T	0.67	0/1342	0.83	4/1816 (0.2%)
7	V	0.53	0/1045	0.66	0/1410
8	W	1.10	3/1151 (0.3%)	1.10	7/1551 (0.5%)
9	X	1.15	0/947	1.20	5/1268 (0.4%)
10	Y	1.30	3/1053 (0.3%)	1.38	12/1403 (0.9%)
11	Z	1.13	2/1092 (0.2%)	1.19	6/1460 (0.4%)
12	a	1.27	3/973 (0.3%)	1.30	9/1301 (0.7%)
13	b	0.84	2/901 (0.2%)	1.08	8/1209 (0.7%)
14	c	1.09	3/927 (0.3%)	1.19	7/1240 (0.6%)
15	d	1.32	4/959 (0.4%)	1.37	15/1278 (1.2%)
16	e	1.08	2/828 (0.2%)	1.08	3/1107 (0.3%)
17	f	1.02	1/864 (0.1%)	1.09	1/1156 (0.1%)
18	g	0.91	0/744	1.01	1/994 (0.1%)
19	h	0.82	1/787 (0.1%)	0.89	0/1051
20	i	0.79	0/765	0.87	0/1025
21	j	1.21	2/575 (0.3%)	1.29	7/762 (0.9%)
22	k	1.09	1/634 (0.2%)	1.15	5/848 (0.6%)
23	l	0.71	0/509	1.04	4/677 (0.6%)
24	m	0.87	0/452	1.08	2/605 (0.3%)
25	n	1.16	2/449 (0.4%)	1.42	7/599 (1.2%)
26	o	1.31	7/416 (1.7%)	0.97	1/554 (0.2%)
27	p	1.38	3/379 (0.8%)	1.76	7/498 (1.4%)
28	q	1.15	1/512 (0.2%)	1.26	6/676 (0.9%)
29	r	1.16	1/302 (0.3%)	1.35	5/397 (1.3%)
30	N	1.24	517/69681 (0.7%)	1.04	339/108706 (0.3%)
31	L	0.60	0/422	0.78	0/565
32	C	0.28	0/1034	0.52	0/1387

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	U	0.29	0/1122	0.58	0/1515
34	M	0.63	3/1779 (0.2%)	0.83	2/2768 (0.1%)
35	x	0.87	8/1035 (0.8%)	1.12	6/1608 (0.4%)
36	0	0.97	133/36966 (0.4%)	0.93	105/57666 (0.2%)
37	1	0.81	2/1729 (0.1%)	0.93	4/2330 (0.2%)
38	2	0.85	1/1651 (0.1%)	0.95	4/2225 (0.2%)
39	3	0.76	0/1664	0.99	5/2227 (0.2%)
40	4	1.11	1/1118 (0.1%)	1.22	7/1504 (0.5%)
41	5	0.90	1/835 (0.1%)	1.03	3/1128 (0.3%)
42	6	0.66	0/1195	0.95	6/1602 (0.4%)
43	7	0.88	0/988	0.99	2/1326 (0.2%)
44	8	0.86	0/1033	1.13	6/1375 (0.4%)
45	9	0.74	0/796	1.01	3/1077 (0.3%)
46	A	0.86	1/892 (0.1%)	1.03	3/1205 (0.2%)
47	B	1.09	3/968 (0.3%)	1.22	7/1300 (0.5%)
48	D	0.85	1/886 (0.1%)	1.11	9/1186 (0.8%)
49	E	0.86	0/784	1.15	7/1043 (0.7%)
50	F	0.94	0/717	1.14	8/959 (0.8%)
51	G	0.94	0/658	1.16	5/884 (0.6%)
52	H	0.82	0/657	1.02	0/881
53	I	0.98	1/462 (0.2%)	1.10	2/621 (0.3%)
54	J	0.81	0/652	1.05	3/877 (0.3%)
55	K	0.89	0/670	1.06	3/888 (0.3%)
56	s	1.07	1/430 (0.2%)	1.25	4/570 (0.7%)
57	t	0.34	0/702	0.44	0/973
58	u	0.66	1/1744 (0.1%)	0.86	0/2716
59	v	0.68	3/1282 (0.2%)	0.67	3/1746 (0.2%)
All	All	1.08	747/162683 (0.5%)	1.02	718/243159 (0.3%)

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	P	0	3
3	Q	0	1
5	S	0	2
7	V	0	1
10	Y	0	2
11	Z	0	2
19	h	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	q	0	1
30	N	0	6
36	0	0	5
37	1	0	2
38	2	0	2
40	4	0	5
41	5	0	2
44	8	0	4
46	A	0	1
47	B	0	2
52	H	0	2
54	J	0	1
55	K	0	1
56	s	0	1
59	v	0	3
All	All	0	50

All (747) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	2873	A	C6-N1	-20.36	1.21	1.35
30	N	2765	A	C6-N1	-18.72	1.22	1.35
30	N	2502	G	P-OP2	16.57	1.77	1.49
30	N	503	A	C6-N1	-15.29	1.24	1.35
30	N	1156	A	P-OP2	15.23	1.74	1.49
36	0	24	U	N3-C4	-13.85	1.25	1.38
36	0	1238	A	C6-N1	-13.75	1.25	1.35
2	P	213	TRP	CD2-CE2	13.70	1.57	1.41
30	N	1333	G	P-OP2	12.85	1.70	1.49
30	N	783	A	P-OP2	12.71	1.70	1.49
30	N	945	A	P-OP2	12.34	1.70	1.49
30	N	1639	C	P-OP1	12.07	1.69	1.49
30	N	1664	A	P-OP2	11.85	1.69	1.49
30	N	945	A	P-OP1	11.84	1.69	1.49
30	N	310	A	C6-N1	-11.67	1.27	1.35
30	N	1670	C	P-OP1	11.51	1.68	1.49
30	N	1141	U	N3-C4	-11.50	1.28	1.38
2	P	213	TRP	CZ3-CH2	11.44	1.58	1.40
30	N	2074	U	P-OP1	11.41	1.68	1.49
36	0	559	A	N1-C2	11.38	1.44	1.34
30	N	234	U	N3-C4	-11.38	1.28	1.38
36	0	368	U	N3-C4	-11.16	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	213	TRP	CB-CG	-11.11	1.30	1.50
36	O	37	U	N3-C4	-11.09	1.28	1.38
30	N	2588	G	P-OP1	10.98	1.67	1.49
30	N	828	U	O3'-P	-10.84	1.48	1.61
30	N	2349	G	O3'-P	-10.77	1.48	1.61
30	N	2005	A	P-OP1	10.71	1.67	1.49
58	u	1	G	OP3-P	-10.71	1.48	1.61
30	N	450	G	P-OP2	10.68	1.67	1.49
30	N	2445	G	O3'-P	-10.64	1.48	1.61
30	N	2272	U	N3-C4	-10.58	1.28	1.38
30	N	827	U	P-OP1	10.57	1.67	1.49
30	N	963	U	O3'-P	-10.46	1.48	1.61
30	N	943	A	P-OP2	10.34	1.66	1.49
30	N	1777	U	O3'-P	-10.28	1.48	1.61
30	N	2589	A	O3'-P	-10.26	1.48	1.61
19	h	68	SER	CB-OG	10.23	1.55	1.42
30	N	932	U	N3-C4	-10.21	1.29	1.38
36	O	757	U	O3'-P	-10.17	1.49	1.61
30	N	2060	A	O3'-P	-10.12	1.49	1.61
36	O	1301	U	N3-C4	10.08	1.47	1.38
30	N	2025	C	P-OP2	10.08	1.66	1.49
36	O	1358	U	N3-C4	-10.06	1.29	1.38
34	M	1	U	OP3-P	-10.06	1.49	1.61
30	N	800	A	P-OP1	10.02	1.66	1.49
36	O	578	C	P-OP1	10.02	1.66	1.49
30	N	567	U	P-OP1	10.00	1.66	1.49
36	O	24	U	C2-N3	10.00	1.44	1.37
30	N	2720	U	C2-N3	9.94	1.44	1.37
30	N	782	A	O3'-P	-9.91	1.49	1.61
26	o	21	TYR	CE2-CZ	-9.86	1.25	1.38
30	N	692	C	O3'-P	-9.81	1.49	1.61
30	N	787	C	O3'-P	-9.77	1.49	1.61
30	N	1968	G	O3'-P	-9.77	1.49	1.61
30	N	1009	A	O3'-P	-9.75	1.49	1.61
30	N	1604	C	P-OP1	9.73	1.65	1.49
30	N	825	A	O3'-P	-9.71	1.49	1.61
30	N	2615	U	P-OP1	9.70	1.65	1.49
30	N	2687	U	O3'-P	-9.69	1.49	1.61
36	O	20	U	O3'-P	-9.69	1.49	1.61
30	N	1774	C	P-OP1	9.66	1.65	1.49
36	O	21	G	P-OP1	9.65	1.65	1.49
30	N	2522	U	C2-N3	9.62	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	585	G	O3'-P	-9.60	1.49	1.61
30	N	1257	C	O3'-P	-9.40	1.49	1.61
30	N	2344	U	N3-C4	-9.40	1.29	1.38
30	N	2019	A	O3'-P	-9.34	1.50	1.61
30	N	1828	G	P-OP2	9.31	1.64	1.49
30	N	963	U	P-OP1	9.29	1.64	1.49
30	N	116	C	O3'-P	-9.25	1.50	1.61
30	N	445	C	O3'-P	-9.24	1.50	1.61
30	N	2025	C	O3'-P	-9.22	1.50	1.61
30	N	809	G	O3'-P	-9.22	1.50	1.61
30	N	554	U	O3'-P	-9.21	1.50	1.61
30	N	576	U	P-OP1	9.21	1.64	1.49
30	N	984	A	O3'-P	-9.17	1.50	1.61
30	N	2593	U	O3'-P	-9.16	1.50	1.61
30	N	2550	G	O3'-P	-9.14	1.50	1.61
30	N	1269	A	P-OP2	9.07	1.64	1.49
30	N	948	C	P-OP1	9.06	1.64	1.49
36	0	667	G	O3'-P	-9.05	1.50	1.61
30	N	2050	C	O3'-P	-9.03	1.50	1.61
30	N	306	U	N3-C4	9.01	1.46	1.38
30	N	2588	G	O3'-P	-8.97	1.50	1.61
36	0	882	C	O3'-P	-8.97	1.50	1.61
30	N	1152	C	O3'-P	-8.96	1.50	1.61
30	N	1375	U	O3'-P	-8.93	1.50	1.61
30	N	673	C	O3'-P	-8.79	1.50	1.61
30	N	397	U	O3'-P	-8.78	1.50	1.61
30	N	2543	G	P-OP1	8.71	1.63	1.49
30	N	2588	G	P-OP2	8.71	1.63	1.49
30	N	859	G	O3'-P	8.69	1.71	1.61
30	N	2635	A	O3'-P	-8.64	1.50	1.61
30	N	2576	G	P-OP1	8.64	1.63	1.49
30	N	1774	C	O3'-P	-8.60	1.50	1.61
36	0	827	U	N3-C4	-8.59	1.30	1.38
30	N	1019	U	O3'-P	-8.58	1.50	1.61
30	N	2052	A	O3'-P	-8.56	1.50	1.61
30	N	120	U	P-OP1	8.56	1.63	1.49
30	N	2698	U	O3'-P	-8.54	1.50	1.61
30	N	2714	G	P-OP2	8.54	1.63	1.49
30	N	1612	C	O3'-P	-8.49	1.50	1.61
30	N	1664	A	P-OP1	8.48	1.63	1.49
30	N	200	U	O3'-P	-8.48	1.50	1.61
29	r	38	GLY	N-CA	8.47	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	1994	C	O3'-P	-8.40	1.51	1.61
30	N	2466	C	O3'-P	-8.40	1.51	1.61
2	P	195	VAL	CB-CG1	-8.38	1.35	1.52
30	N	1658	C	O3'-P	-8.37	1.51	1.61
36	O	1500	A	O3'-P	-8.36	1.51	1.61
30	N	503	A	N1-C2	8.32	1.41	1.34
30	N	499	U	N3-C4	8.30	1.46	1.38
30	N	641	U	O3'-P	-8.29	1.51	1.61
30	N	1751	U	O3'-P	-8.29	1.51	1.61
30	N	2503	A	P-OP2	8.27	1.63	1.49
30	N	1900	A	O3'-P	8.25	1.71	1.61
30	N	2613	U	N3-C4	-8.23	1.31	1.38
30	N	955	U	O3'-P	-8.22	1.51	1.61
30	N	1831	G	O3'-P	-8.19	1.51	1.61
30	N	826	U	P-OP1	8.18	1.62	1.49
30	N	2498	C	P-OP2	8.18	1.62	1.49
36	O	812	G	O3'-P	8.17	1.71	1.61
30	N	453	A	P-OP1	8.16	1.62	1.49
30	N	1780	A	P-OP1	8.14	1.62	1.49
30	N	2740	A	O3'-P	-8.14	1.51	1.61
30	N	2022	U	P-OP1	8.13	1.62	1.49
30	N	1254	A	O3'-P	-8.09	1.51	1.61
10	Y	18	ARG	CZ-NH1	8.08	1.43	1.33
30	N	1353	A	O3'-P	-8.07	1.51	1.61
30	N	2605	U	O3'-P	-8.03	1.51	1.61
30	N	1658	C	P-OP1	7.99	1.62	1.49
30	N	1813	G	O3'-P	-7.98	1.51	1.61
30	N	2489	U	O3'-P	-7.95	1.51	1.61
30	N	2264	C	O3'-P	-7.93	1.51	1.61
30	N	2437	G	O3'-P	-7.89	1.51	1.61
30	N	2502	G	O5'-C5'	-7.86	1.30	1.42
30	N	839	U	O3'-P	-7.86	1.51	1.61
30	N	2265	U	O3'-P	-7.85	1.51	1.61
30	N	2590	A	O3'-P	-7.83	1.51	1.61
30	N	2006	C	P-OP1	7.80	1.62	1.49
30	N	192	C	P-OP1	7.79	1.62	1.49
30	N	2062	A	P-OP2	7.79	1.62	1.49
30	N	1782	U	P-OP1	7.78	1.62	1.49
36	O	726	C	O3'-P	-7.77	1.51	1.61
30	N	733	G	O3'-P	-7.75	1.51	1.61
30	N	1794	A	O3'-P	-7.74	1.51	1.61
30	N	832	U	O3'-P	-7.72	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	192	C	O3'-P	-7.71	1.51	1.61
30	N	515	A	O3'-P	-7.71	1.51	1.61
30	N	1189	A	O3'-P	-7.71	1.51	1.61
30	N	2447	G	O3'-P	-7.70	1.51	1.61
2	P	204	VAL	CB-CG2	-7.67	1.36	1.52
30	N	372	G	O3'-P	7.67	1.70	1.61
30	N	1268	A	P-OP1	7.66	1.61	1.49
30	N	810	U	P-OP1	7.64	1.61	1.49
30	N	2518	A	P-OP2	7.64	1.61	1.49
36	O	884	U	C4-O4	-7.62	1.17	1.23
30	N	2822	G	O3'-P	-7.62	1.52	1.61
30	N	1778	U	O3'-P	-7.61	1.52	1.61
30	N	997	G	O3'-P	-7.60	1.52	1.61
30	N	2572	A	O3'-P	-7.58	1.52	1.61
30	N	1790	C	O3'-P	-7.58	1.52	1.61
36	O	1238	A	N1-C2	7.55	1.41	1.34
30	N	1771	C	O3'-P	-7.54	1.52	1.61
30	N	2620	C	O3'-P	-7.53	1.52	1.61
30	N	254	G	O3'-P	-7.53	1.52	1.61
10	Y	22	GLY	C-O	-7.52	1.11	1.23
30	N	569	U	O3'-P	-7.52	1.52	1.61
30	N	2867	G	O3'-P	7.49	1.70	1.61
30	N	821	A	O3'-P	-7.49	1.52	1.61
30	N	464	U	O3'-P	-7.49	1.52	1.61
30	N	1970	A	P-OP2	7.48	1.61	1.49
10	Y	51	GLU	C-O	7.47	1.37	1.23
30	N	2031	A	P-OP1	-7.47	1.36	1.49
30	N	2272	U	C4-O4	-7.47	1.17	1.23
30	N	676	A	O3'-P	-7.46	1.52	1.61
30	N	1828	G	P-OP1	7.45	1.61	1.49
30	N	1678	A	P-OP2	7.45	1.61	1.49
30	N	2061	G	C2'-O2'	7.45	1.51	1.41
13	b	30	ARG	CZ-NH1	7.43	1.42	1.33
30	N	2081	U	O3'-P	-7.42	1.52	1.61
36	O	1367	C	O3'-P	-7.42	1.52	1.61
41	5	63	ASN	C-O	-7.42	1.09	1.23
30	N	975	A	P-OP2	7.41	1.61	1.49
30	N	566	U	O3'-P	-7.40	1.52	1.61
30	N	2444	G	O3'-P	-7.40	1.52	1.61
30	N	2637	U	O3'-P	-7.39	1.52	1.61
30	N	2625	G	O3'-P	-7.39	1.52	1.61
30	N	2247	A	O3'-P	-7.38	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	1393	U	O3'-P	-7.37	1.52	1.61
30	N	2837	A	O3'-P	-7.33	1.52	1.61
30	N	1822	C	O3'-P	-7.30	1.52	1.61
2	P	221	ARG	CB-CG	-7.28	1.32	1.52
30	N	198	C	O3'-P	-7.28	1.52	1.61
30	N	2072	C	O3'-P	-7.28	1.52	1.61
30	N	2359	C	O3'-P	-7.25	1.52	1.61
30	N	2232	C	O3'-P	-7.25	1.52	1.61
30	N	538	A	O3'-P	-7.24	1.52	1.61
30	N	572	A	P-OP1	7.22	1.61	1.49
30	N	2598	A	O3'-P	-7.22	1.52	1.61
36	0	387	U	O3'-P	-7.21	1.52	1.61
30	N	2542	A	O3'-P	-7.21	1.52	1.61
36	0	22	G	O3'-P	-7.20	1.52	1.61
35	x	435	G	C1'-N9	-7.18	1.36	1.46
30	N	2602	A	O3'-P	7.17	1.69	1.61
26	o	21	TYR	CG-CD1	-7.17	1.29	1.39
30	N	966	G	O3'-P	-7.16	1.52	1.61
30	N	2457	U	O3'-P	-7.16	1.52	1.61
30	N	2419	U	C4-O4	7.16	1.29	1.23
30	N	126	A	O3'-P	-7.15	1.52	1.61
30	N	2013	A	O3'-P	-7.14	1.52	1.61
30	N	1261	C	O3'-P	-7.14	1.52	1.61
30	N	940	G	O3'-P	-7.14	1.52	1.61
30	N	2684	U	O3'-P	-7.13	1.52	1.61
30	N	1298	C	O3'-P	-7.12	1.52	1.61
36	0	505	G	O3'-P	-7.12	1.52	1.61
30	N	29	U	O3'-P	-7.11	1.52	1.61
30	N	1805	A	O3'-P	-7.11	1.52	1.61
30	N	1795	C	O3'-P	-7.09	1.52	1.61
30	N	1681	G	O3'-P	-7.08	1.52	1.61
30	N	2344	U	C2-N3	-7.08	1.32	1.37
30	N	796	C	O3'-P	-7.07	1.52	1.61
30	N	2016	U	O3'-P	-7.07	1.52	1.61
30	N	818	G	P-OP2	7.06	1.60	1.49
36	0	563	A	C6-N6	-7.05	1.28	1.33
26	o	21	TYR	CG-CD2	-7.04	1.29	1.39
30	N	571	U	O3'-P	-7.04	1.52	1.61
47	B	34	CYS	CB-SG	-7.04	1.70	1.82
30	N	25	U	O3'-P	-7.03	1.52	1.61
30	N	2013	A	C6-N6	-7.03	1.28	1.33
30	N	671	C	P-OP2	7.02	1.60	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	2406	A	P-OP1	7.02	1.60	1.49
1	O	83	G	O3'-P	-7.01	1.52	1.61
30	N	773	U	O3'-P	-6.96	1.52	1.61
30	N	1141	U	C2-N3	-6.95	1.32	1.37
30	N	2499	C	P-OP2	6.95	1.60	1.49
30	N	2049	G	O3'-P	-6.95	1.52	1.61
30	N	680	C	O3'-P	-6.94	1.52	1.61
30	N	2385	C	P-OP1	6.93	1.60	1.49
36	O	764	C	O3'-P	-6.92	1.52	1.61
30	N	2332	C	O3'-P	-6.90	1.52	1.61
30	N	730	A	P-OP2	6.89	1.60	1.49
30	N	2829	A	O3'-P	-6.89	1.52	1.61
36	O	980	C	P-OP1	6.89	1.60	1.49
30	N	1949	G	O3'-P	-6.88	1.52	1.61
30	N	2443	C	C4'-C3'	-6.87	1.45	1.53
30	N	1824	G	P-OP2	6.85	1.60	1.49
36	O	1358	U	C4-O4	-6.85	1.18	1.23
12	a	1	MET	C-O	6.84	1.36	1.23
30	N	2436	G	O3'-P	-6.84	1.52	1.61
30	N	688	U	O3'-P	-6.83	1.52	1.61
30	N	784	G	O3'-P	6.83	1.69	1.61
36	O	765	G	O3'-P	-6.82	1.52	1.61
30	N	2051	A	O3'-P	6.78	1.69	1.61
30	N	2516	A	O3'-P	-6.78	1.53	1.61
30	N	2268	A	P-OP1	6.76	1.60	1.49
30	N	927	A	N1-C2	6.74	1.40	1.34
30	N	2572	A	P-OP1	-6.72	1.37	1.49
30	N	239	C	O3'-P	-6.70	1.53	1.61
36	O	814	A	P-OP2	6.69	1.60	1.49
30	N	419	U	O3'-P	-6.69	1.53	1.61
30	N	1394	U	O3'-P	-6.69	1.53	1.61
2	P	10	SER	CA-CB	6.68	1.62	1.52
36	O	864	A	N1-C2	6.66	1.40	1.34
36	O	37	U	C2-N3	-6.66	1.33	1.37
30	N	923	G	O3'-P	-6.65	1.53	1.61
30	N	1662	U	P-OP2	6.65	1.60	1.49
30	N	2048	G	O3'-P	-6.65	1.53	1.61
30	N	1782	U	O3'-P	-6.64	1.53	1.61
30	N	117	G	O3'-P	-6.63	1.53	1.61
30	N	1234	U	O3'-P	-6.63	1.53	1.61
30	N	578	G	P-OP2	6.63	1.60	1.49
30	N	2260	C	O3'-P	-6.63	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	783	A	C4'-O4'	6.61	1.54	1.45
30	N	2694	G	O3'-P	-6.61	1.53	1.61
30	N	2499	C	P-OP1	6.61	1.60	1.49
30	N	2045	C	O3'-P	-6.61	1.53	1.61
30	N	698	C	O3'-P	-6.60	1.53	1.61
30	N	2452	C	O3'-P	-6.60	1.53	1.61
30	N	1977	A	O3'-P	-6.59	1.53	1.61
30	N	2285	C	O3'-P	-6.59	1.53	1.61
30	N	1432	G	O3'-P	-6.59	1.53	1.61
27	p	34	ARG	CG-CD	-6.58	1.35	1.51
30	N	932	U	C4-O4	-6.58	1.18	1.23
2	P	271	ARG	CZ-NH1	6.58	1.41	1.33
30	N	1960	A	O3'-P	-6.57	1.53	1.61
30	N	2074	U	O3'-P	-6.56	1.53	1.61
30	N	761	A	P-OP1	6.55	1.60	1.49
30	N	2072	C	P-OP1	6.54	1.60	1.49
14	c	98	TYR	CE1-CZ	6.54	1.47	1.38
2	P	139	SER	CB-OG	-6.54	1.33	1.42
30	N	2028	U	O3'-P	-6.52	1.53	1.61
30	N	1009	A	P-OP2	6.51	1.60	1.49
30	N	1649	G	O3'-P	-6.51	1.53	1.61
30	N	2426	A	O3'-P	-6.51	1.53	1.61
30	N	393	C	P-OP1	6.51	1.60	1.49
30	N	2723	C	O3'-P	-6.51	1.53	1.61
30	N	2727	A	O3'-P	-6.50	1.53	1.61
30	N	1010	A	P-OP2	6.50	1.59	1.49
30	N	2289	G	O3'-P	-6.50	1.53	1.61
30	N	2248	C	P-OP2	6.49	1.59	1.49
30	N	2699	C	O3'-P	-6.49	1.53	1.61
30	N	499	U	C4-O4	-6.49	1.18	1.23
30	N	1680	U	O3'-P	-6.48	1.53	1.61
30	N	1191	G	O3'-P	-6.48	1.53	1.61
30	N	1677	A	O3'-P	-6.48	1.53	1.61
36	0	1182	G	O3'-P	6.48	1.69	1.61
40	4	127	ALA	C-O	-6.48	1.11	1.23
21	j	42	GLY	N-CA	6.47	1.55	1.46
27	p	38	GLY	CA-C	-6.47	1.41	1.51
36	0	19	A	O3'-P	-6.46	1.53	1.61
36	0	368	U	C2-N3	-6.45	1.33	1.37
36	0	368	U	C4-O4	-6.45	1.18	1.23
30	N	960	A	O3'-P	-6.45	1.53	1.61
30	N	193	U	O3'-P	-6.43	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	2262	U	O3'-P	-6.42	1.53	1.61
15	d	24	TYR	CG-CD1	6.41	1.47	1.39
30	N	28	A	P-O5'	-6.41	1.53	1.59
30	N	1652	A	O3'-P	-6.41	1.53	1.61
30	N	1671	U	P-OP2	6.41	1.59	1.49
30	N	1334	G	O3'-P	-6.40	1.53	1.61
15	d	49	ASP	CB-CG	6.39	1.65	1.51
36	0	1301	U	N1-C2	6.39	1.44	1.38
3	Q	125	TRP	CE3-CZ3	-6.39	1.27	1.38
30	N	1993	U	O5'-C5'	-6.38	1.32	1.42
30	N	694	U	O3'-P	-6.38	1.53	1.61
30	N	1296	G	O3'-P	-6.38	1.53	1.61
36	0	812	G	C3'-C2'	-6.38	1.45	1.52
30	N	1186	G	O3'-P	-6.38	1.53	1.61
30	N	1186	G	P-OP2	6.38	1.59	1.49
30	N	1650	A	O3'-P	-6.38	1.53	1.61
2	P	219	THR	C-O	6.37	1.35	1.23
30	N	632	A	O3'-P	-6.36	1.53	1.61
36	0	884	U	N3-C4	-6.36	1.32	1.38
30	N	2243	U	P-OP1	6.36	1.59	1.49
30	N	1004	U	O3'-P	-6.35	1.53	1.61
26	o	49	TYR	CE1-CZ	-6.34	1.30	1.38
30	N	2502	G	O3'-P	-6.34	1.53	1.61
30	N	1142	A	O3'-P	6.34	1.68	1.61
30	N	745	G	O3'-P	-6.33	1.53	1.61
30	N	783	A	C5-C6	-6.32	1.35	1.41
30	N	208	C	O3'-P	-6.32	1.53	1.61
30	N	1367	A	O3'-P	-6.32	1.53	1.61
30	N	408	G	O3'-P	-6.31	1.53	1.61
36	0	715	A	O3'-P	-6.30	1.53	1.61
30	N	7	G	O3'-P	-6.30	1.53	1.61
30	N	1006	C	O3'-P	-6.30	1.53	1.61
36	0	37	U	C4-O4	-6.29	1.18	1.23
30	N	2554	U	P-OP2	-6.29	1.38	1.49
2	P	213	TRP	CD1-NE1	6.28	1.48	1.38
36	0	787	A	O3'-P	-6.28	1.53	1.61
30	N	1026	G	P-OP2	-6.28	1.38	1.49
30	N	2444	G	C2'-C1'	-6.27	1.46	1.53
8	W	16	TYR	CG-CD1	-6.27	1.31	1.39
30	N	1327	A	P-OP2	6.27	1.59	1.49
30	N	2000	C	O3'-P	-6.25	1.53	1.61
30	N	120	U	P-OP2	6.24	1.59	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	920	U	O3'-P	-6.24	1.53	1.61
30	N	567	U	O3'-P	-6.24	1.53	1.61
30	N	576	U	O3'-P	-6.24	1.53	1.61
30	N	2543	G	O5'-C5'	-6.23	1.32	1.42
36	0	568	G	O3'-P	-6.22	1.53	1.61
36	0	1062	U	O3'-P	-6.21	1.53	1.61
56	s	34	ARG	CZ-NH1	6.21	1.41	1.33
30	N	411	G	P-OP1	6.21	1.59	1.49
36	0	613	C	O3'-P	-6.20	1.53	1.61
30	N	1141	U	C4-O4	-6.20	1.18	1.23
30	N	1816	C	O3'-P	-6.20	1.53	1.61
36	0	356	A	O3'-P	-6.20	1.53	1.61
47	B	23	ALA	N-CA	6.19	1.58	1.46
30	N	247	G	O3'-P	-6.18	1.53	1.61
36	0	1474	U	O3'-P	-6.18	1.53	1.61
30	N	1370	C	O3'-P	-6.18	1.53	1.61
30	N	26	G	O3'-P	-6.17	1.53	1.61
30	N	253	C	O3'-P	-6.17	1.53	1.61
36	0	572	A	P-OP1	6.17	1.59	1.49
14	c	93	ARG	CD-NE	-6.17	1.35	1.46
30	N	593	U	O3'-P	-6.17	1.53	1.61
36	0	581	G	O3'-P	-6.17	1.53	1.61
2	P	214	ARG	CZ-NH1	6.16	1.41	1.33
30	N	1793	C	O3'-P	-6.16	1.53	1.61
30	N	2263	C	O3'-P	-6.15	1.53	1.61
30	N	1827	U	O3'-P	-6.15	1.53	1.61
30	N	1905	C	O3'-P	-6.15	1.53	1.61
30	N	946	C	P-OP2	6.14	1.59	1.49
36	0	439	U	C2-N3	6.14	1.42	1.37
30	N	2035	G	O5'-C5'	-6.14	1.33	1.42
30	N	2277	G	O3'-P	-6.14	1.53	1.61
30	N	1142	A	C5-C6	-6.14	1.35	1.41
30	N	430	A	C6-N6	-6.14	1.29	1.33
30	N	1342	A	P-OP2	6.14	1.59	1.49
30	N	1196	C	O3'-P	-6.12	1.53	1.61
30	N	2682	A	P-OP2	6.12	1.59	1.49
36	0	498	A	N1-C2	6.11	1.39	1.34
30	N	244	A	O3'-P	-6.11	1.53	1.61
30	N	777	G	O3'-P	-6.11	1.53	1.61
30	N	398	C	O3'-P	-6.10	1.53	1.61
36	0	1358	U	C2-N3	-6.10	1.33	1.37
30	N	524	G	O3'-P	-6.10	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	932	U	C2-N3	-6.10	1.33	1.37
30	N	2776	A	C5-C6	-6.10	1.35	1.41
30	N	1636	U	O3'-P	-6.09	1.53	1.61
30	N	725	G	O3'-P	-6.09	1.53	1.61
30	N	1153	C	P-OP2	6.08	1.59	1.49
12	a	2	ARG	C-O	-6.08	1.11	1.23
30	N	1968	G	P-OP1	6.08	1.59	1.49
30	N	123	G	O3'-P	-6.07	1.53	1.61
30	N	1368	G	O3'-P	-6.07	1.53	1.61
36	0	917	G	O3'-P	-6.07	1.53	1.61
30	N	234	U	C2-N3	-6.06	1.33	1.37
36	0	816	A	O3'-P	-6.06	1.53	1.61
36	0	1522	U	O3'-P	-6.05	1.53	1.61
30	N	2442	C	O3'-P	-6.04	1.53	1.61
36	0	1080	A	O3'-P	-6.04	1.53	1.61
30	N	1134	A	O3'-P	6.04	1.68	1.61
30	N	2642	G	O3'-P	-6.03	1.53	1.61
36	0	834	U	O3'-P	-6.03	1.53	1.61
30	N	1756	G	O3'-P	-6.02	1.53	1.61
30	N	1676	A	O3'-P	-6.02	1.53	1.61
30	N	190	A	O3'-P	-6.02	1.53	1.61
36	0	1110	A	P-OP2	6.01	1.59	1.49
30	N	1648	U	P-OP2	6.01	1.59	1.49
36	0	46	G	O3'-P	-6.01	1.53	1.61
30	N	699	A	O3'-P	-6.00	1.53	1.61
30	N	2503	A	P-OP1	6.00	1.59	1.49
30	N	2014	A	O3'-P	-5.99	1.53	1.61
30	N	963	U	P-OP2	5.97	1.59	1.49
30	N	1610	A	O3'-P	-5.96	1.53	1.61
4	R	80	SER	C-O	-5.96	1.12	1.23
30	N	2003	A	O3'-P	-5.96	1.54	1.61
30	N	727	A	P-OP1	5.95	1.59	1.49
30	N	1957	C	O3'-P	-5.95	1.54	1.61
30	N	2626	C	O3'-P	-5.95	1.54	1.61
36	0	559	A	C2-N3	5.95	1.39	1.33
30	N	2847	U	O3'-P	-5.94	1.54	1.61
30	N	2250	G	C5-C6	-5.93	1.36	1.42
30	N	2571	U	O3'-P	-5.93	1.54	1.61
36	0	1513	A	O3'-P	-5.93	1.54	1.61
36	0	888	G	O3'-P	-5.93	1.54	1.61
30	N	1187	G	P-OP2	5.93	1.59	1.49
30	N	1323	C	O3'-P	-5.93	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	1324	G	O3'-P	-5.92	1.54	1.61
30	N	2639	A	O3'-P	-5.92	1.54	1.61
30	N	1205	A	O3'-P	5.92	1.68	1.61
36	0	879	C	O3'-P	-5.92	1.54	1.61
36	0	813	U	P-O5'	-5.92	1.53	1.59
30	N	1676	A	P-OP2	5.91	1.58	1.49
30	N	577	G	O3'-P	-5.91	1.54	1.61
36	0	500	G	O3'-P	-5.91	1.54	1.61
59	v	89	ARG	C-N	5.90	1.43	1.33
30	N	1007	C	O3'-P	-5.89	1.54	1.61
30	N	1264	A	O3'-P	-5.87	1.54	1.61
36	0	1054	C	P-OP2	5.87	1.58	1.49
34	M	72	G	O3'-P	-5.86	1.54	1.61
36	0	118	U	O3'-P	-5.86	1.54	1.61
30	N	1602	U	C4-O4	5.85	1.28	1.23
38	2	2	GLY	N-CA	5.85	1.54	1.46
30	N	1665	A	P-OP2	5.85	1.58	1.49
30	N	580	U	O3'-P	-5.84	1.54	1.61
36	0	1363	A	C6-N6	-5.82	1.29	1.33
30	N	1369	G	O3'-P	-5.82	1.54	1.61
30	N	2238	G	O3'-P	5.82	1.68	1.61
36	0	498	A	C2-N3	5.82	1.38	1.33
30	N	605	G	O3'-P	-5.81	1.54	1.61
30	N	2779	U	O3'-P	-5.81	1.54	1.61
36	0	804	U	O3'-P	-5.80	1.54	1.61
36	0	116	A	P-OP2	5.80	1.58	1.49
30	N	2545	G	O3'-P	-5.79	1.54	1.61
36	0	24	U	C4-O4	-5.79	1.19	1.23
30	N	310	A	C5-C6	-5.79	1.35	1.41
30	N	774	G	C2'-O2'	5.79	1.49	1.41
36	0	788	U	O3'-P	-5.79	1.54	1.61
30	N	2541	A	O3'-P	-5.78	1.54	1.61
30	N	2025	C	O5'-C5'	-5.78	1.33	1.42
30	N	2072	C	O5'-C5'	-5.78	1.33	1.42
30	N	2612	C	O3'-P	-5.78	1.54	1.61
30	N	562	U	O3'-P	-5.78	1.54	1.61
30	N	2272	U	O3'-P	-5.77	1.54	1.61
30	N	1796	U	O3'-P	-5.77	1.54	1.61
36	0	1430	A	O3'-P	-5.77	1.54	1.61
30	N	628	G	O3'-P	-5.77	1.54	1.61
30	N	499	U	O3'-P	-5.76	1.54	1.61
30	N	2011	U	O3'-P	-5.75	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	570	G	O3'-P	-5.74	1.54	1.61
36	O	323	U	O3'-P	-5.74	1.54	1.61
30	N	382	A	O3'-P	-5.73	1.54	1.61
30	N	2509	G	O3'-P	-5.72	1.54	1.61
36	O	439	U	C4-O4	-5.72	1.19	1.23
36	O	545	C	O3'-P	-5.72	1.54	1.61
30	N	2272	U	C2-N3	-5.72	1.33	1.37
30	N	1605	C	O3'-P	-5.71	1.54	1.61
36	O	786	G	O3'-P	-5.71	1.54	1.61
22	k	29	PHE	CG-CD2	-5.71	1.30	1.38
36	O	750	C	O3'-P	-5.71	1.54	1.61
30	N	1647	U	P-OP2	5.70	1.58	1.49
30	N	2688	G	O3'-P	-5.70	1.54	1.61
30	N	2054	A	O3'-P	-5.70	1.54	1.61
2	P	213	TRP	CE3-CZ3	5.70	1.48	1.38
30	N	310	A	N1-C2	5.70	1.39	1.34
36	O	1068	G	O3'-P	-5.69	1.54	1.61
25	n	29	SER	CB-OG	-5.69	1.34	1.42
36	O	1238	A	C5-C6	-5.69	1.35	1.41
36	O	868	C	O3'-P	-5.68	1.54	1.61
36	O	404	G	O3'-P	-5.68	1.54	1.61
30	N	565	C	O3'-P	-5.67	1.54	1.61
30	N	28	A	O3'-P	-5.67	1.54	1.61
36	O	319	G	O3'-P	-5.67	1.54	1.61
8	W	30	THR	CB-CG2	-5.67	1.33	1.52
30	N	2429	G	P-OP2	5.66	1.58	1.49
2	P	221	ARG	CA-C	-5.66	1.38	1.52
30	N	2503	A	O3'-P	-5.66	1.54	1.61
30	N	536	G	O3'-P	-5.66	1.54	1.61
30	N	1338	G	O3'-P	-5.65	1.54	1.61
30	N	691	C	O3'-P	-5.62	1.54	1.61
30	N	1790	C	N1-C2	-5.62	1.34	1.40
30	N	1742	U	O3'-P	-5.62	1.54	1.61
36	O	570	G	O3'-P	-5.62	1.54	1.61
36	O	233	C	O3'-P	-5.61	1.54	1.61
30	N	810	U	O3'-P	-5.60	1.54	1.61
30	N	464	U	C4'-O4'	-5.60	1.38	1.45
30	N	2448	A	P-OP1	5.60	1.58	1.49
2	P	222	GLY	C-O	-5.60	1.14	1.23
8	W	16	TYR	CE1-CZ	-5.60	1.31	1.38
30	N	2732	G	C3'-O3'	5.60	1.50	1.42
30	N	234	U	C4-O4	-5.59	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	238	ARG	C-O	5.59	1.33	1.23
4	R	81	GLY	N-CA	-5.59	1.37	1.46
30	N	2732	G	C2'-O2'	5.59	1.49	1.41
30	N	2560	A	O3'-P	-5.58	1.54	1.61
30	N	784	G	C4'-C3'	-5.58	1.47	1.52
36	0	878	A	O3'-P	-5.58	1.54	1.61
30	N	1328	A	O3'-P	-5.57	1.54	1.61
30	N	1446	C	O3'-P	-5.57	1.54	1.61
36	0	895	G	O3'-P	-5.56	1.54	1.61
30	N	2821	A	P-O5'	-5.55	1.54	1.59
30	N	1670	C	O3'-P	-5.54	1.54	1.61
30	N	1351	C	O3'-P	-5.54	1.54	1.61
36	0	907	A	O3'-P	-5.54	1.54	1.61
30	N	1802	A	C5-C6	-5.53	1.36	1.41
30	N	2685	G	O3'-P	-5.53	1.54	1.61
36	0	547	A	P-OP1	5.53	1.58	1.49
30	N	824	U	O3'-P	-5.53	1.54	1.61
30	N	2591	C	O3'-P	-5.52	1.54	1.61
30	N	375	G	P-OP1	5.52	1.58	1.49
36	0	826	C	O3'-P	-5.52	1.54	1.61
17	f	101	SER	CB-OG	-5.51	1.35	1.42
30	N	1568	G	O3'-P	-5.51	1.54	1.61
30	N	2645	G	O3'-P	-5.50	1.54	1.61
15	d	45	TYR	CG-CD1	-5.50	1.31	1.39
30	N	1189	A	P-OP2	5.49	1.58	1.49
35	x	439	A	C1'-N9	-5.49	1.39	1.46
36	0	528	C	O3'-P	-5.49	1.54	1.61
30	N	1770	G	O3'-P	-5.49	1.54	1.61
30	N	1783	A	O3'-P	-5.49	1.54	1.61
30	N	2445	G	P-OP2	5.48	1.58	1.49
30	N	246	C	O3'-P	-5.48	1.54	1.61
36	0	927	G	O3'-P	-5.48	1.54	1.61
12	a	43	GLU	CG-CD	5.47	1.60	1.51
30	N	2266	A	P-OP1	5.47	1.58	1.49
30	N	2643	G	O3'-P	-5.47	1.54	1.61
36	0	827	U	C4-O4	-5.46	1.19	1.23
36	0	885	G	O3'-P	-5.46	1.54	1.61
30	N	468	G	O3'-P	-5.46	1.54	1.61
30	N	1973	G	O3'-P	-5.45	1.54	1.61
59	v	77	PRO	N-CD	5.44	1.55	1.47
30	N	990	A	P-OP2	5.44	1.58	1.49
30	N	693	A	O3'-P	-5.44	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	840	C	O3'-P	-5.44	1.54	1.61
59	v	94	PRO	N-CD	5.44	1.55	1.47
30	N	973	A	O3'-P	-5.44	1.54	1.61
30	N	1995	U	P-OP1	5.43	1.58	1.49
30	N	2720	U	C4-O4	-5.42	1.19	1.23
36	0	963	G	O3'-P	-5.42	1.54	1.61
30	N	1648	U	O3'-P	-5.42	1.54	1.61
30	N	2062	A	O5'-C5'	-5.41	1.34	1.42
34	M	73	C	O3'-P	-5.41	1.54	1.61
36	0	887	G	O3'-P	-5.41	1.54	1.61
30	N	528	A	C5-C6	-5.40	1.36	1.41
30	N	783	A	N9-C4	-5.39	1.34	1.37
30	N	2274	A	O3'-P	-5.39	1.54	1.61
30	N	742	A	O3'-P	-5.39	1.54	1.61
30	N	787	C	P-OP1	5.38	1.58	1.49
25	n	20	ASP	CB-CG	5.38	1.63	1.51
36	0	24	U	O3'-P	-5.38	1.54	1.61
30	N	1272	A	O3'-P	-5.37	1.54	1.61
30	N	1708	C	O3'-P	-5.37	1.54	1.61
30	N	2005	A	O3'-P	-5.37	1.54	1.61
30	N	1993	U	P-O5'	-5.36	1.54	1.59
30	N	66	C	O3'-P	-5.36	1.54	1.61
36	0	373	A	O3'-P	-5.36	1.54	1.61
30	N	771	G	O3'-P	-5.36	1.54	1.61
30	N	973	A	P-O5'	-5.36	1.54	1.59
35	x	469	U	C1'-N1	5.36	1.56	1.48
30	N	561	G	O3'-P	-5.35	1.54	1.61
36	0	1497	G	O3'-P	-5.35	1.54	1.61
30	N	1832	C	O3'-P	-5.35	1.54	1.61
30	N	2023	C	O3'-P	-5.35	1.54	1.61
30	N	1136	G	P-OP1	5.35	1.58	1.49
30	N	1265	A	P-O5'	-5.35	1.54	1.59
30	N	2715	C	O3'-P	-5.34	1.54	1.61
13	b	102	ARG	CZ-NH2	5.34	1.40	1.33
11	Z	39	GLY	C-O	-5.33	1.15	1.23
30	N	1786	A	O3'-P	-5.33	1.54	1.61
30	N	1934	C	O3'-P	-5.33	1.54	1.61
30	N	2724	U	O3'-P	-5.33	1.54	1.61
30	N	188	G	O3'-P	-5.33	1.54	1.61
30	N	2445	G	C2-N2	5.33	1.39	1.34
36	0	1507	A	O3'-P	-5.32	1.54	1.61
36	0	1322	C	O3'-P	5.32	1.67	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	1990	C	C2'-C1'	-5.31	1.47	1.53
30	N	2549	G	O3'-P	-5.31	1.54	1.61
30	N	1837	C	O3'-P	-5.30	1.54	1.61
30	N	385	C	O3'-P	-5.30	1.54	1.61
21	j	41	ARG	CG-CD	5.29	1.65	1.51
30	N	2243	U	N3-C4	-5.29	1.33	1.38
30	N	1255	U	O5'-C5'	-5.29	1.34	1.42
30	N	1141	U	C2-O2	-5.29	1.17	1.22
36	0	391	G	O3'-P	-5.29	1.54	1.61
53	I	20	GLU	CD-OE1	5.29	1.31	1.25
30	N	261	G	O3'-P	-5.28	1.54	1.61
30	N	1833	C	O3'-P	-5.28	1.54	1.61
30	N	1021	A	C6-N6	-5.28	1.29	1.33
48	D	101	ARG	CZ-NH1	5.27	1.40	1.33
30	N	2766	A	O3'-P	-5.27	1.54	1.61
30	N	2500	U	O3'-P	-5.27	1.54	1.61
37	1	213	TYR	CB-CG	-5.26	1.43	1.51
36	0	291	U	O3'-P	-5.26	1.54	1.61
30	N	927	A	C2-N3	5.26	1.38	1.33
2	P	11	PRO	N-CA	5.25	1.56	1.47
3	Q	127	PHE	CE1-CZ	-5.25	1.27	1.37
36	0	816	A	P-OP1	5.25	1.57	1.49
30	N	2845	U	O3'-P	-5.25	1.54	1.61
36	0	123	U	O3'-P	-5.25	1.54	1.61
36	0	554	A	O3'-P	-5.25	1.54	1.61
2	P	48	ARG	C-O	-5.24	1.13	1.23
14	c	53	ARG	CG-CD	-5.24	1.38	1.51
30	N	1327	A	O3'-P	-5.24	1.54	1.61
30	N	1632	A	O3'-P	-5.24	1.54	1.61
30	N	1637	A	O3'-P	-5.24	1.54	1.61
36	0	886	G	O3'-P	-5.24	1.54	1.61
36	0	397	A	C6-N6	-5.24	1.29	1.33
15	d	24	TYR	CE2-CZ	5.24	1.45	1.38
30	N	430	A	C6-N1	-5.24	1.31	1.35
30	N	787	C	P-O5'	-5.24	1.54	1.59
30	N	2592	G	O3'-P	-5.24	1.54	1.61
30	N	2430	A	P-OP2	5.23	1.57	1.49
47	B	38	TYR	CB-CG	-5.23	1.43	1.51
36	0	1301	U	C2-N3	5.23	1.41	1.37
36	0	751	U	O3'-P	-5.22	1.54	1.61
36	0	964	A	P-OP1	5.22	1.57	1.49
30	N	2024	G	O3'-P	-5.22	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	2036	C	O3'-P	-5.22	1.54	1.61
36	0	1500	A	P-OP2	5.22	1.57	1.49
11	Z	91	TYR	CE1-CZ	-5.21	1.31	1.38
30	N	989	G	C3'-O3'	5.21	1.49	1.42
30	N	2241	A	O3'-P	-5.21	1.54	1.61
4	R	77	ILE	CB-CG1	-5.21	1.39	1.54
36	0	938	A	O3'-P	-5.21	1.54	1.61
30	N	978	G	O3'-P	-5.21	1.54	1.61
30	N	981	A	P-OP1	5.21	1.57	1.49
2	P	234	GLY	C-O	-5.20	1.15	1.23
36	0	924	C	O3'-P	-5.20	1.54	1.61
27	p	39	ARG	NE-CZ	5.20	1.39	1.33
26	o	49	TYR	CE2-CZ	-5.19	1.31	1.38
36	0	18	C	O3'-P	-5.19	1.54	1.61
26	o	21	TYR	CE1-CZ	-5.19	1.31	1.38
36	0	318	G	O3'-P	-5.19	1.54	1.61
30	N	664	G	O3'-P	-5.19	1.54	1.61
30	N	2839	G	O3'-P	-5.19	1.54	1.61
35	x	437	C	O3'-P	-5.18	1.54	1.61
30	N	976	G	O3'-P	-5.18	1.54	1.61
30	N	1991	U	O3'-P	-5.18	1.54	1.61
30	N	2267	A	P-OP1	5.18	1.57	1.49
30	N	1864	U	O3'-P	-5.18	1.54	1.61
16	e	80	ARG	CB-CG	-5.18	1.38	1.52
30	N	469	G	O3'-P	-5.18	1.54	1.61
30	N	784	G	P-OP1	5.18	1.57	1.49
30	N	2267	A	C6-N1	-5.18	1.31	1.35
30	N	223	A	O3'-P	-5.17	1.54	1.61
30	N	1254	A	C2'-O2'	5.17	1.48	1.41
46	A	65	VAL	CB-CG1	-5.17	1.42	1.52
30	N	1817	G	O3'-P	-5.17	1.54	1.61
30	N	1308	A	O3'-P	-5.17	1.54	1.61
36	0	25	C	O3'-P	-5.16	1.54	1.61
35	x	468	G	O3'-P	-5.16	1.54	1.61
35	x	464	G	O3'-P	-5.16	1.54	1.61
30	N	604	G	O3'-P	-5.16	1.54	1.61
35	x	441	U	O3'-P	-5.15	1.54	1.61
36	0	386	C	O3'-P	-5.15	1.54	1.61
36	0	881	G	O3'-P	-5.15	1.54	1.61
30	N	2490	G	O3'-P	-5.15	1.54	1.61
2	P	213	TRP	CA-C	-5.15	1.39	1.52
30	N	69	C	O3'-P	-5.14	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	872	A	C6-N6	-5.14	1.29	1.33
36	0	951	G	O3'-P	-5.14	1.54	1.61
30	N	467	G	O3'-P	-5.14	1.54	1.61
30	N	1202	G	O3'-P	-5.14	1.54	1.61
30	N	503	A	O3'-P	5.13	1.67	1.61
36	0	586	C	O3'-P	-5.13	1.54	1.61
30	N	1638	C	P-O5'	-5.12	1.54	1.59
36	0	783	C	O3'-P	-5.12	1.55	1.61
30	N	2448	A	P-OP2	5.11	1.57	1.49
36	0	1408	A	O3'-P	-5.11	1.55	1.61
2	P	235	GLY	CA-C	-5.11	1.43	1.51
30	N	1985	C	O3'-P	-5.11	1.55	1.61
30	N	1666	G	O3'-P	-5.11	1.55	1.61
30	N	752	A	P-O5'	-5.11	1.54	1.59
36	0	1434	A	O3'-P	-5.09	1.55	1.61
30	N	800	A	N9-C4	-5.09	1.34	1.37
30	N	2611	C	P-OP2	5.09	1.57	1.49
35	x	472	U	C1'-N1	5.09	1.56	1.48
30	N	419	U	P-OP1	5.08	1.57	1.49
30	N	587	C	O3'-P	-5.08	1.55	1.61
30	N	296	U	O3'-P	-5.08	1.55	1.61
3	Q	113	SER	CB-OG	-5.08	1.35	1.42
36	0	506	G	O3'-P	-5.08	1.55	1.61
30	N	1679	A	O3'-P	-5.07	1.55	1.61
36	0	296	U	O3'-P	-5.07	1.55	1.61
26	o	49	TYR	CG-CD1	-5.07	1.32	1.39
30	N	2838	G	O3'-P	-5.07	1.55	1.61
30	N	1998	A	C2'-C1'	-5.07	1.47	1.53
30	N	2706	A	O3'-P	-5.07	1.55	1.61
30	N	513	A	P-O5'	-5.06	1.54	1.59
30	N	1313	U	P-OP1	5.06	1.57	1.49
30	N	2387	U	O3'-P	-5.06	1.55	1.61
36	0	827	U	C2-N3	-5.06	1.34	1.37
30	N	1826	G	O3'-P	-5.05	1.55	1.61
30	N	1250	G	P-OP1	5.05	1.57	1.49
30	N	2875	C	O3'-P	-5.05	1.55	1.61
30	N	948	C	N1-C2	-5.04	1.35	1.40
30	N	2440	C	O3'-P	-5.04	1.55	1.61
30	N	2551	C	P-OP2	5.04	1.57	1.49
30	N	2580	U	O3'-P	-5.04	1.55	1.61
30	N	449	A	O3'-P	-5.04	1.55	1.61
30	N	2092	U	O3'-P	5.04	1.67	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	96	TRP	CG-CD1	5.03	1.43	1.36
28	q	8	ARG	CB-CG	-5.03	1.39	1.52
36	0	1526	G	O3'-P	-5.03	1.55	1.61
30	N	954	G	O3'-P	-5.03	1.55	1.61
30	N	2078	C	O3'-P	-5.02	1.55	1.61
36	0	979	C	O3'-P	-5.02	1.55	1.61
16	e	53	PHE	CG-CD1	5.02	1.46	1.38
30	N	2361	G	O3'-P	-5.01	1.55	1.61
30	N	1972	G	O3'-P	-5.01	1.55	1.61
2	P	236	GLU	CD-OE2	5.00	1.31	1.25
30	N	666	A	O3'-P	-5.00	1.55	1.61

All (718) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	2506[A]	U	OP1-P-O3'	17.16	142.95	105.20
30	N	2506[B]	U	OP1-P-O3'	17.16	142.95	105.20
27	p	39	ARG	NE-CZ-NH1	16.07	128.33	120.30
27	p	39	ARG	NE-CZ-NH2	-14.77	112.92	120.30
34	M	73	C	O3'-P-O5'	14.34	131.24	104.00
30	N	2720	U	C2-N3-C4	-13.72	118.77	127.00
30	N	2522	U	C2-N3-C4	-13.67	118.80	127.00
30	N	2062	A	O5'-P-OP1	-13.29	93.74	105.70
30	N	467	G	O5'-P-OP1	-13.13	93.89	105.70
30	N	2836	U	O5'-P-OP1	-12.80	94.17	105.70
54	J	5	LEU	CB-CG-CD2	12.68	132.56	111.00
15	d	53	ARG	NE-CZ-NH1	12.39	126.49	120.30
21	j	41	ARG	NE-CZ-NH1	12.34	126.47	120.30
30	N	1996	C	O5'-P-OP2	-12.26	94.67	105.70
30	N	2506[A]	U	O3'-P-O5'	-12.25	80.72	104.00
30	N	2506[B]	U	O3'-P-O5'	-12.25	80.72	104.00
30	N	2873	A	N1-C6-N6	-12.19	111.29	118.60
30	N	499	U	C2-N3-C4	-11.98	119.81	127.00
30	N	2821	A	O5'-P-OP1	-11.77	95.11	105.70
10	Y	18	ARG	NE-CZ-NH2	-11.76	114.42	120.30
22	k	28	ARG	NE-CZ-NH2	-11.69	114.45	120.30
25	n	20	ASP	CB-CG-OD1	11.48	128.63	118.30
36	0	559	A	C6-N1-C2	-11.35	111.79	118.60
36	0	1301	U	C2-N3-C4	-11.31	120.21	127.00
30	N	1665	A	O5'-P-OP1	-11.18	95.64	105.70
30	N	2505	G	P-O3'-C3'	-11.03	106.46	119.70
30	N	228	C	O5'-P-OP1	-11.02	95.78	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	p	34	ARG	NE-CZ-NH1	-10.99	114.80	120.30
36	0	752	G	O5'-P-OP1	-10.87	95.92	105.70
11	Z	16	ARG	NE-CZ-NH2	-10.84	114.88	120.30
30	N	2447	G	O5'-P-OP1	-10.83	95.95	105.70
8	W	116	ARG	NE-CZ-NH2	-10.82	114.89	120.30
30	N	2765	A	N1-C6-N6	-10.75	112.15	118.60
30	N	1941	C	O5'-P-OP1	-10.69	96.08	105.70
46	A	122	ARG	NE-CZ-NH1	10.69	125.64	120.30
2	P	214	ARG	NE-CZ-NH2	-10.66	114.97	120.30
48	D	109	ARG	NE-CZ-NH1	10.56	125.58	120.30
30	N	27	G	O5'-P-OP1	-10.50	96.25	105.70
30	N	2067	G	O5'-P-OP1	-10.50	96.25	105.70
15	d	53	ARG	NE-CZ-NH2	-10.48	115.06	120.30
36	0	16	A	O5'-P-OP1	-10.42	96.32	105.70
36	0	1497	G	O5'-P-OP2	-10.38	96.36	105.70
56	s	34	ARG	NE-CZ-NH2	-10.30	115.15	120.30
3	Q	13	ARG	NE-CZ-NH2	10.22	125.41	120.30
30	N	1965	C	O5'-P-OP2	-10.09	96.62	105.70
15	d	6	ARG	NE-CZ-NH2	10.06	125.33	120.30
30	N	474	G	O5'-P-OP1	-9.97	96.73	105.70
30	N	953	G	O5'-P-OP1	-9.94	96.76	105.70
37	1	21	ARG	NE-CZ-NH1	9.87	125.23	120.30
36	0	21	G	O5'-P-OP1	9.86	122.54	110.70
30	N	2060	A	O5'-P-OP1	-9.84	96.84	105.70
30	N	2059	A	O5'-P-OP2	-9.82	96.86	105.70
30	N	2072	C	O5'-P-OP1	-9.81	96.87	105.70
30	N	306	U	C2-N3-C4	-9.77	121.14	127.00
30	N	801	G	O5'-P-OP2	-9.65	97.02	105.70
30	N	537	G	O5'-P-OP1	-9.56	97.09	105.70
13	b	102	ARG	NE-CZ-NH2	9.55	125.07	120.30
30	N	2873	A	C5-C6-N6	9.55	131.34	123.70
30	N	1809	A	O5'-P-OP1	-9.54	97.11	105.70
42	6	109	ARG	NE-CZ-NH1	9.54	125.07	120.30
30	N	2726	A	O5'-P-OP1	-9.54	97.11	105.70
29	r	36	ARG	NE-CZ-NH1	-9.45	115.58	120.30
36	0	795	C	O5'-P-OP1	-9.43	97.22	105.70
30	N	2776	A	C8-N9-C1'	-9.41	110.75	127.70
30	N	2776	A	C4-N9-C1'	9.34	143.10	126.30
10	Y	47	ARG	NE-CZ-NH2	9.31	124.95	120.30
30	N	2543	G	O5'-P-OP1	-9.30	97.33	105.70
30	N	805	G	O5'-P-OP1	-9.27	97.36	105.70
2	P	258	ARG	NE-CZ-NH1	-9.23	115.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	1190	G	O5'-P-OP2	9.23	121.78	110.70
30	N	2044	C	O5'-P-OP1	-9.22	97.41	105.70
30	N	2711	A	O5'-P-OP2	9.21	121.75	110.70
40	4	111	MET	CG-SD-CE	-9.13	85.59	100.20
14	c	72	ARG	NE-CZ-NH2	-9.11	115.75	120.30
30	N	1253	A	O5'-P-OP1	-9.10	97.51	105.70
30	N	2022	U	O5'-P-OP1	-9.10	97.51	105.70
22	k	57	ARG	NE-CZ-NH2	9.06	124.83	120.30
30	N	2513	A	O5'-P-OP2	-9.05	97.55	105.70
30	N	1639	C	O5'-P-OP1	-9.04	97.56	105.70
30	N	2456	C	O5'-P-OP1	-9.02	97.58	105.70
13	b	102	ARG	NE-CZ-NH1	-8.93	115.83	120.30
48	D	92	ARG	NE-CZ-NH1	8.89	124.74	120.30
37	1	21	ARG	NE-CZ-NH2	-8.87	115.87	120.30
36	0	968	A	O5'-P-OP2	-8.83	97.76	105.70
13	b	30	ARG	NE-CZ-NH2	-8.81	115.90	120.30
30	N	1798	U	O5'-P-OP2	-8.72	97.85	105.70
30	N	2725	A	O5'-P-OP1	-8.67	97.89	105.70
10	Y	78	ARG	NE-CZ-NH2	8.67	124.64	120.30
30	N	684	G	O5'-P-OP1	-8.66	97.90	105.70
50	F	54	ARG	NE-CZ-NH2	-8.65	115.97	120.30
2	P	270	ARG	NE-CZ-NH2	-8.63	115.99	120.30
59	v	175	GLU	O-C-N	-8.58	108.97	122.70
30	N	2497	A	O5'-P-OP2	8.57	120.98	110.70
14	c	21	ARG	NE-CZ-NH1	-8.55	116.03	120.30
36	0	816	A	O5'-P-OP1	-8.53	98.02	105.70
51	G	70	ARG	NE-CZ-NH1	8.51	124.55	120.30
30	N	1994	C	O5'-P-OP1	-8.50	98.05	105.70
1	O	90	C	O5'-P-OP1	-8.45	98.09	105.70
12	a	69	ARG	NE-CZ-NH2	8.45	124.52	120.30
55	K	10	ARG	CB-CG-CD	-8.44	89.66	111.60
40	4	157	ARG	NE-CZ-NH1	-8.41	116.09	120.30
28	q	8	ARG	NE-CZ-NH1	8.39	124.50	120.30
49	E	9	ARG	NE-CZ-NH1	8.36	124.48	120.30
36	0	726	C	O5'-P-OP1	-8.32	98.21	105.70
2	P	271	ARG	NE-CZ-NH2	-8.28	116.16	120.30
13	b	30	ARG	NE-CZ-NH1	8.27	124.43	120.30
9	X	78	ARG	NE-CZ-NH2	-8.23	116.18	120.30
2	P	221	ARG	CG-CD-NE	-8.23	94.52	111.80
30	N	2248	C	O5'-P-OP1	-8.18	98.34	105.70
30	N	234	U	N3-C4-O4	-8.17	113.68	119.40
36	0	1358	U	N3-C4-O4	-8.12	113.71	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	1141	U	N3-C4-O4	-8.12	113.72	119.40
30	N	2267	A	O5'-P-OP2	-8.12	98.40	105.70
30	N	812	C	O5'-P-OP2	-8.10	98.41	105.70
48	D	92	ARG	NE-CZ-NH2	-8.10	116.25	120.30
30	N	671	C	O5'-P-OP1	-8.08	98.43	105.70
15	d	13	ARG	NE-CZ-NH2	8.06	124.33	120.30
4	R	49	ARG	NE-CZ-NH1	-8.05	116.27	120.30
34	M	73	C	OP1-P-O3'	-8.05	87.49	105.20
36	0	674	G	O5'-P-OP1	-8.02	98.48	105.70
40	4	38	VAL	CG1-CB-CG2	-7.99	98.11	110.90
8	W	116	ARG	NE-CZ-NH1	7.98	124.29	120.30
15	d	51	ARG	NE-CZ-NH2	-7.97	116.31	120.30
4	R	61	ARG	NE-CZ-NH1	7.96	124.28	120.30
30	N	234	U	C5-C4-O4	7.96	130.67	125.90
25	n	7	LYS	CD-CE-NZ	7.95	129.98	111.70
30	N	2222	C	O5'-P-OP1	-7.92	98.57	105.70
15	d	51	ARG	NE-CZ-NH1	7.91	124.26	120.30
30	N	1141	U	C5-C4-O4	7.91	130.64	125.90
36	0	439	U	C2-N3-C4	-7.89	122.27	127.00
38	2	156	ARG	NE-CZ-NH1	7.89	124.25	120.30
36	0	1191	A	O5'-P-OP1	-7.88	98.61	105.70
30	N	704	G	O5'-P-OP1	-7.86	98.63	105.70
15	d	3	ARG	NE-CZ-NH1	-7.85	116.37	120.30
36	0	1054	C	O5'-P-OP2	7.84	120.11	110.70
47	B	12	ARG	NE-CZ-NH1	-7.83	116.39	120.30
15	d	58	ARG	NE-CZ-NH2	-7.82	116.39	120.30
30	N	2061	G	O4'-C1'-N9	7.80	114.44	108.20
30	N	2277	G	O5'-P-OP1	-7.78	98.70	105.70
41	5	79	ARG	NE-CZ-NH1	7.77	124.19	120.30
30	N	974	G	N9-C1'-C2'	7.77	124.09	114.00
4	R	69	ARG	NE-CZ-NH2	-7.76	116.42	120.30
30	N	2847	U	O5'-P-OP1	-7.76	98.71	105.70
30	N	581	C	O5'-P-OP1	-7.74	98.73	105.70
30	N	1136	G	P-O5'-C5'	-7.72	108.54	120.90
30	N	927	A	C6-N1-C2	-7.72	113.97	118.60
42	6	3	ARG	NE-CZ-NH1	7.72	124.16	120.30
30	N	1611	C	O5'-P-OP2	-7.70	98.77	105.70
30	N	2344	U	N3-C4-O4	-7.69	114.01	119.40
30	N	2544	G	O5'-P-OP2	-7.69	98.78	105.70
30	N	1255	U	O5'-P-OP2	7.69	119.92	110.70
44	8	49	ARG	NE-CZ-NH1	7.68	124.14	120.30
30	N	813	U	O5'-P-OP2	-7.67	98.79	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	2765	A	C5-C6-N6	7.67	129.84	123.70
23	l	52	ARG	NE-CZ-NH1	-7.67	116.47	120.30
30	N	787	C	O5'-P-OP1	7.64	119.87	110.70
36	0	368	U	N3-C4-O4	-7.64	114.06	119.40
30	N	2022	U	OP1-P-OP2	7.63	131.05	119.60
30	N	2729	G	O5'-P-OP1	-7.62	98.84	105.70
30	N	430	A	N1-C6-N6	-7.62	114.03	118.60
36	0	571	U	C2-N3-C4	-7.62	122.43	127.00
39	3	5	LEU	CA-CB-CG	7.61	132.80	115.30
30	N	1255	U	O5'-P-OP1	-7.60	98.86	105.70
30	N	2447	G	P-O3'-C3'	7.59	128.81	119.70
30	N	698	C	O5'-P-OP2	-7.58	98.88	105.70
30	N	512	G	P-O3'-C3'	7.57	128.79	119.70
36	0	37	U	N3-C4-O4	-7.55	114.12	119.40
36	0	567	G	O5'-P-OP1	-7.53	98.93	105.70
2	P	177	ARG	NE-CZ-NH1	-7.51	116.54	120.30
30	N	2060	A	O5'-P-OP2	7.51	119.72	110.70
30	N	784	G	C2'-C3'-O3'	7.49	125.98	109.50
49	E	85	ARG	NE-CZ-NH1	7.46	124.03	120.30
36	0	498	A	C6-N1-C2	-7.43	114.14	118.60
30	N	2693	G	O5'-P-OP1	-7.43	99.01	105.70
30	N	1900	A	P-O3'-C3'	7.42	128.60	119.70
36	0	1331	G	O5'-P-OP1	-7.42	99.03	105.70
30	N	1930	G	O5'-P-OP1	-7.41	99.03	105.70
36	0	1363	A	N1-C6-N6	-7.40	114.16	118.60
30	N	1639	C	O5'-P-OP2	7.38	119.56	110.70
30	N	1932	A	O5'-P-OP1	-7.38	99.06	105.70
30	N	932	U	N3-C4-O4	-7.37	114.24	119.40
36	0	501	C	O5'-P-OP1	-7.36	99.08	105.70
30	N	784	G	P-O3'-C3'	7.34	128.51	119.70
30	N	2256	G	O5'-P-OP1	-7.34	99.09	105.70
30	N	850	U	C2-N3-C4	-7.32	122.61	127.00
43	7	80	ARG	NE-CZ-NH2	-7.32	116.64	120.30
10	Y	29	LYS	CD-CE-NZ	-7.32	94.87	111.70
30	N	2542	A	O5'-P-OP2	-7.31	99.12	105.70
30	N	2072	C	O5'-P-OP2	7.31	119.47	110.70
30	N	2692	G	O5'-P-OP2	-7.28	99.15	105.70
36	0	1507	A	O5'-P-OP1	-7.27	99.16	105.70
30	N	2497	A	C5'-C4'-C3'	-7.23	104.42	116.00
30	N	2714	G	O5'-P-OP2	7.23	119.38	110.70
23	l	29	ARG	NE-CZ-NH1	-7.23	116.69	120.30
30	N	795	C	O5'-P-OP1	-7.21	99.21	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	0	368	U	C5-C4-O4	7.20	130.22	125.90
30	N	760	G	OP1-P-O3'	7.19	121.03	105.20
21	j	14	ARG	CG-CD-NE	-7.19	96.71	111.80
55	K	74	ARG	NE-CZ-NH1	7.19	123.89	120.30
30	N	1026	G	O5'-P-OP2	-7.17	99.25	105.70
4	R	81	GLY	C-N-CA	-7.16	107.26	122.30
30	N	1145	C	O5'-P-OP1	-7.14	99.27	105.70
30	N	2344	U	C5-C4-O4	7.14	130.18	125.90
30	N	2506[A]	U	OP2-P-O3'	-7.14	89.50	105.20
30	N	2506[B]	U	OP2-P-O3'	-7.14	89.50	105.20
10	Y	82	LEU	CA-CB-CG	7.13	131.71	115.30
10	Y	59	ARG	NE-CZ-NH1	7.12	123.86	120.30
30	N	510	C	O5'-P-OP2	-7.10	99.31	105.70
30	N	2344	U	O5'-P-OP1	-7.07	99.34	105.70
30	N	2637	U	O5'-P-OP1	-7.07	99.34	105.70
54	J	5	LEU	CB-CG-CD1	-7.07	98.99	111.00
36	0	6	G	O5'-P-OP2	-7.06	99.34	105.70
36	0	827	U	N3-C4-O4	-7.04	114.47	119.40
30	N	1962	C	O5'-P-OP1	-7.01	99.39	105.70
30	N	1236	G	P-O3'-C3'	6.99	128.09	119.70
30	N	1790	C	O5'-P-OP1	-6.99	99.41	105.70
30	N	740	C	O5'-P-OP1	-6.98	99.42	105.70
30	N	578	G	O5'-P-OP1	6.97	119.06	110.70
30	N	967	U	O5'-P-OP1	-6.96	99.44	105.70
36	0	24	U	N1-C2-O2	-6.95	117.93	122.80
30	N	1944	U	O5'-P-OP2	-6.94	99.45	105.70
30	N	2304	G	O5'-P-OP1	-6.94	99.45	105.70
42	6	109	ARG	CG-CD-NE	-6.93	97.25	111.80
30	N	196	A	O5'-P-OP1	-6.92	99.48	105.70
30	N	2711	A	O5'-P-OP1	-6.91	99.48	105.70
39	3	3	ARG	NE-CZ-NH1	6.90	123.75	120.30
30	N	2021	C	O5'-P-OP2	-6.90	99.49	105.70
30	N	2311	A	P-O3'-C3'	6.89	127.97	119.70
30	N	1021	A	N1-C6-N6	-6.87	114.48	118.60
53	I	43	ARG	NE-CZ-NH1	6.87	123.73	120.30
3	Q	156	PHE	CB-CG-CD2	-6.86	116.00	120.80
30	N	2059	A	O5'-P-OP1	6.86	118.93	110.70
36	0	37	U	C5-C4-O4	6.86	130.01	125.90
14	c	93	ARG	CG-CD-NE	-6.86	97.40	111.80
28	q	13	ARG	NE-CZ-NH1	-6.83	116.88	120.30
30	N	630	G	O5'-P-OP1	-6.83	99.55	105.70
4	R	77	ILE	CG1-CB-CG2	-6.83	96.38	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	q	8	ARG	CD-NE-CZ	-6.83	114.04	123.60
12	a	4	ARG	NE-CZ-NH2	-6.81	116.89	120.30
2	P	101	ARG	NE-CZ-NH2	-6.80	116.90	120.30
21	j	41	ARG	CD-NE-CZ	6.80	133.12	123.60
30	N	1607	C	O5'-P-OP1	-6.79	99.59	105.70
30	N	1836	C	O5'-P-OP1	-6.76	99.62	105.70
30	N	2543	G	P-O5'-C5'	-6.76	110.08	120.90
36	0	1349	A	O5'-P-OP2	6.76	118.81	110.70
27	p	14	ARG	NE-CZ-NH1	-6.75	116.92	120.30
36	0	904	U	O5'-P-OP1	-6.75	99.62	105.70
36	0	1343	G	O5'-P-OP1	-6.75	99.62	105.70
36	0	865	A	O5'-P-OP1	-6.75	99.63	105.70
30	N	2272	U	N3-C4-O4	-6.74	114.69	119.40
30	N	512	G	O4'-C1'-N9	6.73	113.59	108.20
30	N	932	U	C5-C4-O4	6.73	129.94	125.90
10	Y	59	ARG	NE-CZ-NH2	-6.72	116.94	120.30
36	0	812	G	P-O3'-C3'	6.72	127.76	119.70
18	g	12	ARG	NE-CZ-NH1	6.71	123.66	120.30
30	N	679	C	O5'-P-OP1	-6.69	99.68	105.70
30	N	2576	G	O5'-P-OP2	-6.69	99.68	105.70
36	0	738	C	O5'-P-OP1	-6.68	99.69	105.70
36	0	1280	A	O5'-P-OP2	-6.67	99.70	105.70
49	E	53	ARG	NE-CZ-NH1	-6.64	116.98	120.30
36	0	1358	U	C5-C4-O4	6.62	129.87	125.90
36	0	864	A	C6-N1-C2	-6.62	114.63	118.60
36	0	261	U	O5'-P-OP1	-6.62	99.75	105.70
30	N	961	C	O5'-P-OP2	-6.59	99.77	105.70
13	b	25	ARG	NE-CZ-NH1	-6.58	117.01	120.30
30	N	1666	G	O4'-C4'-C3'	-6.57	97.44	104.00
41	5	24	ARG	NE-CZ-NH1	6.56	123.58	120.30
30	N	2656	U	C2-N1-C1'	6.54	125.55	117.70
30	N	51	G	O4'-C1'-N9	6.54	113.43	108.20
30	N	188	G	O5'-P-OP1	-6.54	99.82	105.70
30	N	2060	A	O3'-P-O5'	6.53	116.41	104.00
38	2	172	ARG	NE-CZ-NH2	-6.53	117.04	120.30
30	N	729	G	O5'-P-OP2	-6.51	99.84	105.70
30	N	1648	U	P-O5'-C5'	-6.51	110.48	120.90
6	T	3	ARG	NE-CZ-NH2	6.50	123.55	120.30
30	N	204	A	O5'-P-OP2	-6.49	99.86	105.70
30	N	1902	C	O5'-P-OP1	-6.49	99.86	105.70
30	N	1439	A	O5'-P-OP1	-6.49	99.86	105.70
30	N	2516	A	O5'-P-OP1	-6.49	99.86	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	963	U	O5'-P-OP2	6.49	118.48	110.70
29	r	24	ARG	NE-CZ-NH2	6.48	123.54	120.30
48	D	3	ARG	NE-CZ-NH1	6.45	123.52	120.30
30	N	2048	G	O5'-P-OP1	-6.44	99.90	105.70
30	N	555	G	O5'-P-OP1	-6.44	99.90	105.70
36	0	829	G	O5'-P-OP1	-6.44	99.91	105.70
8	W	99	ARG	NE-CZ-NH1	6.43	123.52	120.30
36	0	1279	G	N9-C1'-C2'	6.43	122.36	114.00
11	Z	40	ARG	NE-CZ-NH2	6.41	123.51	120.30
30	N	1664	A	O5'-P-OP2	6.41	118.39	110.70
56	s	34	ARG	NE-CZ-NH1	6.41	123.50	120.30
21	j	41	ARG	NH1-CZ-NH2	-6.41	112.36	119.40
30	N	752	A	N9-C1'-C2'	6.40	122.31	114.00
54	J	37	ARG	NE-CZ-NH1	6.40	123.50	120.30
2	P	87	ARG	NE-CZ-NH2	6.39	123.50	120.30
30	N	2522	U	N1-C2-O2	-6.39	118.33	122.80
30	N	1933	G	O5'-P-OP1	-6.38	99.96	105.70
36	0	827	U	C5-C4-O4	6.38	129.73	125.90
30	N	2725	A	C3'-C2'-O2'	-6.37	94.82	113.30
30	N	2055	C	O5'-P-OP1	-6.37	99.97	105.70
30	N	1299	G	O5'-P-OP1	-6.37	99.97	105.70
30	N	747	U	O5'-P-OP1	-6.37	99.97	105.70
30	N	1313	U	C2-N1-C1'	6.37	125.34	117.70
30	N	2074	U	O5'-P-OP2	-6.36	99.97	105.70
2	P	229	ASP	CB-CG-OD1	-6.36	112.58	118.30
30	N	650	C	O5'-P-OP1	-6.36	99.98	105.70
13	b	13	ARG	NE-CZ-NH1	6.36	123.48	120.30
17	f	88	ARG	NE-CZ-NH1	-6.35	117.12	120.30
30	N	310	A	O5'-P-OP1	-6.35	99.98	105.70
30	N	2061	G	O5'-P-OP1	-6.34	99.99	105.70
30	N	792	A	O5'-P-OP1	-6.33	100.00	105.70
47	B	9	ARG	NE-CZ-NH1	6.33	123.47	120.30
9	X	71	ARG	NE-CZ-NH1	6.33	123.46	120.30
30	N	1967	C	O5'-P-OP1	-6.33	100.01	105.70
12	a	69	ARG	NE-CZ-NH1	-6.32	117.14	120.30
30	N	2443	C	O4'-C4'-C3'	-6.32	97.68	104.00
25	n	20	ASP	CB-CG-OD2	-6.31	112.62	118.30
42	6	95	ARG	NE-CZ-NH1	6.30	123.45	120.30
25	n	17	ARG	NE-CZ-NH2	-6.29	117.16	120.30
15	d	48	ARG	NE-CZ-NH2	6.29	123.44	120.30
30	N	995	C	C4'-C3'-O3'	-6.28	96.21	109.40
48	D	90	ARG	NE-CZ-NH2	-6.27	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	0	397	A	N1-C6-N6	-6.27	114.84	118.60
30	N	2423	U	O5'-P-OP2	-6.27	100.06	105.70
36	0	890	G	O4'-C1'-N9	6.26	113.21	108.20
30	N	1141	U	N3-C2-O2	-6.25	117.82	122.20
36	0	880	C	O5'-P-OP2	-6.25	100.08	105.70
47	B	83	ARG	NE-CZ-NH1	6.25	123.42	120.30
36	0	131	A	O5'-P-OP1	-6.24	100.08	105.70
36	0	563	A	N1-C6-N6	-6.24	114.86	118.60
24	m	11	ARG	NE-CZ-NH2	6.24	123.42	120.30
30	N	1205	A	P-O3'-C3'	6.23	127.18	119.70
30	N	2364	C	O4'-C4'-C3'	-6.23	97.77	104.00
30	N	140	C	C2-N1-C1'	6.22	125.64	118.80
30	N	1936	A	C4'-C3'-O3'	-6.20	96.39	109.40
30	N	983	A	C5'-C4'-O4'	-6.19	101.67	109.10
11	Z	81	ARG	NE-CZ-NH2	-6.19	117.21	120.30
30	N	1865	U	O5'-P-OP1	-6.18	100.14	105.70
30	N	1313	U	N1-C1'-C2'	6.17	122.02	114.00
50	F	63	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	P	229	ASP	CB-CG-OD2	6.16	123.85	118.30
46	A	122	ARG	NE-CZ-NH2	-6.16	117.22	120.30
30	N	2243	U	O5'-P-OP2	6.15	118.08	110.70
39	3	3	ARG	NE-CZ-NH2	-6.15	117.22	120.30
36	0	1238	A	C6-C5-N7	-6.15	127.99	132.30
28	q	25	LYS	CD-CE-NZ	-6.14	97.57	111.70
36	0	540	G	O5'-P-OP1	-6.14	100.17	105.70
30	N	1264	A	O5'-P-OP1	-6.13	100.19	105.70
2	P	228	VAL	CG1-CB-CG2	-6.12	101.12	110.90
30	N	2258	C	O5'-P-OP1	-6.12	100.19	105.70
30	N	503	A	C4-C5-C6	6.11	120.06	117.00
36	0	576	C	O5'-P-OP2	-6.10	100.21	105.70
30	N	310	A	C6-C5-N7	-6.10	128.03	132.30
30	N	1844	C	O5'-P-OP1	-6.10	100.21	105.70
30	N	1501	G	O5'-P-OP1	-6.09	100.22	105.70
36	0	687	A	O5'-P-OP1	-6.09	100.22	105.70
36	0	1356	G	O5'-P-OP1	-6.09	100.22	105.70
1	O	94	A	O5'-P-OP1	-6.08	100.22	105.70
30	N	91	A	O5'-P-OP2	-6.08	100.23	105.70
30	N	2725	A	O5'-P-OP2	6.08	117.99	110.70
36	0	1054	C	O5'-P-OP1	-6.07	100.23	105.70
53	I	57	ARG	CA-CB-CG	6.05	126.71	113.40
23	l	6	LEU	CB-CG-CD1	6.03	121.26	111.00
30	N	2603	G	O5'-P-OP1	-6.03	100.27	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	948	C	O5'-P-OP1	6.03	117.94	110.70
12	a	54	LEU	CB-CG-CD1	-6.02	100.77	111.00
36	0	31	G	O5'-P-OP2	-6.01	100.29	105.70
8	W	37	ARG	NE-CZ-NH2	6.01	123.31	120.30
3	Q	109	VAL	CG1-CB-CG2	-6.01	101.29	110.90
30	N	670	A	P-O3'-C3'	6.00	126.91	119.70
36	0	529	G	O5'-P-OP2	-6.00	100.30	105.70
36	0	762	U	O5'-P-OP1	-6.00	100.30	105.70
15	d	28	ARG	NE-CZ-NH1	5.99	123.30	120.30
36	0	2	A	O5'-P-OP1	-5.99	100.31	105.70
6	T	153	ARG	NE-CZ-NH2	5.97	123.29	120.30
44	8	12	ARG	NE-CZ-NH2	-5.97	117.31	120.30
30	N	2576	G	O5'-P-OP1	5.97	117.86	110.70
45	9	60	ASP	CB-CG-OD2	5.97	123.67	118.30
30	N	2246	G	O4'-C4'-C3'	-5.96	98.04	104.00
30	N	1328	A	O5'-P-OP1	5.95	117.84	110.70
49	E	59	ARG	NE-CZ-NH1	5.95	123.28	120.30
2	P	177	ARG	CG-CD-NE	-5.95	99.30	111.80
12	a	69	ARG	CG-CD-NE	5.95	124.29	111.80
44	8	45	ARG	NE-CZ-NH1	5.94	123.27	120.30
36	0	1182	G	P-O3'-C3'	5.94	126.83	119.70
36	0	1347	G	P-O3'-C3'	5.94	126.83	119.70
30	N	2699	C	O5'-P-OP1	-5.94	100.36	105.70
30	N	536	G	O5'-P-OP2	-5.93	100.36	105.70
30	N	1795	C	O5'-P-OP1	-5.93	100.36	105.70
30	N	2512	C	O5'-P-OP1	-5.93	100.36	105.70
30	N	404	A	P-O3'-C3'	5.92	126.81	119.70
30	N	310	A	C4-C5-C6	5.92	119.96	117.00
30	N	2503	A	OP1-P-OP2	-5.92	110.73	119.60
30	N	2267	A	N1-C6-N6	-5.91	115.05	118.60
36	0	1301	U	N1-C1'-C2'	5.91	121.69	114.00
36	0	1238	A	C4-C5-C6	5.91	119.95	117.00
40	4	138	ARG	NE-CZ-NH1	-5.91	117.35	120.30
28	q	8	ARG	CG-CD-NE	5.91	124.20	111.80
44	8	18	ARG	CB-CG-CD	-5.91	96.25	111.60
30	N	466	A	O5'-P-OP1	5.90	117.78	110.70
30	N	673	C	O5'-P-OP1	5.90	117.78	110.70
26	o	10	LYS	CD-CE-NZ	5.90	125.27	111.70
36	0	388	G	P-O3'-C3'	5.90	126.78	119.70
4	R	81	GLY	O-C-N	-5.89	113.18	123.20
25	n	52	ARG	NE-CZ-NH2	5.89	123.25	120.30
9	X	23	LYS	CD-CE-NZ	-5.88	98.17	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	0	59	A	O5'-P-OP1	5.88	117.76	110.70
48	D	107	ARG	NE-CZ-NH2	-5.88	117.36	120.30
11	Z	136	MET	CG-SD-CE	5.87	109.59	100.20
4	R	65	THR	C-N-CA	-5.86	109.99	122.30
28	q	45	ARG	NE-CZ-NH1	5.86	123.23	120.30
30	N	27	G	C5'-C4'-O4'	-5.86	102.07	109.10
36	0	9	G	O5'-P-OP1	5.86	117.73	110.70
30	N	2028	U	O5'-P-OP1	-5.86	100.43	105.70
30	N	820	A	O4'-C4'-C3'	-5.85	98.15	104.00
30	N	2273	A	O5'-P-OP1	-5.85	100.43	105.70
39	3	91	LEU	CB-CG-CD1	-5.84	101.07	111.00
10	Y	30	THR	N-CA-CB	5.84	121.39	110.30
30	N	2272	U	C5-C4-O4	5.83	129.40	125.90
2	P	133	ARG	NE-CZ-NH2	5.83	123.21	120.30
30	N	1134	A	P-O3'-C3'	5.83	126.69	119.70
30	N	2383	G	O5'-P-OP2	-5.82	100.46	105.70
27	p	12	ARG	NE-CZ-NH1	-5.81	117.39	120.30
27	p	12	ARG	CA-CB-CG	5.81	126.18	113.40
30	N	1427	A	O5'-P-OP1	-5.81	100.47	105.70
30	N	2689	U	OP1-P-OP2	5.81	128.31	119.60
30	N	775	G	O5'-P-OP1	-5.80	100.48	105.70
39	3	70	ARG	NE-CZ-NH1	5.80	123.20	120.30
30	N	1617	C	O5'-P-OP2	-5.80	100.48	105.70
30	N	1673	G	O5'-P-OP2	5.80	117.66	110.70
30	N	503	A	C6-C5-N7	-5.79	128.24	132.30
30	N	578	G	O5'-P-OP2	-5.79	100.49	105.70
30	N	679	C	OP1-P-OP2	5.79	128.29	119.60
30	N	675	A	O5'-P-OP2	5.79	117.64	110.70
47	B	14	ARG	NE-CZ-NH1	5.79	123.19	120.30
30	N	859	G	P-O3'-C3'	5.79	126.64	119.70
36	0	884	U	N3-C4-O4	-5.78	115.36	119.40
30	N	1348	C	O5'-P-OP1	-5.77	100.51	105.70
30	N	504	A	O5'-P-OP2	-5.76	100.51	105.70
30	N	2682	A	O5'-P-OP2	5.76	117.61	110.70
36	0	1201	A	P-O3'-C3'	5.76	126.61	119.70
22	k	37	ARG	NE-CZ-NH2	5.75	123.18	120.30
30	N	301	G	C4-N9-C1'	-5.75	119.03	126.50
12	a	49	GLU	OE1-CD-OE2	-5.74	116.41	123.30
30	N	1843	C	O5'-P-OP1	-5.74	100.53	105.70
50	F	54	ARG	NE-CZ-NH1	5.74	123.17	120.30
30	N	477	A	O5'-P-OP2	-5.73	100.54	105.70
30	N	1130	U	O5'-P-OP1	-5.72	100.55	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	4	69	ARG	NE-CZ-NH1	5.72	123.16	120.30
41	5	90	MET	C-N-CA	5.71	135.98	121.70
3	Q	124	ARG	NE-CZ-NH1	5.71	123.15	120.30
50	F	43	PHE	CB-CG-CD1	-5.70	116.81	120.80
30	N	783	A	O5'-P-OP2	-5.70	100.57	105.70
30	N	242	G	C4'-C3'-O3'	5.70	124.40	113.00
30	N	780	G	O5'-P-OP2	-5.70	100.57	105.70
30	N	1676	A	O5'-P-OP2	5.70	117.54	110.70
30	N	1565	C	C5'-C4'-C3'	-5.70	106.89	116.00
49	E	61	ARG	NE-CZ-NH2	-5.69	117.45	120.30
50	F	70	LEU	CB-CG-CD2	-5.69	101.33	111.00
56	s	17	ARG	NE-CZ-NH2	-5.69	117.46	120.30
30	N	1570	A	O5'-P-OP1	-5.68	100.58	105.70
36	0	1331	G	O4'-C1'-N9	5.68	112.75	108.20
30	N	2688	G	O5'-P-OP1	-5.68	100.59	105.70
2	P	130	LEU	CA-CB-CG	5.67	128.34	115.30
36	0	176	C	O5'-P-OP1	-5.67	100.60	105.70
30	N	2645	G	C5'-C4'-C3'	-5.67	106.93	116.00
30	N	2873	A	C3'-C2'-C1'	5.66	106.03	101.50
1	O	44	G	N9-C1'-C2'	5.66	121.36	114.00
36	0	1254	A	O5'-P-OP1	-5.65	100.61	105.70
16	e	80	ARG	NE-CZ-NH2	-5.65	117.47	120.30
30	N	1788	C	OP1-P-O3'	5.65	117.62	105.20
30	N	860	U	OP1-P-OP2	-5.64	111.14	119.60
30	N	2499	C	O5'-P-OP1	5.63	117.46	110.70
44	8	99	ARG	NE-CZ-NH2	-5.63	117.48	120.30
35	x	439	A	C1'-C2'-O2'	-5.63	93.71	110.60
38	2	132	ARG	NE-CZ-NH1	5.63	123.11	120.30
35	x	466	C	C1'-C2'-O2'	-5.62	93.73	110.60
15	d	28	ARG	NE-CZ-NH2	-5.61	117.50	120.30
44	8	123	ARG	NE-CZ-NH1	5.60	123.10	120.30
40	4	138	ARG	N-CA-CB	5.60	120.68	110.60
15	d	6	ARG	NE-CZ-NH1	-5.60	117.50	120.30
30	N	1143	A	O5'-P-OP2	-5.60	100.66	105.70
36	0	1067	A	O5'-P-OP1	-5.59	100.67	105.70
30	N	2720	U	N3-C4-C5	5.59	117.95	114.60
30	N	1688	U	O5'-P-OP1	-5.59	100.67	105.70
30	N	1261	C	O4'-C4'-C3'	-5.58	98.42	104.00
30	N	205	G	O4'-C1'-N9	5.58	112.67	108.20
30	N	1952	A	O5'-P-OP1	-5.58	100.68	105.70
30	N	2720	U	N1-C2-O2	-5.58	118.89	122.80
30	N	2498	C	OP1-P-OP2	5.58	127.97	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	187	ASP	CB-CG-OD1	5.57	123.31	118.30
14	c	21	ARG	NH1-CZ-NH2	5.57	125.52	119.40
36	0	1474	U	O5'-P-OP1	-5.57	100.69	105.70
30	N	528	A	C8-N9-C1'	5.56	137.71	127.70
30	N	2776	A	C2'-C3'-O3'	5.56	122.59	113.70
30	N	372	G	P-O3'-C3'	5.56	126.37	119.70
30	N	1612	C	O5'-P-OP1	-5.55	100.71	105.70
14	c	89	ARG	NE-CZ-NH2	5.54	123.07	120.30
30	N	790	U	O5'-P-OP2	-5.54	100.71	105.70
30	N	1029	A	O5'-P-OP1	-5.54	100.71	105.70
36	0	567	G	OP1-P-OP2	5.54	127.92	119.60
30	N	2725	A	C5'-C4'-O4'	-5.54	102.45	109.10
4	R	88	ARG	NE-CZ-NH1	-5.54	117.53	120.30
30	N	803	U	O5'-P-OP1	-5.53	100.72	105.70
12	a	46	ARG	NE-CZ-NH1	-5.53	117.53	120.30
36	0	37	U	N3-C2-O2	-5.53	118.33	122.20
8	W	39	LYS	CD-CE-NZ	-5.52	99.00	111.70
2	P	232	HIS	O-C-N	-5.52	113.82	123.20
36	0	734	G	O5'-P-OP1	-5.51	100.74	105.70
30	N	2260	C	O5'-P-OP1	-5.51	100.74	105.70
30	N	2543	G	C5'-C4'-C3'	-5.51	107.18	116.00
2	P	156	ARG	NE-CZ-NH1	5.51	123.05	120.30
2	P	156	ARG	CG-CD-NE	5.50	123.36	111.80
30	N	2452	C	O5'-P-OP2	-5.50	100.75	105.70
23	l	48	ARG	NE-CZ-NH2	-5.50	117.55	120.30
30	N	573	U	P-O3'-C3'	5.50	126.30	119.70
30	N	670	A	C2'-C3'-O3'	5.50	122.49	113.70
30	N	1695	G	O5'-P-OP2	-5.50	100.75	105.70
30	N	1990	C	O5'-P-OP1	-5.50	100.75	105.70
30	N	2580	U	O5'-P-OP2	-5.50	100.75	105.70
30	N	871	U	P-O5'-C5'	-5.49	112.11	120.90
36	0	818	G	N9-C1'-C2'	5.49	121.14	114.00
30	N	2514	U	O5'-P-OP2	-5.49	100.76	105.70
30	N	2359	C	O5'-P-OP1	-5.47	100.77	105.70
2	P	239	ASN	N-CA-C	5.47	125.78	111.00
30	N	825	A	O5'-P-OP2	-5.47	100.78	105.70
6	T	149	ARG	NE-CZ-NH2	-5.46	117.57	120.30
13	b	33	ARG	NE-CZ-NH2	-5.45	117.58	120.30
30	N	514	A	O5'-P-OP1	-5.45	100.80	105.70
30	N	463	G	O5'-P-OP2	-5.45	100.80	105.70
30	N	1322	A	O5'-P-OP1	-5.44	100.80	105.70
48	D	109	ARG	NE-CZ-NH2	-5.44	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	234	U	N3-C2-O2	-5.44	118.39	122.20
36	0	330	C	P-O5'-C5'	-5.44	112.20	120.90
30	N	301	G	C8-N9-C1'	5.44	134.07	127.00
30	N	774	G	C1'-C2'-O2'	-5.44	94.29	110.60
30	N	2037	A	C5'-C4'-O4'	-5.44	102.57	109.10
36	0	653	U	O5'-P-OP1	-5.44	100.81	105.70
45	9	92	LEU	CA-CB-CG	5.44	127.81	115.30
11	Z	40	ARG	NE-CZ-NH1	-5.42	117.59	120.30
30	N	2266	A	C4'-C3'-O3'	-5.42	98.01	109.40
30	N	2405	G	P-O3'-C3'	5.42	126.20	119.70
36	0	368	U	N3-C2-O2	-5.42	118.41	122.20
25	n	16	ARG	NE-CZ-NH1	-5.41	117.59	120.30
36	0	886	G	O5'-P-OP1	-5.41	100.83	105.70
8	W	124	VAL	CG1-CB-CG2	-5.41	102.25	110.90
30	N	1325	U	O5'-P-OP2	-5.41	100.83	105.70
24	m	54	MET	CG-SD-CE	-5.41	91.55	100.20
30	N	2872	A	O5'-P-OP1	-5.40	100.84	105.70
50	F	64	ARG	CG-CD-NE	-5.40	100.46	111.80
30	N	1669	A	C8-N9-C1'	-5.40	117.99	127.70
30	N	2873	A	P-O5'-C5'	-5.40	112.27	120.90
15	d	92	ARG	NE-CZ-NH2	5.39	123.00	120.30
30	N	748	G	O5'-P-OP2	-5.39	100.85	105.70
36	0	880	C	O5'-P-OP1	5.39	117.17	110.70
36	0	816	A	O5'-P-OP2	5.38	117.16	110.70
38	2	157	LEU	CA-CB-CG	5.38	127.68	115.30
13	b	94	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	O	48	U	O5'-P-OP1	-5.38	100.86	105.70
30	N	2848	G	O5'-P-OP1	-5.38	100.86	105.70
10	Y	52	GLY	C-N-CA	-5.37	111.02	122.30
35	x	469	U	O4'-C1'-C2'	-5.37	100.43	105.80
47	B	38	TYR	CB-CG-CD1	-5.37	117.78	121.00
30	N	1142	A	P-O3'-C3'	5.36	126.14	119.70
35	x	442	G	O4'-C1'-C2'	-5.36	100.44	105.80
3	Q	146	ILE	CG1-CB-CG2	-5.36	99.61	111.40
36	0	976	G	O5'-P-OP2	5.36	117.13	110.70
30	N	430	A	C5-C6-N6	5.35	127.98	123.70
36	0	1301	U	C6-N1-C1'	-5.35	113.71	121.20
2	P	195	VAL	CG1-CB-CG2	-5.34	102.36	110.90
36	0	1500	A	O5'-P-OP2	-5.34	100.90	105.70
2	P	84	ASP	CB-CG-OD1	5.34	123.10	118.30
30	N	1031	G	O5'-P-OP2	-5.33	100.90	105.70
30	N	1256	G	O4'-C1'-N9	-5.33	103.93	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	0	804	U	O5'-P-OP1	-5.33	100.90	105.70
30	N	2286	G	P-O3'-C3'	5.33	126.09	119.70
10	Y	78	ARG	NE-CZ-NH1	-5.33	117.64	120.30
30	N	1783	A	O5'-P-OP1	5.32	117.09	110.70
2	P	217	ARG	NE-CZ-NH1	-5.32	117.64	120.30
42	6	3	ARG	NE-CZ-NH2	-5.32	117.64	120.30
3	Q	154	LYS	CD-CE-NZ	-5.32	99.47	111.70
30	N	2613	U	N3-C4-O4	-5.32	115.68	119.40
48	D	98	ARG	CG-CD-NE	5.32	122.97	111.80
36	0	1504	G	O5'-P-OP2	-5.31	100.92	105.70
36	0	560	A	O5'-P-OP1	-5.30	100.93	105.70
43	7	99	LEU	CB-CG-CD1	-5.30	101.99	111.00
30	N	2848	G	O4'-C1'-N9	5.30	112.44	108.20
30	N	528	A	C4-N9-C1'	-5.30	116.77	126.30
30	N	1669	A	C4-N9-C1'	5.30	135.83	126.30
29	r	1	MET	CB-CG-SD	-5.29	96.52	112.40
36	0	96	U	C2'-C3'-O3'	5.29	122.17	113.70
36	0	574	A	O5'-P-OP1	-5.29	100.94	105.70
30	N	2832	U	P-O3'-C3'	5.29	126.05	119.70
30	N	1142	A	C3'-C2'-C1'	5.29	105.73	101.50
36	0	1319	A	O5'-P-OP1	-5.29	100.94	105.70
56	s	16	LEU	CA-CB-CG	5.29	127.46	115.30
2	P	221	ARG	N-CA-CB	5.29	120.11	110.60
30	N	1021	A	C5-C6-N6	5.29	127.93	123.70
36	0	728	A	O5'-P-OP2	-5.29	100.94	105.70
36	0	822	U	O5'-P-OP1	-5.29	100.94	105.70
47	B	61	PHE	CB-CG-CD1	5.29	124.50	120.80
30	N	2884	U	O4'-C1'-N1	5.28	112.42	108.20
36	0	1363	A	C5-C6-N6	5.28	127.92	123.70
21	j	41	ARG	CB-CG-CD	5.28	125.32	111.60
12	a	17	ARG	NE-CZ-NH2	5.28	122.94	120.30
30	N	771	G	O5'-P-OP1	-5.27	100.95	105.70
25	n	10	ARG	NE-CZ-NH2	5.27	122.94	120.30
14	c	109	ARG	NE-CZ-NH2	5.26	122.93	120.30
30	N	932	U	N3-C2-O2	-5.26	118.52	122.20
51	G	51	ARG	NE-CZ-NH1	5.26	122.93	120.30
9	X	23	LYS	N-CA-CB	5.26	120.06	110.60
30	N	611	C	O5'-P-OP1	-5.26	100.97	105.70
30	N	140	C	C6-N1-C1'	-5.25	114.49	120.80
8	W	99	ARG	NE-CZ-NH2	-5.25	117.67	120.30
30	N	1829	A	O5'-P-OP2	-5.25	100.97	105.70
30	N	532	A	O5'-P-OP2	-5.25	100.98	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r	36	ARG	CG-CD-NE	-5.25	100.78	111.80
30	N	1271	G	O5'-P-OP1	5.25	116.99	110.70
36	0	890	G	P-O3'-C3'	5.25	125.99	119.70
22	k	28	ARG	NH1-CZ-NH2	5.24	125.17	119.40
30	N	2831	G	O5'-P-OP1	-5.24	100.98	105.70
30	N	2765	A	C2-N3-C4	-5.24	107.98	110.60
36	0	108	G	O4'-C1'-N9	5.24	112.39	108.20
30	N	2394	C	O4'-C4'-C3'	-5.23	98.77	104.00
30	N	1800	C	O5'-P-OP2	-5.22	101.00	105.70
36	0	163	C	O5'-P-OP1	-5.22	101.00	105.70
2	P	14	ARG	NE-CZ-NH1	5.21	122.91	120.30
15	d	3	ARG	NE-CZ-NH2	5.21	122.91	120.30
29	r	3	VAL	CG1-CB-CG2	-5.21	102.56	110.90
30	N	752	A	O4'-C1'-N9	5.21	112.37	108.20
30	N	2243	U	O5'-P-OP1	-5.20	101.02	105.70
36	0	558	G	O5'-P-OP1	5.20	116.94	110.70
30	N	1313	U	C6-N1-C1'	-5.20	113.92	121.20
3	Q	124	ARG	NE-CZ-NH2	-5.20	117.70	120.30
40	4	138	ARG	NE-CZ-NH2	-5.20	117.70	120.30
15	d	33	ARG	CB-CG-CD	-5.19	98.10	111.60
30	N	825	A	OP1-P-O3'	5.19	116.62	105.20
30	N	2007	U	O5'-P-OP2	-5.19	101.03	105.70
30	N	1815	A	C5'-C4'-O4'	-5.19	102.88	109.10
37	1	103	ASN	N-CA-CB	5.18	119.93	110.60
30	N	2867	G	P-O3'-C3'	5.18	125.92	119.70
59	v	174	VAL	O-C-N	-5.18	114.42	122.70
59	v	78	ASP	CB-CG-OD2	5.17	122.96	118.30
30	N	1606	C	O5'-P-OP2	-5.17	101.05	105.70
30	N	499	U	N3-C4-C5	5.17	117.70	114.60
36	0	1125	U	C2-N1-C1'	5.16	123.89	117.70
36	0	595	A	P-O3'-C3'	5.16	125.89	119.70
30	N	915	C	O5'-P-OP2	-5.15	101.06	105.70
11	Z	18	ARG	NE-CZ-NH2	5.15	122.88	120.30
16	e	79	ARG	CD-NE-CZ	-5.15	116.39	123.60
2	P	156	ARG	CB-CG-CD	-5.15	98.22	111.60
30	N	2049	G	O4'-C4'-C3'	-5.15	98.85	104.00
30	N	2645	G	P-O5'-C5'	-5.14	112.67	120.90
49	E	13	ARG	NE-CZ-NH2	-5.14	117.73	120.30
30	N	140	C	N1-C1'-C2'	5.14	120.68	114.00
49	E	85	ARG	NE-CZ-NH2	-5.13	117.73	120.30
6	T	149	ARG	NE-CZ-NH1	5.13	122.87	120.30
22	k	57	ARG	NE-CZ-NH1	-5.13	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	1950	G	O5'-P-OP1	-5.13	101.08	105.70
30	N	2874	C	O5'-P-OP2	-5.13	101.08	105.70
30	N	1288	G	C4-N9-C1'	5.13	133.17	126.50
47	B	22	PRO	O-C-N	-5.12	114.50	122.70
30	N	1667	G	O5'-P-OP2	5.12	116.84	110.70
36	0	887	G	O5'-P-OP2	-5.12	101.09	105.70
35	x	438	C	C1'-O4'-C4'	-5.11	105.81	109.90
51	G	70	ARG	CG-CD-NE	5.11	122.53	111.80
30	N	1998	A	O4'-C4'-C3'	-5.11	98.89	104.00
48	D	3	ARG	CD-NE-CZ	5.11	130.75	123.60
2	P	217	ARG	CG-CD-NE	-5.11	101.08	111.80
36	0	1358	U	N3-C2-O2	-5.11	118.63	122.20
50	F	66	LEU	CB-CG-CD2	-5.11	102.32	111.00
14	c	53	ARG	CB-CG-CD	-5.10	98.33	111.60
30	N	1764	C	O5'-P-OP1	-5.10	101.11	105.70
37	1	74	ARG	NE-CZ-NH1	5.10	122.85	120.30
3	Q	114	LYS	CA-CB-CG	5.10	124.61	113.40
30	N	1997	C	O4'-C4'-C3'	-5.10	98.90	104.00
4	R	65	THR	O-C-N	-5.09	114.54	123.20
12	a	86	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	P	24	LEU	CB-CG-CD1	-5.09	102.34	111.00
30	N	830	G	O4'-C1'-N9	-5.09	104.13	108.20
51	G	8	ARG	NE-CZ-NH1	5.09	122.85	120.30
30	N	555	G	P-O3'-C3'	5.09	125.81	119.70
30	N	2215	C	O5'-P-OP1	-5.09	101.12	105.70
30	N	1020	A	P-O3'-C3'	5.08	125.80	119.70
30	N	1270	C	O5'-P-OP1	-5.08	101.13	105.70
30	N	953	G	OP1-P-OP2	5.08	127.22	119.60
16	e	81	LYS	CD-CE-NZ	5.08	123.38	111.70
30	N	578	G	OP1-P-OP2	-5.08	111.98	119.60
30	N	997	G	O5'-P-OP1	-5.08	101.13	105.70
30	N	651	G	O5'-P-OP2	-5.07	101.13	105.70
35	x	465	U	C1'-O4'-C4'	-5.07	105.84	109.90
46	A	126	LYS	CB-CA-C	5.07	120.54	110.40
30	N	2049	G	OP1-P-OP2	-5.07	112.00	119.60
30	N	2656	U	C6-N1-C1'	-5.07	114.11	121.20
50	F	58	ARG	NE-CZ-NH1	5.06	122.83	120.30
10	Y	3	LEU	CB-CG-CD1	-5.05	102.41	111.00
36	0	502	A	O5'-P-OP2	-5.05	101.15	105.70
36	0	103	U	O5'-P-OP1	-5.05	101.15	105.70
30	N	658	U	O5'-P-OP2	-5.05	101.16	105.70
30	N	2765	A	C4-N9-C1'	5.05	135.38	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	0	85	U	P-O3'-C3'	5.05	125.76	119.70
1	O	52	A	P-O3'-C3'	5.04	125.75	119.70
30	N	1026	G	O5'-P-OP1	5.04	116.75	110.70
51	G	14	ARG	NE-CZ-NH2	-5.04	117.78	120.30
30	N	278	A	C4-N9-C1'	5.04	135.37	126.30
21	j	79	PHE	CB-CG-CD1	5.04	124.33	120.80
30	N	1236	G	C5'-C4'-O4'	-5.04	103.06	109.10
27	p	33	ARG	NE-CZ-NH1	5.03	122.82	120.30
30	N	704	G	O4'-C1'-N9	5.03	112.23	108.20
30	N	2267	A	N9-C1'-C2'	5.03	120.54	114.00
45	9	17	LEU	CB-CG-CD2	-5.03	102.45	111.00
55	K	69	LYS	N-CA-C	5.03	124.58	111.00
10	Y	2	ARG	NE-CZ-NH1	5.03	122.81	120.30
36	0	578	C	O5'-P-OP1	5.03	116.73	110.70
9	X	71	ARG	NE-CZ-NH2	-5.01	117.79	120.30
21	j	77	ARG	NE-CZ-NH2	-5.01	117.79	120.30
30	N	2006	C	O5'-P-OP1	5.01	116.72	110.70
42	6	95	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	O	15	A	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	0	24	U	Sidechain
36	0	368	U	Sidechain
36	0	559	A	Sidechain
36	0	571	U	Sidechain
36	0	864	A	Sidechain
37	1	102	THR	Peptide
37	1	14	VAL	Peptide
38	2	79	LYS	Peptide
38	2	80	LYS	Peptide
40	4	102	GLY	Peptide
40	4	136	VAL	Peptide
40	4	137	VAL	Peptide
40	4	142	ASP	Peptide
40	4	89	HIS	Peptide
41	5	52	ASN	Peptide
41	5	93	LYS	Peptide
44	8	128	SER	Peptide
44	8	53	GLU	Peptide

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Mol	Chain	Res	Type	Group
44	8	54	LEU	Peptide
44	8	55	VAL	Peptide
46	A	125	LYS	Peptide
47	B	22	PRO	Peptide
47	B	77	HIS	Peptide
52	H	17	MET	Peptide
52	H	69	LYS	Peptide
54	J	37	ARG	Peptide
55	K	3	ASN	Peptide
30	N	1802	A	Sidechain
30	N	2522	U	Sidechain
30	N	2765	A	Sidechain
30	N	586	A	Sidechain
30	N	850	U	Sidechain
30	N	927	A	Sidechain
2	P	195	VAL	Peptide
2	P	234	GLY	Peptide
2	P	238	ARG	Peptide
3	Q	151	THR	Peptide
5	S	174	ASP	Peptide
5	S	175	PHE	Peptide
7	V	11	LEU	Peptide
10	Y	114	GLY	Peptide
10	Y	82	LEU	Peptide
11	Z	57	VAL	Peptide,Mainchain
19	h	52	LEU	Peptide
28	q	31	HIS	Peptide
56	s	34	ARG	Peptide
59	v	174	VAL	Mainchain
59	v	175	GLU	Mainchain
59	v	22	THR	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	269/273 (98%)	247 (92%)	18 (7%)	4 (2%)	8	39
3	Q	207/209 (99%)	195 (94%)	11 (5%)	1 (0%)	25	64
4	R	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
5	S	175/179 (98%)	163 (93%)	11 (6%)	1 (1%)	22	60
6	T	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
7	V	139/142 (98%)	112 (81%)	27 (19%)	0	100	100
8	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
9	X	120/123 (98%)	109 (91%)	9 (8%)	2 (2%)	7	36
10	Y	141/144 (98%)	121 (86%)	16 (11%)	4 (3%)	4	24
11	Z	134/136 (98%)	118 (88%)	11 (8%)	5 (4%)	2	20
12	a	118/127 (93%)	102 (86%)	14 (12%)	2 (2%)	7	36
13	b	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
14	c	112/115 (97%)	104 (93%)	8 (7%)	0	100	100
15	d	115/118 (98%)	115 (100%)	0	0	100	100
16	e	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	13	49
17	f	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14	51
18	g	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	5	29
19	h	100/104 (96%)	84 (84%)	14 (14%)	2 (2%)	6	31
20	i	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
21	j	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
22	k	75/78 (96%)	71 (95%)	3 (4%)	1 (1%)	10	42
23	l	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
24	m	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
25	n	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	6	32
26	o	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
27	p	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
28	q	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	8	37
29	r	36/55 (66%)	35 (97%)	1 (3%)	0	100	100
31	L	52/70 (74%)	44 (85%)	7 (14%)	1 (2%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	C	130/223 (58%)	123 (95%)	7 (5%)	0	100	100
33	U	147/149 (99%)	124 (84%)	21 (14%)	2 (1%)	9	40
37	1	216/239 (90%)	188 (87%)	27 (12%)	1 (0%)	25	64
38	2	204/218 (94%)	186 (91%)	16 (8%)	2 (1%)	13	49
39	3	203/206 (98%)	182 (90%)	21 (10%)	0	100	100
40	4	148/162 (91%)	116 (78%)	30 (20%)	2 (1%)	9	40
41	5	98/131 (75%)	81 (83%)	11 (11%)	6 (6%)	1	13
42	6	149/152 (98%)	139 (93%)	10 (7%)	0	100	100
43	7	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
44	8	125/130 (96%)	103 (82%)	20 (16%)	2 (2%)	8	37
45	9	96/103 (93%)	84 (88%)	9 (9%)	3 (3%)	3	22
46	A	115/129 (89%)	102 (89%)	13 (11%)	0	100	100
47	B	121/124 (98%)	104 (86%)	15 (12%)	2 (2%)	7	36
48	D	112/118 (95%)	103 (92%)	8 (7%)	1 (1%)	14	51
49	E	92/101 (91%)	77 (84%)	14 (15%)	1 (1%)	12	46
50	F	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
51	G	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	10	42
52	H	78/84 (93%)	66 (85%)	9 (12%)	3 (4%)	2	19
53	I	53/75 (71%)	49 (92%)	3 (6%)	1 (2%)	6	32
54	J	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
55	K	83/87 (95%)	78 (94%)	4 (5%)	1 (1%)	11	44
56	s	49/71 (69%)	40 (82%)	9 (18%)	0	100	100
57	t	139/557 (25%)	115 (83%)	21 (15%)	3 (2%)	5	29
59	v	173/182 (95%)	168 (97%)	3 (2%)	2 (1%)	11	44
All	All	6111/6981 (88%)	5521 (90%)	528 (9%)	62 (1%)	16	49

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	239	ASN
10	Y	36	LYS
11	Z	58	LYS
16	e	53	PHE
25	n	55	ILE

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Mol	Chain	Res	Type
28	q	32	ILE
33	U	9	VAL
41	5	53	LYS
45	9	58	ASN
51	G	44	SER
52	H	70	THR
11	Z	59	ARG
12	a	3	HIS
33	U	11	ASN
38	2	81	GLY
41	5	56	LYS
41	5	91	ARG
44	8	55	VAL
47	B	23	ALA
52	H	18	GLU
55	K	69	LYS
57	t	33	LYS
2	P	235	GLY
11	Z	39	GLY
18	g	78	SER
19	h	99	ASN
22	k	3	ARG
38	2	80	LYS
41	5	54	LEU
41	5	94	HIS
45	9	43	PRO
47	B	78	SER
52	H	71	LYS
53	I	48	ARG
59	v	78	ASP
2	P	10	SER
2	P	238	ARG
3	Q	149	ASN
5	S	175	PHE
9	X	93	GLN
10	Y	29	LYS
10	Y	30	THR
10	Y	31	GLY
11	Z	69	PRO
18	g	77	ARG
31	L	3	LYS
40	4	51	GLY

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Mol	Chain	Res	Type
41	5	86	ARG
48	D	66	GLU
57	t	116	VAL
12	a	88	ALA
17	f	64	ALA
19	h	53	ASN
37	l	194	ASP
40	4	90	THR
49	E	4	GLN
57	t	89	ALA
59	v	175	GLU
11	Z	87	GLY
45	9	42	LEU
9	X	119	ALA
44	8	10	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	
2	P	216/218 (99%)	215 (100%)	1 (0%)	86	89
3	Q	164/164 (100%)	161 (98%)	3 (2%)	54	71
4	R	165/165 (100%)	161 (98%)	4 (2%)	44	62
5	S	145/150 (97%)	145 (100%)	0	100	100
6	T	137/138 (99%)	137 (100%)	0	100	100
7	V	109/110 (99%)	108 (99%)	1 (1%)	75	83
8	W	116/116 (100%)	116 (100%)	0	100	100
9	X	103/104 (99%)	103 (100%)	0	100	100
10	Y	102/103 (99%)	102 (100%)	0	100	100
11	Z	109/109 (100%)	108 (99%)	1 (1%)	75	83
12	a	100/102 (98%)	97 (97%)	3 (3%)	36	55
13	b	86/87 (99%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	c	98/100 (98%)	95 (97%)	3 (3%)	35	54
15	d	89/90 (99%)	88 (99%)	1 (1%)	70	79
16	e	84/84 (100%)	82 (98%)	2 (2%)	44	62
17	f	93/93 (100%)	93 (100%)	0	100	100
18	g	80/85 (94%)	80 (100%)	0	100	100
19	h	83/85 (98%)	82 (99%)	1 (1%)	67	78
20	i	78/78 (100%)	78 (100%)	0	100	100
21	j	56/63 (89%)	55 (98%)	1 (2%)	54	71
22	k	67/68 (98%)	67 (100%)	0	100	100
23	l	55/55 (100%)	55 (100%)	0	100	100
24	m	48/49 (98%)	48 (100%)	0	100	100
25	n	47/48 (98%)	46 (98%)	1 (2%)	48	66
26	o	45/49 (92%)	45 (100%)	0	100	100
27	p	38/38 (100%)	38 (100%)	0	100	100
28	q	51/52 (98%)	49 (96%)	2 (4%)	27	48
29	r	34/50 (68%)	34 (100%)	0	100	100
31	L	48/63 (76%)	48 (100%)	0	100	100
32	C	110/174 (63%)	110 (100%)	0	100	100
33	U	114/114 (100%)	113 (99%)	1 (1%)	75	83
37	1	179/198 (90%)	177 (99%)	2 (1%)	70	79
38	2	170/178 (96%)	169 (99%)	1 (1%)	84	88
39	3	172/173 (99%)	171 (99%)	1 (1%)	84	88
40	4	113/123 (92%)	110 (97%)	3 (3%)	40	58
41	5	87/112 (78%)	86 (99%)	1 (1%)	70	79
42	6	124/125 (99%)	123 (99%)	1 (1%)	79	84
43	7	104/105 (99%)	104 (100%)	0	100	100
44	8	105/107 (98%)	104 (99%)	1 (1%)	73	81
45	9	86/90 (96%)	85 (99%)	1 (1%)	67	78
46	A	90/98 (92%)	89 (99%)	1 (1%)	70	79
47	B	103/104 (99%)	103 (100%)	0	100	100
48	D	91/96 (95%)	90 (99%)	1 (1%)	70	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	E	79/83 (95%)	79 (100%)	0	100	100
50	F	75/77 (97%)	74 (99%)	1 (1%)	65	76
51	G	65/65 (100%)	65 (100%)	0	100	100
52	H	74/77 (96%)	73 (99%)	1 (1%)	62	75
53	I	48/66 (73%)	48 (100%)	0	100	100
54	J	70/80 (88%)	68 (97%)	2 (3%)	37	56
55	K	65/66 (98%)	65 (100%)	0	100	100
56	s	44/61 (72%)	43 (98%)	1 (2%)	45	64
59	v	108/156 (69%)	108 (100%)	0	100	100
All	All	4922/5244 (94%)	4879 (99%)	43 (1%)	74	83

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	218	PRO
3	Q	73	VAL
3	Q	105	LYS
3	Q	205	PRO
4	R	61	ARG
4	R	69	ARG
4	R	149	ILE
4	R	163	ASN
7	V	65	ARG
11	Z	128	THR
12	a	2	ARG
12	a	50	PRO
12	a	70	THR
14	c	53	ARG
14	c	73	VAL
14	c	93	ARG
15	d	33	ARG
16	e	49	ILE
16	e	53	PHE
19	h	68	SER
21	j	41	ARG
25	n	28	LEU
28	q	2	PRO
28	q	32	ILE
33	U	101	ASP

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Mol	Chain	Res	Type
37	1	11	LYS
37	1	207	ILE
38	2	55	ILE
39	3	5	LEU
40	4	15	LEU
40	4	115	LEU
40	4	157	ARG
41	5	9	MET
42	6	25	LYS
44	8	120	LYS
45	9	17	LEU
46	A	93	ARG
48	D	98	ARG
50	F	70	LEU
52	H	61	ILE
54	J	5	LEU
54	J	49	ILE
56	s	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
2	P	53	HIS
2	P	86	ASN
2	P	134	ASN
2	P	260	ASN
3	Q	49	GLN
3	Q	149	ASN
3	Q	150	GLN
4	R	163	ASN
4	R	165	HIS
6	T	22	GLN
6	T	143	GLN
7	V	12	GLN
8	W	40	HIS
13	b	38	GLN
14	c	12	GLN
15	d	37	GLN
15	d	44	GLN
17	f	15	GLN
23	l	27	ASN
23	l	58	ASN

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Mol	Chain	Res	Type
25	n	6	ASN
26	o	19	HIS
31	L	20	ASN
32	C	57	GLN
32	C	58	ASN
32	C	172	HIS
33	U	2	GLN
33	U	18	GLN
33	U	28	ASN
33	U	43	ASN
37	1	177	ASN
40	4	89	HIS
41	5	3	HIS
41	5	11	HIS
41	5	14	GLN
41	5	55	HIS
42	6	28	ASN
44	8	32	GLN
46	A	118	HIS
48	D	8	ASN
49	E	49	GLN
51	G	63	GLN
52	H	31	HIS
53	I	52	GLN
59	v	51	GLN
59	v	56	HIS
59	v	151	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	O	117/120 (97%)	21 (17%)	1 (0%)
30	N	2894/2903 (99%)	521 (18%)	34 (1%)
34	M	74/75 (98%)	11 (14%)	0
35	x	43/692 (6%)	34 (79%)	0
36	0	1538/1539 (99%)	280 (18%)	21 (1%)
58	u	72/73 (98%)	19 (26%)	0
All	All	4738/5402 (87%)	886 (18%)	56 (1%)

All (886) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	O	13	G
1	O	25	U
1	O	31	C
1	O	35	C
1	O	41	G
1	O	44	G
1	O	45	A
1	O	51	G
1	O	53	A
1	O	56	G
1	O	57	A
1	O	64	G
1	O	66	A
1	O	67	G
1	O	88	C
1	O	89	U
1	O	90	C
1	O	91	C
1	O	99	A
1	O	108	A
1	O	109	A
30	N	10	A
30	N	23	G
30	N	28	A
30	N	35	G
30	N	36	G
30	N	42	A
30	N	46	G
30	N	51	G
30	N	55	G
30	N	60	G
30	N	63	A
30	N	71	A
30	N	74	A
30	N	75	G
30	N	84	A
30	N	96	C
30	N	101	A
30	N	102	U
30	N	103	A
30	N	118	A
30	N	119	A
30	N	120	U

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Mol	Chain	Res	Type
30	N	125	A
30	N	138	U
30	N	139	U
30	N	140	C
30	N	141	G
30	N	142	A
30	N	162	U
30	N	163	C
30	N	165	A
30	N	166	U
30	N	188	G
30	N	196	A
30	N	199	A
30	N	201	C
30	N	215	G
30	N	216	A
30	N	221	A
30	N	222	A
30	N	223	A
30	N	224	U
30	N	228	C
30	N	241	A
30	N	242	G
30	N	243	U
30	N	248	G
30	N	255	A
30	N	265	A
30	N	266	G
30	N	267	C
30	N	271	G
30	N	272	A
30	N	276	U
30	N	278	A
30	N	281	C
30	N	284	U
30	N	294	A
30	N	301	G
30	N	311	A
30	N	323	C
30	N	329	G
30	N	330	A
30	N	332	A

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Mol	Chain	Res	Type
30	N	346	A
30	N	361	G
30	N	362	A
30	N	371	A
30	N	372	G
30	N	373	U
30	N	386	G
30	N	396	G
30	N	399	U
30	N	403	U
30	N	404	A
30	N	405	U
30	N	406	G
30	N	411	G
30	N	412	A
30	N	421	C
30	N	422	A
30	N	424	G
30	N	435	C
30	N	447	A
30	N	455	C
30	N	456	C
30	N	457	A
30	N	467	G
30	N	471	A
30	N	473	G
30	N	481	G
30	N	491	G
30	N	501	A
30	N	504	A
30	N	505	A
30	N	509	C
30	N	513	A
30	N	529	A
30	N	531	C
30	N	532	A
30	N	543	G
30	N	544	C
30	N	546	U
30	N	548	G
30	N	549	G
30	N	550	C

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Mol	Chain	Res	Type
30	N	556	A
30	N	563	A
30	N	573	U
30	N	575	A
30	N	578	G
30	N	586	A
30	N	603	A
30	N	613	A
30	N	614	A
30	N	616	A
30	N	622	G
30	N	627	A
30	N	637	A
30	N	645	C
30	N	646	U
30	N	647	G
30	N	648	G
30	N	654	A
30	N	655	A
30	N	669	G
30	N	670	A
30	N	671	C
30	N	677	A
30	N	686	U
30	N	695	G
30	N	696	G
30	N	717	C
30	N	729	G
30	N	730	A
30	N	738	G
30	N	747	U
30	N	764	A
30	N	765	C
30	N	775	G
30	N	776	G
30	N	782	A
30	N	783	A
30	N	784	G
30	N	785	G
30	N	792	A
30	N	800	A
30	N	805	G

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Mol	Chain	Res	Type
30	N	806	C
30	N	812	C
30	N	819	A
30	N	827	U
30	N	828	U
30	N	829	A
30	N	845	A
30	N	846	U
30	N	858	G
30	N	860	U
30	N	866	A
30	N	869	G
30	N	878	A
30	N	885	C
30	N	896	A
30	N	897	C
30	N	907	G
30	N	910	A
30	N	914	G
30	N	919	U
30	N	932	U
30	N	941	A
30	N	945	A
30	N	946	C
30	N	953	G
30	N	961	C
30	N	973	A
30	N	974	G
30	N	983	A
30	N	985	C
30	N	989	G
30	N	995	C
30	N	996	A
30	N	997	G
30	N	1004	U
30	N	1012	U
30	N	1013	C
30	N	1020	A
30	N	1021	A
30	N	1022	G
30	N	1023	U
30	N	1025	G

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Mol	Chain	Res	Type
30	N	1026	G
30	N	1033	U
30	N	1046	A
30	N	1047	G
30	N	1057	A
30	N	1060	U
30	N	1062	G
30	N	1064	C
30	N	1066	U
30	N	1067	A
30	N	1068	G
30	N	1070	A
30	N	1077	A
30	N	1082	U
30	N	1083	U
30	N	1088	A
30	N	1089	A
30	N	1090	A
30	N	1094	U
30	N	1096	A
30	N	1097	U
30	N	1100	C
30	N	1104	C
30	N	1110	G
30	N	1111	A
30	N	1112	G
30	N	1119	U
30	N	1122	G
30	N	1130	U
30	N	1132	U
30	N	1133	A
30	N	1135	C
30	N	1136	G
30	N	1141	U
30	N	1142	A
30	N	1143	A
30	N	1155	A
30	N	1168	G
30	N	1171	G
30	N	1173	U
30	N	1174	U
30	N	1175	A

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Mol	Chain	Res	Type
30	N	1180	U
30	N	1186	G
30	N	1195	G
30	N	1204	A
30	N	1205	A
30	N	1206	G
30	N	1210	G
30	N	1212	G
30	N	1237	A
30	N	1238	G
30	N	1250	G
30	N	1251	C
30	N	1253	A
30	N	1256	G
30	N	1257	C
30	N	1265	A
30	N	1266	G
30	N	1268	A
30	N	1271	G
30	N	1272	A
30	N	1275	A
30	N	1300	G
30	N	1301	A
30	N	1321	A
30	N	1329	U
30	N	1332	G
30	N	1345	C
30	N	1352	U
30	N	1365	A
30	N	1368	G
30	N	1376	C
30	N	1379	U
30	N	1383	A
30	N	1386	C
30	N	1395	A
30	N	1403	A
30	N	1416	G
30	N	1419	A
30	N	1420	A
30	N	1421	G
30	N	1427	A
30	N	1428	C

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Mol	Chain	Res	Type
30	N	1434	A
30	N	1437	C
30	N	1453	A
30	N	1458	U
30	N	1461	C
30	N	1478	G
30	N	1482	G
30	N	1504	A
30	N	1508	A
30	N	1509	A
30	N	1515	A
30	N	1524	G
30	N	1529	G
30	N	1535	A
30	N	1536	C
30	N	1537	G
30	N	1538	G
30	N	1554	U
30	N	1565	C
30	N	1566	A
30	N	1569	A
30	N	1578	U
30	N	1583	A
30	N	1584	U
30	N	1585	C
30	N	1587	G
30	N	1607	C
30	N	1608	A
30	N	1610	A
30	N	1613	G
30	N	1622	G
30	N	1647	U
30	N	1648	U
30	N	1651	G
30	N	1674	G
30	N	1675	C
30	N	1676	A
30	N	1698	A
30	N	1699	G
30	N	1713	A
30	N	1715	G
30	N	1728	C

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Mol	Chain	Res	Type
30	N	1729	U
30	N	1730	C
30	N	1733	G
30	N	1738	G
30	N	1757	A
30	N	1758	U
30	N	1760	C
30	N	1764	C
30	N	1773	A
30	N	1784	A
30	N	1787	A
30	N	1800	C
30	N	1801	A
30	N	1802	A
30	N	1808	A
30	N	1811	G
30	N	1816	C
30	N	1829	A
30	N	1833	C
30	N	1835	G
30	N	1857	G
30	N	1869	G
30	N	1870	C
30	N	1900	A
30	N	1901	A
30	N	1905	C
30	N	1906	G
30	N	1913	A
30	N	1919	A
30	N	1927	A
30	N	1929	G
30	N	1930	G
30	N	1931	U
30	N	1938	A
30	N	1955	U
30	N	1964	G
30	N	1967	C
30	N	1970	A
30	N	1971	U
30	N	1972	G
30	N	1991	U
30	N	1993	U

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Mol	Chain	Res	Type
30	N	1997	C
30	N	2004	G
30	N	2006	C
30	N	2020	A
30	N	2022	U
30	N	2023	C
30	N	2031	A
30	N	2033	A
30	N	2043	C
30	N	2046	G
30	N	2055	C
30	N	2056	G
30	N	2060	A
30	N	2061	G
30	N	2062	A
30	N	2063	C
30	N	2069	G
30	N	2072	C
30	N	2077	A
30	N	2092	U
30	N	2094	A
30	N	2097	A
30	N	2099	U
30	N	2110	G
30	N	2111	U
30	N	2112	G
30	N	2113	U
30	N	2118	U
30	N	2119	A
30	N	2132	U
30	N	2133	G
30	N	2145	C
30	N	2147	A
30	N	2162	G
30	N	2171	A
30	N	2172	U
30	N	2173	A
30	N	2190	G
30	N	2191	A
30	N	2194	U
30	N	2198	A
30	N	2200	C

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Mol	Chain	Res	Type
30	N	2203	U
30	N	2204	G
30	N	2211	A
30	N	2212	A
30	N	2214	C
30	N	2225	A
30	N	2226	C
30	N	2238	G
30	N	2239	G
30	N	2266	A
30	N	2278	A
30	N	2279	G
30	N	2283	C
30	N	2286	G
30	N	2287	A
30	N	2288	A
30	N	2297	A
30	N	2305	U
30	N	2307	G
30	N	2309	A
30	N	2312	U
30	N	2325	G
30	N	2333	A
30	N	2334	U
30	N	2345	G
30	N	2347	C
30	N	2350	C
30	N	2354	C
30	N	2357	G
30	N	2361	G
30	N	2383	G
30	N	2385	C
30	N	2391	G
30	N	2402	U
30	N	2403	C
30	N	2406	A
30	N	2407	A
30	N	2422	C
30	N	2423	U
30	N	2425	A
30	N	2426	A
30	N	2427	C

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Mol	Chain	Res	Type
30	N	2429	G
30	N	2430	A
30	N	2431	U
30	N	2435	A
30	N	2441	U
30	N	2448	A
30	N	2470	G
30	N	2476	A
30	N	2498	C
30	N	2502	G
30	N	2503	A
30	N	2504	U
30	N	2505	G
30	N	2507	C
30	N	2518	A
30	N	2520	C
30	N	2529	G
30	N	2535	G
30	N	2547	A
30	N	2554	U
30	N	2566	A
30	N	2567	G
30	N	2572	A
30	N	2573	C
30	N	2574	G
30	N	2578	G
30	N	2585	U
30	N	2602	A
30	N	2603	G
30	N	2609	U
30	N	2613	U
30	N	2615	U
30	N	2629	U
30	N	2630	G
30	N	2636	C
30	N	2645	G
30	N	2646	C
30	N	2655	G
30	N	2656	U
30	N	2661	G
30	N	2663	G
30	N	2682	A

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Mol	Chain	Res	Type
30	N	2689	U
30	N	2690	U
30	N	2714	G
30	N	2716	C
30	N	2718	G
30	N	2724	U
30	N	2727	A
30	N	2733	A
30	N	2748	A
30	N	2751	G
30	N	2752	C
30	N	2765	A
30	N	2776	A
30	N	2777	G
30	N	2778	A
30	N	2779	U
30	N	2791	G
30	N	2792	A
30	N	2798	U
30	N	2801	G
30	N	2818	U
30	N	2820	A
30	N	2833	U
30	N	2834	G
30	N	2836	U
30	N	2849	U
30	N	2850	A
30	N	2859	G
30	N	2867	G
30	N	2868	A
30	N	2872	A
30	N	2873	A
30	N	2880	C
30	N	2884	U
30	N	2887	A
30	N	2891	U
30	N	2903	U
34	M	9	C
34	M	10	G
34	M	15	G
34	M	16	C
34	M	17	G

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Mol	Chain	Res	Type
34	M	19	U
34	M	20	A
34	M	42	G
34	M	47	C
34	M	74	C
34	M	75	A
35	x	435	G
35	x	436	A
35	x	437	C
35	x	438	C
35	x	442	G
35	x	443	C
35	x	444	C
35	x	445	A
35	x	446	U
35	x	448	U
35	x	449	A
35	x	450	C
35	x	451	G
35	x	452	U
35	x	453	C
35	x	455	C
35	x	457	C
35	x	458	U
35	x	459	C
35	x	460	A
35	x	461	A
35	x	462	U
35	x	463	A
35	x	464	G
35	x	465	U
35	x	469	U
35	x	470	U
35	x	471	U
35	x	472	U
35	x	473	C
35	x	474	U
35	x	475	G
35	x	476	C
35	x	477	A
36	0	4	U
36	0	6	G

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Mol	Chain	Res	Type
36	0	9	G
36	0	32	A
36	0	39	G
36	0	44	A
36	0	47	C
36	0	48	C
36	0	50	A
36	0	51	A
36	0	52	C
36	0	58	C
36	0	65	A
36	0	69	G
36	0	71	A
36	0	72	A
36	0	83	C
36	0	84	U
36	0	85	U
36	0	86	G
36	0	87	C
36	0	92	U
36	0	97	G
36	0	108	G
36	0	115	G
36	0	116	A
36	0	122	G
36	0	130	A
36	0	141	G
36	0	143	A
36	0	144	G
36	0	149	A
36	0	156	C
36	0	163	C
36	0	174	A
36	0	177	G
36	0	182	A
36	0	183	C
36	0	184	G
36	0	197	A
36	0	209	U
36	0	210	C
36	0	211	G
36	0	226	G

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Mol	Chain	Res	Type
36	0	245	U
36	0	247	G
36	0	251	G
36	0	266	G
36	0	267	C
36	0	280	C
36	0	281	G
36	0	289	G
36	0	298	A
36	0	306	A
36	0	321	A
36	0	328	C
36	0	332	G
36	0	347	G
36	0	351	G
36	0	352	C
36	0	354	G
36	0	358	U
36	0	367	U
36	0	372	C
36	0	375	U
36	0	384	G
36	0	389	A
36	0	397	A
36	0	398	U
36	0	406	G
36	0	412	A
36	0	413	G
36	0	421	U
36	0	422	C
36	0	423	G
36	0	424	G
36	0	429	U
36	0	430	A
36	0	439	U
36	0	451	A
36	0	458	U
36	0	459	A
36	0	467	U
36	0	468	A
36	0	474	G
36	0	478	A

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Mol	Chain	Res	Type
36	0	479	U
36	0	481	G
36	0	484	G
36	0	485	U
36	0	486	U
36	0	495	A
36	0	497	G
36	0	511	C
36	0	518	C
36	0	519	C
36	0	521	G
36	0	527	G
36	0	531	U
36	0	532	A
36	0	533	A
36	0	547	A
36	0	559	A
36	0	562	U
36	0	572	A
36	0	573	A
36	0	576	C
36	0	596	A
36	0	607	A
36	0	633	G
36	0	639	G
36	0	650	G
36	0	652	U
36	0	665	A
36	0	675	A
36	0	688	G
36	0	695	A
36	0	701	U
36	0	702	A
36	0	703	G
36	0	718	A
36	0	721	G
36	0	723	U
36	0	724	G
36	0	731	G
36	0	734	G
36	0	747	A
36	0	755	G

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Mol	Chain	Res	Type
36	0	760	G
36	0	777	A
36	0	793	U
36	0	794	A
36	0	813	U
36	0	815	A
36	0	817	C
36	0	818	G
36	0	819	A
36	0	821	G
36	0	828	U
36	0	832	G
36	0	836	G
36	0	841	C
36	0	843	U
36	0	844	G
36	0	846	G
36	0	849	G
36	0	859	G
36	0	864	A
36	0	885	G
36	0	889	A
36	0	890	G
36	0	891	U
36	0	902	G
36	0	914	A
36	0	926	G
36	0	934	C
36	0	935	A
36	0	960	U
36	0	965	U
36	0	966	G
36	0	969	A
36	0	971	G
36	0	972	C
36	0	975	A
36	0	976	G
36	0	977	A
36	0	989	U
36	0	993	G
36	0	996	A
36	0	999	C

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Mol	Chain	Res	Type
36	0	1000	A
36	0	1004	A
36	0	1008	U
36	0	1009	U
36	0	1017	U
36	0	1018	G
36	0	1020	G
36	0	1022	A
36	0	1024	G
36	0	1025	U
36	0	1026	G
36	0	1027	C
36	0	1030	U
36	0	1031	C
36	0	1032	G
36	0	1043	G
36	0	1044	A
36	0	1053	G
36	0	1056	U
36	0	1065	U
36	0	1085	U
36	0	1092	A
36	0	1094	G
36	0	1095	U
36	0	1101	A
36	0	1125	U
36	0	1130	A
36	0	1132	C
36	0	1136	C
36	0	1137	C
36	0	1138	G
36	0	1139	G
36	0	1140	C
36	0	1146	A
36	0	1158	C
36	0	1159	U
36	0	1168	U
36	0	1171	A
36	0	1182	G
36	0	1183	U
36	0	1184	G
36	0	1190	G

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Mol	Chain	Res	Type
36	0	1196	A
36	0	1200	C
36	0	1201	A
36	0	1202	U
36	0	1212	U
36	0	1213	A
36	0	1227	A
36	0	1238	A
36	0	1253	G
36	0	1256	A
36	0	1257	A
36	0	1258	G
36	0	1260	G
36	0	1261	A
36	0	1274	A
36	0	1275	A
36	0	1278	G
36	0	1280	A
36	0	1281	C
36	0	1287	A
36	0	1297	G
36	0	1298	U
36	0	1300	G
36	0	1301	U
36	0	1302	C
36	0	1305	G
36	0	1317	C
36	0	1318	A
36	0	1319	A
36	0	1320	C
36	0	1322	C
36	0	1323	G
36	0	1331	G
36	0	1332	A
36	0	1340	A
36	0	1346	A
36	0	1347	G
36	0	1348	U
36	0	1353	G
36	0	1363	A
36	0	1364	U
36	0	1370	G

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Mol	Chain	Res	Type
36	0	1379	G
36	0	1383	C
36	0	1394	A
36	0	1400	C
36	0	1419	G
36	0	1422	G
36	0	1433	A
36	0	1441	A
36	0	1446	A
36	0	1451	U
36	0	1452	C
36	0	1487	G
36	0	1491	G
36	0	1492	A
36	0	1493	A
36	0	1497	G
36	0	1503	A
36	0	1506	U
36	0	1517	G
36	0	1519	A
36	0	1529	G
36	0	1530	G
36	0	1531	A
36	0	1534	A
36	0	1535	C
36	0	1537	U
58	u	13	C
58	u	14	A
58	u	16	U
58	u	17	C
58	u	18	G
58	u	19	G
58	u	20	U
58	u	21	A
58	u	22	G
58	u	36	A
58	u	45	U
58	u	46	G
58	u	47	U
58	u	48	C
58	u	52	G
58	u	61	C

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Mol	Chain	Res	Type
58	u	62	C
58	u	63	G
58	u	73	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	O	52	A
30	N	60	G
30	N	227	A
30	N	242	G
30	N	249	C
30	N	372	G
30	N	404	A
30	N	421	C
30	N	446	G
30	N	456	C
30	N	474	G
30	N	503	A
30	N	512	G
30	N	555	G
30	N	670	A
30	N	774	G
30	N	784	G
30	N	859	G
30	N	995	C
30	N	1020	A
30	N	1134	A
30	N	1141	U
30	N	1142	A
30	N	1236	G
30	N	1900	A
30	N	2062	A
30	N	2225	A
30	N	2282	G
30	N	2286	G
30	N	2311	A
30	N	2405	G
30	N	2655	G
30	N	2776	A
30	N	2867	G
30	N	2873	A

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Mol	Chain	Res	Type
36	0	64	G
36	0	85	U
36	0	96	U
36	0	115	G
36	0	388	G
36	0	429	U
36	0	518	C
36	0	595	A
36	0	812	G
36	0	890	G
36	0	965	U
36	0	1124	G
36	0	1145	A
36	0	1182	G
36	0	1190	G
36	0	1201	A
36	0	1300	G
36	0	1345	U
36	0	1347	G
36	0	1491	G
36	0	1528	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

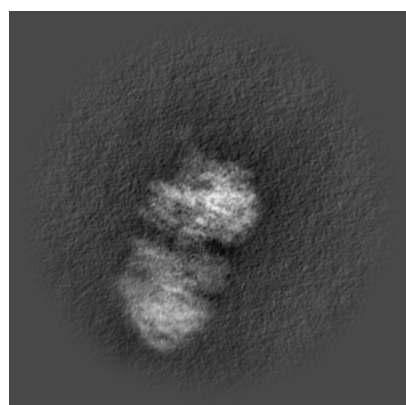
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13958. These allow visual inspection of the internal detail of the map and identification of artifacts.

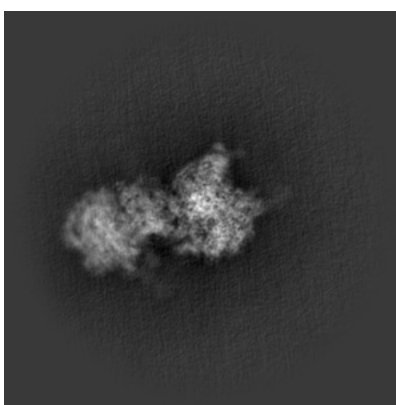
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

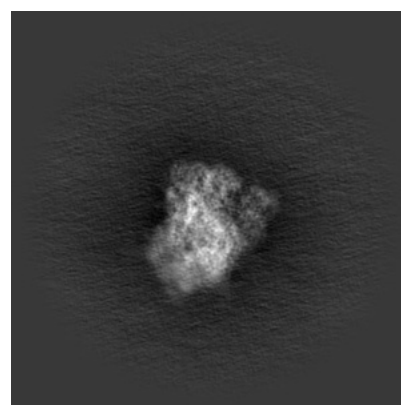
6.1.1 Primary map



X



Y

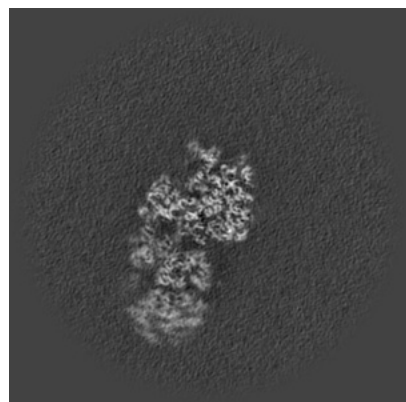


Z

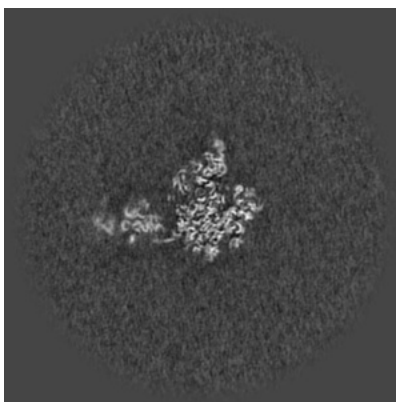
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

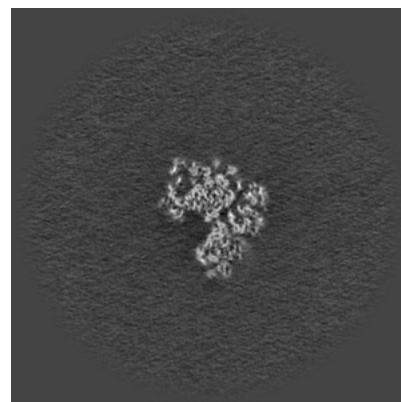
6.2.1 Primary map



X Index: 300



Y Index: 300

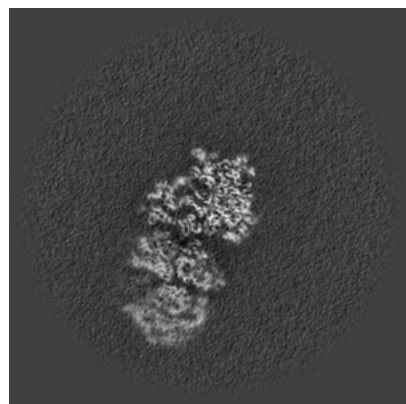


Z Index: 300

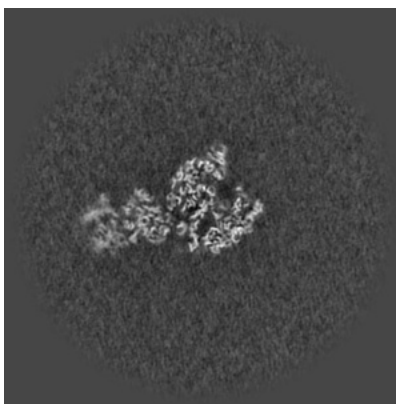
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

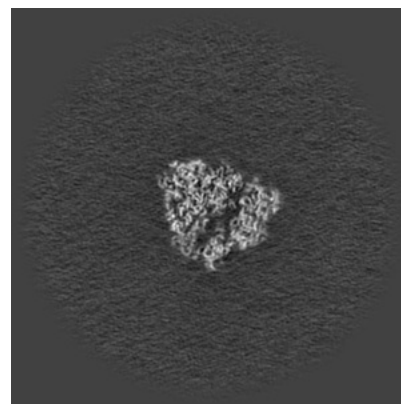
6.3.1 Primary map



X Index: 293



Y Index: 289

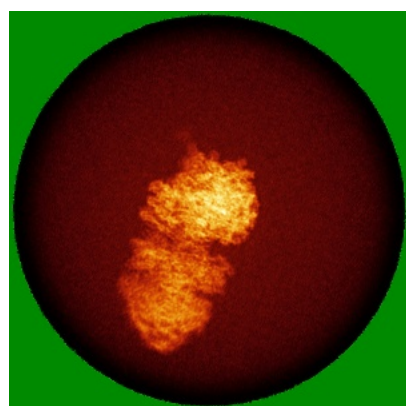


Z Index: 321

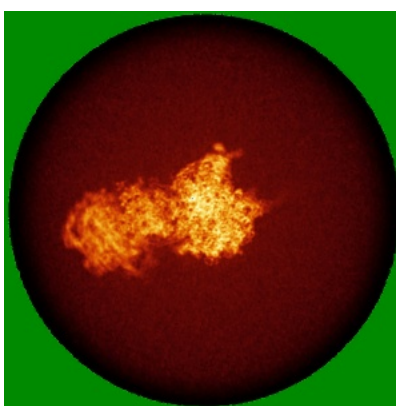
The images above show the largest variance slices of the map in three orthogonal directions.

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

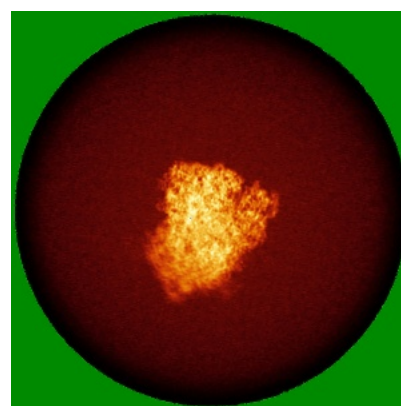
6.4.1 Primary map



X



Y

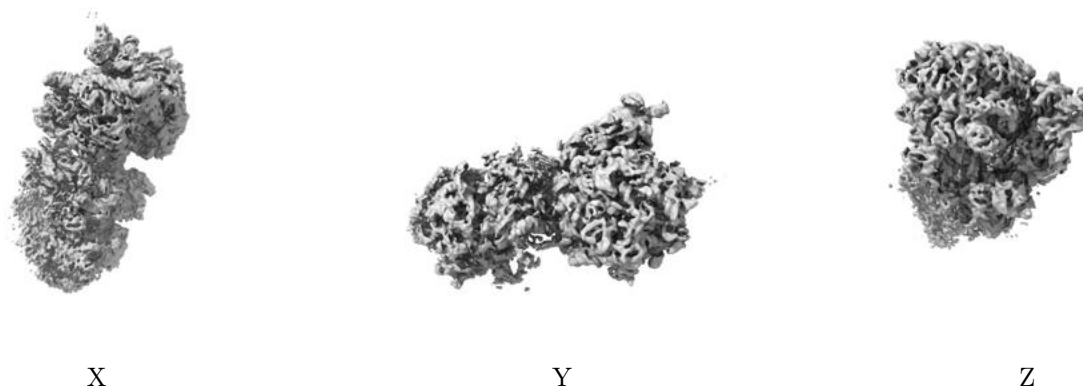


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

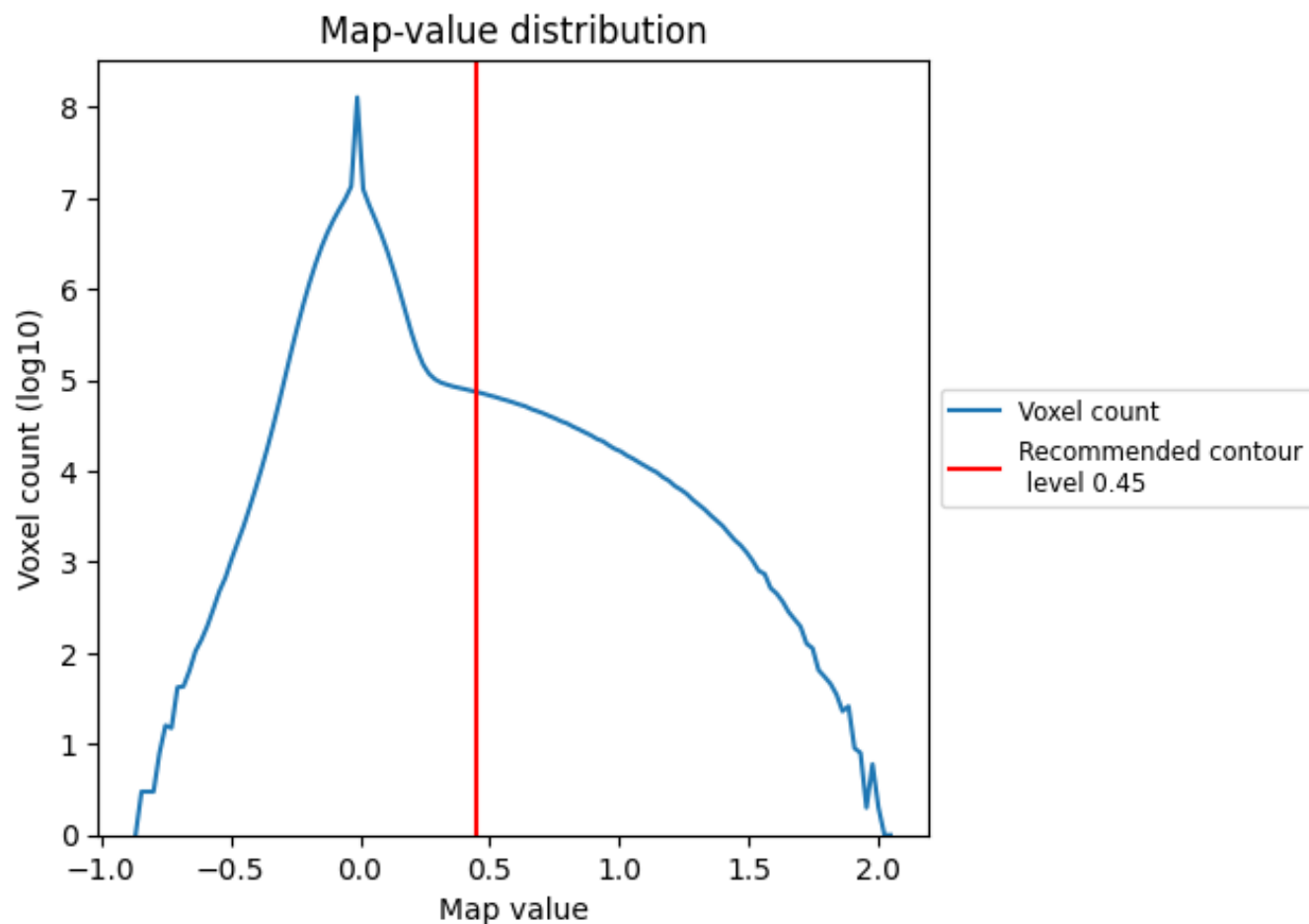
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

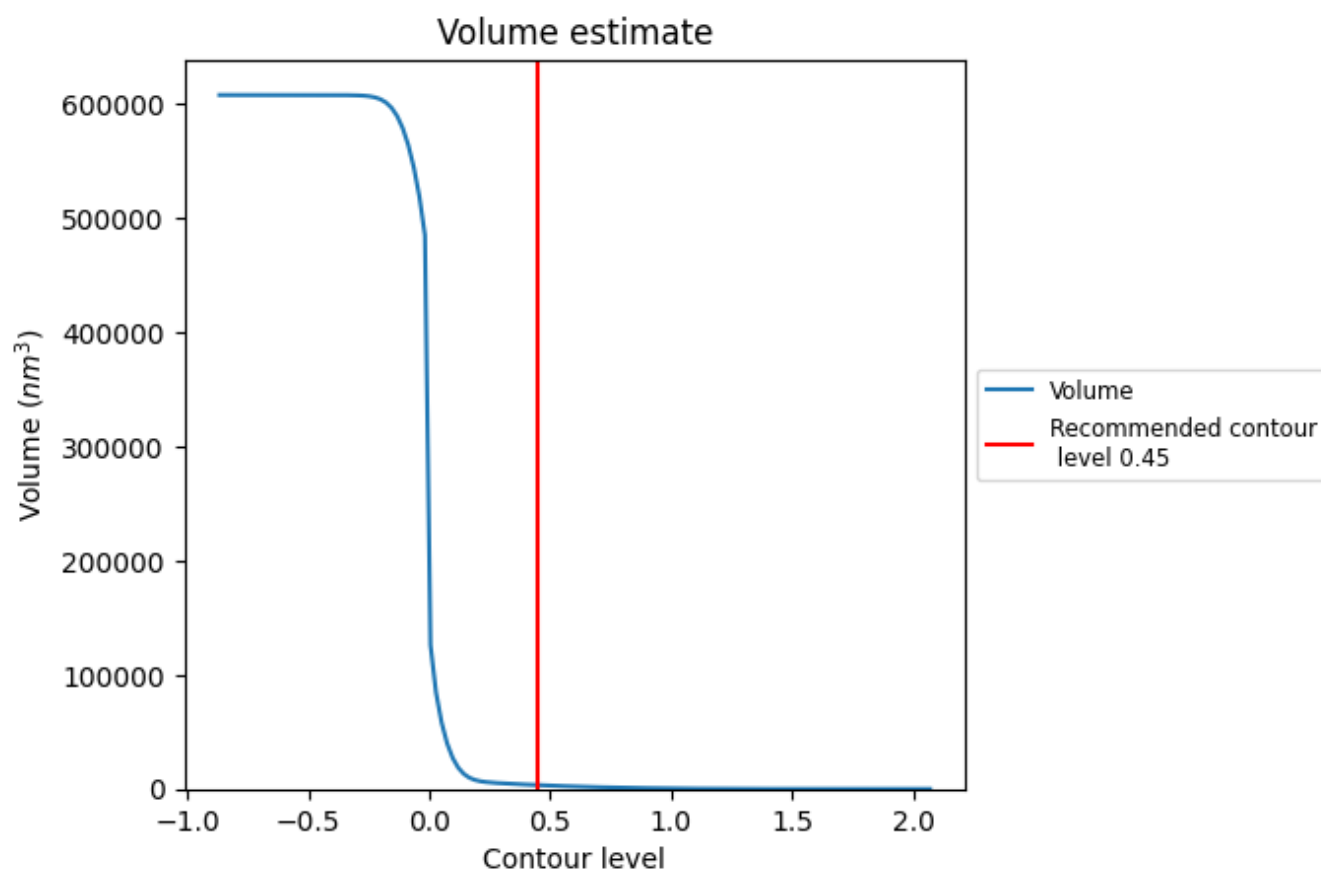
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

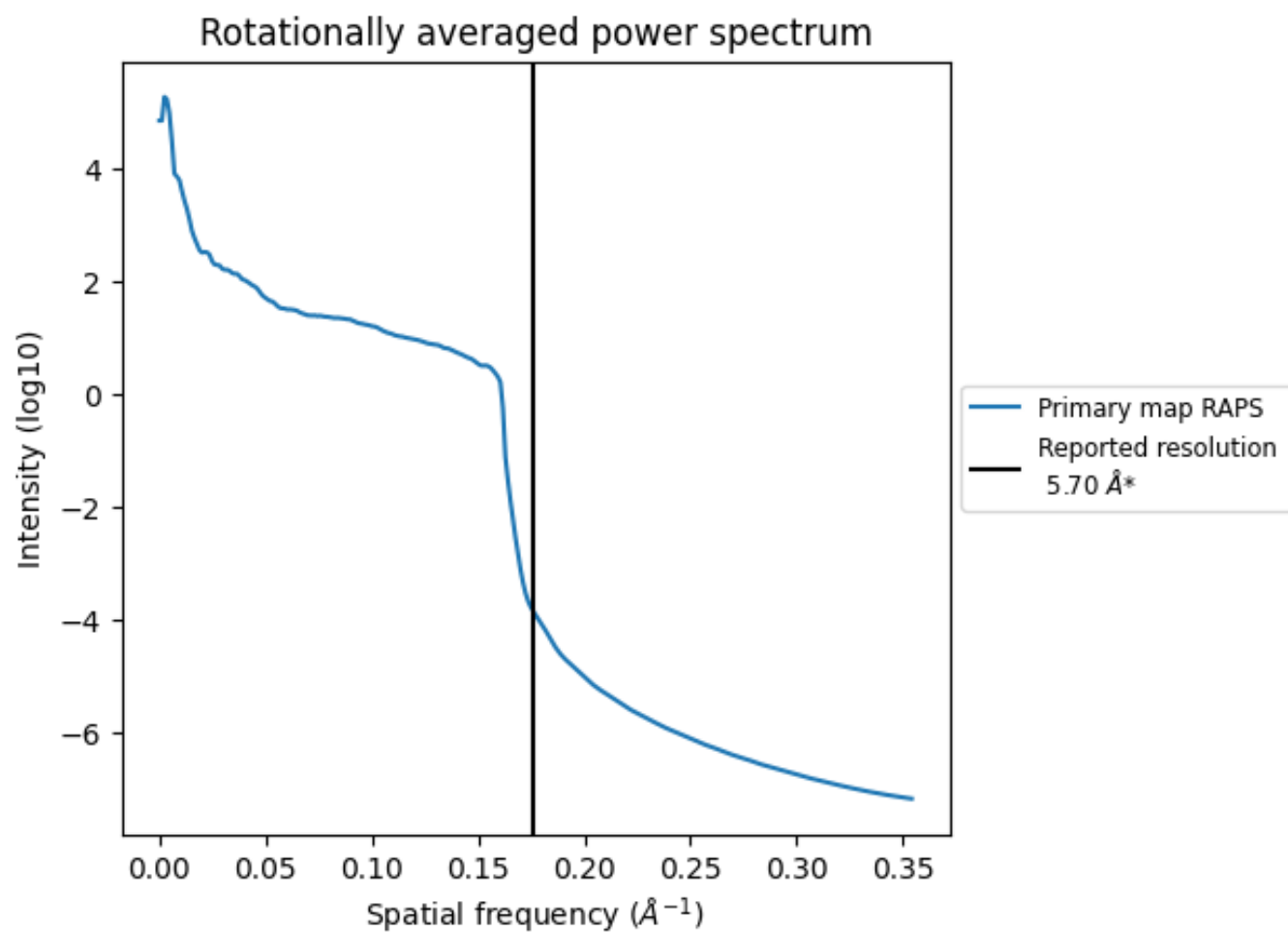
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3383 nm³; this corresponds to an approximate mass of 3056 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

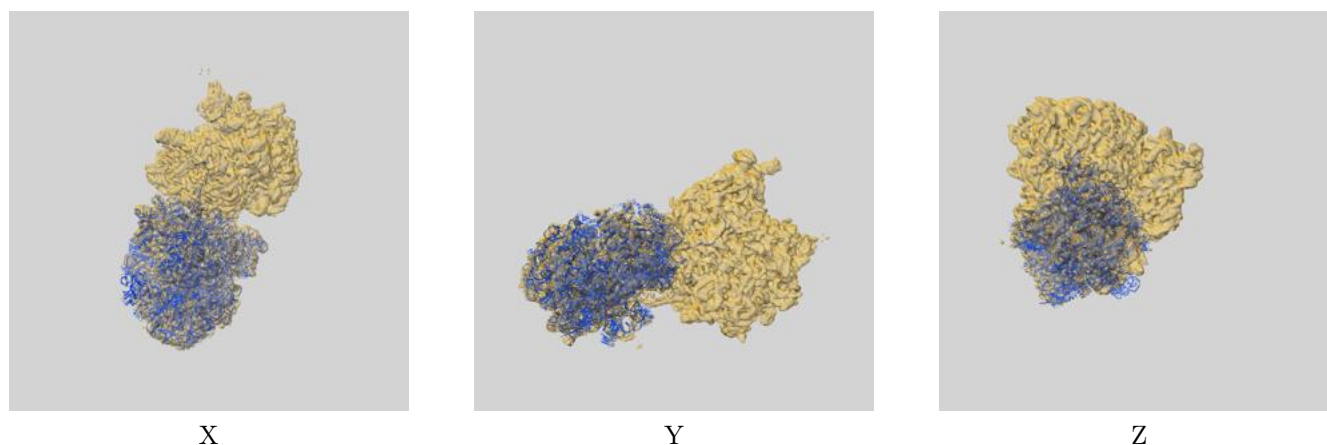
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

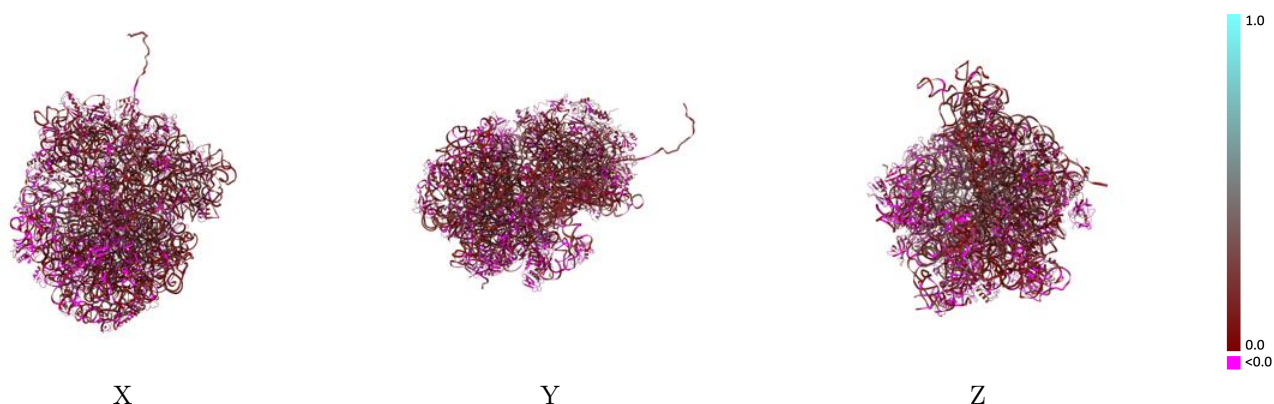
This section contains information regarding the fit between EMDB map EMD-13958 and PDB model 7QGR. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



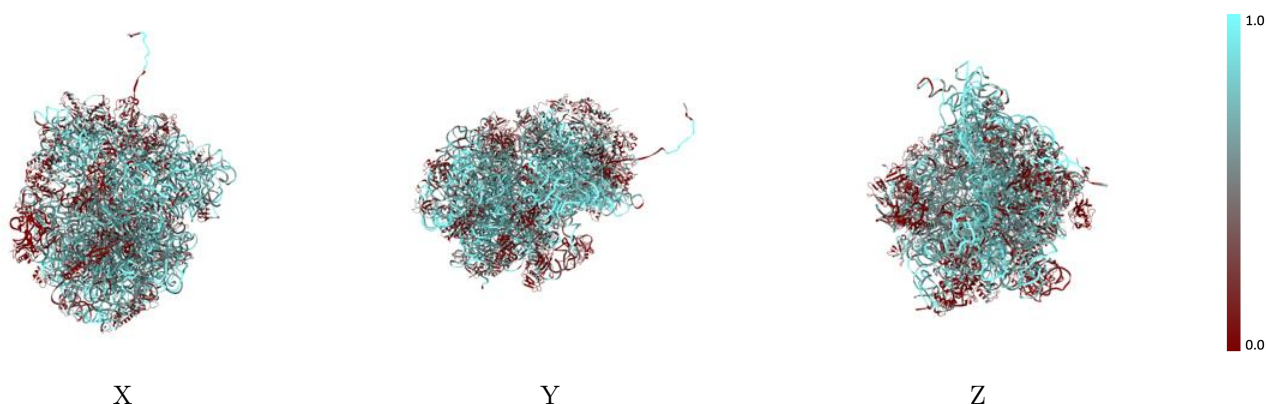
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



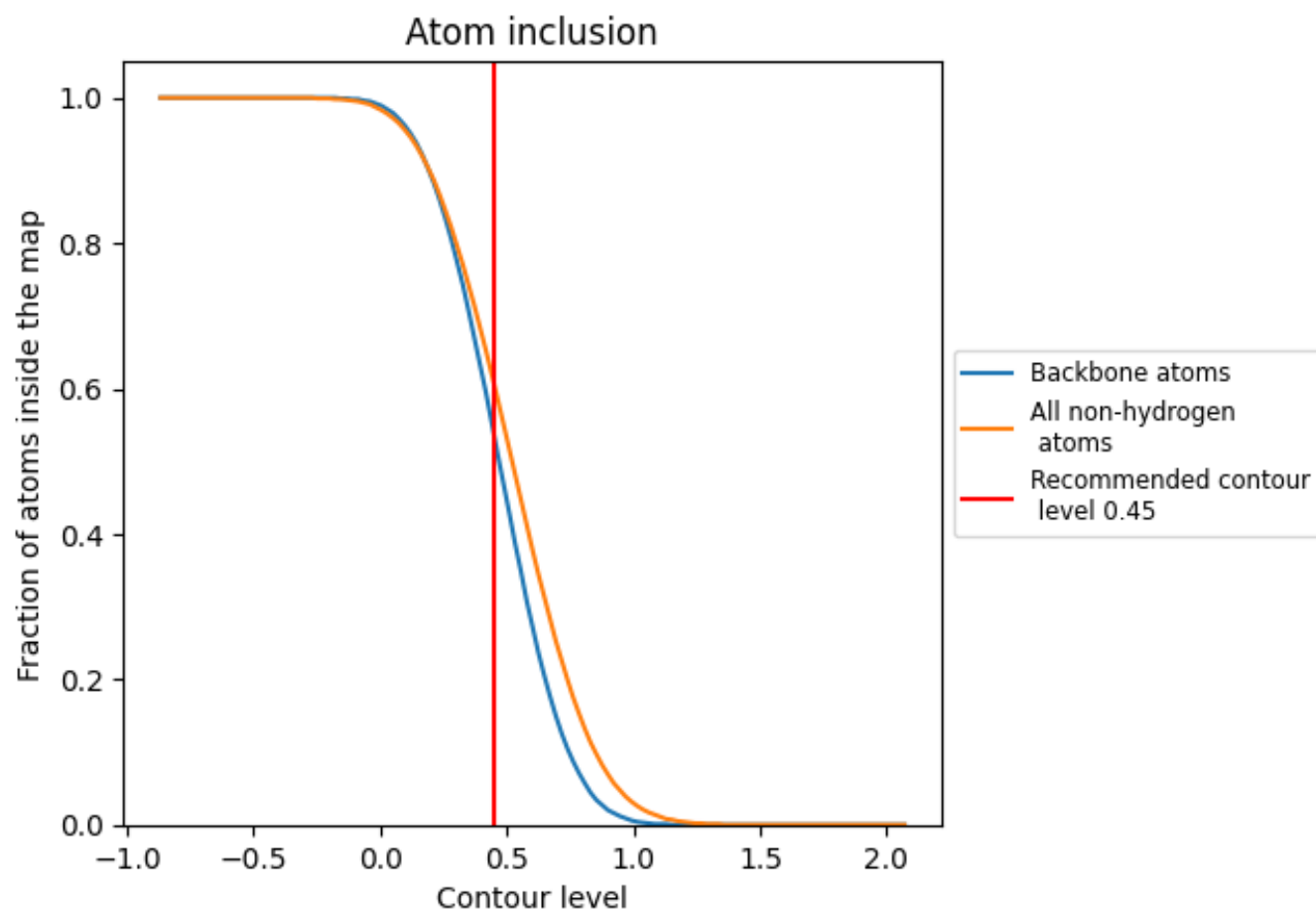
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary



















































The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6060	 0.1120
0	 0.8330	 0.1680
1	 0.3620	 0.1410
2	 0.2970	 0.1100
3	 0.2500	 0.0970
4	 0.2750	 0.1150
5	 0.3430	 0.0910
6	 0.3930	 0.0880
7	 0.4510	 0.0910
8	 0.3530	 0.0620
9	 0.3170	 0.0750
A	 0.2630	 0.0770
B	 0.4250	 0.1380
C	 0.0010	 0.0310
D	 0.3240	 0.0920
E	 0.3620	 0.0880
F	 0.5200	 0.1100
G	 0.4790	 0.1000
H	 0.4510	 0.0900
I	 0.3920	 0.0760
J	 0.3610	 0.0700
K	 0.4750	 0.1070
L	 0.0050	 0.0850
M	 0.3450	 0.1300
N	 0.7260	 0.1120
O	 0.6460	 0.0810
P	 0.2350	 0.0630
Q	 0.2930	 0.0460
R	 0.3730	 0.0600
S	 0.1120	 0.0550
T	 0.1350	 0.0410
U	 0.0090	 -0.0030
V	 0.0680	 0.0050
W	 0.4510	 0.0470
X	 0.1770	 0.0770



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Chain	Atom inclusion	Q-score
Y	 0.3190	 -0.0160
Z	 0.3300	 0.0750
a	 0.3730	 0.1000
b	 0.2510	 0.0340
c	 0.1850	 0.0390
d	 0.3980	 0.0380
e	 0.2400	 0.0540
f	 0.2510	 0.0750
g	 0.2580	 0.0730
h	 0.3640	 0.0510
i	 0.4480	 0.0630
j	 0.6900	 0.0690
k	 0.4020	 0.0460
l	 0.2760	 0.0520
m	 0.4500	 0.0680
n	 0.5130	 0.1020
o	 0.2020	 0.0300
p	 0.3930	 0.0730
q	 0.4710	 0.0590
r	 0.2650	 0.0610
s	 0.3620	 0.1080
t	 0.0070	 0.0240
u	 0.4900	 0.1310
v	 0.1890	 0.1340
x	 0.5100	 0.1920