



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 12:03 PM UTC

PDB ID : 3JBO / pdb_00003jbo
EMDB ID : EMD-6452
Title : Cryo-electron microscopy reconstruction of the Plasmodium falciparum 80S ribosome bound to P/E-tRNA
Authors : Sun, M.; Li, W.; Blomqvist, K.; Das, S.; Hashem, Y.; Dvorin, J.D.; Frank, J.
Deposited on : 2015-09-16
Resolution : 5.80 Å(reported)
Based on initial models : 3J79, 3J7A

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

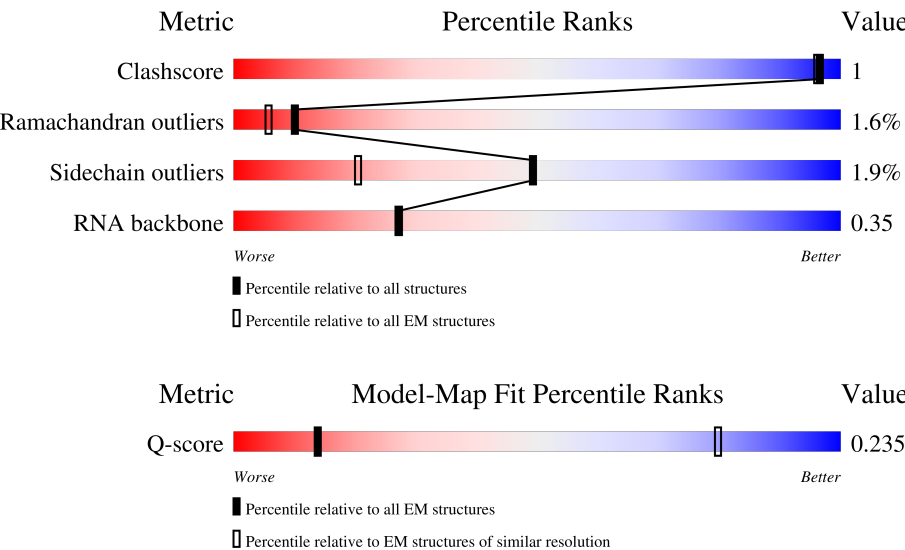
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 5.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	511 (5.30 - 6.30)

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

Mol	Chain	Length	Quality of chain
1	A	1608	58% 32% 8% .
2	7	75	47% 37% 16%
3	Q	144	17% 92% 8% .

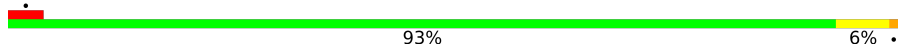
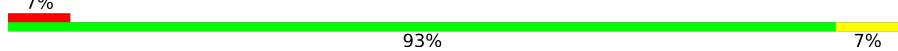
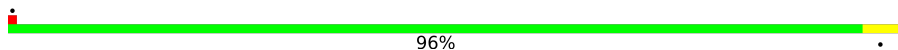
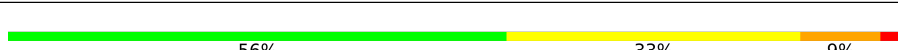
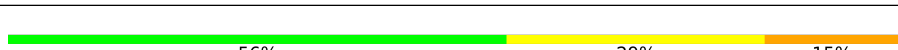
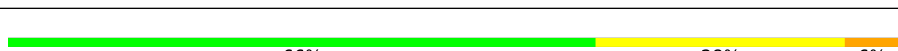
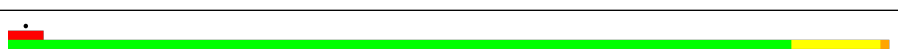
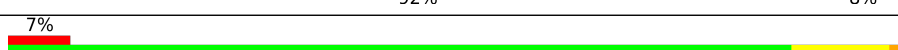
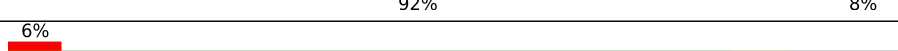
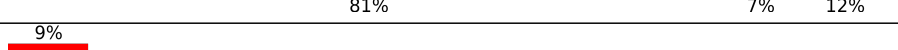
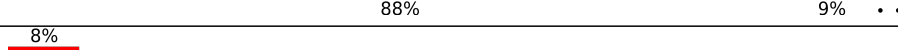
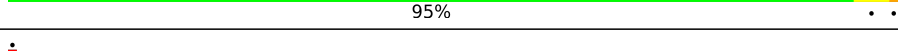
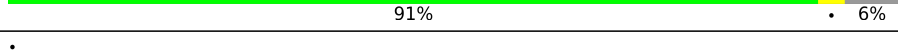
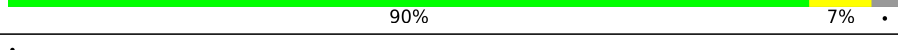
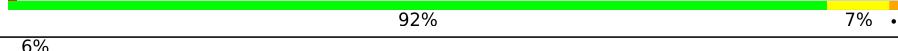
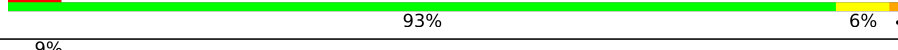
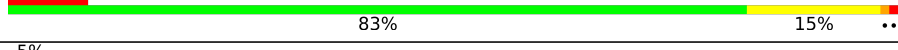
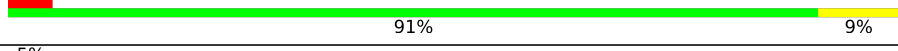
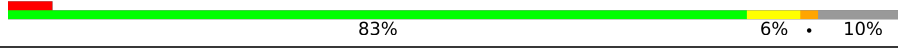
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Mol	Chain	Length	Quality of chain
4	S	128	
5	T	48	
6	M	138	
7	U	149	
8	V	156	
9	E	185	
10	X	103	
11	G	224	
12	W	108	
13	R	114	
14	I	189	
15	O	79	
16	Y	154	
17	Z	72	
18	1	120	
19	2	68	
20	C	195	
21	3	95	
22	4	76	
23	5	65	
24	6	43	
25	B	210	
26	D	209	
27	F	257	
28	H	214	

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Mol	Chain	Length	Quality of chain
29	K	129	
30	J	188	
31	N	98	
32	P	127	
33	L	214	
34	AA	3192	
35	AC	151	
36	AB	118	
37	AL	211	
38	A0	62	
39	AO	147	
40	Ai	95	
41	A2	118	
42	A4	66	
43	A6	98	
44	A7	102	
45	A1	145	
46	AN	146	
47	A8	125	
48	A9	103	
49	Aa	106	
50	Ab	105	
51	Ad	76	
52	Ae	50	
53	Af	51	

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Mol	Chain	Length	Quality of chain
54	AP	204	
55	Ah	85	
56	AI	213	
57	Ac	89	
58	AK	201	
59	AM	132	
60	AS	186	
61	AQ	205	
62	AR	289	
63	AW	170	
64	AY	101	
65	AT	181	
66	AZ	121	
67	A3	119	
68	A5	223	
69	AD	247	
70	AE	380	
71	AF	390	
72	AG	159	
73	AU	180	
74	AH	185	
75	AV	155	
76	Ag	37	
77	AX	97	
78	AJ	244	

2 Entry composition

There are 78 unique types of molecules in this entry. The entry contains 193017 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1608	Total	C	N	O	P	0	0
			34207	15346	6106	11169	1586		

- Molecule 2 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	75	Total	C	N	O	P	0	0
			1598	713	290	521	74		

- Molecule 3 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	144	Total	C	N	O	S	0	0
			1129	712	222	193	2		

- Molecule 4 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	128	Total	C	N	O	S	0	0
			1047	657	205	181	4		

- Molecule 5 is a protein called 40S ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	48	Total	C	N	O	S	0	0
			405	252	85	64	4		

- Molecule 6 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	138	Total	C	N	O	S	0	0
			1099	704	200	194	1		

- Molecule 7 is a protein called 40S ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	149	Total	C	N	O	S	0	0
			1202	769	220	210	3		

- Molecule 8 is a protein called 40S ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	146	Total	C	N	O	S	0	0
			1206	772	227	200	7		

- Molecule 9 is a protein called 40S ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	185	Total	C	N	O	S	0	0
			1515	962	290	261	2		

- Molecule 10 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	96	Total	C	N	O	S	0	0
			777	497	137	139	4		

- Molecule 11 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	224	Total	C	N	O	S	0	0
			1758	1132	307	310	9		

- Molecule 12 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	95	Total	C	N	O	S	0	0
			786	498	149	136	3		

- Molecule 13 is a protein called 40S ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	98	Total	C	N	O	S	0	0
			747	474	123	146	4		

- Molecule 14 is a protein called 40S ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	180	Total	C	N	O	S	0	0
			1424	893	263	258	10		

- Molecule 15 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	79	Total	C	N	O	S	0	0
			687	450	116	119	2		

- Molecule 16 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	154	Total	C	N	O	S	0	0
			1267	811	239	215	2		

- Molecule 17 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	72	Total	C	N	O	S	0	0
			557	346	102	105	4		

- Molecule 18 is a protein called 40S ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1	120	Total	C	N	O	S	0	0
			986	632	189	163	2		

- Molecule 19 is a protein called 40S ribosomal protein eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	2	41	Total	C	N	O	0	0
			321	208	56	57		

- Molecule 20 is a protein called 40S ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	195	Total	C	N	O	S	0	0
			1539	990	266	274	9		

- Molecule 21 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3	95	Total	C	N	O	S	0	0
			782	478	169	129	6		

- Molecule 22 is a protein called 40S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4	76	Total	C	N	O	S	0	0
			586	368	102	107	9		

- Molecule 23 is a protein called 40S ribosomal protein eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	5	58	Total	C	N	O	0	0
			458	285	93	80		

- Molecule 24 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	6	43	Total	C	N	O	0	0
			346	213	75	58		

- Molecule 25 is a protein called 40S ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	210	Total	C	N	O	S	0	0
			1714	1097	301	304	12		

- Molecule 26 is a protein called 40S ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	D	157	Total	C	N	O	S	0	0
			1229	782	225	215	7		

- Molecule 27 is a protein called 40S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	257	Total	C	N	O	S	0	0
			2062	1320	377	357	8		

- Molecule 28 is a protein called 40S ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	204	Total	C	N	O	S	0	0
			1648	1045	313	284	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	158	ILE	-	insertion	UNP Q8IDR9
H	195	ASP	GLU	conflict	UNP Q8IDR9

- Molecule 29 is a protein called 40S ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	K	129	Total	C	N	O	S	0	0
			1037	665	189	178	5		

- Molecule 30 is a protein called 40S ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	J	188	Total	C	N	O	S	0	0
			1529	982	264	279	4		

- Molecule 31 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	N	98	Total	C	N	O	S	0	0
			772	484	135	148	5		

- Molecule 32 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	P	127	Total	C	N	O	S	0	0
			954	591	184	176	3		

- Molecule 33 is a protein called 40S ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	171	Total	C	N	O	S	0	0
			1383	872	264	243	4		

- Molecule 34 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AA	3192	Total	C	N	O	P	0	0
			67862	30436	12049	22217	3160		

- Molecule 35 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AC	151	Total	C	N	O	P	0	0
			3215	1444	589	1034	148		

- Molecule 36 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AB	118	Total	C	N	O	P	0	0
			2522	1128	461	816	117		

- Molecule 37 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AL	211	Total	C	N	O	S	0	0
			1757	1116	346	291	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	19	HIS	ARG	conflict	UNP Q8IAX6
AL	20	ARG	HIS	conflict	UNP Q8IAX6
AL	201	CYS	ARG	conflict	UNP Q8IAX6

- Molecule 38 is a protein called 60S ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A0	62	Total	C	N	O	S	0	0
			522	336	97	88	1		

- Molecule 39 is a protein called 60S ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AO	147	Total	C	N	O	S	0	0
			1172	747	232	189	4		

- Molecule 40 is a protein called 60S ribosomal protein eL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ai	95	Total	C	N	O	S	0	0
			779	490	152	128	9		

- Molecule 41 is a protein called 60S ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	A2	104	Total	C	N	O	S	0	0
			831	529	151	148	3		

- Molecule 42 is a protein called 60S ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	A4	66	Total	C	N	O	S	0	0
			555	347	116	90	2		

- Molecule 43 is a protein called 60S ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	A6	98	Total	C	N	O	S	0	0
			741	462	132	140	7		

- Molecule 44 is a protein called 60S ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	A7	96	Total	C	N	O	S	0	0
			794	508	151	130	5		

- Molecule 45 is a protein called 60S ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	A1	140	Total	C	N	O	S	0	0
			1134	736	204	191	3		

- Molecule 46 is a protein called 60S ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AN	146	Total	C	N	O	S	0	0
			1202	781	210	205	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	?	-	LYS	deletion	UNP Q8ILE8

- Molecule 47 is a protein called 60S ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	A8	125	Total	C	N	O	S	0	0
			1037	660	206	164	7		

- Molecule 48 is a protein called 60S ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A9	103	Total	C	N	O	S	0	0
			845	543	163	136	3		

- Molecule 49 is a protein called 60S ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Aa	106	Total	C	N	O	S	0	0
			859	530	184	139	6		

- Molecule 50 is a protein called 60S ribosomal protein eL36.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	Ab	95	Total	C	N	O	0	0
			757	477	150	130		

- Molecule 51 is a protein called 60S ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ad	72	Total	C	N	O	S	0	0
			604	395	107	100	2		

- Molecule 52 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Ae	43	Total	C	N	O	S	0	0
			388	243	92	52	1		

- Molecule 53 is a protein called 60S ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Af	51	Total	C	N	O	S	0	0
			414	255	87	67	5		

- Molecule 54 is a protein called 60S ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AP	204	Total	C	N	O	S	0	0
			1697	1075	351	267	4		

- Molecule 55 is a protein called 60S ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Ah	85	Total	C	N	O	S	0	0
			659	417	127	108	7		

- Molecule 56 is a protein called 60S ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AI	207	Total	C	N	O	S	0	0
			1685	1096	298	286	5		

- Molecule 57 is a protein called 60S ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ac	89	Total	C	N	O	S	0	0
			710	441	150	114	5		

- Molecule 58 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AK	201	Total	C	N	O	S	0	0
			1660	1064	311	277	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	109	ALA	TYR	conflict	UNP Q8IJZ7

- Molecule 59 is a protein called 60S ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AM	132	Total	C	N	O	S	0	0
			996	631	179	178	8		

- Molecule 60 is a protein called 60S ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AS	186	Total	C	N	O	S	0	0
			1503	958	299	241	5		

- Molecule 61 is a protein called 60S ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AQ	189	Total	C	N	O	S	0	0
			1545	984	291	262	8		

- Molecule 62 is a protein called 60S ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AR	252	Total	C	N	O	S	0	0
			2050	1300	385	359	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	?	-	LYS	deletion	UNP Q8ILL3

- Molecule 63 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AW	170	Total	C	N	O	S	0	0
			1319	824	266	222	7		

- Molecule 64 is a protein called 60S ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AY	101	Total	C	N	O	S	0	0
			797	502	144	145	6		

- Molecule 65 is a protein called 60S ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AT	181	Total	C	N	O	S	0	0
			1509	952	309	244	4		

- Molecule 66 is a protein called 60S ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AZ	121	Total	C	N	O	S	0	0
			1001	626	206	166	3		

- Molecule 67 is a protein called 60S ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	A3	119	Total	C	N	O	S	0	0
			995	635	194	164	2		

- Molecule 68 is a protein called 60S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	A5	223	Total	C	N	O	S	0	0
			1879	1211	357	306	5		

- Molecule 69 is a protein called 60S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AD	247	Total	C	N	O	S	0	0
			1867	1166	374	318	9		

- Molecule 70 is a protein called 60S ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AE	380	Total	C	N	O	S	0	0
			3062	1948	575	522	17		

- Molecule 71 is a protein called 60S ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AF	390	Total	C	N	O	S	0	0
			3095	1962	594	528	11		

- Molecule 72 is a protein called 60S ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AG	124	Total	C	N	O	S	0	0
			1011	636	197	172	6		

- Molecule 73 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AU	180	Total	C	N	O	S	0	0
			1497	946	289	255	7		

- Molecule 74 is a protein called 60S ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AH	185	Total	C	N	O	S	0	0
			1476	950	264	256	6		

- Molecule 75 is a protein called 60S ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AV	155	Total	C	N	O	S	0	0
			1276	814	241	215	6		

- Molecule 76 is a protein called 60S ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Ag	37	Total	C	N	O	S	0	0
			343	210	86	45	2		

- Molecule 77 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AX	97	Total	C	N	O	S	0	0
			825	548	135	140	2		

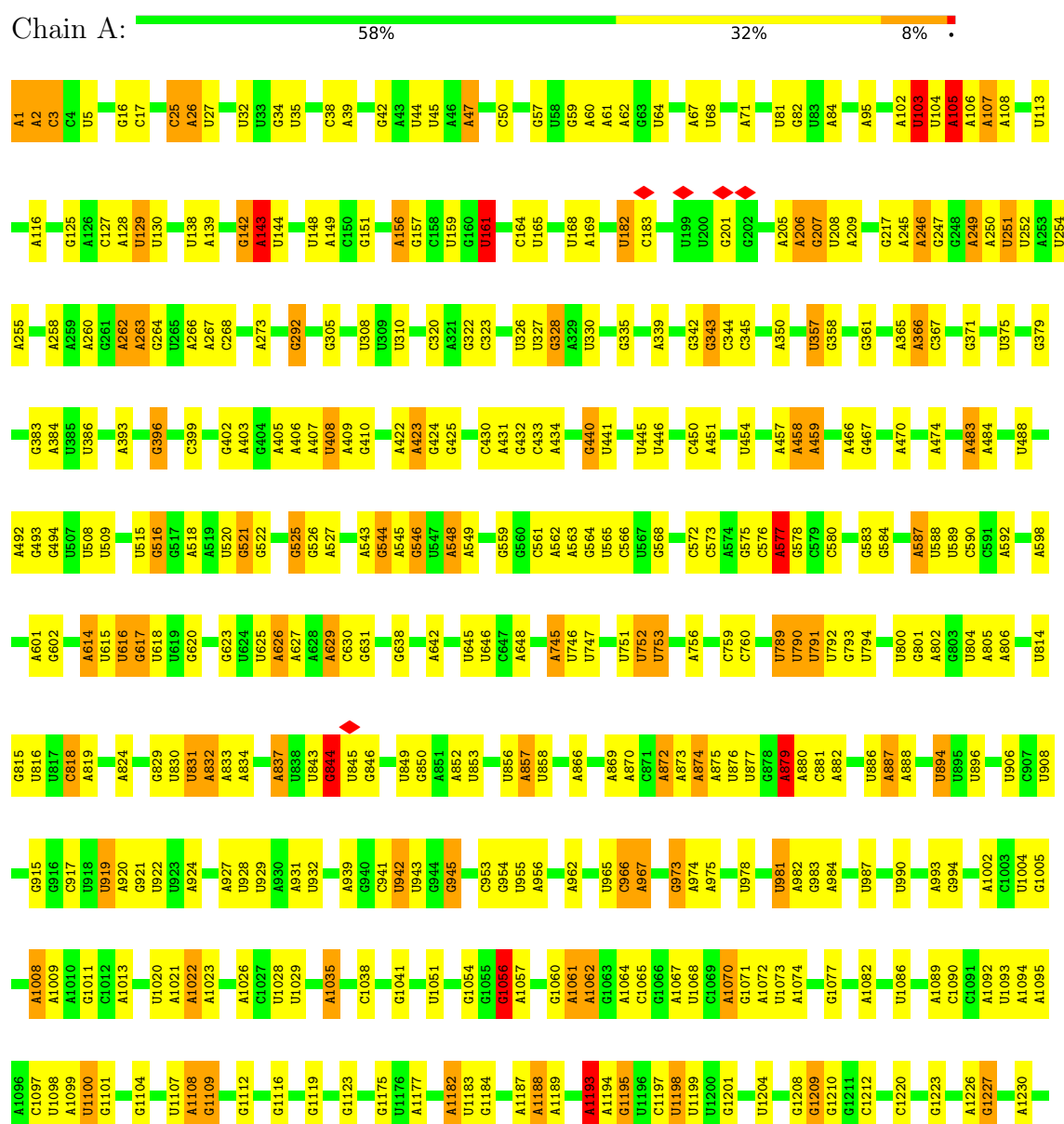
- Molecule 78 is a protein called 60S ribosomal protein eL8.

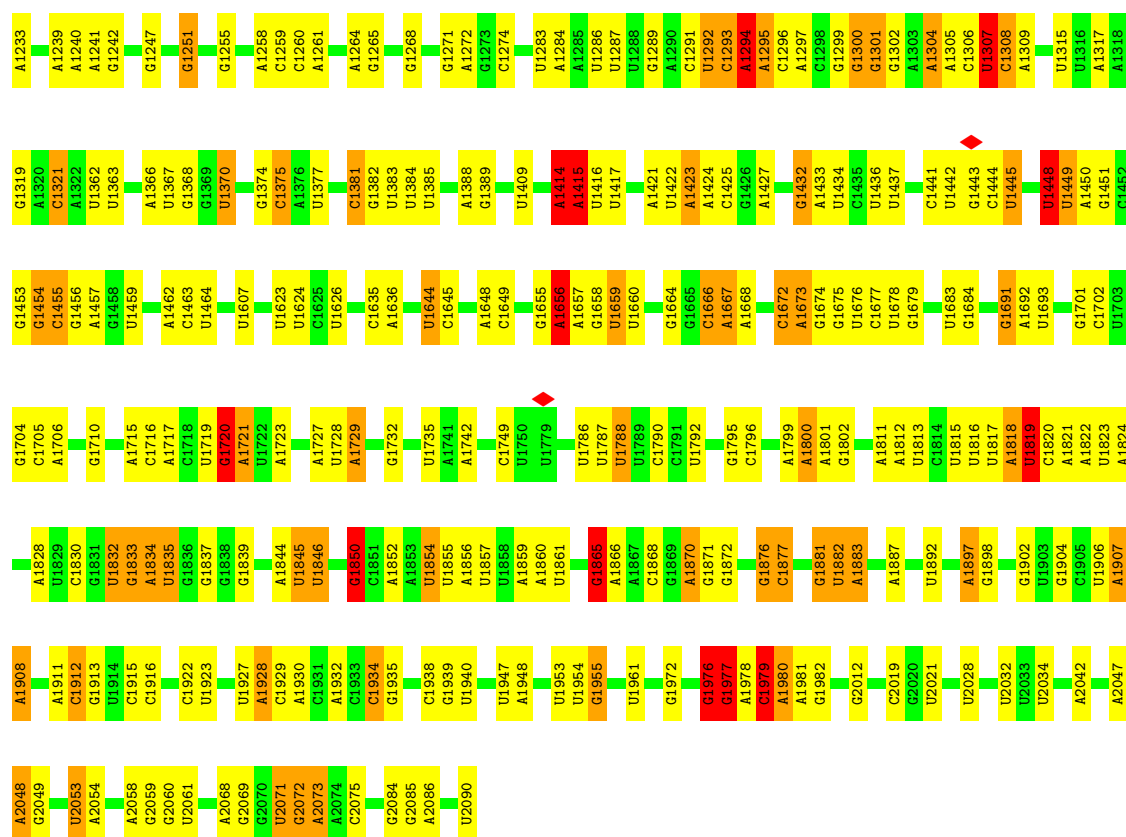
Mol	Chain	Residues	Atoms					AltConf	Trace
78	AJ	222	Total	C	N	O	S	0	0
			1813	1174	323	309	7		

3 Residue-property plots

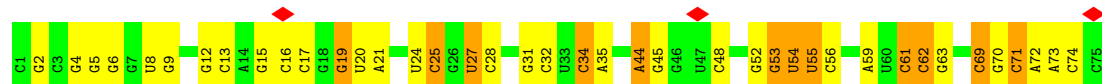
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 18S ribosomal RNA

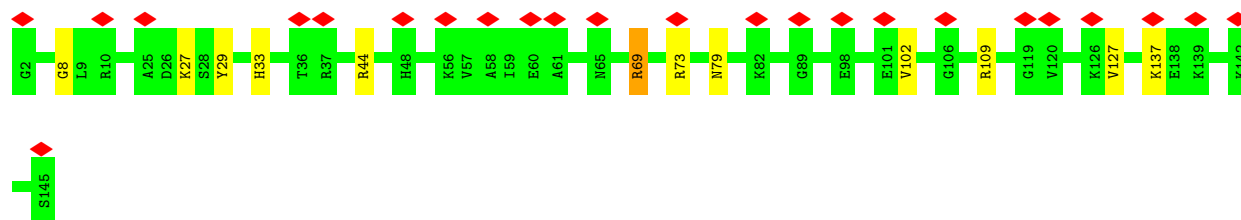
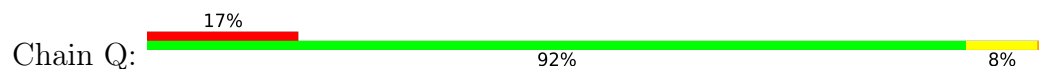




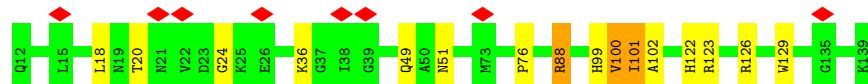
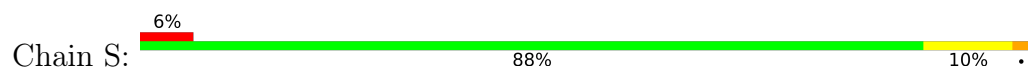
• Molecule 2: P/E-tRNA



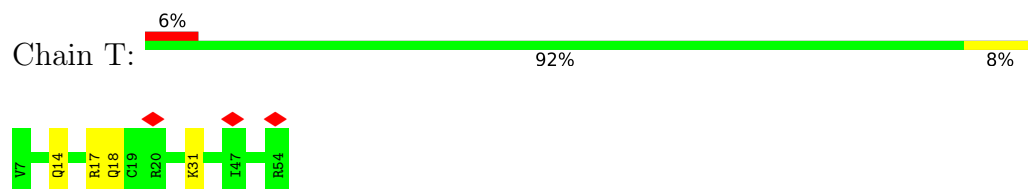
• Molecule 3: 40S ribosomal protein uS12



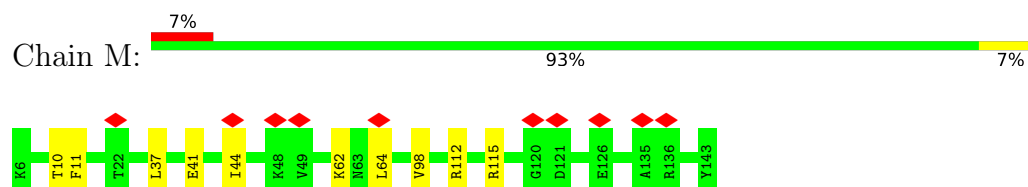
• Molecule 4: 40S ribosomal protein uS13



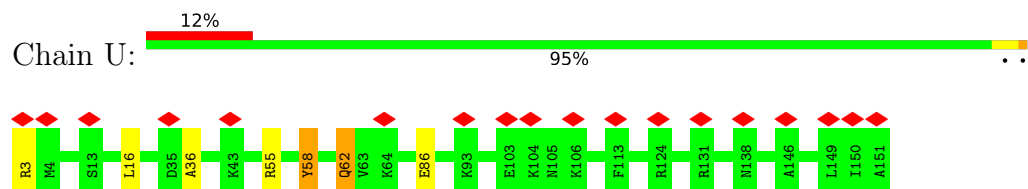
- Molecule 5: 40S ribosomal protein uS14



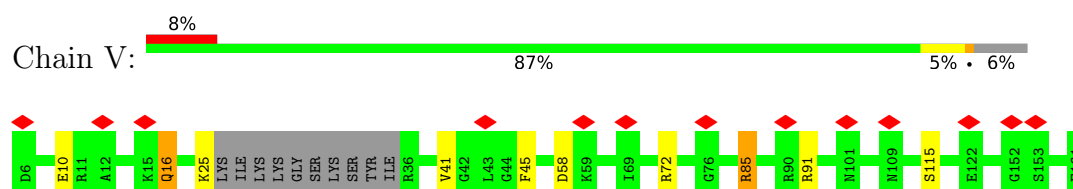
- Molecule 6: 40S ribosomal protein uS9



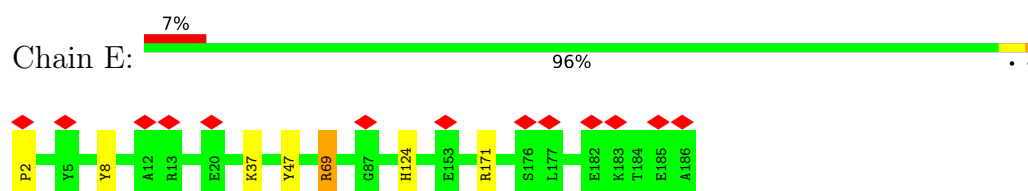
- Molecule 7: 40S ribosomal protein uS15



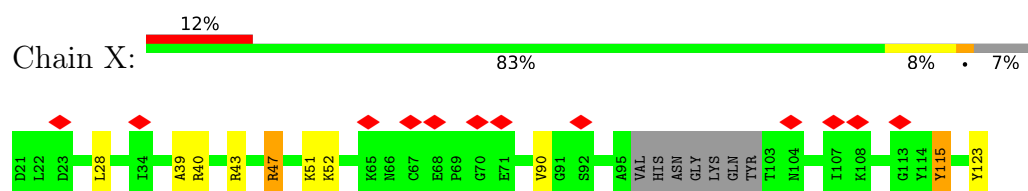
- Molecule 8: 40S ribosomal protein uS17



- Molecule 9: 40S ribosomal protein uS4

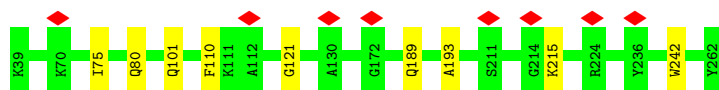


- Molecule 10: 40S ribosomal protein uS19

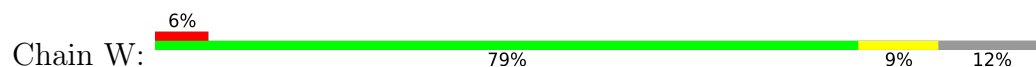


- Molecule 11: 40S ribosomal protein uS5

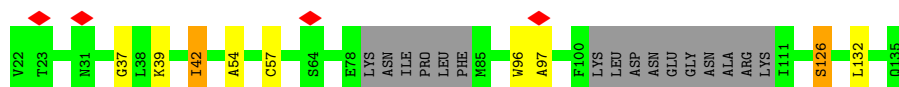
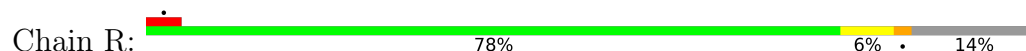




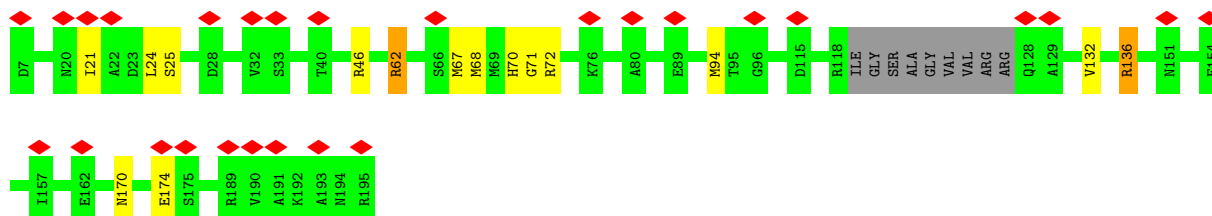
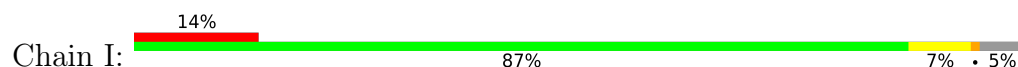
- Molecule 12: 40S ribosomal protein eS17



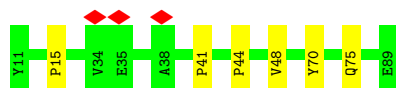
- Molecule 13: 40S ribosomal protein eS12



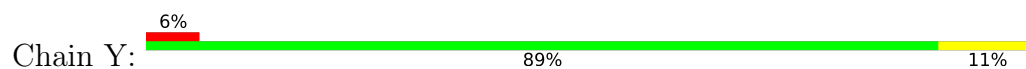
- Molecule 14: 40S ribosomal protein uS7



- Molecule 15: 40S ribosomal protein eS10

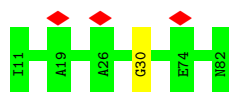


- Molecule 16: 40S ribosomal protein eS19

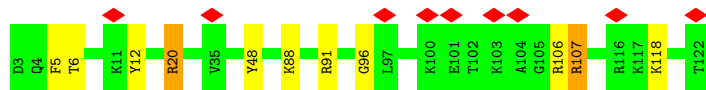
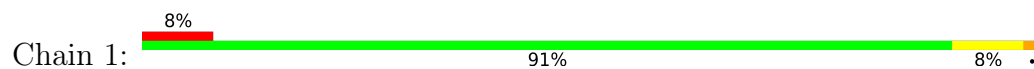


- Molecule 17: 40S ribosomal protein eS21

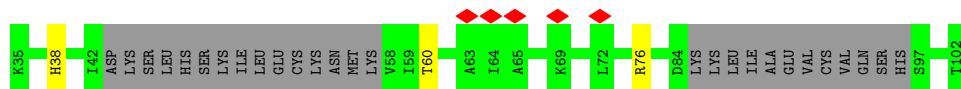




- Molecule 18: 40S ribosomal protein eS24



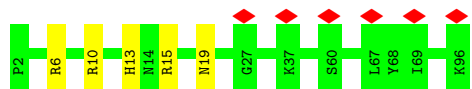
- Molecule 19: 40S ribosomal protein eS25



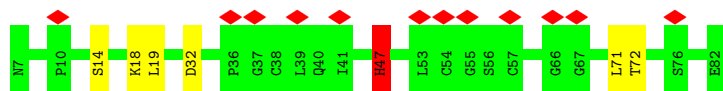
- Molecule 20: 40S ribosomal protein uS2



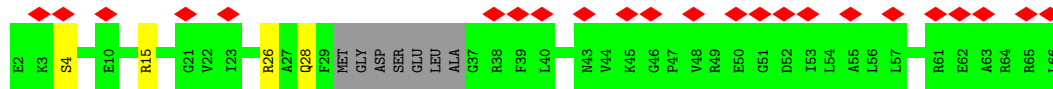
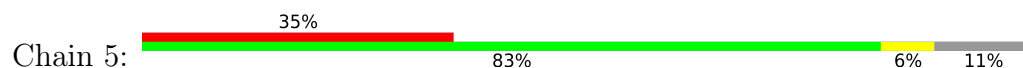
- Molecule 21: 40S ribosomal protein eS26



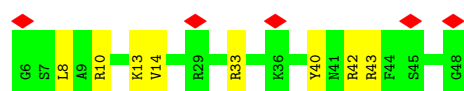
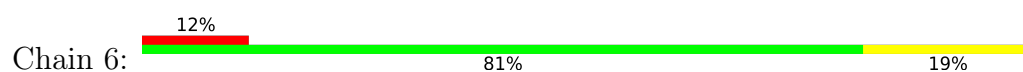
- Molecule 22: 40S ribosomal protein eS27



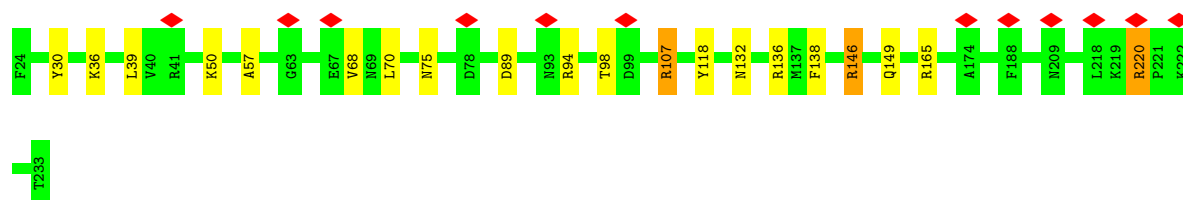
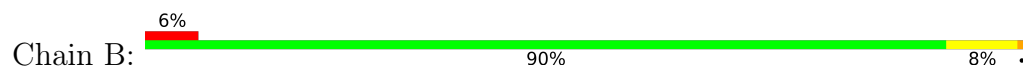
- Molecule 23: 40S ribosomal protein eS28



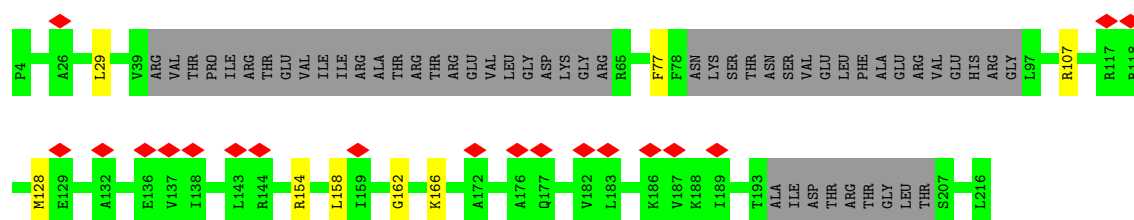
- Molecule 24: 40S ribosomal protein eS30



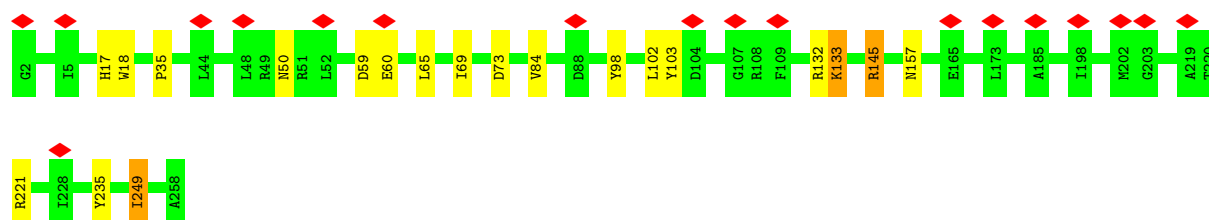
- Molecule 25: 40S ribosomal protein eS1



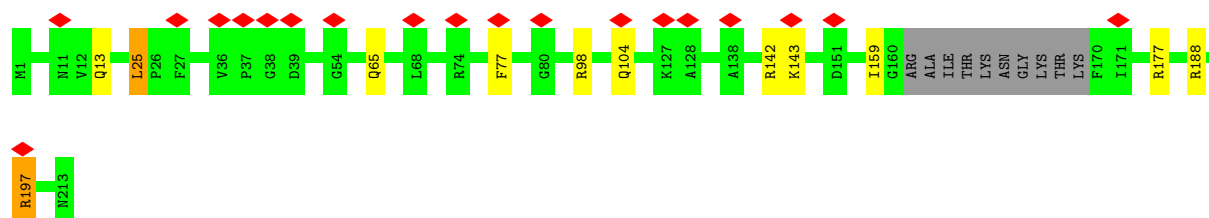
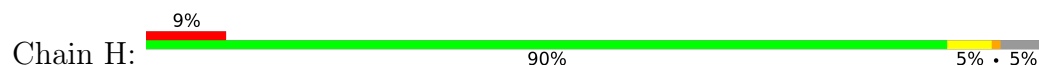
- Molecule 26: 40S ribosomal protein uS3



- Molecule 27: 40S ribosomal protein eS4



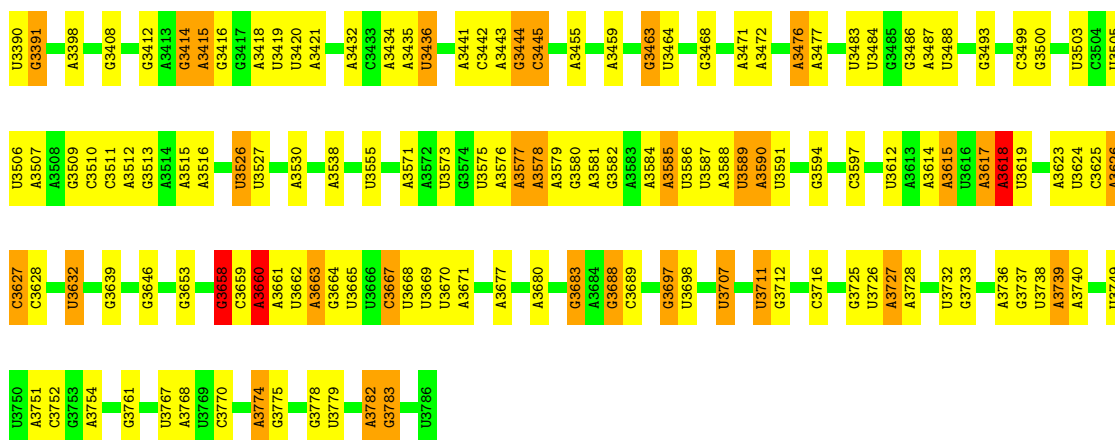
- Molecule 28: 40S ribosomal protein eS6



- | | |
|------|------|
| G10 | A11 | U12 | G13 | U14 | U15 | A16 | G17 | G18 | A19 | G20 | A25 | A26 | G30 | G31 | G32 | A33 | A34 | A35 | U36 | U37 | A38 | A39 | A40 | A41 | G42 | A43 | U44 | A45 | U46 | U49 | C54 | G55 | G56 | A57 | A58 | G59 | A60 | A61 | A62 | A63 | G64 | A65 | A66 | U69 | A70 | A71 | G72 | U73 | A74 | U75 | G76 | U83 | A84 | A85 | G86 | A87 | A88 | G89 | A90 | A91 | A92 | A93 | A94 | A95 | A96 | A97 | A98 | A99 | G100 | A101 | A102 | A103 | A104 | A105 | A106 | A107 | A108 | A109 | A110 | A111 | A112 | A113 | A114 | A115 | A116 | A117 | A118 | A119 | A120 | A121 | A122 | A123 | A124 | A125 | A126 | A127 | A128 | A129 | A130 | A131 | A132 | A133 | A134 | A135 | A136 | A137 | A138 | A139 | A140 | A141 | A142 | A143 | A144 | A145 | A146 | A147 | A148 | A149 | A150 | A151 | A152 | A153 | A154 | A155 | A156 | A157 | A158 | A159 | A160 | A161 | A162 | A163 | A164 | A165 | A166 | A167 | A168 | A169 | A170 | A171 | A172 | A173 | A174 | A175 | A176 | A177 | A178 | A179 | A180 | A181 | A182 | A183 | A184 | A185 | A186 | A187 | A188 | A189 | A190 | A191 | A192 | A193 | A194 | A195 | A196 | A197 | A198 | A199 | A200 | A201 | A202 | A203 | A204 | A205 | A206 | A207 | A208 | A209 | A210 | A211 | A212 | A213 | A214 | A215 | A216 | A217 | A218 | A219 | A220 | A221 | A222 | A223 | A224 | A225 | A226 | A227 | A228 | A229 | A230 | A231 | A232 | A233 | A234 | A235 | A236 | A237 | A238 | A239 | A240 | A241 | A242 | A243 | A244 | A245 | A246 | A247 | A248 | A249 | A250 | A251 | A252 | A253 | A254 | A255 | A256 | A257 | A258 | A259 | A260 | A261 | A262 | A263 | A264 | A265 | A266 | A267 | A268 | A269 | A270 | A271 | A272 | A273 | A274 | A275 | A276 | A277 | A278 | A279 | A280 | A281 | A282 | A283 | A284 | A285 | A286 | A287 | A288 | A289 | A290 | A291 | A292 | A293 | A294 | A295 | A296 | A297 | A298 | A299 | A300 | A301 | A302 | A303 | A304 | A305 | A306 | A307 | A308 | A309 | A310 | A311 | A312 | A313 | A314 | A315 | A316 | A317 | A318 | A319 | A320 | A321 | A322 | A323 | A324 | A325 | A326 | A327 | A328 | A329 | A330 | A331 | A332 | A333 | A334 | A335 | A336 | A337 | A338 | A339 | A340 | A341 | A342 | A343 | A344 | A345 | A346 | A347 | A348 | A349 | A350 | A351 | A352 | A353 | A354 | A355 | A356 | A357 | A358 | A359 | A360 | A361 | A362 | A363 | A364 | A365 | A366 | A367 | A368 | A369 | A370 | A371 | A372 | A373 | A374 | A375 | A376 | A377 | A378 | A379 | A380 | A381 | A382 | A383 | A384 | A385 | A386 | A387 | A388 | A389 | A390 | A391 | A392 | A393 | A394 | A395 | A396 | A397 | A398 | A399 | A400 | A401 | A402 | A403 | A404 | A405 | A406 | A407 | A408 | A409 | A410 | A411 | A412 | A413 | A414 | A415 | A416 | A417 | A418 | A419 | A420 | A421 | A422 | A423 | A424 | A425 | A426 | A427 | A428 | A429 | A430 | A431 | A432 | A433 | A434 | A435 | A436 | A437 | A438 | A439 | A440 | A441 | A442 | A443 | A444 | A445 | A446 | A447 | A448 | A449 | A450 | A451 | A452 | A453 | A454 | A455 | A456 | A457 | A458 | A459 | A460 | A461 | A462 | A463 | A464 | A465 | A466 | A467 | A468 | A469 | A470 | A471 | A472 | A473 | A474 | A475 | A476 | A477 | A478 | A479 | A480 | A481 | A482 | A483 | A484 | A485 | A486 | A487 | A488 | A489 | A490 | A491 | A492 | A493 | A494 | A495 | A496 | A497 | A498 | A499 | A500 | A501 | A502 | A503 | A504 | A505 | A506 | A507 | A508 | A509 | A510 | A511 | A512 | A513 | A514 | A515 | A516 | A517 | A518 | A519 | A520 | A521 | A522 | A523 | A524 | A525 | A526 | A527 | A528 | A529 | A530 | A531 | A532 | A533 | A534 | A535 | A536 | A537 | A538 | A539 | A540 | A541 | A542 | A543 | A544 | A545 | A546 | A547 | A548 |
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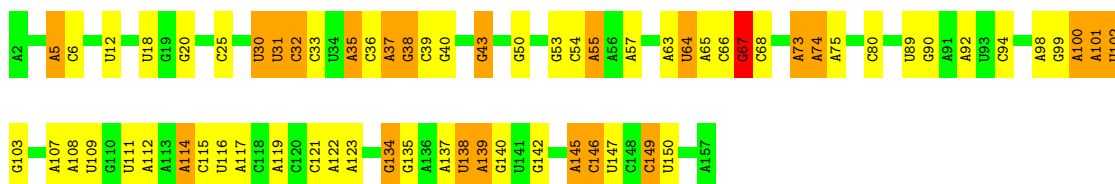
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A1468	U1210	U1109	U1209	U1110	U1013	G915	A799	C621	U530	G435	U336	U254	A168	U87
U1459	U1211	G1111	U1211	A1111	C1014	U916	A800	U622	U531	G436	U337	U255	U173	A88
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A1479	U1218	G1121	C1218	G1121	U1121	G924	A809	U636	A542	A447	G349	U264	A185	A109
G1480	U1219	A1122	G1026	U1122	G1026	G925	U810	U637	U543	A448	G353	U265	A186	G110
A1481	U1223	A1124	G1028	U1123	G1028	A926	A811	U641	U544	A449	C268	U266	U189	C111
A1486	U1224	A1125	G1031	U1124	G1031	A927	U812	U642	C544	A450	C354	U267	G190	U112
U1497	A1225	A1032	G1032	A1128	A1032	G934	C821	G643	C545	A451	A355	U270	A191	C113
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C1506	U1232	C1042	U1232	G1141	C1042	G941	U834	U648	U574	G462	U367	U278	U198	A122
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G1516	A1240	U1063	A1240	G1159	U1063	A951	C859	A652	C579	A488	G379	U281	G201	G130
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U1534	G1244	U1065	G1244	G1161	U1065	A955	U869	U658	C582	U492	A382	U283	A206	U132
G1535	U1255	U1066	U1255	G1170	U1066	A956	A874	U665	C592	U493	A383	U284	A207	U133
U1536	U1256	U1067	U1256	G1171	U1067	G964	A880	U666	A593	U494	A384	U285	G214	G136
U1538	A1257	U1068	A1257	G1172	U1068	A965	A884	U667	C594	U495	A385	U286	C215	G138
G1540	U1258	U1069	U1258	G1173	U1069	A966	A885	U668	C595	U496	A386	U287	C216	A139
U1549	G1259	U1070	G1259	G1174	U1070	A967	U888	U669	A500	U497	C386	U288	A217	A140
A1550	U1263	U1071	A1263	G1184	U1071	G968	A889	U670	A501	U498	G387	U289	U218	A141
G1552	A1264	U1072	A1264	G1185	U1072	A969	U890	U671	A502	U499	A388	U290	A219	C142
U1556	U1272	U1073	U1272	G1186	U1073	G976	U893	U672	A503	U500	G389	U291	G220	G143
U1560	G1273	U1074	G1273	G1187	U1074	A970	U894	U673	A504	U501	A390	U292	U144	U145
U1563	A1274	U1075	A1274	G1188	U1075	A971	U895	U674	A505	U502	A391	U293	U146	U147
G1564	U1278	U1076	U1278	G1189	U1076	A972	U896	U675	A506	U503	A392	U294	A229	A149
U1565	A1279	U1077	A1279	G1190	U1077	A973	U897	U676	A507	U504	A393	U295	G230	G152
A1567	U1280	U1078	U1280	G1191	U1078	A974	U898	U677	A508	U505	A394	U296	G231	A153
C1568	C1281	U1079	C1281	G1192	U1079	A975	U899	U678	A509	U506	A395	U297	A235	A154
U1571	U1282	U1080	U1282	G1193	U1080	A976	U900	U679	A606	U507	A396	U298	U240	U155
U1577	C1283	U1081	C1283	G1194	U1081	A977	U901	U680	A607	U508	A397	U299	C241	G157
C1578	U1284	U1082	U1284	G1195	U1082	A978	U902	U681	A608	U509	A398	U300	U242	U162
U1580	A1285	U1083	A1285	G1196	U1083	A979	U903	U682	A609	U510	A399	U301	U246	G163
U1583	U1286	U1084	U1286	G1197	U1084	A980	U904	U683	A610	U511	A400	U302	U247	A164
G1584	C1286	U1085	C1286	G1198	U1085	A981	U905	U684	A611	U512	A401	U303	U248	A165
U1587	U1287	U1086	U1287	G1199	U1086	A982	U906	U685	A612	U513	A402	U304	U249	
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U1633	A1304	U1104	A1304	G1217	U1104	A1000	U924	U703	A630	U531	A420	U322	U267	
U1636	U1305	U1105	U1305	G1218	U1105	A1001	U925	U704	A631	U532	A421	U323	U268	
U1639	A1306	U1106	A1306	G1219	U1106	A1002	U926	U705	A632	U533	A422	U324	U269	
U1642	U1307	U1107	U1307	G1220	U1107	A1003	U927	U706	A633	U534	A423	U325	U270	
U1645	A1308	U1108	A1308	G1221	U1108	A1004	U928	U707	A634	U535	A424	U326	U271	
U1648	U1309	U1109	U1309	G1222	U1109	A1005	U929	U708	A635	U536	A425	U327	U272	
U1651	A1310	U1110	A1310	G1223	U1110	A1006	U930	U709	A636	U537	A426	U328	U273	
U1654	U1311	U1111	U1311	G1224	U1111	A1007	U931	U710	A637	U538	A427	U329	U274	
U1657	A1312	U1112	A1312	G1225	U1112	A1008	U932	U711	A638	U539	A428	U330	U275	
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U1666	U1315	U1115	U1315	G1228	U1115	A1011	U935	U714	A641	U542	A431	U333	U278	
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U1672	U1317	U1117	U1317	G1230	U1117	A1013	U937	U716	A643	U544	A433	U335	U280	
U1675	A1318	U1118	A1318	G1231	U1118	A1014	U938	U717	A644	U545	A434	U336	U281	
U1678	U1319	U1119	U1319	G1232	U1119	A1015	U939	U718	A645	U546	A435	U337	U282	
U1681	A1320	U1120	A1320	G1233	U1120	A1016	U940	U719	A646	U547	A436	U338	U283	
U1684	U1321	U1121	U1321	G1234	U1121	A1017	U941	U720	A647	U548	A437	U339	U284	
U1687	A1322	U1122	A1322	G1235	U1122	A1018	U942	U721	A648	U549	A438	U340	U285	
U1690	U1323	U1123	U1323	G1236	U1123	A1019	U943	U722	A649	U550	A439	U341	U286	
U1693	A1324	U1124	A1324	G1237	U1124	A1020	U944	U723	A650	U551	A440	U342	U287	
U1696	U1325	U1125	U1325	G1238	U1125	A1021	U945	U724	A651	U552	A441	U343	U288	
U1699	A1326	U1126	A1326	G1239	U1126	A1022	U946	U725	A652	U553	A442	U344	U289	
U1702	U1327	U1127	U1327	G1240	U1127	A1023	U947	U726	A653	U554	A443	U345	U290	
U1705	A1328	U1128	A1328	G1241	U1128	A1024	U948	U727	A654	U555	A444	U346	U291	
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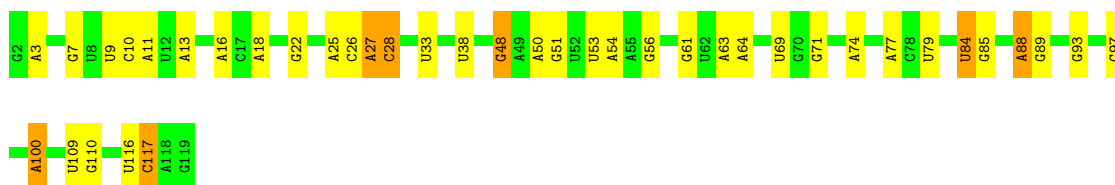
• Molecule 35: 5.8S ribosomal RNA

Chain AC: 56% 29% 15%



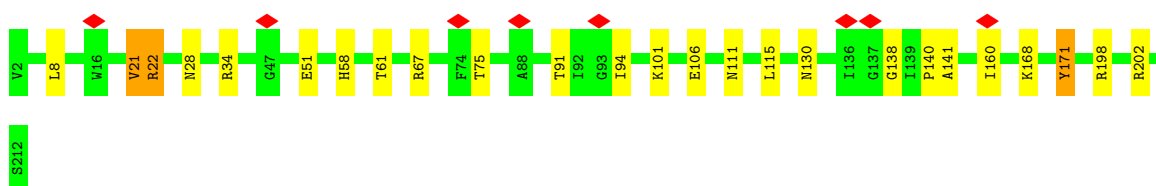
• Molecule 36: 5S ribosomal RNA

Chain AB: 66% 28% 6%



• Molecule 37: 60S ribosomal protein eL13

Chain AL: 88% 10%

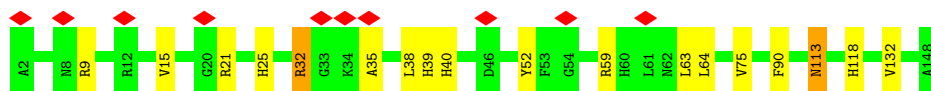
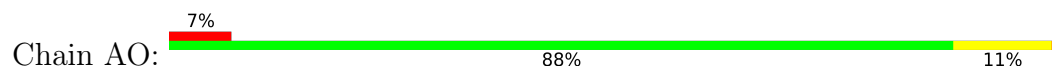


• Molecule 38: 60S ribosomal protein eL24

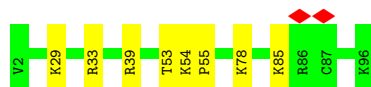
Chain A0: 6% 92% 8%



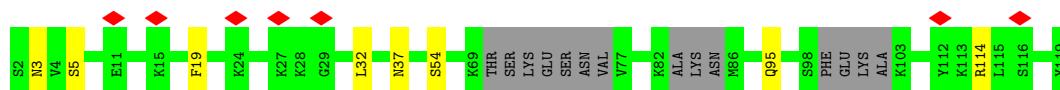
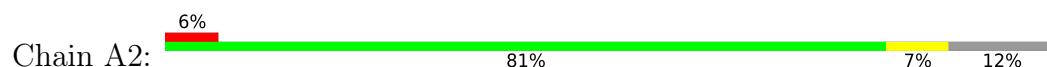
- Molecule 39: 60S ribosomal protein uL15



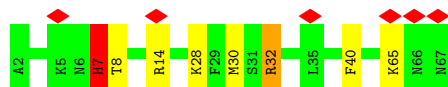
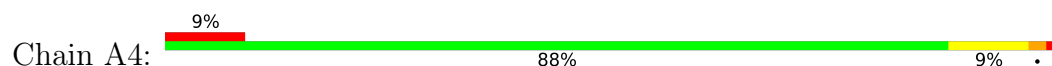
- Molecule 40: 60S ribosomal protein eL44



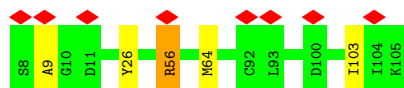
- Molecule 41: 60S ribosomal protein eL28



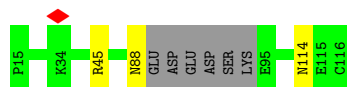
- Molecule 42: 60S ribosomal protein eL29



- Molecule 43: 60S ribosomal protein eL30

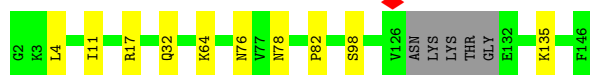


- Molecule 44: 60S ribosomal protein eL31



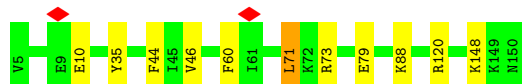
- Molecule 45: 60S ribosomal protein eL27

Chain A1:  90% 7%

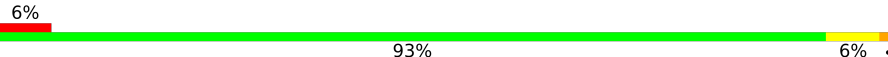


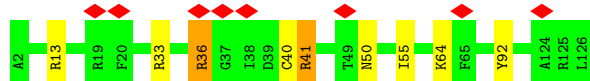
- Molecule 46: 60S ribosomal protein eL14

Chain AN:  92% 7%



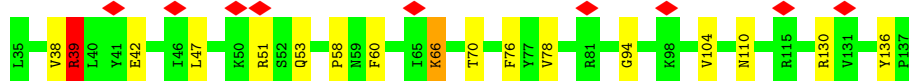
- Molecule 47: 60S ribosomal protein eL32

Chain A8:  6% 93% 6%



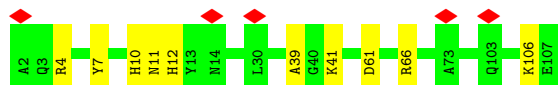
- Molecule 48: 60S ribosomal protein eL33

Chain A9:  9% 83% 15%



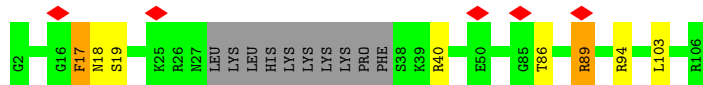
- Molecule 49: 60S ribosomal protein eL34

Chain Aa:  5% 91% 9%



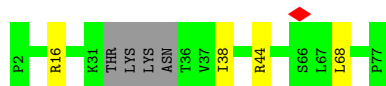
- Molecule 50: 60S ribosomal protein eL36

Chain Ab:  5% 83% 6% 10%

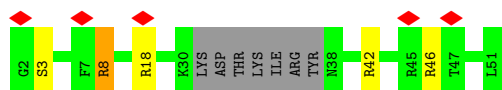
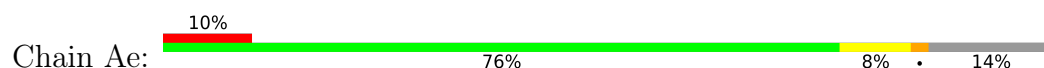


- Molecule 51: 60S ribosomal protein eL38

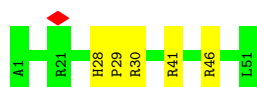
Chain Ad:  89% 5% 5%



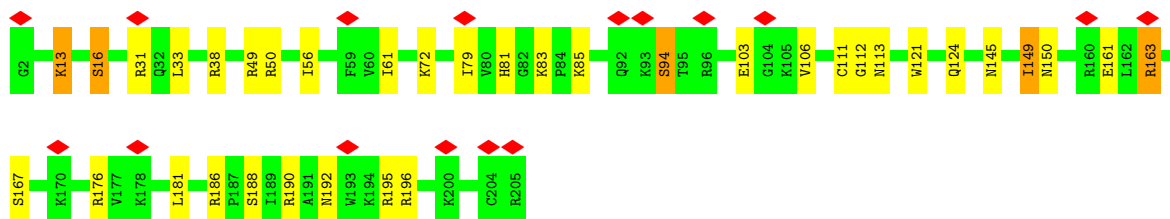
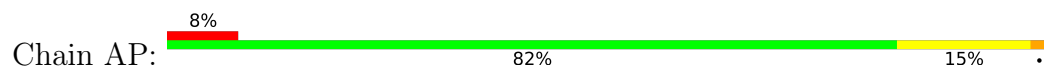
- Molecule 52: 60S ribosomal protein eL39



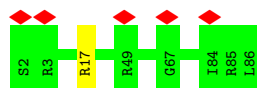
- Molecule 53: 60S ribosomal protein eL40



- Molecule 54: 60S ribosomal protein eL15



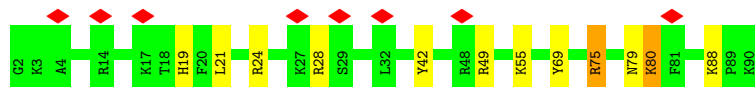
- Molecule 55: 60S ribosomal protein eL43



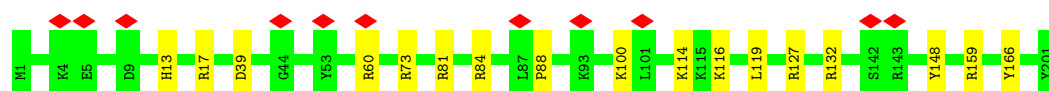
- Molecule 56: 60S ribosomal protein eL6



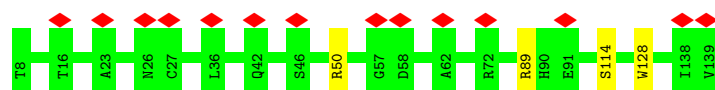
- Molecule 57: 60S ribosomal protein eL37



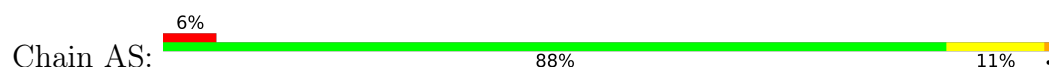
- Molecule 58: 60S ribosomal protein uL13



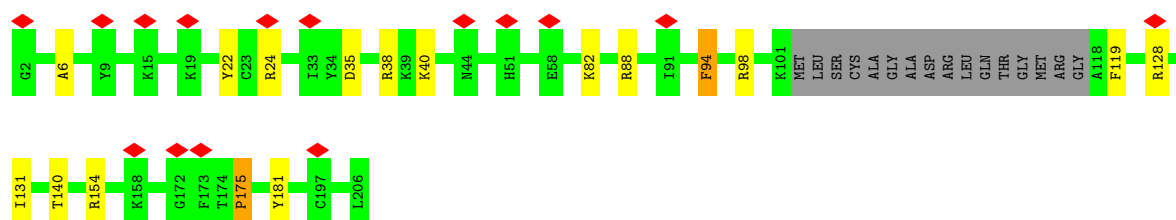
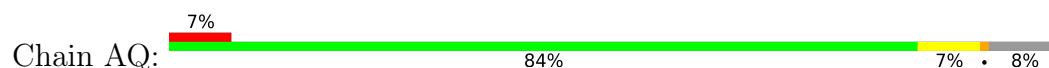
- Molecule 59: 60S ribosomal protein uL14



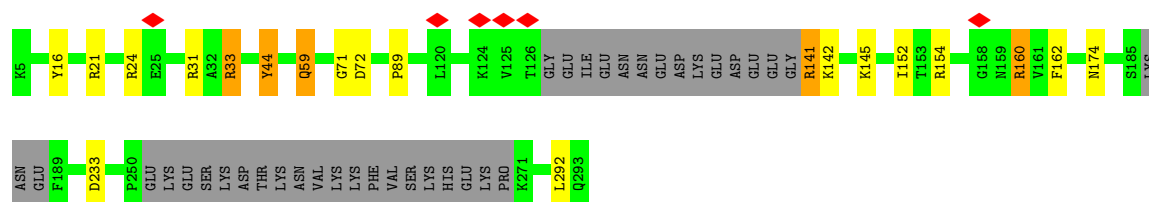
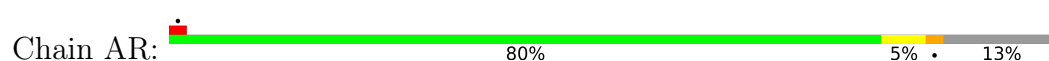
- Molecule 60: 60S ribosomal protein eL18



- Molecule 61: 60S ribosomal protein uL16



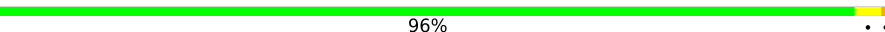
- Molecule 62: 60S ribosomal protein uL18

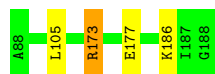


- Molecule 63: 60S ribosomal protein uL22

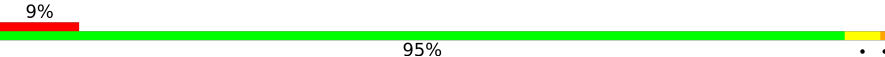


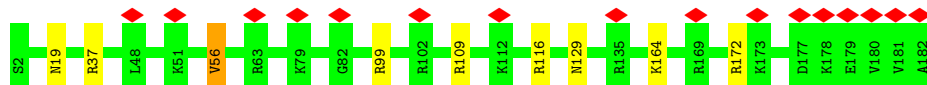
- Molecule 64: 60S ribosomal protein uL23

Chain AY:  96% ..

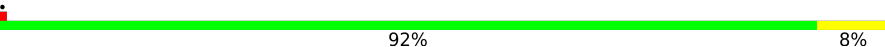


- Molecule 65: 60S ribosomal protein eL19

Chain AT:  95% ..



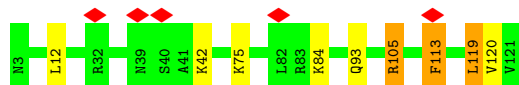
- Molecule 66: 60S ribosomal protein uL24

Chain AZ:  92% 8%

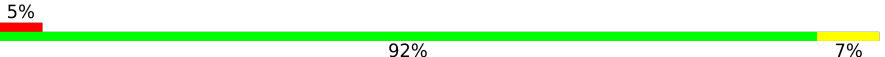


- Molecule 67: 60S ribosomal protein uL29

Chain A3:  92% 5%

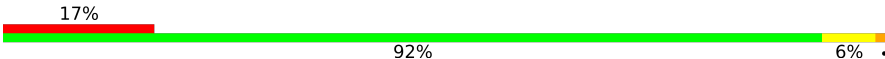


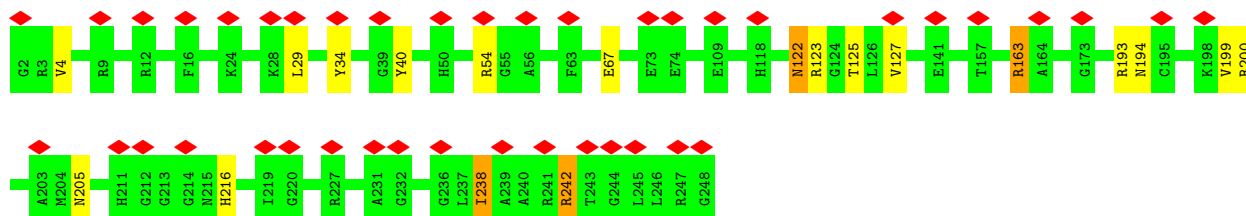
- Molecule 68: 60S ribosomal protein uL30

Chain A5:  92% 7%

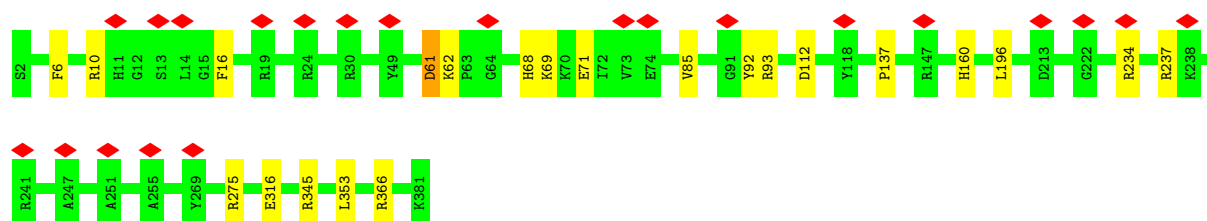


- Molecule 69: 60S ribosomal protein uL2

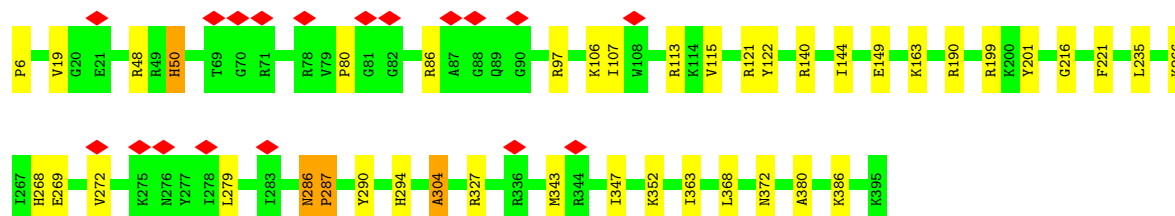
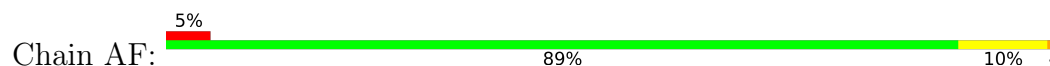
Chain AD:  92% 6%



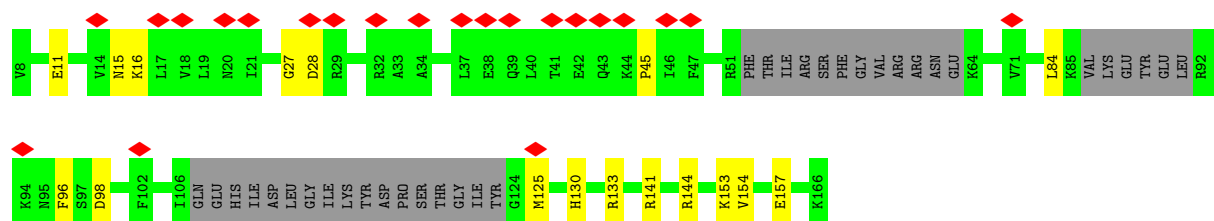
- Molecule 70: 60S ribosomal protein uL3



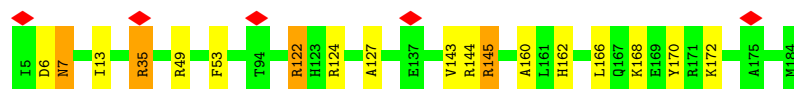
- Molecule 71: 60S ribosomal protein uL4



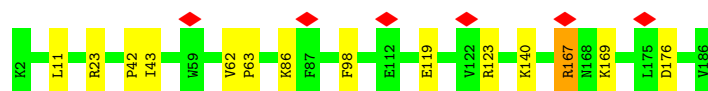
- Molecule 72: 60S ribosomal protein uL5



- Molecule 73: 60S ribosomal protein eL20



- Molecule 74: 60S ribosomal protein uL6

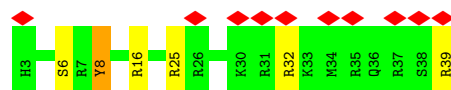
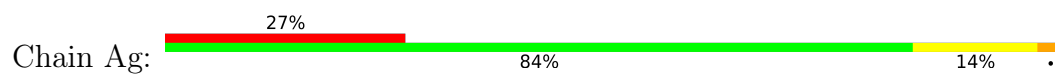


- Molecule 75: 60S ribosomal protein eL21





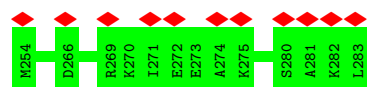
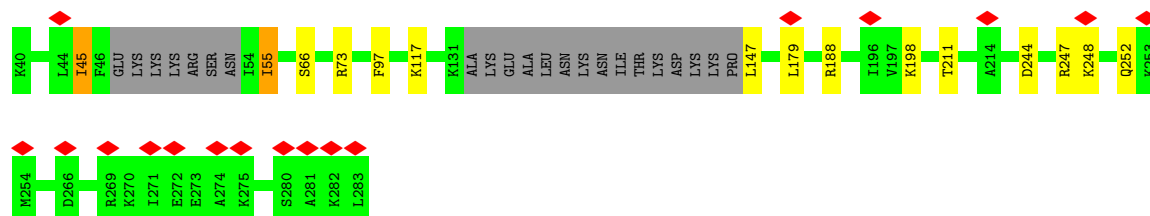
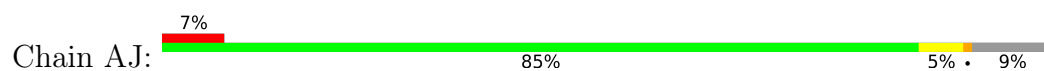
- Molecule 76: 60S ribosomal protein eL41



- Molecule 77: 60S ribosomal protein eL22



- Molecule 78: 60S ribosomal protein eL8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22793	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	30120	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	491.36, 491.36, 491.36	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.66, 1.66, 1.66	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	A	0.95	0/38275	1.12	124/59596 (0.2%)
2	7	0.97	0/1785	1.25	16/2782 (0.6%)
3	Q	0.85	0/1149	1.46	1/1532 (0.1%)
4	S	0.87	0/1063	1.63	6/1425 (0.4%)
5	T	0.94	0/412	1.46	1/544 (0.2%)
6	M	0.83	0/1114	1.48	5/1487 (0.3%)
7	U	0.81	0/1223	1.56	4/1634 (0.2%)
8	V	0.86	0/1233	1.40	1/1645 (0.1%)
9	E	0.85	0/1539	1.53	1/2055 (0.0%)
10	X	0.84	0/788	1.61	5/1050 (0.5%)
11	G	0.80	0/1800	1.48	3/2429 (0.1%)
12	W	0.86	0/793	1.59	8/1053 (0.8%)
13	R	0.89	0/755	1.65	8/1013 (0.8%)
14	I	0.86	0/1443	1.56	8/1936 (0.4%)
15	O	0.86	0/706	1.47	1/950 (0.1%)
16	Y	0.85	0/1295	1.59	8/1742 (0.5%)
17	Z	0.83	0/565	1.42	0/758
18	1	0.85	0/999	1.48	4/1321 (0.3%)
19	2	0.93	0/324	1.53	0/435
20	C	0.82	0/1570	1.54	10/2129 (0.5%)
21	3	0.93	0/794	1.51	2/1055 (0.2%)
22	4	0.81	0/597	1.45	3/801 (0.4%)
23	5	0.87	0/459	1.30	1/606 (0.2%)
24	6	0.88	0/349	1.72	6/458 (1.3%)
25	B	0.82	0/1738	1.49	11/2321 (0.5%)
26	D	0.89	0/1241	1.44	4/1652 (0.2%)
27	F	0.84	0/2098	1.48	4/2819 (0.1%)
28	H	0.83	0/1665	1.47	9/2210 (0.4%)
29	K	0.86	0/1054	1.50	3/1411 (0.2%)
30	J	0.82	0/1545	1.46	6/2064 (0.3%)
31	N	0.84	0/780	1.53	4/1053 (0.4%)
32	P	0.87	0/966	1.56	6/1295 (0.5%)
33	L	0.86	0/1407	1.43	5/1879 (0.3%)
34	AA	0.96	7/75922 (0.0%)	1.12	262/118216 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	AC	0.93	0/3599	1.16	20/5603 (0.4%)
36	AB	0.95	0/2823	1.06	6/4400 (0.1%)
37	AL	0.84	0/1789	1.57	8/2381 (0.3%)
38	A0	0.83	0/534	1.48	4/711 (0.6%)
39	AO	0.85	0/1199	1.58	15/1597 (0.9%)
40	Ai	0.81	0/789	1.39	2/1032 (0.2%)
41	A2	0.86	0/840	1.46	4/1114 (0.4%)
42	A4	0.86	0/564	1.71	6/737 (0.8%)
43	A6	0.85	0/749	1.53	2/1001 (0.2%)
44	A7	0.88	0/806	1.47	1/1073 (0.1%)
45	A1	0.82	0/1151	1.45	8/1531 (0.5%)
46	AN	0.81	0/1218	1.45	5/1621 (0.3%)
47	A8	0.85	0/1054	1.53	5/1399 (0.4%)
48	A9	0.86	0/865	1.50	9/1160 (0.8%)
49	Aa	0.86	0/872	1.54	6/1161 (0.5%)
50	Ab	0.88	0/763	1.53	2/1008 (0.2%)
51	Ad	0.84	0/612	1.45	0/812
52	Ae	0.96	0/396	1.64	3/521 (0.6%)
53	Af	0.83	0/419	1.45	0/556
54	AP	0.89	0/1735	1.62	20/2320 (0.9%)
55	Ah	0.83	0/668	1.46	0/887
56	AI	0.81	0/1708	1.56	12/2274 (0.5%)
57	Ac	0.87	0/723	1.62	11/951 (1.2%)
58	AK	0.84	0/1690	1.48	3/2260 (0.1%)
59	AM	0.81	0/1012	1.42	3/1363 (0.2%)
60	AS	0.86	0/1531	1.49	12/2040 (0.6%)
61	AQ	0.86	0/1580	1.48	4/2113 (0.2%)
62	AR	0.85	0/2079	1.53	7/2777 (0.3%)
63	AW	0.87	0/1244	1.49	2/1663 (0.1%)
64	AY	0.81	0/806	1.41	1/1074 (0.1%)
65	AT	0.85	0/1525	1.56	8/2016 (0.4%)
66	AZ	0.86	0/1013	1.49	2/1339 (0.1%)
67	A3	0.83	0/1005	1.60	7/1329 (0.5%)
68	A5	0.86	0/1917	1.53	7/2562 (0.3%)
69	AD	0.85	0/1902	1.48	7/2544 (0.3%)
70	AE	0.83	0/3130	1.50	8/4195 (0.2%)
71	AF	0.85	0/3145	1.55	23/4205 (0.5%)
72	AG	0.90	0/1021	1.63	11/1349 (0.8%)
73	AU	0.85	0/1527	1.51	12/2043 (0.6%)
74	AH	0.82	0/1501	1.52	10/2025 (0.5%)
75	AV	0.83	0/1301	1.52	5/1732 (0.3%)
76	Ag	1.01	0/348	1.66	3/448 (0.7%)
77	AX	0.81	0/842	1.46	5/1125 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
78	AJ	1.19	1/1840 (0.1%)	1.57	7/2456 (0.3%)
All	All	0.92	8/207281 (0.0%)	1.28	836/303864 (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
1	A	0	141
2	7	1	5
3	Q	0	4
5	T	0	1
6	M	0	2
7	U	0	1
8	V	0	3
9	E	0	3
10	X	0	2
12	W	0	3
14	I	0	3
16	Y	0	2
18	1	0	3
19	2	0	1
21	3	0	2
23	5	0	1
24	6	0	4
25	B	1	4
27	F	0	4
28	H	0	4
29	K	0	1
32	P	0	5
33	L	0	2
34	AA	1	328
35	AC	0	13
36	AB	0	8
37	AL	0	7
38	A0	0	1
39	AO	0	1
40	Ai	0	3
41	A2	2	0
42	A4	0	5
43	A6	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
44	A7	0	1
46	AN	0	3
47	A8	0	3
48	A9	0	3
49	Aa	0	2
50	Ab	0	3
51	Ad	0	2
52	Ae	0	2
53	Af	0	2
54	AP	0	7
55	Ah	0	1
56	AI	0	2
57	Ac	0	3
58	AK	0	8
60	AS	0	9
61	AQ	0	6
62	AR	0	7
63	AW	0	4
64	AY	0	1
65	AT	0	3
66	AZ	0	4
67	A3	0	1
68	A5	0	5
69	AD	0	4
70	AE	0	6
71	AF	0	10
72	AG	0	3
73	AU	0	5
74	AH	0	2
75	AV	0	6
76	Ag	0	3
77	AX	0	1
78	AJ	0	2
All	All	5	692

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	AJ	55	ILE	CG1-CD1	36.58	2.94	1.51
34	AA	2915	U	C4-C5	30.17	2.03	1.43
34	AA	2915	U	N1-C2	27.44	1.93	1.38
34	AA	2915	U	N1-C6	25.70	1.89	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AA	2915	U	N3-C4	25.41	1.89	1.38
34	AA	2915	U	C2-N3	24.78	1.87	1.37
34	AA	2915	U	C5-C6	16.85	1.67	1.34
34	AA	1202	C	O3'-P	-5.02	1.53	1.61

All (836) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	AB	27	A	O3'-P-O5'	-11.35	86.98	104.00
34	AA	181	C	P-O3'-C3'	11.22	137.03	120.20
1	A	981	U	P-O3'-C3'	11.07	136.81	120.20
1	A	844	G	P-O3'-C3'	10.86	136.49	120.20
1	A	1912	C	P-O3'-C3'	10.85	136.47	120.20
34	AA	1202	C	P-O3'-C3'	10.82	136.44	120.20
1	A	1300	G	P-O3'-C3'	10.65	136.18	120.20
36	AB	28	C	P-O5'-C5'	10.49	136.63	120.90
34	AA	2810	A	P-O3'-C3'	10.31	135.66	120.20
34	AA	581	C	P-O3'-C3'	10.18	135.46	120.20
34	AA	2219	A	P-O3'-C3'	10.02	135.22	120.20
1	A	249	A	P-O3'-C3'	9.90	135.05	120.20
1	A	1056	G	P-O3'-C3'	9.89	135.04	120.20
1	A	1381	C	P-O3'-C3'	9.69	134.74	120.20
1	A	789	U	P-O3'-C3'	9.68	134.72	120.20
34	AA	257	U	P-O3'-C3'	9.62	134.63	120.20
1	A	1897	A	P-O3'-C3'	9.61	134.61	120.20
34	AA	2563	A	P-O3'-C3'	9.60	134.60	120.20
1	A	1865	G	P-O3'-C3'	9.58	134.57	120.20
34	AA	674	U	P-O3'-C3'	9.57	134.56	120.20
34	AA	3019	A	P-O3'-C3'	9.57	134.56	120.20
34	AA	1101	A	P-O3'-C3'	9.54	134.52	120.20
34	AA	270	U	P-O3'-C3'	9.45	134.38	120.20
78	AJ	55	ILE	CB-CG1-CD1	9.44	133.63	113.80
34	AA	1989	A	P-O3'-C3'	9.35	134.22	120.20
34	AA	580	A	P-O3'-C3'	9.24	134.06	120.20
34	AA	900	G	P-O5'-C5'	9.18	134.67	120.90
34	AA	2219	A	C2'-C3'-O3'	9.12	123.18	109.50
34	AA	764	G	P-O3'-C3'	9.11	133.87	120.20
1	A	544	G	P-O3'-C3'	9.06	133.80	120.20
34	AA	1224	A	P-O3'-C3'	9.04	133.75	120.20
35	AC	37	A	P-O3'-C3'	9.01	133.71	120.20
35	AC	35	A	P-O3'-C3'	8.94	133.62	120.20
2	7	55	U	P-O3'-C3'	8.87	133.51	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	53	G	P-O3'-C3'	8.86	133.50	120.20
34	AA	255	C	P-O5'-C5'	8.80	134.09	120.90
34	AA	1217	U	P-O3'-C3'	8.79	133.39	120.20
34	AA	579	C	P-O3'-C3'	8.76	133.34	120.20
34	AA	270	U	C2'-C3'-O3'	8.75	122.62	109.50
34	AA	646	A	P-O5'-C5'	8.58	133.78	120.90
34	AA	3688	G	P-O3'-C3'	8.51	132.97	120.20
34	AA	500	A	P-O3'-C3'	8.51	132.96	120.20
34	AA	2810	A	C2'-C3'-O3'	8.50	122.25	109.50
34	AA	697	A	P-O3'-C3'	8.48	132.93	120.20
34	AA	2013	U	O3'-P-O5'	-8.39	91.41	104.00
1	A	1448	U	P-O3'-C3'	8.30	132.65	120.20
34	AA	3140	U	P-O3'-C3'	8.28	132.61	120.20
34	AA	3658	G	P-O3'-C3'	8.24	132.56	120.20
46	AN	60	PHE	CA-CB-CG	-8.19	105.61	113.80
2	7	31	G	C2'-C3'-O3'	8.14	125.91	113.70
1	A	1455	C	P-O3'-C3'	8.10	132.35	120.20
47	A8	41	ARG	NE-CZ-NH2	8.05	126.44	119.20
34	AA	1881	C	P-O3'-C3'	7.95	132.12	120.20
34	AA	1873	U	P-O3'-C3'	7.94	132.11	120.20
18	1	106	ARG	NE-CZ-NH2	7.93	126.34	119.20
34	AA	218	U	P-O3'-C3'	7.88	132.02	120.20
34	AA	621	C	P-O3'-C3'	7.83	131.94	120.20
49	Aa	106	LYS	N-CA-C	7.82	119.80	111.28
7	U	55	ARG	NE-CZ-NH2	7.79	126.21	119.20
1	A	246	A	P-O3'-C3'	7.78	131.87	120.20
34	AA	121	U	P-O3'-C3'	7.77	131.85	120.20
34	AA	2695	A	P-O5'-C5'	7.77	132.55	120.90
34	AA	1873	U	C2'-C3'-O3'	7.76	121.14	109.50
34	AA	698	G	P-O3'-C3'	7.75	131.83	120.20
34	AA	3476	A	P-O3'-C3'	7.74	131.82	120.20
34	AA	1538	U	C2'-C3'-O3'	7.70	121.05	109.50
56	AI	202	HIS	CA-CB-CG	-7.62	106.18	113.80
1	A	2053	U	C2'-C3'-O3'	7.62	120.92	109.50
41	A2	54	SER	CA-C-N	7.61	134.46	122.74
41	A2	54	SER	C-N-CA	7.61	134.46	122.74
34	AA	715	U	P-O3'-C3'	7.59	131.59	120.20
34	AA	811	A	P-O3'-C3'	7.59	131.59	120.20
34	AA	859	C	P-O3'-C3'	7.58	131.56	120.20
34	AA	1035	G	P-O3'-C3'	7.56	131.54	120.20
20	C	106	MET	N-CA-C	7.55	119.50	111.28
34	AA	2822	U	P-O3'-C3'	7.54	131.51	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	G	P-O3'-C3'	7.54	131.50	120.20
1	A	1907	A	C4'-C3'-C2'	-7.44	95.16	102.60
34	AA	254	U	O3'-P-O5'	-7.43	92.85	104.00
34	AA	3476	A	C2'-C3'-O3'	7.43	120.64	109.50
77	AX	67	LYS	N-CA-C	7.42	119.16	111.14
1	A	105	A	C2'-C3'-O3'	7.42	120.63	109.50
1	A	1976	G	P-O3'-C3'	7.42	131.33	120.20
34	AA	3381	A	C2'-C3'-O3'	7.42	120.62	109.50
34	AA	1574	C	P-O3'-C3'	7.41	131.32	120.20
34	AA	597	A	P-O3'-C3'	7.41	131.31	120.20
34	AA	2394	C	P-O3'-C3'	7.41	131.31	120.20
34	AA	1435	G	P-O3'-C3'	7.38	131.26	120.20
34	AA	858	C	P-O3'-C3'	7.36	131.24	120.20
34	AA	205	G	P-O3'-C3'	7.34	131.21	120.20
34	AA	1503	A	P-O3'-C3'	7.33	131.19	120.20
1	A	790	U	C2'-C3'-O3'	7.31	120.47	109.50
34	AA	3027	U	P-O3'-C3'	7.31	131.16	120.20
34	AA	1881	C	C2'-C3'-O3'	7.29	120.44	109.50
34	AA	289	A	P-O3'-C3'	7.28	131.12	120.20
34	AA	1537	G	P-O5'-C5'	7.28	131.82	120.90
1	A	1818	A	C1'-O4'-C4'	-7.28	102.42	109.70
34	AA	2095	U	P-O3'-C3'	7.27	131.11	120.20
1	A	1414	A	P-O3'-C3'	7.23	131.04	120.20
1	A	981	U	C2'-C3'-O3'	7.18	120.28	109.50
34	AA	146	U	C2'-C3'-O3'	7.18	120.27	109.50
1	A	1691	G	P-O3'-C3'	7.14	130.90	120.20
34	AA	3361	U	C2'-C3'-O3'	7.14	120.20	109.50
34	AA	721	U	P-O3'-C3'	7.13	130.90	120.20
78	AJ	97	PHE	CA-CB-CG	-7.13	106.67	113.80
34	AA	860	A	P-O5'-C5'	7.13	131.59	120.90
34	AA	607	A	P-O3'-C3'	7.12	130.87	120.20
34	AA	162	U	P-O3'-C3'	7.11	130.86	120.20
34	AA	504	A	P-O3'-C3'	7.09	130.84	120.20
39	AO	52	TYR	N-CA-C	7.09	118.66	111.07
34	AA	337	A	C2'-C3'-O3'	7.08	120.12	109.50
69	AD	122	ASN	CA-CB-CG	-7.08	105.53	112.60
34	AA	1904	U	P-O3'-C3'	7.07	130.81	120.20
56	AI	132	ASP	CA-C-N	7.06	129.75	120.28
56	AI	132	ASP	C-N-CA	7.06	129.75	120.28
34	AA	620	U	P-O3'-C3'	7.05	130.78	120.20
2	7	61	C	P-O3'-C3'	7.00	130.71	120.20
1	A	752	U	P-O3'-C3'	6.99	130.68	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	1805	U	P-O3'-C3'	6.98	130.67	120.20
62	AR	162	PHE	CA-CB-CG	-6.97	106.83	113.80
27	F	69	ILE	N-CA-C	6.97	117.73	110.62
34	AA	620	U	C2'-C3'-O3'	6.95	119.92	109.50
33	L	65	PHE	CA-CB-CG	-6.94	106.86	113.80
1	A	2053	U	P-O3'-C3'	6.92	130.58	120.20
12	W	82	LEU	N-CA-C	6.90	118.80	111.28
35	AC	134	G	P-O3'-C3'	6.89	130.54	120.20
35	AC	145	A	P-O3'-C3'	6.89	130.54	120.20
34	AA	337	A	P-O3'-C3'	6.89	130.54	120.20
1	A	1667	A	C2'-C3'-O3'	6.88	119.81	109.50
1	A	423	A	P-O3'-C3'	6.87	130.51	120.20
72	AG	27	GLY	CA-C-N	6.87	129.37	120.44
72	AG	27	GLY	C-N-CA	6.87	129.37	120.44
1	A	2071	U	P-O3'-C3'	6.86	130.49	120.20
34	AA	2816	U	P-O3'-C3'	6.86	130.49	120.20
31	N	105	ILE	N-CA-C	6.85	120.37	110.09
34	AA	1999	A	P-O3'-C3'	6.85	130.47	120.20
34	AA	3019	A	C2'-C3'-O3'	6.84	119.77	109.50
34	AA	353	G	P-O3'-C3'	6.82	130.44	120.20
34	AA	1904	U	C4'-C3'-C2'	-6.82	95.78	102.60
1	A	752	U	C2'-C3'-O3'	6.81	119.71	109.50
14	I	68	MET	N-CA-C	6.81	119.54	111.71
39	AO	15	VAL	N-CA-C	6.81	117.56	110.62
48	A9	76	PHE	CA-CB-CG	6.80	120.60	113.80
34	AA	62	A	P-O3'-C3'	6.79	130.39	120.20
34	AA	2041	U	P-O5'-C5'	6.76	131.03	120.90
34	AA	61	A	P-O3'-C3'	6.75	130.33	120.20
78	AJ	247	ARG	N-CA-C	6.75	118.29	111.07
1	A	818	C	P-O3'-C3'	6.74	130.31	120.20
34	AA	3660	A	P-O3'-C3'	6.72	130.28	120.20
1	A	1870	A	P-O3'-C3'	6.71	130.27	120.20
1	A	1070	A	P-O3'-C3'	6.71	130.26	120.20
34	AA	681	U	C5'-C4'-C3'	-6.70	105.95	116.00
34	AA	138	C	P-O3'-C3'	6.70	130.25	120.20
6	M	11	PHE	CA-C-N	6.70	127.82	121.46
6	M	11	PHE	C-N-CA	6.70	127.82	121.46
34	AA	501	U	P-O3'-C3'	6.69	130.24	120.20
34	AA	215	C	P-O3'-C3'	6.68	130.22	120.20
34	AA	1705	A	C2'-C3'-O3'	6.65	119.48	109.50
71	AF	272	VAL	N-CA-C	6.65	116.78	110.53
65	AT	19	ASN	CA-CB-CG	-6.64	105.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	124	HIS	CA-CB-CG	6.64	120.44	113.80
34	AA	3577	A	P-O3'-C3'	6.64	130.16	120.20
42	A4	7	HIS	CA-CB-CG	6.62	120.42	113.80
1	A	1442	U	C5'-C4'-C3'	-6.61	106.08	116.00
34	AA	3663	A	P-O3'-C3'	6.61	130.11	120.20
34	AA	2696	G	P-O3'-C3'	6.60	130.10	120.20
34	AA	821	C	C2'-C3'-O3'	6.60	119.40	109.50
34	AA	1996	C	P-O3'-C3'	6.60	130.10	120.20
70	AE	61	ASP	CA-C-O	6.59	121.76	117.94
34	AA	3085	A	P-O3'-C3'	6.58	130.08	120.20
1	A	1294	A	P-O3'-C3'	6.58	130.07	120.20
34	AA	1703	U	C2'-C3'-O3'	6.56	119.34	109.50
67	A3	42	LYS	CA-C-N	6.56	129.95	120.38
67	A3	42	LYS	C-N-CA	6.56	129.95	120.38
71	AF	221	PHE	CA-CB-CG	-6.56	107.24	113.80
34	AA	3361	U	P-O3'-C3'	6.54	130.02	120.20
10	X	47	ARG	NE-CZ-NH2	6.53	125.08	119.20
34	AA	3043	A	C2'-C3'-O3'	6.53	119.30	109.50
1	A	1109	G	P-O5'-C5'	6.51	130.66	120.90
34	AA	1204	A	P-O3'-C3'	6.51	129.96	120.20
56	AI	212	ASN	CA-C-N	6.50	128.99	120.28
56	AI	212	ASN	C-N-CA	6.50	128.99	120.28
35	AC	100	A	P-O3'-C3'	6.50	129.94	120.20
1	A	25	C	P-O3'-C3'	6.49	129.94	120.20
2	7	55	U	C2'-C3'-O3'	6.49	119.23	109.50
34	AA	3667	C	C2'-C3'-O3'	6.49	119.23	109.50
34	AA	697	A	C2'-C3'-O3'	6.48	119.22	109.50
54	AP	94	SER	CA-C-N	6.48	128.97	120.28
54	AP	94	SER	C-N-CA	6.48	128.97	120.28
1	A	206	A	P-O3'-C3'	6.45	129.87	120.20
1	A	156	A	P-O3'-C3'	6.44	129.86	120.20
69	AD	205	ASN	CA-CB-CG	-6.44	106.16	112.60
34	AA	10	G	P-O3'-C3'	6.44	129.85	120.20
34	AA	1750	U	C2'-C3'-O3'	6.43	119.15	109.50
34	AA	1605	A	P-O3'-C3'	6.43	129.84	120.20
34	AA	3590	A	C2'-C3'-O3'	6.43	119.14	109.50
36	AB	28	C	C5'-C4'-C3'	6.42	125.64	116.00
34	AA	2932	A	P-O3'-C3'	6.42	129.83	120.20
24	6	13	LYS	N-CA-C	6.42	118.85	111.02
34	AA	3578	A	C2'-C3'-O3'	6.41	119.12	109.50
34	AA	317	U	P-O5'-C5'	6.41	130.51	120.90
8	V	45	PHE	CA-CB-CG	-6.40	107.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	2070	U	P-O5'-C5'	6.40	130.50	120.90
1	A	872	A	P-O3'-C3'	6.39	129.79	120.20
37	AL	28	ASN	CA-CB-CG	-6.39	106.21	112.60
34	AA	1197	U	P-O3'-C3'	6.37	129.75	120.20
14	I	21	ILE	N-CA-C	6.36	117.11	110.62
35	AC	54	C	P-O3'-C3'	6.35	129.73	120.20
29	K	22	ARG	N-CA-C	6.35	118.20	111.28
2	7	44	A	C5'-C4'-C3'	-6.32	106.52	116.00
57	Ac	80	LYS	CA-C-N	6.31	129.60	120.38
57	Ac	80	LYS	C-N-CA	6.31	129.60	120.38
1	A	879	A	C2'-C3'-O3'	6.30	118.96	109.50
34	AA	359	A	P-O5'-C5'	6.29	130.34	120.90
31	N	40	LYS	CA-C-N	6.29	126.96	119.98
31	N	40	LYS	C-N-CA	6.29	126.96	119.98
36	AB	84	U	C2'-C3'-O3'	6.28	118.92	109.50
1	A	1644	U	C2'-C3'-O3'	6.28	118.92	109.50
2	7	31	G	O4'-C4'-C3'	-6.28	97.72	104.00
34	AA	1217	U	C2'-C3'-O3'	6.28	118.92	109.50
61	AQ	6	ALA	CA-C-N	6.28	128.69	120.28
61	AQ	6	ALA	C-N-CA	6.28	128.69	120.28
71	AF	286	ASN	O-C-N	-6.27	117.43	121.88
54	AP	38	ARG	NE-CZ-NH2	6.26	124.83	119.20
1	A	832	A	P-O3'-C3'	6.25	129.57	120.20
73	AU	122	ARG	NE-CZ-NH2	6.24	124.81	119.20
34	AA	889	U	C2'-C3'-O3'	6.24	118.85	109.50
2	7	31	G	C4'-C3'-C2'	6.23	108.83	102.60
78	AJ	198	LYS	N-CA-C	6.23	118.07	111.28
52	Ae	3	SER	CA-C-N	6.23	128.91	120.63
52	Ae	3	SER	C-N-CA	6.23	128.91	120.63
34	AA	1319	U	C2'-C3'-O3'	6.22	118.83	109.50
34	AA	3754	A	O4'-C1'-N9	6.21	117.81	108.50
34	AA	162	U	C2'-C3'-O3'	6.21	118.81	109.50
48	A9	78	VAL	N-CA-C	6.20	116.94	110.62
45	A1	4	LEU	N-CA-C	6.19	117.83	111.14
34	AA	1705	A	P-O3'-C3'	6.18	129.47	120.20
34	AA	3291	U	P-O3'-C3'	6.18	129.47	120.20
34	AA	308	U	C2'-C3'-O3'	6.18	118.77	109.50
42	A4	8	THR	N-CA-C	6.17	119.30	110.10
12	W	13	ALA	CA-C-N	6.17	128.46	120.44
12	W	13	ALA	C-N-CA	6.17	128.46	120.44
33	L	32	PRO	N-CA-C	6.16	118.22	110.70
48	A9	110	ASN	CA-CB-CG	-6.16	106.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	124	ARG	NE-CZ-NH2	6.14	124.73	119.20
1	A	747	U	P-O5'-C5'	6.14	130.11	120.90
34	AA	3161	A	P-O3'-C3'	6.13	129.40	120.20
34	AA	3034	A	C2'-C3'-O3'	6.13	118.69	109.50
34	AA	1568	C	O3'-P-O5'	-6.13	94.81	104.00
16	Y	59	PHE	CA-CB-CG	-6.12	107.68	113.80
44	A7	114	ASN	CA-CB-CG	-6.11	106.49	112.60
1	A	1870	A	C2'-C3'-O3'	6.11	118.66	109.50
2	7	69	C	P-O3'-C3'	6.09	129.33	120.20
46	AN	44	PHE	CA-CB-CG	-6.08	107.72	113.80
14	I	94	MET	N-CA-C	6.08	117.91	111.28
1	A	1064	A	O3'-P-O5'	-6.07	94.89	104.00
34	AA	3027	U	C2'-C3'-O3'	6.07	118.60	109.50
71	AF	86	ARG	NE-CZ-NH2	6.06	124.66	119.20
34	AA	1208	G	P-O5'-C5'	6.06	129.99	120.90
34	AA	1169	A	P-O5'-C5'	6.05	129.98	120.90
1	A	2	A	C2'-C3'-O3'	6.05	118.58	109.50
34	AA	596	A	P-O3'-C3'	6.04	129.27	120.20
39	AO	21	ARG	NE-CZ-NH2	6.04	124.64	119.20
75	AV	13	ARG	NE-CZ-NH2	6.04	124.63	119.20
54	AP	106	VAL	CA-C-N	6.03	126.78	120.03
54	AP	106	VAL	C-N-CA	6.03	126.78	120.03
35	AC	67	G	O4'-C1'-N9	6.03	117.24	108.20
68	A5	84	PHE	CA-CB-CG	-6.03	107.77	113.80
56	AI	18	LYS	N-CA-C	6.02	117.84	111.28
72	AG	157	GLU	N-CA-C	6.01	117.51	111.07
34	AA	65	A	P-O3'-C3'	6.00	129.21	120.20
34	AA	3067	G	O3'-P-O5'	-6.00	95.01	104.00
69	AD	216	HIS	CA-CB-CG	-6.00	107.81	113.80
1	A	103	U	C2'-C3'-O3'	5.99	122.69	113.70
34	AA	3067	G	C1'-O4'-C4'	-5.99	103.91	109.90
39	AO	90	PHE	CA-CB-CG	-5.99	107.81	113.80
1	A	1321	C	C5'-C4'-C3'	-5.99	107.02	116.00
34	AA	703	U	P-O3'-C3'	5.99	129.18	120.20
34	AA	2039	U	C5'-C4'-C3'	5.98	124.97	116.00
35	AC	145	A	C2'-C3'-O3'	5.98	122.67	113.70
69	AD	163	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	A	1934	C	P-O3'-C3'	5.96	129.15	120.20
34	AA	1273	G	P-O5'-C5'	5.96	129.84	120.90
34	AA	3587	U	P-O3'-C3'	5.96	129.14	120.20
67	A3	113	PHE	CA-CB-CG	5.96	119.76	113.80
34	AA	2695	A	O5'-C5'-C4'	5.96	120.63	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	3140	U	C2'-C3'-O3'	5.96	118.43	109.50
1	A	844	G	P-O5'-C5'	5.95	129.83	120.90
26	D	77	PHE	CA-CB-CG	-5.95	107.85	113.80
1	A	894	U	P-O3'-C3'	-5.93	111.30	120.20
34	AA	1780	G	P-O5'-C5'	5.93	129.80	120.90
21	3	6	ARG	NE-CZ-NH2	5.93	124.54	119.20
41	A2	19	PHE	CA-CB-CG	-5.92	107.88	113.80
1	A	142	G	C2'-C3'-O3'	5.92	118.38	109.50
58	AK	100	LYS	N-CA-C	5.92	117.73	111.28
1	A	102	A	P-O3'-C3'	5.92	129.08	120.20
1	A	1980	A	C2'-C3'-O3'	5.91	118.37	109.50
34	AA	2665	A	C2'-C3'-O3'	5.91	118.36	109.50
60	AS	166	VAL	N-CA-C	5.91	121.63	109.34
35	AC	100	A	C4'-C3'-C2'	-5.91	96.69	102.60
1	A	753	U	C2'-C3'-O3'	5.90	118.35	109.50
34	AA	184	U	P-O3'-C3'	5.90	129.05	120.20
34	AA	3663	A	C2'-C3'-O3'	5.90	118.35	109.50
67	A3	105	ARG	NE-CZ-NH2	5.89	124.50	119.20
34	AA	683	A	P-O3'-C3'	5.88	129.03	120.20
34	AA	998	U	C2'-C3'-O3'	5.88	118.32	109.50
34	AA	3526	U	C2'-C3'-O3'	5.88	118.32	109.50
34	AA	3020	U	O5'-C5'-C4'	5.87	120.31	111.50
54	AP	16	SER	N-CA-CB	5.87	120.41	110.49
34	AA	811	A	C2'-C3'-O3'	5.87	118.30	109.50
29	K	3	ARG	N-CA-C	5.86	117.67	111.28
34	AA	1990	A	P-O3'-C3'	5.86	129.00	120.20
1	A	129	U	C2'-C3'-O3'	5.86	118.29	109.50
1	A	1729	A	P-O5'-C5'	-5.85	112.12	120.90
77	AX	121	ARG	NE-CZ-NH2	5.84	124.46	119.20
34	AA	833	G	P-O5'-C5'	5.84	129.66	120.90
34	AA	3230	G	P-O3'-C3'	5.84	128.96	120.20
34	AA	2932	A	O5'-C5'-C4'	5.84	120.45	111.70
57	Ac	79	ASN	CA-CB-CG	-5.83	106.77	112.60
30	J	189	PRO	N-CA-C	5.83	117.81	110.70
49	Aa	61	ASP	CA-CB-CG	-5.82	106.78	112.60
34	AA	521	U	C2'-C3'-O3'	5.82	118.23	109.50
54	AP	33	LEU	N-CA-C	5.81	117.92	109.84
1	A	1819	U	C2'-C3'-O3'	5.81	118.22	109.50
57	Ac	79	ASN	CA-C-N	5.79	132.61	121.54
57	Ac	79	ASN	C-N-CA	5.79	132.61	121.54
35	AC	38	G	C2'-C3'-O3'	5.79	118.19	109.50
34	AA	500	A	C2'-C3'-O3'	5.79	118.19	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	AC	55	A	P-O5'-C5'	-5.78	112.22	120.90
25	B	220	ARG	NE-CZ-NH2	5.78	124.40	119.20
34	AA	3441	A	C2'-C3'-O3'	5.78	118.17	109.50
34	AA	1279	U	P-O5'-C5'	5.78	129.56	120.90
73	AU	172	LYS	N-CA-C	5.77	117.74	110.24
34	AA	683	A	C4'-C3'-O3'	5.76	118.04	109.40
34	AA	1904	U	C2'-C3'-O3'	5.76	118.13	109.50
34	AA	2966	C	C2'-C3'-O3'	5.76	118.13	109.50
34	AA	3107	U	P-O3'-C3'	5.76	128.83	120.20
34	AA	33	G	O3'-P-O5'	-5.75	95.37	104.00
34	AA	2409	G	C2'-C3'-O3'	5.75	118.13	109.50
45	A1	78	ASN	CA-CB-CG	-5.75	106.85	112.60
34	AA	215	C	C2'-C3'-O3'	5.75	122.32	113.70
1	A	1193	A	C2'-C3'-O3'	5.74	118.11	109.50
34	AA	2695	A	C5'-C4'-C3'	-5.73	106.61	115.20
34	AA	2917	C	P-O5'-C5'	-5.73	112.31	120.90
57	Ac	69	TYR	N-CA-C	-5.72	106.34	113.55
34	AA	1762	A	C2'-C3'-O3'	5.72	118.08	109.50
34	AA	3363	U	C5'-C4'-C3'	-5.72	107.42	116.00
38	A0	66	ASN	CA-CB-CG	-5.72	106.88	112.60
1	A	1659	U	P-O3'-C3'	5.71	128.77	120.20
34	AA	3379	A	P-O5'-C5'	5.71	129.47	120.90
34	AA	3506	U	P-O5'-C5'	-5.71	112.33	120.90
34	AA	3697	G	P-O5'-C5'	5.70	129.46	120.90
1	A	1292	U	P-O3'-C3'	5.70	128.75	120.20
34	AA	3577	A	C2'-C3'-O3'	5.70	118.05	109.50
4	S	102	ALA	N-CA-C	5.70	116.43	108.00
34	AA	580	A	C5'-C4'-C3'	5.69	124.54	116.00
1	A	251	U	C2'-C3'-O3'	5.69	118.04	109.50
28	H	143	LYS	CA-C-N	5.69	127.91	120.28
28	H	143	LYS	C-N-CA	5.69	127.91	120.28
34	AA	2883	U	C2'-C3'-O3'	5.69	118.03	109.50
1	A	831	U	P-O3'-C3'	5.69	128.73	120.20
34	AA	3017	A	P-O3'-C3'	5.69	128.73	120.20
1	A	1441	C	P-O5'-C5'	5.69	129.43	120.90
32	P	141	ARG	NE-CZ-NH2	5.68	124.31	119.20
34	AA	54	C	P-O5'-C5'	5.67	129.41	120.90
34	AA	579	C	C2'-C3'-O3'	5.67	118.01	109.50
68	A5	229	ALA	CA-C-N	5.67	128.15	120.38
68	A5	229	ALA	C-N-CA	5.67	128.15	120.38
34	AA	768	C	C2'-C3'-O3'	5.67	118.00	109.50
73	AU	127	ALA	CA-C-N	5.66	128.14	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	AU	127	ALA	C-N-CA	5.66	128.14	120.38
1	A	251	U	C1'-O4'-C4'	-5.66	104.04	109.70
45	A1	76	ASN	CA-CB-CG	5.66	118.26	112.60
76	Ag	39	ARG	NE-CZ-NH2	5.66	124.29	119.20
34	AA	3617	A	C2'-C3'-O3'	5.65	117.98	109.50
1	A	1854	U	C2'-C3'-O3'	5.65	117.97	109.50
34	AA	702	U	O4'-C1'-N1	5.65	116.97	108.50
39	AO	63	LEU	N-CA-C	5.64	117.11	111.07
34	AA	3658	G	C4'-C3'-O3'	5.64	117.86	109.40
1	A	371	G	C5'-C4'-C3'	-5.63	107.55	116.00
34	AA	432	A	P-O3'-C3'	5.63	128.65	120.20
71	AF	380	ALA	CA-C-N	5.63	127.83	120.28
71	AF	380	ALA	C-N-CA	5.63	127.83	120.28
70	AE	112	ASP	CA-CB-CG	-5.62	106.98	112.60
34	AA	1457	G	P-O3'-C3'	5.62	128.63	120.20
16	Y	31	ASP	CA-CB-CG	-5.62	106.98	112.60
1	A	548	A	P-O3'-C3'	-5.62	111.78	120.20
34	AA	1435	G	C2'-C3'-O3'	5.61	117.92	109.50
47	A8	36	ARG	NE-CZ-NH2	5.61	124.25	119.20
34	AA	500	A	C4'-C3'-O3'	5.61	117.81	109.40
34	AA	2955	C	P-O5'-C5'	5.61	129.31	120.90
5	T	14	GLN	N-CA-C	5.61	118.11	111.33
34	AA	3017	A	C2'-C3'-O3'	5.61	117.91	109.50
2	7	62	C	P-O5'-C5'	5.60	129.31	120.90
25	B	70	LEU	CA-C-N	5.60	127.79	120.28
25	B	70	LEU	C-N-CA	5.60	127.79	120.28
34	AA	86	G	C2'-C3'-O3'	5.60	117.91	109.50
45	A1	64	LYS	CA-C-N	5.60	127.72	120.44
45	A1	64	LYS	C-N-CA	5.60	127.72	120.44
47	A8	55	ILE	CA-C-N	5.60	127.19	120.13
47	A8	55	ILE	C-N-CA	5.60	127.19	120.13
32	P	109	GLY	CA-C-N	5.60	125.26	119.05
32	P	109	GLY	C-N-CA	5.60	125.26	119.05
34	AA	2883	U	P-O3'-C3'	5.60	128.60	120.20
54	AP	49	ARG	CB-CA-C	-5.60	102.09	110.88
34	AA	353	G	C2'-C3'-O3'	5.60	122.09	113.70
34	AA	3585	A	C2'-C3'-O3'	5.60	117.90	109.50
39	AO	32	ARG	N-CA-C	5.60	117.96	110.35
1	A	357	U	P-O3'-C3'	5.59	128.59	120.20
34	AA	273	C	P-O3'-C3'	-5.59	111.82	120.20
61	AQ	24	ARG	NE-CZ-NH2	5.59	124.23	119.20
36	AB	88	A	P-O3'-C3'	5.58	128.57	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1108	A	C2'-C3'-O3'	5.58	117.87	109.50
18	1	91	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	127	C	C2'-C3'-O3'	5.57	117.86	109.50
45	A1	17	ARG	NE-CZ-NH2	5.57	124.22	119.20
56	AI	102	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	A	1295	A	C4'-C3'-C2'	-5.57	97.03	102.60
27	F	50	ASN	CA-CB-CG	-5.56	107.04	112.60
34	AA	803	A	O4'-C1'-N9	5.56	116.84	108.50
75	AV	36	ASN	N-CA-C	5.56	116.76	108.31
60	AS	173	PHE	CA-C-N	5.56	132.15	121.54
60	AS	173	PHE	C-N-CA	5.56	132.15	121.54
71	AF	48	ARG	NE-CZ-NH2	5.55	124.20	119.20
34	AA	773	A	C2'-C3'-O3'	5.55	117.83	109.50
1	A	1907	A	C2'-C3'-O3'	5.55	117.82	109.50
12	W	67	ARG	N-CA-C	5.55	117.69	110.43
2	7	34	C	C2'-C3'-O3'	5.54	117.81	109.50
48	A9	66	LYS	N-CA-C	5.54	118.03	111.33
1	A	1448	U	O4'-C1'-N1	5.54	116.81	108.50
2	7	31	G	O3'-P-O5'	5.54	112.30	104.00
34	AA	3231	A	P-O3'-C3'	-5.54	111.90	120.20
67	A3	12	LEU	N-CA-C	5.54	117.88	110.35
1	A	973	G	C1'-O4'-C4'	-5.53	104.17	109.70
60	AS	173	PHE	CA-CB-CG	-5.53	108.27	113.80
61	AQ	181	TYR	CB-CA-C	-5.53	102.20	110.88
16	Y	47	LEU	CA-C-N	5.53	127.69	120.28
16	Y	47	LEU	C-N-CA	5.53	127.69	120.28
34	AA	1171	A	C2'-C3'-O3'	5.53	117.79	109.50
37	AL	168	LYS	N-CA-C	5.53	117.52	109.84
1	A	1	A	C2'-C3'-O3'	5.53	117.79	109.50
4	S	88	ARG	NE-CZ-NH2	5.52	124.17	119.20
34	AA	3300	A	P-O3'-C3'	5.52	128.48	120.20
59	AM	128	TRP	CA-C-N	5.52	124.98	119.24
59	AM	128	TRP	C-N-CA	5.52	124.98	119.24
34	AA	1101	A	C4'-C3'-O3'	5.52	117.68	109.40
73	AU	144	ARG	NE-CZ-NH2	5.52	124.17	119.20
67	A3	93	GLN	N-CA-C	5.52	117.66	110.43
1	A	1832	U	P-O3'-C3'	5.51	128.47	120.20
13	R	126	SER	N-CA-C	5.51	119.46	109.32
39	AO	75	VAL	N-CA-C	5.51	116.24	110.62
2	7	32	C	P-O5'-C5'	5.51	129.16	120.90
1	A	2	A	P-O3'-C3'	5.50	128.46	120.20
13	R	54	ALA	N-CA-C	5.50	117.28	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	3086	A	C2'-C3'-O3'	5.50	117.75	109.50
67	A3	105	ARG	NE-CZ-NH1	-5.50	116.00	121.50
6	M	37	LEU	CA-C-N	5.50	127.91	120.38
6	M	37	LEU	C-N-CA	5.50	127.91	120.38
57	Ac	21	LEU	N-CA-C	5.50	116.95	111.07
34	AA	3381	A	P-O3'-C3'	5.49	128.44	120.20
18	1	20	ARG	NE-CZ-NH2	5.49	124.14	119.20
34	AA	652	A	C2'-C3'-O3'	5.49	121.94	113.70
24	6	42	ARG	CA-C-N	5.48	128.08	120.29
24	6	42	ARG	C-N-CA	5.48	128.08	120.29
35	AC	74	A	C5'-C4'-C3'	-5.48	107.78	116.00
72	AG	154	VAL	N-CA-C	5.48	116.26	110.72
27	F	157	ASN	CA-CB-CG	-5.48	107.12	112.60
71	AF	343	MET	N-CA-C	5.48	117.05	111.14
25	B	57	ALA	CA-C-N	5.47	127.93	120.54
25	B	57	ALA	C-N-CA	5.47	127.93	120.54
34	AA	2727	U	O4'-C1'-N1	5.47	116.41	108.20
34	AA	3229	C	C2'-C3'-O3'	5.47	117.71	109.50
60	AS	74	HIS	CA-CB-CG	-5.47	108.33	113.80
34	AA	3711	U	P-O3'-C3'	5.47	128.41	120.20
1	A	26	A	C4'-C3'-C2'	-5.47	97.13	102.60
34	AA	1805	U	C2'-C3'-O3'	5.47	121.90	113.70
45	A1	98	SER	CA-C-N	5.46	127.92	120.54
45	A1	98	SER	C-N-CA	5.46	127.92	120.54
46	AN	79	GLU	N-CA-C	5.46	118.15	110.23
27	F	65	LEU	N-CA-C	5.46	117.23	111.28
34	AA	33	G	C5'-C4'-C3'	-5.46	107.81	116.00
26	D	154	ARG	NE-CZ-NH2	5.46	124.11	119.20
72	AG	11	GLU	N-CA-C	5.46	117.77	110.35
1	A	837	A	C5'-C4'-C3'	5.45	124.18	116.00
7	U	86	GLU	CA-C-N	5.45	127.52	120.44
7	U	86	GLU	C-N-CA	5.45	127.52	120.44
1	A	1381	C	C2'-C3'-O3'	5.45	121.87	113.70
20	C	148	ASP	CA-C-N	5.45	127.89	120.54
20	C	148	ASP	C-N-CA	5.45	127.89	120.54
34	AA	3137	U	P-O3'-C3'	5.44	128.36	120.20
78	AJ	244	ASP	CA-CB-CG	-5.44	107.16	112.60
78	AJ	252	GLN	N-CA-C	5.44	117.75	110.35
39	AO	59	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	A	1100	U	C4'-C3'-O3'	5.44	117.56	109.40
43	A6	56	ARG	NE-CZ-NH2	5.44	124.09	119.20
34	AA	941	G	C5'-C4'-C3'	5.44	124.16	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1976	G	C5'-C4'-C3'	-5.43	107.85	116.00
28	H	77	PHE	CA-CB-CG	-5.43	108.36	113.80
39	AO	38	LEU	CA-C-N	5.43	127.83	120.44
39	AO	38	LEU	C-N-CA	5.43	127.83	120.44
37	AL	22	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	A	1788	U	O4'-C1'-N1	5.43	116.64	108.50
73	AU	7	ASN	N-CA-C	-5.43	107.66	114.56
1	A	1182	A	P-O3'-C3'	5.43	128.34	120.20
58	AK	81	ARG	NE-CZ-NH2	5.43	124.08	119.20
34	AA	3711	U	C2'-C3'-O3'	5.42	117.64	109.50
65	AT	37	ARG	NE-CZ-NH2	5.42	124.08	119.20
34	AA	803	A	P-O3'-C3'	5.42	128.33	120.20
18	1	91	ARG	NE-CZ-NH1	-5.42	116.08	121.50
34	AA	685	U	O3'-P-O5'	-5.41	95.88	104.00
34	AA	2092	G	O3'-P-O5'	-5.41	95.88	104.00
35	AC	37	A	C2'-C3'-O3'	5.41	121.82	113.70
72	AG	98	ASP	CA-C-N	5.41	127.53	120.28
72	AG	98	ASP	C-N-CA	5.41	127.53	120.28
73	AU	53	PHE	CA-CB-CG	-5.41	108.39	113.80
16	Y	158	PHE	CA-CB-CG	-5.40	108.40	113.80
57	Ac	19	HIS	CA-CB-CG	-5.40	108.40	113.80
30	J	37	THR	CA-C-N	5.40	127.52	120.28
30	J	37	THR	C-N-CA	5.40	127.52	120.28
1	A	1701	G	P-O3'-C3'	-5.39	112.11	120.20
37	AL	21	VAL	N-CA-C	5.39	120.56	109.34
60	AS	57	ARG	NE-CZ-NH2	5.39	124.05	119.20
75	AV	39	ASP	N-CA-C	5.39	118.04	110.23
20	C	129	ASP	CA-C-N	5.39	127.50	120.28
20	C	129	ASP	C-N-CA	5.39	127.50	120.28
37	AL	141	ALA	N-CA-C	5.38	119.06	111.52
1	A	1857	U	O4'-C1'-N1	5.38	116.57	108.50
34	AA	2574	A	C1'-O4'-C4'	-5.38	104.32	109.70
68	A5	218	PHE	CA-CB-CG	-5.38	108.42	113.80
28	H	65	GLN	N-CA-C	5.38	117.14	111.28
1	A	1375	C	O4'-C1'-N1	5.38	116.26	108.20
7	U	62	GLN	N-CA-C	5.38	117.66	110.35
24	6	14	VAL	N-CA-C	5.38	116.10	110.62
60	AS	78	ILE	CA-C-N	5.38	128.48	120.95
60	AS	78	ILE	C-N-CA	5.38	128.48	120.95
1	A	1251	G	O4'-C1'-N9	5.37	116.56	108.50
1	A	1666	C	C2'-C3'-O3'	5.37	117.56	109.50
2	7	25	C	O5'-C5'-C4'	5.37	119.56	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	79	ARG	CA-C-N	5.37	124.83	119.24
20	C	79	ARG	C-N-CA	5.37	124.83	119.24
68	A5	64	TYR	N-CA-CB	5.37	117.80	110.01
34	AA	25	A	C2'-C3'-O3'	5.37	117.56	109.50
54	AP	195	ARG	NE-CZ-NH2	5.37	124.03	119.20
75	AV	8	LYS	N-CA-C	5.37	116.94	111.14
71	AF	149	GLU	CA-C-N	5.37	123.62	120.24
71	AF	149	GLU	C-N-CA	5.37	123.62	120.24
13	R	97	ALA	N-CA-C	5.37	119.09	112.54
73	AU	145	ARG	N-CA-C	5.37	117.20	109.48
54	AP	103	GLU	CA-C-N	5.36	125.93	119.98
54	AP	103	GLU	C-N-CA	5.36	125.93	119.98
65	AT	37	ARG	NE-CZ-NH1	-5.36	116.14	121.50
39	AO	118	HIS	N-CA-C	5.36	117.64	110.35
34	AA	257	U	C2'-C3'-O3'	5.36	121.73	113.70
69	AD	200	ARG	NE-CZ-NH2	5.35	124.02	119.20
77	AX	117	ARG	CA-C-N	5.35	128.85	120.82
77	AX	117	ARG	C-N-CA	5.35	128.85	120.82
34	AA	1027	G	P-O5'-C5'	-5.35	112.87	120.90
35	AC	138	U	P-O3'-C3'	5.35	128.23	120.20
63	AW	127	ARG	NE-CZ-NH2	5.35	124.01	119.20
30	J	77	GLN	N-CA-C	5.34	117.11	111.28
54	AP	81	HIS	N-CA-C	5.34	117.83	110.35
71	AF	163	LYS	CA-C-N	5.34	127.44	120.28
71	AF	163	LYS	C-N-CA	5.34	127.44	120.28
1	A	1818	A	O4'-C1'-N9	5.34	116.21	108.20
70	AE	316	GLU	CA-C-N	5.34	128.67	120.82
70	AE	316	GLU	C-N-CA	5.34	128.67	120.82
34	AA	2095	U	C2'-C3'-O3'	5.33	117.50	109.50
71	AF	86	ARG	NE-CZ-NH1	-5.33	116.17	121.50
10	X	28	LEU	N-CA-C	5.33	117.60	110.35
1	A	1659	U	C2'-C3'-O3'	5.33	117.49	109.50
34	AA	2038	U	C5'-C4'-C3'	5.32	123.98	116.00
34	AA	3097	A	C2'-C3'-O3'	5.32	117.48	109.50
15	O	48	VAL	N-CA-C	5.32	114.76	108.96
1	A	932	U	P-O5'-C5'	5.32	128.88	120.90
14	I	62	ARG	NE-CZ-NH2	5.32	123.98	119.20
37	AL	171	TYR	N-CA-C	5.32	122.12	110.80
71	AF	352	LYS	CA-C-N	5.32	127.40	120.28
71	AF	352	LYS	C-N-CA	5.32	127.40	120.28
1	A	1710	G	C5'-C4'-C3'	-5.31	108.03	116.00
20	C	101	ARG	NE-CZ-NH2	5.31	123.98	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	AR	16	TYR	N-CA-C	5.31	117.93	110.23
34	AA	3617	A	P-O3'-C3'	5.31	128.16	120.20
42	A4	28	LYS	N-CA-C	5.31	117.57	110.35
23	5	15	ARG	NE-CZ-NH2	5.30	123.97	119.20
34	AA	1278	A	O4'-C1'-N9	5.30	116.45	108.50
34	AA	1017	U	O3'-P-O5'	-5.30	96.05	104.00
1	A	874	A	P-O3'-C3'	5.29	128.14	120.20
57	Ac	75	ARG	N-CA-CB	5.29	119.44	110.49
25	B	39	LEU	N-CA-C	5.29	117.04	111.28
34	AA	3751	A	C5'-C4'-C3'	-5.29	108.07	116.00
1	A	919	U	P-O3'-C3'	5.28	128.12	120.20
26	D	128	MET	CA-C-N	5.28	127.36	120.28
26	D	128	MET	C-N-CA	5.28	127.36	120.28
21	3	19	ASN	N-CA-C	5.28	116.35	109.64
34	AA	1157	U	C5'-C4'-C3'	5.28	123.92	116.00
10	X	43	ARG	NE-CZ-NH2	5.28	123.95	119.20
69	AD	194	ASN	CA-CB-CG	-5.28	107.33	112.60
28	H	142	ARG	CA-C-N	5.27	127.29	120.44
28	H	142	ARG	C-N-CA	5.27	127.29	120.44
34	AA	121	U	C2'-C3'-O3'	5.27	117.41	109.50
34	AA	3246	A	C5'-C4'-C3'	5.27	123.11	115.20
73	AU	35	ARG	NE-CZ-NH2	5.27	123.95	119.20
34	AA	1040	A	C2'-C3'-O3'	5.27	117.40	109.50
34	AA	641	G	C2'-C3'-O3'	5.27	117.40	109.50
64	AY	186	LYS	N-CA-C	5.27	116.70	111.07
70	AE	16	PHE	CA-CB-CG	-5.27	108.53	113.80
14	I	24	LEU	CA-C-N	5.26	127.34	120.28
14	I	24	LEU	C-N-CA	5.26	127.34	120.28
1	A	16	G	C5'-C4'-C3'	5.26	123.89	116.00
1	A	143	A	C2'-C3'-O3'	5.26	117.39	109.50
10	X	40	ARG	CA-C-N	5.26	127.28	120.44
10	X	40	ARG	C-N-CA	5.26	127.28	120.44
35	AC	139	A	C2'-C3'-O3'	5.26	117.39	109.50
34	AA	895	A	C5'-C4'-C3'	-5.25	108.12	116.00
46	AN	148	LYS	CA-C-N	5.25	127.32	120.28
46	AN	148	LYS	C-N-CA	5.25	127.32	120.28
56	AI	50	LEU	N-CA-C	5.25	117.06	110.24
1	A	26	A	C2'-C3'-O3'	5.25	117.37	109.50
1	A	1198	U	O4'-C1'-N1	5.25	116.07	108.20
1	A	1454	G	P-O5'-C5'	5.24	128.76	120.90
34	AA	3257	G	C2'-C3'-O3'	5.24	117.37	109.50
34	AA	3414	G	P-O3'-C3'	5.24	128.07	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	A6	9	ALA	N-CA-C	5.24	116.68	111.07
54	AP	167	SER	CA-C-N	5.24	127.30	120.28
54	AP	167	SER	C-N-CA	5.24	127.30	120.28
1	A	577	A	C4'-C3'-C2'	-5.24	97.36	102.60
2	7	69	C	C2'-C3'-O3'	5.24	117.36	109.50
38	A0	16	SER	CA-C-N	5.24	127.30	120.28
38	A0	16	SER	C-N-CA	5.24	127.30	120.28
76	Ag	6	SER	CA-C-N	5.24	127.30	120.28
76	Ag	6	SER	C-N-CA	5.24	127.30	120.28
25	B	36	LYS	CA-C-N	5.23	127.29	120.28
25	B	36	LYS	C-N-CA	5.23	127.29	120.28
54	AP	145	ASN	CA-CB-CG	-5.23	107.37	112.60
74	AH	98	PHE	N-CA-C	5.23	116.28	109.64
48	A9	58	PRO	CA-C-N	5.23	127.81	120.28
48	A9	58	PRO	C-N-CA	5.23	127.81	120.28
30	J	78	ARG	NE-CZ-NH2	5.22	123.90	119.20
34	AA	1243	G	C2'-C3'-O3'	5.22	117.34	109.50
1	A	919	U	C2'-C3'-O3'	5.22	121.53	113.70
71	AF	304	ALA	N-CA-C	5.22	117.66	110.35
1	A	525	G	C2'-C3'-O3'	5.22	121.53	113.70
34	AA	312	A	P-O3'-C3'	-5.22	112.38	120.20
63	AW	62	LYS	N-CA-C	-5.22	107.47	113.88
74	AH	119	GLU	N-CA-C	5.22	117.71	111.71
1	A	516	G	C2'-C3'-O3'	5.21	117.32	109.50
34	AA	1680	C	C5'-C4'-C3'	-5.21	108.18	116.00
70	AE	234	ARG	NE-CZ-NH2	5.21	123.89	119.20
4	S	123	ARG	CA-C-N	5.21	125.73	119.94
4	S	123	ARG	C-N-CA	5.21	125.73	119.94
31	N	78	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	1035	A	P-O5'-C5'	5.21	128.71	120.90
1	A	1100	U	P-O3'-C3'	5.21	128.01	120.20
1	A	1979	C	O4'-C1'-N1	5.21	116.01	108.20
1	A	1432	G	P-O3'-C3'	5.20	128.00	120.20
34	AA	1724	G	P-O5'-C5'	5.20	128.71	120.90
34	AA	3782	A	P-O5'-C5'	5.20	128.70	120.90
37	AL	198	ARG	NE-CZ-NH2	5.20	123.88	119.20
39	AO	59	ARG	NE-CZ-NH1	-5.20	116.30	121.50
73	AU	124	ARG	NE-CZ-NH2	5.20	123.88	119.20
32	P	38	ASN	CA-CB-CG	-5.20	107.40	112.60
34	AA	577	U	P-O5'-C5'	5.20	128.69	120.90
1	A	1932	A	P-O3'-C3'	-5.20	112.41	120.20
6	M	11	PHE	N-CA-C	5.20	116.19	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R	57	CYS	N-CA-C	5.20	117.42	110.35
72	AG	11	GLU	CA-C-N	5.20	127.46	120.50
72	AG	11	GLU	C-N-CA	5.20	127.46	120.50
68	A5	250	ASN	CA-CB-CG	-5.19	107.41	112.60
28	H	25	LEU	N-CA-C	5.19	121.28	109.81
34	AA	2809	A	C2'-C3'-O3'	5.19	117.29	109.50
34	AA	1218	C	C5'-C4'-C3'	-5.19	108.22	116.00
39	AO	113	ASN	N-CA-C	5.19	117.41	110.35
34	AA	888	A	C2'-C3'-O3'	5.19	117.28	109.50
34	AA	1436	A	P-O5'-C5'	5.19	128.68	120.90
34	AA	3774	A	P-O5'-C5'	5.19	128.68	120.90
12	W	24	LEU	N-CA-C	5.18	117.40	110.35
1	A	789	U	C2'-C3'-O3'	5.18	121.47	113.70
14	I	170	ASN	CA-CB-CG	-5.18	107.42	112.60
39	AO	39	HIS	N-CA-C	5.18	116.74	111.14
74	AH	140	LYS	N-CA-C	5.17	116.92	111.28
34	AA	2144	U	P-O5'-C5'	5.17	128.66	120.90
62	AR	292	LEU	N-CA-C	5.17	116.60	111.07
1	A	25	C	C2'-C3'-O3'	5.17	117.25	109.50
42	A4	40	PHE	CA-CB-CG	-5.17	108.63	113.80
54	AP	149	ILE	CA-C-N	5.17	131.41	121.54
54	AP	149	ILE	C-N-CA	5.17	131.41	121.54
32	P	58	GLY	CA-C-N	5.16	126.59	120.14
32	P	58	GLY	C-N-CA	5.16	126.59	120.14
54	AP	13	LYS	N-CA-C	5.16	116.59	111.07
48	A9	70	THR	CA-C-N	5.16	127.50	120.54
48	A9	70	THR	C-N-CA	5.16	127.50	120.54
35	AC	67	G	C4'-C3'-C2'	-5.16	97.44	102.60
71	AF	368	LEU	CA-C-N	5.16	127.19	120.28
71	AF	368	LEU	C-N-CA	5.16	127.19	120.28
77	AX	117	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	A	1845	U	C5'-C4'-C3'	-5.15	108.27	116.00
34	AA	2590	U	C2'-C3'-O3'	5.15	117.23	109.50
74	AH	43	ILE	N-CA-C	5.15	117.92	109.78
66	AZ	62	ASN	CA-CB-CG	-5.15	107.45	112.60
34	AA	122	A	O5'-C5'-C4'	5.15	119.42	111.70
34	AA	3782	A	P-O3'-C3'	5.15	127.92	120.20
1	A	492	A	P-O5'-C5'	5.15	128.62	120.90
4	S	49	GLN	CA-C-N	5.15	127.17	120.28
4	S	49	GLN	C-N-CA	5.15	127.17	120.28
48	A9	60	PHE	CA-CB-CG	-5.14	108.66	113.80
65	AT	164	LYS	CA-C-N	5.14	127.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	AT	164	LYS	C-N-CA	5.14	127.17	120.28
34	AA	904	G	C2'-C3'-O3'	5.14	117.21	109.50
34	AA	2146	A	C2'-C3'-O3'	5.14	117.21	109.50
34	AA	3408	G	C2'-C3'-O3'	5.14	117.21	109.50
34	AA	3782	A	C2'-C3'-O3'	5.14	117.21	109.50
35	AC	67	G	C2'-C3'-O3'	5.14	117.21	109.50
34	AA	1574	C	O4'-C1'-N1	5.14	116.21	108.50
56	AI	102	ARG	NE-CZ-NH1	-5.14	116.36	121.50
24	6	8	LEU	CA-C-N	5.13	127.16	120.28
24	6	8	LEU	C-N-CA	5.13	127.16	120.28
34	AA	3129	U	P-O3'-C3'	5.13	127.90	120.20
50	Ab	103	LEU	CA-C-N	5.13	127.16	120.28
50	Ab	103	LEU	C-N-CA	5.13	127.16	120.28
62	AR	233	ASP	CA-CB-CG	-5.13	107.47	112.60
56	AI	113	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	1300	G	C2'-C3'-O3'	5.13	121.39	113.70
34	AA	2220	U	O5'-C5'-C4'	5.13	119.19	111.50
34	AA	3617	A	O4'-C1'-N9	5.13	115.89	108.20
74	AH	42	PRO	CA-C-N	5.13	127.48	120.35
74	AH	42	PRO	C-N-CA	5.13	127.48	120.35
34	AA	207	A	O3'-P-O5'	-5.12	96.32	104.00
1	A	1980	A	C4'-C3'-C2'	-5.12	97.48	102.60
69	AD	242	ARG	NE-CZ-NH2	5.12	123.81	119.20
71	AF	343	MET	CA-C-N	5.12	127.39	120.38
71	AF	343	MET	C-N-CA	5.12	127.39	120.38
70	AE	137	PRO	N-CA-C	5.12	119.25	111.11
13	R	96	TRP	N-CA-C	5.12	116.86	111.28
20	C	130	ALA	N-CA-C	5.12	116.86	111.28
1	A	32	U	P-O3'-C3'	-5.11	112.53	120.20
42	A4	7	HIS	CB-CA-C	-5.11	102.16	110.85
28	H	188	ARG	CA-C-N	5.11	127.13	120.28
28	H	188	ARG	C-N-CA	5.11	127.13	120.28
73	AU	168	LYS	CA-C-N	5.11	127.38	120.38
73	AU	168	LYS	C-N-CA	5.11	127.38	120.38
34	AA	2033	C	P-O3'-C3'	5.11	127.86	120.20
34	AA	890	G	P-O5'-C5'	5.11	128.56	120.90
66	AZ	11	ARG	NE-CZ-NH1	-5.11	116.39	121.50
12	W	10	LYS	CA-C-N	5.10	127.08	120.44
12	W	10	LYS	C-N-CA	5.10	127.08	120.44
74	AH	176	ASP	N-CA-C	5.10	117.49	110.35
13	R	132	LEU	CA-C-N	5.10	127.12	120.28
13	R	132	LEU	C-N-CA	5.10	127.12	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	I	67	MET	N-CA-C	5.10	116.53	111.07
42	A4	65	LYS	N-CA-C	5.10	116.92	111.36
25	B	50	LYS	CA-C-N	5.10	127.11	120.28
25	B	50	LYS	C-N-CA	5.10	127.11	120.28
60	AS	55	PRO	CA-C-N	5.10	127.37	120.38
60	AS	55	PRO	C-N-CA	5.10	127.37	120.38
25	B	138	PHE	CA-CB-CG	-5.09	108.71	113.80
29	K	64	ASN	CA-CB-CG	-5.09	107.51	112.60
34	AA	2807	U	P-O5'-C5'	5.09	128.54	120.90
52	Ae	46	ARG	NE-CZ-NH1	-5.09	116.41	121.50
72	AG	28	ASP	CA-C-N	5.09	127.10	120.28
72	AG	28	ASP	C-N-CA	5.09	127.10	120.28
34	AA	109	A	P-O3'-C3'	5.09	127.83	120.20
11	G	110	PHE	CA-CB-CG	-5.08	108.72	113.80
34	AA	3195	C	O4'-C1'-N1	5.08	115.83	108.20
60	AS	23	ASN	CA-C-N	5.08	124.26	118.97
60	AS	23	ASN	C-N-CA	5.08	124.26	118.97
34	AA	59	G	P-O5'-C5'	5.08	128.52	120.90
20	C	35	ARG	NE-CZ-NH2	5.08	123.77	119.20
34	AA	197	G	C2'-C3'-O3'	5.08	117.12	109.50
35	AC	134	G	C2'-C3'-O3'	5.08	121.32	113.70
57	Ac	88	LYS	CA-C-N	5.08	125.07	119.89
57	Ac	88	LYS	C-N-CA	5.08	125.07	119.89
3	Q	79	ASN	CA-CB-CG	-5.07	107.53	112.60
34	AA	2039	U	P-O3'-C3'	5.07	127.81	120.20
34	AA	773	A	C4'-C3'-C2'	-5.07	97.53	102.60
34	AA	2215	G	P-O3'-C3'	5.07	127.81	120.20
34	AA	2125	A	C2'-C3'-O3'	5.07	117.10	109.50
78	AJ	117	LYS	N-CA-C	5.07	116.88	109.84
49	Aa	39	ALA	CA-C-N	5.06	124.91	120.10
49	Aa	39	ALA	C-N-CA	5.06	124.91	120.10
47	A8	64	LYS	N-CA-C	5.06	119.72	111.37
65	AT	172	ARG	CA-C-N	5.06	127.06	120.28
65	AT	172	ARG	C-N-CA	5.06	127.06	120.28
71	AF	363	ILE	N-CA-C	5.06	115.28	110.42
34	AA	62	A	C2'-C3'-O3'	5.05	121.28	113.70
37	AL	111	ASN	CA-CB-CG	-5.05	107.55	112.60
62	AR	59	GLN	N-CA-CB	5.05	119.03	110.49
41	A2	3	ASN	N-CA-C	5.05	116.79	111.28
16	Y	74	ASP	CA-C-N	5.05	127.05	120.28
16	Y	74	ASP	C-N-CA	5.05	127.05	120.28
22	4	47	HIS	CA-CB-CG	5.05	118.85	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	AF	50	HIS	CB-CA-C	-5.05	104.10	109.85
30	J	132	SER	N-CA-C	5.04	120.96	109.81
33	L	29	LEU	N-CA-C	5.04	121.54	110.80
34	AA	1223	U	C2'-C3'-O3'	5.04	121.26	113.70
1	A	1370	U	C1'-O4'-C4'	-5.04	104.66	109.70
33	L	188	ARG	CA-C-N	5.04	125.06	119.32
33	L	188	ARG	C-N-CA	5.04	125.06	119.32
62	AR	71	GLY	CA-C-N	5.04	127.92	120.82
62	AR	71	GLY	C-N-CA	5.04	127.92	120.82
65	AT	56	VAL	N-CA-C	5.04	119.82	109.34
75	AV	51	LYS	N-CA-C	5.04	116.85	111.36
1	A	614	A	C2'-C3'-O3'	5.04	117.05	109.50
35	AC	114	A	C4'-C3'-O3'	5.03	116.95	109.40
58	AK	114	LYS	N-CA-C	5.03	117.59	110.50
34	AA	3390	U	P-O5'-C5'	-5.03	113.36	120.90
74	AH	167	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	A	1056	G	C2'-C3'-O3'	5.03	121.24	113.70
68	A5	231	ARG	NE-CZ-NH2	5.03	123.72	119.20
74	AH	63	PRO	CA-C-N	5.03	126.97	120.44
74	AH	63	PRO	C-N-CA	5.03	126.97	120.44
56	AI	87	GLY	CA-C-N	5.02	126.12	119.84
56	AI	87	GLY	C-N-CA	5.02	126.12	119.84
59	AM	50	ARG	N-CA-C	5.02	117.18	110.35
1	A	1108	A	C4'-C3'-C2'	-5.02	97.58	102.60
49	Aa	41	LYS	CA-C-N	5.02	125.02	119.90
49	Aa	41	LYS	C-N-CA	5.02	125.02	119.90
71	AF	372	ASN	CA-CB-CG	-5.02	107.58	112.60
1	A	107	A	P-O3'-C3'	5.02	127.72	120.20
2	7	25	C	C5'-C4'-O4'	-5.02	102.27	109.80
22	4	14	SER	CA-C-N	5.02	127.51	120.28
22	4	14	SER	C-N-CA	5.02	127.51	120.28
35	AC	43	G	C2'-C3'-O3'	5.01	117.02	109.50
36	AB	109	U	C2'-C3'-O3'	5.01	117.02	109.50
39	AO	35	ALA	N-CA-C	5.01	116.75	111.28
12	W	53	PHE	CA-CB-CG	-5.01	108.79	113.80
13	R	42	ILE	N-CA-C	5.01	119.76	109.34
40	Ai	53	THR	CA-C-N	5.01	128.26	120.60
40	Ai	53	THR	C-N-CA	5.01	128.26	120.60
34	AA	521	U	P-O3'-C3'	5.01	127.71	120.20
70	AE	6	PHE	CA-CB-CG	-5.01	108.79	113.80
1	A	745	A	C4'-C3'-O3'	5.01	116.91	109.40
11	G	193	ALA	CA-C-N	5.00	126.09	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	193	ALA	C-N-CA	5.00	126.09	119.84
38	A0	18	TYR	N-CA-C	5.00	116.98	110.43
54	AP	83	LYS	CA-C-N	5.00	125.02	119.32
54	AP	83	LYS	C-N-CA	5.00	125.02	119.32

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	7	31	G	C3'
25	B	225	ILE	CB
34	AA	3018	A	C3'
41	A2	55	THR	CA
41	A2	116	SER	CA

All (692) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	1	107	ARG	Sidechain
18	1	12	TYR	Sidechain
18	1	88	LYS	Peptide
19	2	76	ARG	Sidechain
21	3	10	ARG	Sidechain
21	3	15	ARG	Sidechain
23	5	26	ARG	Sidechain
24	6	10	ARG	Sidechain
24	6	33	ARG	Sidechain
24	6	40	TYR	Sidechain
24	6	43	ARG	Peptide
2	7	12	G	Sidechain
2	7	19	G	Sidechain
2	7	27	U	Sidechain
2	7	54	U	Sidechain
2	7	69	C	Sidechain
1	A	1008	A	Sidechain
1	A	1022	A	Sidechain
1	A	1026	A	Sidechain
1	A	103	U	Sidechain
1	A	1041	G	Sidechain
1	A	1056	G	Sidechain
1	A	1060	G	Sidechain
1	A	1068	U	Sidechain
1	A	1077	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1086	U	Sidechain
1	A	1104	G	Sidechain
1	A	1123	G	Sidechain
1	A	1188	A	Sidechain
1	A	1193	A	Sidechain
1	A	1195	G	Sidechain
1	A	1198	U	Sidechain
1	A	1201	G	Sidechain
1	A	1204	U	Sidechain
1	A	1208	G	Sidechain
1	A	1209	G	Sidechain
1	A	1220	C	Sidechain
1	A	1223	G	Sidechain
1	A	1240	A	Sidechain
1	A	1241	A	Sidechain
1	A	1242	G	Sidechain
1	A	1258	A	Sidechain
1	A	1264	A	Sidechain
1	A	1272	A	Sidechain
1	A	1283	U	Sidechain
1	A	1289	G	Sidechain
1	A	1307	U	Sidechain
1	A	1308	C	Sidechain
1	A	1362	U	Sidechain
1	A	1368	G	Sidechain
1	A	1377	U	Sidechain
1	A	1414	A	Sidechain
1	A	1415	A	Sidechain
1	A	1423	A	Sidechain
1	A	143	A	Sidechain
1	A	1436	U	Sidechain
1	A	1445	U	Sidechain
1	A	1457	A	Sidechain
1	A	148	U	Sidechain
1	A	161	U	Sidechain
1	A	1655	G	Sidechain
1	A	1656	A	Sidechain
1	A	1658	G	Sidechain
1	A	168	U	Sidechain
1	A	1683	U	Sidechain
1	A	1684	G	Sidechain
1	A	1719	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1720	G	Sidechain
1	A	1800	A	Sidechain
1	A	1819	U	Sidechain
1	A	182	U	Sidechain
1	A	1823	U	Sidechain
1	A	1828	A	Sidechain
1	A	1834	A	Sidechain
1	A	1835	U	Sidechain
1	A	1839	G	Sidechain
1	A	1845	U	Sidechain
1	A	1850	G	Sidechain
1	A	1865	G	Sidechain
1	A	1872	G	Sidechain
1	A	1876	G	Sidechain
1	A	1877	C	Sidechain
1	A	1881	G	Sidechain
1	A	1882	U	Sidechain
1	A	1906	U	Sidechain
1	A	1928	A	Sidechain
1	A	1939	G	Sidechain
1	A	1940	U	Sidechain
1	A	1953	U	Sidechain
1	A	1955	G	Sidechain
1	A	1972	G	Sidechain
1	A	1977	G	Sidechain
1	A	1979	C	Sidechain
1	A	201	G	Sidechain
1	A	2032	U	Sidechain
1	A	2059	G	Sidechain
1	A	207	G	Sidechain
1	A	2072	G	Sidechain
1	A	2073	A	Sidechain
1	A	245	A	Sidechain
1	A	263	A	Sidechain
1	A	292	G	Sidechain
1	A	3	C	Sidechain
1	A	310	U	Sidechain
1	A	328	G	Sidechain
1	A	343	G	Sidechain
1	A	38	C	Sidechain
1	A	39	A	Sidechain
1	A	393	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	396	G	Sidechain
1	A	402	G	Sidechain
1	A	403	A	Sidechain
1	A	408	U	Sidechain
1	A	440	G	Sidechain
1	A	441	U	Sidechain
1	A	457	A	Sidechain
1	A	47	A	Sidechain
1	A	493	G	Sidechain
1	A	522	G	Sidechain
1	A	546	G	Sidechain
1	A	559	G	Sidechain
1	A	573	C	Sidechain
1	A	577	A	Sidechain
1	A	580	C	Sidechain
1	A	583	G	Sidechain
1	A	587	A	Sidechain
1	A	589	U	Sidechain
1	A	598	A	Sidechain
1	A	616	U	Sidechain
1	A	617	G	Sidechain
1	A	62	A	Sidechain
1	A	620	G	Sidechain
1	A	623	G	Sidechain
1	A	625	U	Sidechain
1	A	626	A	Sidechain
1	A	629	A	Sidechain
1	A	638	G	Sidechain
1	A	64	U	Sidechain
1	A	751	U	Sidechain
1	A	759	C	Sidechain
1	A	791	U	Sidechain
1	A	802	A	Sidechain
1	A	814	U	Sidechain
1	A	829	G	Sidechain
1	A	850	G	Sidechain
1	A	857	A	Sidechain
1	A	879	A	Sidechain
1	A	894	U	Sidechain
1	A	939	A	Sidechain
1	A	942	U	Sidechain
1	A	943	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	953	C	Sidechain
1	A	954	G	Sidechain
1	A	966	C	Sidechain
1	A	967	A	Sidechain
1	A	975	A	Sidechain
1	A	987	U	Sidechain
38	A0	38	TYR	Sidechain
67	A3	105	ARG	Sidechain
42	A4	14	ARG	Sidechain
42	A4	30	MET	Peptide
42	A4	32	ARG	Sidechain
42	A4	7	HIS	Sidechain,Peptide
68	A5	109	ARG	Sidechain
68	A5	164	ARG	Sidechain
68	A5	222	PRO	Peptide
68	A5	245	ARG	Sidechain
68	A5	255	ARG	Sidechain
43	A6	56	ARG	Sidechain
44	A7	45	ARG	Sidechain
47	A8	13	ARG	Sidechain
47	A8	36	ARG	Sidechain
47	A8	92	TYR	Sidechain
48	A9	130	ARG	Sidechain
48	A9	39	ARG	Sidechain
48	A9	51	ARG	Sidechain
34	AA	1013	U	Sidechain
34	AA	1053	U	Sidechain
34	AA	1065	U	Sidechain
34	AA	1073	G	Sidechain
34	AA	109	A	Sidechain
34	AA	1095	U	Sidechain
34	AA	1096	G	Sidechain
34	AA	1101	A	Sidechain
34	AA	1103	A	Sidechain
34	AA	1109	U	Sidechain
34	AA	1115	G	Sidechain
34	AA	1116	G	Sidechain
34	AA	1122	A	Sidechain
34	AA	1135	G	Sidechain
34	AA	1141	G	Sidechain
34	AA	1158	G	Sidechain
34	AA	116	A	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	1172	C	Sidechain
34	AA	1188	A	Sidechain
34	AA	1193	G	Sidechain
34	AA	1196	A	Sidechain
34	AA	1204	A	Sidechain
34	AA	1224	A	Sidechain
34	AA	1243	G	Sidechain
34	AA	1255	G	Sidechain
34	AA	1256	U	Sidechain
34	AA	1264	A	Sidechain
34	AA	1274	A	Sidechain
34	AA	1280	G	Sidechain
34	AA	1282	U	Sidechain
34	AA	1294	G	Sidechain
34	AA	132	U	Sidechain
34	AA	1321	A	Sidechain
34	AA	1329	U	Sidechain
34	AA	1330	A	Sidechain
34	AA	1331	A	Sidechain
34	AA	136	U	Sidechain
34	AA	1429	A	Sidechain
34	AA	1436	A	Sidechain
34	AA	1443	U	Sidechain
34	AA	1445	A	Sidechain
34	AA	1446	A	Sidechain
34	AA	1447	G	Sidechain
34	AA	1458	A	Sidechain
34	AA	147	C	Sidechain
34	AA	1470	A	Sidechain
34	AA	1476	A	Sidechain
34	AA	1497	U	Sidechain
34	AA	1510	U	Sidechain
34	AA	1516	G	Sidechain
34	AA	153	A	Sidechain
34	AA	1534	U	Sidechain
34	AA	1538	U	Sidechain
34	AA	1540	G	Sidechain
34	AA	1552	G	Sidechain
34	AA	156	U	Sidechain
34	AA	1560	U	Sidechain
34	AA	1563	U	Sidechain
34	AA	1565	G	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	1575	C	Sidechain
34	AA	1586	C	Sidechain
34	AA	1588	U	Sidechain
34	AA	1595	A	Sidechain
34	AA	1597	U	Sidechain
34	AA	1613	G	Sidechain
34	AA	1618	C	Sidechain
34	AA	1619	U	Sidechain
34	AA	1628	U	Sidechain
34	AA	1629	G	Sidechain
34	AA	1643	U	Sidechain
34	AA	1644	U	Sidechain
34	AA	1645	U	Sidechain
34	AA	1647	U	Sidechain
34	AA	1650	U	Sidechain
34	AA	1661	U	Sidechain
34	AA	1674	G	Sidechain
34	AA	1695	A	Sidechain
34	AA	1703	U	Sidechain
34	AA	1735	G	Sidechain
34	AA	1740	A	Sidechain
34	AA	1763	G	Sidechain
34	AA	1784	G	Sidechain
34	AA	1785	U	Sidechain
34	AA	1786	A	Sidechain
34	AA	1797	A	Sidechain
34	AA	1820	U	Sidechain
34	AA	1821	U	Sidechain
34	AA	183	U	Sidechain
34	AA	1844	G	Sidechain
34	AA	1848	U	Sidechain
34	AA	1849	U	Sidechain
34	AA	1853	C	Sidechain
34	AA	1855	U	Sidechain
34	AA	1867	U	Sidechain
34	AA	1870	G	Sidechain
34	AA	1896	C	Sidechain
34	AA	1899	U	Sidechain
34	AA	190	G	Sidechain
34	AA	1902	A	Sidechain
34	AA	191	A	Sidechain
34	AA	1913	A	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	193	C	Sidechain
34	AA	1964	G	Sidechain
34	AA	1997	G	Sidechain
34	AA	20	G	Sidechain
34	AA	2004	U	Sidechain
34	AA	201	G	Sidechain
34	AA	2040	G	Sidechain
34	AA	205	G	Sidechain
34	AA	2081	U	Sidechain
34	AA	2084	U	Sidechain
34	AA	2102	A	Sidechain
34	AA	2104	C	Sidechain
34	AA	2107	C	Sidechain
34	AA	2109	A	Sidechain
34	AA	211	U	Sidechain
34	AA	2125	A	Sidechain
34	AA	2153	A	Sidechain
34	AA	2157	G	Sidechain
34	AA	2172	C	Sidechain
34	AA	2176	A	Sidechain
34	AA	219	A	Sidechain
34	AA	2202	G	Sidechain
34	AA	2207	G	Sidechain
34	AA	2219	A	Sidechain
34	AA	240	U	Sidechain
34	AA	2403	G	Sidechain
34	AA	2409	G	Sidechain
34	AA	2423	G	Sidechain
34	AA	2429	U	Sidechain
34	AA	2435	A	Sidechain
34	AA	2450	G	Sidechain
34	AA	2452	A	Sidechain
34	AA	246	U	Sidechain
34	AA	2460	A	Sidechain
34	AA	2473	A	Sidechain
34	AA	2481	A	Sidechain
34	AA	2497	U	Sidechain
34	AA	2498	U	Sidechain
34	AA	25	A	Sidechain
34	AA	2514	G	Sidechain
34	AA	2515	A	Sidechain
34	AA	2551	U	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	2554	G	Sidechain
34	AA	2562	U	Sidechain
34	AA	2564	A	Sidechain
34	AA	2565	G	Sidechain
34	AA	2590	U	Sidechain
34	AA	26	A	Sidechain
34	AA	261	A	Sidechain
34	AA	2614	A	Sidechain
34	AA	265	U	Sidechain
34	AA	2652	C	Sidechain
34	AA	2654	A	Sidechain
34	AA	2657	G	Sidechain
34	AA	2660	A	Sidechain
34	AA	2665	A	Sidechain
34	AA	2669	G	Sidechain
34	AA	2679	A	Sidechain
34	AA	2693	G	Sidechain
34	AA	2698	C	Sidechain
34	AA	2727	U	Sidechain
34	AA	2728	G	Sidechain
34	AA	2809	A	Sidechain
34	AA	2835	G	Sidechain
34	AA	2838	A	Sidechain
34	AA	2917	C	Sidechain
34	AA	293	U	Sidechain
34	AA	2932	A	Sidechain
34	AA	2945	G	Sidechain
34	AA	2956	U	Sidechain
34	AA	2963	G	Sidechain
34	AA	297	G	Sidechain
34	AA	2981	A	Sidechain
34	AA	3011	G	Sidechain
34	AA	3016	G	Sidechain
34	AA	3017	A	Sidechain
34	AA	3033	A	Sidechain
34	AA	3035	A	Sidechain
34	AA	3036	A	Sidechain
34	AA	3037	G	Sidechain
34	AA	304	U	Sidechain
34	AA	3062	U	Sidechain
34	AA	3063	U	Sidechain
34	AA	3066	A	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	308	U	Sidechain
34	AA	3082	G	Sidechain
34	AA	3084	G	Sidechain
34	AA	309	G	Sidechain
34	AA	3091	U	Sidechain
34	AA	3097	A	Sidechain
34	AA	3108	A	Sidechain
34	AA	3138	A	Sidechain
34	AA	3152	G	Sidechain
34	AA	3155	G	Sidechain
34	AA	3160	A	Sidechain
34	AA	3186	U	Sidechain
34	AA	319	U	Sidechain
34	AA	3192	U	Sidechain
34	AA	3195	C	Sidechain
34	AA	3209	G	Sidechain
34	AA	3210	A	Sidechain
34	AA	3220	U	Sidechain
34	AA	3222	G	Sidechain
34	AA	3227	U	Sidechain
34	AA	3239	U	Sidechain
34	AA	3245	U	Sidechain
34	AA	325	A	Sidechain
34	AA	3257	G	Sidechain
34	AA	3260	G	Sidechain
34	AA	3268	A	Sidechain
34	AA	3271	G	Sidechain
34	AA	3283	U	Sidechain
34	AA	3300	A	Sidechain
34	AA	331	A	Sidechain
34	AA	3313	U	Sidechain
34	AA	3325	G	Sidechain
34	AA	3341	A	Sidechain
34	AA	3388	U	Sidechain
34	AA	3391	G	Sidechain
34	AA	3412	G	Sidechain
34	AA	3415	A	Sidechain
34	AA	3436	U	Sidechain
34	AA	344	A	Sidechain
34	AA	3455	A	Sidechain
34	AA	346	A	Sidechain
34	AA	3463	G	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	3484	U	Sidechain
34	AA	349	G	Sidechain
34	AA	3499	C	Sidechain
34	AA	3503	U	Sidechain
34	AA	3505	U	Sidechain
34	AA	3509	G	Sidechain
34	AA	3538	A	Sidechain
34	AA	3589	U	Sidechain
34	AA	36	U	Sidechain
34	AA	3614	A	Sidechain
34	AA	3618	A	Sidechain
34	AA	3639	G	Sidechain
34	AA	3646	G	Sidechain
34	AA	3658	G	Sidechain
34	AA	3660	A	Sidechain
34	AA	367	U	Sidechain
34	AA	368	G	Sidechain
34	AA	3683	G	Sidechain
34	AA	3707	U	Sidechain
34	AA	3725	G	Sidechain
34	AA	3738	U	Sidechain
34	AA	3739	A	Sidechain
34	AA	3749	U	Sidechain
34	AA	3783	G	Sidechain
34	AA	379	G	Sidechain
34	AA	38	U	Sidechain
34	AA	380	A	Sidechain
34	AA	401	A	Sidechain
34	AA	41	G	Sidechain
34	AA	416	G	Sidechain
34	AA	436	G	Sidechain
34	AA	440	A	Sidechain
34	AA	441	A	Sidechain
34	AA	458	A	Sidechain
34	AA	46	U	Sidechain
34	AA	467	U	Sidechain
34	AA	497	U	Sidechain
34	AA	500	A	Sidechain
34	AA	503	A	Sidechain
34	AA	525	U	Sidechain
34	AA	527	A	Sidechain
34	AA	528	A	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	582	U	Sidechain
34	AA	583	U	Sidechain
34	AA	599	G	Sidechain
34	AA	606	A	Sidechain
34	AA	61	A	Sidechain
34	AA	632	U	Sidechain
34	AA	633	U	Sidechain
34	AA	643	G	Sidechain
34	AA	644	G	Sidechain
34	AA	652	A	Sidechain
34	AA	673	U	Sidechain
34	AA	684	G	Sidechain
34	AA	685	U	Sidechain
34	AA	688	U	Sidechain
34	AA	69	U	Sidechain
34	AA	70	A	Sidechain
34	AA	702	U	Sidechain
34	AA	706	U	Sidechain
34	AA	707	U	Sidechain
34	AA	708	A	Sidechain
34	AA	71	A	Sidechain
34	AA	716	C	Sidechain
34	AA	729	G	Sidechain
34	AA	734	A	Sidechain
34	AA	744	G	Sidechain
34	AA	746	A	Sidechain
34	AA	76	G	Sidechain
34	AA	760	A	Sidechain
34	AA	765	A	Sidechain
34	AA	769	U	Sidechain
34	AA	795	G	Sidechain
34	AA	802	U	Sidechain
34	AA	824	U	Sidechain
34	AA	825	G	Sidechain
34	AA	86	G	Sidechain
34	AA	869	A	Sidechain
34	AA	87	U	Sidechain
34	AA	884	A	Sidechain
34	AA	910	A	Sidechain
34	AA	911	U	Sidechain
34	AA	912	U	Sidechain
34	AA	913	U	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	915	G	Sidechain
34	AA	917	A	Sidechain
34	AA	919	G	Sidechain
34	AA	92	G	Sidechain
34	AA	924	G	Sidechain
34	AA	925	A	Sidechain
34	AA	926	G	Sidechain
34	AA	938	U	Sidechain
34	AA	939	A	Sidechain
34	AA	94	G	Sidechain
34	AA	943	G	Sidechain
34	AA	954	G	Sidechain
34	AA	964	G	Sidechain
34	AA	967	A	Sidechain
34	AA	976	G	Sidechain
34	AA	981	U	Sidechain
34	AA	988	G	Sidechain
36	AB	11	A	Sidechain
36	AB	117	C	Sidechain
36	AB	48	G	Sidechain
36	AB	50	A	Sidechain
36	AB	56	G	Sidechain
36	AB	61	G	Sidechain
36	AB	79	U	Sidechain
36	AB	9	U	Sidechain
35	AC	103	G	Sidechain
35	AC	12	U	Sidechain
35	AC	121	C	Sidechain
35	AC	18	U	Sidechain
35	AC	20	G	Sidechain
35	AC	30	U	Sidechain
35	AC	31	U	Sidechain
35	AC	32	C	Sidechain
35	AC	40	G	Sidechain
35	AC	5	A	Sidechain
35	AC	64	U	Sidechain
35	AC	67	G	Sidechain
35	AC	89	U	Sidechain
69	AD	122	ASN	Peptide
69	AD	123	ARG	Sidechain
69	AD	163	ARG	Sidechain
69	AD	193	ARG	Sidechain

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Mol	Chain	Res	Type	Group
70	AE	10	ARG	Sidechain
70	AE	275	ARG	Sidechain
70	AE	345	ARG	Sidechain
70	AE	366	ARG	Sidechain
70	AE	92	TYR	Sidechain
70	AE	93	ARG	Sidechain
71	AF	113	ARG	Sidechain
71	AF	121	ARG	Sidechain
71	AF	140	ARG	Sidechain
71	AF	190	ARG	Sidechain
71	AF	199	ARG	Sidechain
71	AF	201	TYR	Peptide
71	AF	286	ASN	Peptide
71	AF	327	ARG	Sidechain
71	AF	50	HIS	Peptide
71	AF	97	ARG	Sidechain
72	AG	133	ARG	Sidechain
72	AG	141	ARG	Sidechain
72	AG	144	ARG	Sidechain
74	AH	123	ARG	Sidechain
74	AH	23	ARG	Sidechain
56	AI	102	ARG	Sidechain
56	AI	48	ARG	Sidechain
78	AJ	188	ARG	Sidechain
78	AJ	73	ARG	Sidechain
58	AK	132	ARG	Sidechain
58	AK	148	TYR	Sidechain
58	AK	159	ARG	Sidechain
58	AK	166	TYR	Sidechain
58	AK	17	ARG	Sidechain
58	AK	60	ARG	Sidechain
58	AK	73	ARG	Sidechain
58	AK	84	ARG	Sidechain
37	AL	138	GLY	Peptide
37	AL	140	PRO	Peptide
37	AL	202	ARG	Sidechain
37	AL	22	ARG	Sidechain
37	AL	34	ARG	Sidechain
37	AL	67	ARG	Sidechain
37	AL	8	LEU	Peptide
46	AN	120	ARG	Sidechain
46	AN	35	TYR	Sidechain

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Mol	Chain	Res	Type	Group
46	AN	73	ARG	Sidechain
39	AO	9	ARG	Sidechain
54	AP	111	CYS	Peptide
54	AP	112	GLY	Peptide
54	AP	163	ARG	Sidechain
54	AP	176	ARG	Sidechain
54	AP	186	ARG	Sidechain
54	AP	196	ARG	Sidechain
54	AP	50	ARG	Sidechain
61	AQ	128	ARG	Sidechain
61	AQ	154	ARG	Sidechain
61	AQ	22	TYR	Sidechain
61	AQ	38	ARG	Sidechain
61	AQ	88	ARG	Sidechain
61	AQ	98	ARG	Sidechain
62	AR	141	ARG	Sidechain
62	AR	154	ARG	Sidechain
62	AR	160	ARG	Sidechain
62	AR	21	ARG	Sidechain
62	AR	24	ARG	Sidechain
62	AR	31	ARG	Sidechain
62	AR	33	ARG	Sidechain
60	AS	10	ARG	Sidechain
60	AS	103	ARG	Sidechain
60	AS	111	ARG	Sidechain
60	AS	145	ARG	Sidechain
60	AS	165	TYR	Sidechain
60	AS	183	ARG	Sidechain
60	AS	27	ARG	Sidechain
60	AS	39	ARG	Sidechain
60	AS	59	ARG	Sidechain
65	AT	109	ARG	Sidechain
65	AT	116	ARG	Sidechain
65	AT	99	ARG	Sidechain
73	AU	122	ARG	Sidechain
73	AU	145	ARG	Sidechain
73	AU	170	TYR	Sidechain
73	AU	35	ARG	Sidechain
73	AU	49	ARG	Sidechain
75	AV	31	TYR	Sidechain,Peptide
75	AV	33	GLU	Peptide
75	AV	40	TYR	Sidechain

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Mol	Chain	Res	Type	Group
75	AV	71	ARG	Sidechain
75	AV	80	ARG	Sidechain
63	AW	113	ARG	Sidechain
63	AW	123	ARG	Sidechain
63	AW	135	ARG	Sidechain
63	AW	61	ARG	Sidechain
77	AX	117	ARG	Sidechain
64	AY	173	ARG	Sidechain
66	AZ	120	ARG	Sidechain
66	AZ	26	ARG	Sidechain
66	AZ	50	ARG	Sidechain
66	AZ	59	ARG	Sidechain
49	Aa	4	ARG	Sidechain
49	Aa	66	ARG	Sidechain
50	Ab	40	ARG	Sidechain
50	Ab	89	ARG	Sidechain
50	Ab	94	ARG	Sidechain
57	Ac	24	ARG	Sidechain
57	Ac	28	ARG	Sidechain
57	Ac	49	ARG	Sidechain
51	Ad	16	ARG	Sidechain
51	Ad	44	ARG	Sidechain
52	Ae	18	ARG	Sidechain
52	Ae	8	ARG	Sidechain
53	Af	41	ARG	Sidechain
53	Af	46	ARG	Sidechain
76	Ag	16	ARG	Sidechain
76	Ag	25	ARG	Sidechain
76	Ag	32	ARG	Sidechain
55	Ah	17	ARG	Sidechain
40	Ai	33	ARG	Sidechain
40	Ai	39	ARG	Sidechain
40	Ai	54	LYS	Peptide
25	B	107	ARG	Sidechain
25	B	118	TYR	Sidechain
25	B	136	ARG	Sidechain
25	B	165	ARG	Sidechain
9	E	171	ARG	Sidechain
9	E	69	ARG	Sidechain
9	E	8	TYR	Sidechain
27	F	145	ARG	Sidechain
27	F	221	ARG	Sidechain

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Mol	Chain	Res	Type	Group
27	F	235	TYR	Sidechain
27	F	98	TYR	Sidechain
28	H	104	GLN	Peptide
28	H	177	ARG	Sidechain
28	H	197	ARG	Sidechain
28	H	98	ARG	Sidechain
14	I	136	ARG	Sidechain
14	I	46	ARG	Sidechain
14	I	72	ARG	Sidechain
29	K	118	ARG	Sidechain
33	L	25	ARG	Sidechain
33	L	47	ARG	Sidechain
6	M	112	ARG	Sidechain
6	M	115	ARG	Sidechain
32	P	128	ARG	Sidechain
32	P	141	ARG	Sidechain
32	P	146	ARG	Sidechain
32	P	147	ARG	Sidechain
32	P	50	ARG	Sidechain
3	Q	109	ARG	Sidechain
3	Q	44	ARG	Sidechain
3	Q	69	ARG	Sidechain
3	Q	73	ARG	Sidechain
5	T	17	ARG	Sidechain
7	U	58	TYR	Sidechain
8	V	72	ARG	Sidechain
8	V	85	ARG	Sidechain
8	V	91	ARG	Sidechain
12	W	45	ARG	Sidechain
12	W	60	ARG	Sidechain
12	W	78	ARG	Sidechain
10	X	115	TYR	Sidechain
10	X	123	TYR	Sidechain
16	Y	53	TYR	Peptide
16	Y	79	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34207	0	17266	43	0
2	7	1598	0	816	1	0
3	Q	1129	0	1196	3	0
4	S	1047	0	1101	2	0
5	T	405	0	419	0	0
6	M	1099	0	1183	1	0
7	U	1202	0	1299	1	0
8	V	1206	0	1239	1	0
9	E	1515	0	1605	0	0
10	X	777	0	832	2	0
11	G	1758	0	1811	1	0
12	W	786	0	858	0	0
13	R	747	0	754	0	0
14	I	1424	0	1471	0	0
15	O	687	0	695	0	0
16	Y	1267	0	1316	0	0
17	Z	557	0	558	0	0
18	1	986	0	1076	1	0
19	2	321	0	338	0	0
20	C	1539	0	1600	0	0
21	3	782	0	820	1	0
22	4	586	0	604	1	0
23	5	458	0	496	0	0
24	6	346	0	381	0	0
25	B	1714	0	1838	3	0
26	D	1229	0	1311	0	0
27	F	2062	0	2200	3	0
28	H	1648	0	1803	0	0
29	K	1037	0	1099	2	0
30	J	1529	0	1680	1	0
31	N	772	0	813	0	0
32	P	954	0	997	1	0
33	L	1383	0	1434	0	0
34	AA	67862	0	34233	154	0
35	AC	3215	0	1633	6	0
36	AB	2522	0	1275	2	0
37	AL	1757	0	1888	1	0
38	A0	522	0	539	0	0
39	AO	1172	0	1230	1	0
40	Ai	779	0	861	0	0
41	A2	831	0	887	1	0
42	A4	555	0	599	3	0
43	A6	741	0	763	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	A7	794	0	869	0	0
45	A1	1134	0	1245	1	0
46	AN	1202	0	1316	1	0
47	A8	1037	0	1139	1	0
48	A9	845	0	886	1	0
49	Aa	859	0	912	2	0
50	Ab	757	0	842	1	0
51	Ad	604	0	686	0	0
52	Ae	388	0	421	0	0
53	Af	414	0	452	1	0
54	AP	1697	0	1802	2	0
55	Ah	659	0	727	0	0
56	AI	1685	0	1849	0	0
57	Ac	710	0	761	0	0
58	AK	1660	0	1785	1	0
59	AM	996	0	1044	0	0
60	AS	1503	0	1636	0	0
61	AQ	1545	0	1582	0	0
62	AR	2050	0	2140	2	0
63	AW	1319	0	1303	0	0
64	AY	797	0	850	0	0
65	AT	1509	0	1682	0	0
66	AZ	1001	0	1099	1	0
67	A3	995	0	1121	1	0
68	A5	1879	0	2005	0	0
69	AD	1867	0	1964	1	0
70	AE	3062	0	3205	6	0
71	AF	3095	0	3333	3	0
72	AG	1011	0	1073	1	0
73	AU	1497	0	1556	2	0
74	AH	1476	0	1574	0	0
75	AV	1276	0	1355	1	0
76	Ag	343	0	388	0	0
77	AX	825	0	882	1	0
78	AJ	1813	0	1985	25	0
All	All	193017	0	144286	254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AA:2915:U:C5	34:AA:2915:U:C4	2.03	1.46
34:AA:2915:U:N3	34:AA:2915:U:C2	1.87	1.42
34:AA:2915:U:N1	34:AA:2915:U:C6	1.89	1.39
34:AA:2915:U:C4	34:AA:2915:U:N3	1.89	1.37
34:AA:2915:U:C2	34:AA:2915:U:N1	1.93	1.35
34:AA:2915:U:C4	78:AJ:55:ILE:CD1	2.35	1.09
34:AA:2915:U:C5	78:AJ:55:ILE:CD1	2.35	1.09
34:AA:2915:U:C6	78:AJ:55:ILE:CD1	2.36	1.08
34:AA:2915:U:C2	78:AJ:55:ILE:CD1	2.38	1.06
34:AA:2915:U:C5	78:AJ:55:ILE:CG1	2.39	1.05
34:AA:2915:U:C4	78:AJ:55:ILE:CG1	2.39	1.05
34:AA:2915:U:C2	78:AJ:55:ILE:CG1	2.42	1.02
34:AA:2915:U:C6	78:AJ:55:ILE:CG1	2.41	1.02
34:AA:2915:U:C6	78:AJ:55:ILE:HG12	2.03	0.92
34:AA:2915:U:N3	78:AJ:55:ILE:CD1	2.38	0.87
34:AA:2915:U:C2	78:AJ:55:ILE:HG13	2.10	0.87
34:AA:2915:U:N1	78:AJ:55:ILE:CD1	2.39	0.85
34:AA:2915:U:C5	78:AJ:55:ILE:HG12	2.09	0.85
34:AA:2915:U:N3	78:AJ:55:ILE:CG1	2.42	0.83
34:AA:2915:U:C5	78:AJ:55:ILE:HD13	2.13	0.82
34:AA:2915:U:C4	78:AJ:55:ILE:HD13	2.14	0.82
34:AA:2915:U:C6	78:AJ:55:ILE:HD11	2.14	0.82
34:AA:2915:U:N1	78:AJ:55:ILE:CG1	2.43	0.81
34:AA:2915:U:C2	78:AJ:55:ILE:HD12	2.16	0.81
34:AA:2838:A:N1	34:AA:2916:C:N3	2.40	0.69
34:AA:2915:U:C4	78:AJ:55:ILE:CB	2.77	0.68
34:AA:2915:U:N3	78:AJ:55:ILE:HD12	2.09	0.65
34:AA:2915:U:N1	78:AJ:55:ILE:HD11	2.10	0.65
34:AA:2915:U:N1	78:AJ:55:ILE:HG13	2.10	0.65
34:AA:1072:A:H4'	34:AA:1073:G:H21	1.63	0.63
70:AE:68:HIS:CG	70:AE:69:LYS:H	2.19	0.60
34:AA:2838:A:C2	34:AA:2916:C:C2	2.89	0.59
66:AZ:108:LEU:H	66:AZ:108:LEU:HD23	1.69	0.57
34:AA:123:A:H3'	34:AA:124:U:H5''	1.85	0.57
34:AA:1273:G:H2'	34:AA:1274:A:C8	2.40	0.57
34:AA:1204:A:N6	62:AR:141:ARG:HH22	2.02	0.57
34:AA:3626:A:H3'	34:AA:3627:C:H5''	1.86	0.57
34:AA:3726:U:H4'	34:AA:3727:A:H5''	1.86	0.56
1:A:458:A:H3'	1:A:459:A:C5'	2.35	0.56
4:S:122:HIS:CE1	4:S:126:ARG:HE	2.23	0.56
34:AA:799:A:N6	39:AO:113:ASN:HD21	2.04	0.56
34:AA:2915:U:C4	78:AJ:55:ILE:HB	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AA:2083:U:H2'	34:AA:2084:U:C6	2.43	0.54
34:AA:1263:A:H4'	42:A4:7:HIS:CG	2.43	0.54
34:AA:2981:A:C4	42:A4:7:HIS:CE1	2.96	0.53
34:AA:746:A:H2'	34:AA:747:A:C8	2.43	0.53
34:AA:2657:G:H22	34:AA:2689:G:H1'	1.74	0.53
34:AA:681:U:C6	34:AA:681:U:H5''	2.44	0.53
54:AP:181:LEU:H	54:AP:181:LEU:HD12	1.75	0.52
1:A:1061:A:C2	1:A:1062:A:C8	2.98	0.52
34:AA:2838:A:C6	34:AA:2916:C:N3	2.77	0.52
69:AD:238:ILE:H	69:AD:238:ILE:HD12	1.74	0.52
34:AA:445:A:C2	34:AA:446:G:C4	2.98	0.51
1:A:1672:C:H3'	1:A:1673:A:H5''	1.91	0.51
34:AA:1727:U:H2'	34:AA:1728:C:C6	2.45	0.51
29:K:115:GLU:CD	29:K:118:ARG:HH12	2.19	0.51
34:AA:2084:U:H5''	34:AA:2084:U:H6	1.74	0.51
34:AA:3632:U:H3	34:AA:3653:G:H1	1.59	0.51
6:M:44:ILE:HD12	6:M:44:ILE:H	1.76	0.50
34:AA:909:U:H2'	34:AA:910:A:C8	2.46	0.50
43:A6:103:ILE:HD12	43:A6:103:ILE:H	1.77	0.50
71:AF:268:HIS:CG	71:AF:269:GLU:H	2.30	0.50
1:A:1307:U:H2'	1:A:1308:C:C5	2.46	0.50
34:AA:967:A:C5	34:AA:968:G:H1'	2.47	0.50
1:A:1022:A:H2'	1:A:1023:A:C8	2.47	0.50
34:AA:1822:A:N1	34:AA:2004:U:C4	2.80	0.50
34:AA:2915:U:C2	34:AA:2915:U:C1'	2.89	0.49
34:AA:3035:A:H2'	34:AA:3036:A:C8	2.47	0.49
34:AA:2669:G:H2'	34:AA:2670:G:C8	2.46	0.49
34:AA:3257:G:H3'	34:AA:3258:C:C5'	2.42	0.49
35:AC:149:C:H2'	35:AC:150:U:C6	2.48	0.49
35:AC:30:U:H2'	35:AC:31:U:C6	2.47	0.49
70:AE:68:HIS:CG	70:AE:69:LYS:N	2.79	0.48
1:A:1187:A:H2'	1:A:1188:A:C8	2.49	0.48
34:AA:2496:U:H2'	34:AA:2497:U:C6	2.48	0.48
34:AA:173:A:H3'	34:AA:174:U:H5''	1.95	0.48
34:AA:715:U:H2'	34:AA:716:C:C5	2.49	0.48
1:A:886:U:H2'	1:A:887:A:C8	2.47	0.48
34:AA:34:A:H2'	34:AA:35:A:C8	2.48	0.48
34:AA:445:A:N1	34:AA:702:U:C4	2.81	0.48
34:AA:1644:U:C4	34:AA:2102:A:N1	2.82	0.48
1:A:1832:U:H4'	1:A:1833:G:C4	2.48	0.48
67:A3:119:LEU:HD13	67:A3:120:VAL:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1859:A:H2'	1:A:1860:A:C8	2.49	0.48
34:AA:440:A:H2'	34:AA:441:A:C8	2.48	0.47
34:AA:1758:C:H2'	34:AA:1759:A:C8	2.49	0.47
34:AA:642:A:C5	34:AA:684:G:C8	3.02	0.47
34:AA:2838:A:C2	34:AA:2916:C:N3	2.82	0.47
1:A:2047:A:H3'	1:A:2048:A:H5'	1.96	0.47
25:B:107:ARG:HH21	32:P:131:ASP:CG	2.22	0.47
34:AA:506:A:H2'	34:AA:507:G:C8	2.50	0.47
34:AA:1257:A:H2'	34:AA:1258:A:C8	2.50	0.47
34:AA:2106:A:H5'	34:AA:2107:C:C5	2.49	0.47
27:F:249:ILE:HD12	27:F:249:ILE:H	1.79	0.47
34:AA:916:U:H2'	34:AA:917:A:C8	2.50	0.47
1:A:843:U:H2'	1:A:844:G:C8	2.49	0.46
1:A:1424:A:H2'	1:A:1425:C:C6	2.50	0.46
34:AA:912:U:H2'	34:AA:913:U:C6	2.50	0.46
34:AA:1506:C:H2'	34:AA:1507:U:C6	2.50	0.46
78:AJ:55:ILE:CD1	78:AJ:55:ILE:CG1	2.94	0.46
34:AA:2589:A:H2'	34:AA:2590:U:H5'	1.98	0.46
34:AA:525:U:H2'	34:AA:526:U:C6	2.51	0.46
49:Aa:7:TYR:HB3	49:Aa:12:HIS:CD2	2.51	0.46
1:A:955:U:H2'	1:A:956:A:C8	2.51	0.46
4:S:100:VAL:HG23	4:S:101:ILE:H	1.81	0.46
34:AA:939:A:H2'	34:AA:940:A:C8	2.51	0.46
49:Aa:10:HIS:CD2	49:Aa:11:ASN:H	2.35	0.46
34:AA:3615:A:C6	34:AA:3618:A:C5	3.04	0.45
73:AU:6:ASP:CG	73:AU:7:ASN:H	2.24	0.45
34:AA:2008:G:H2'	34:AA:2009:A:C8	2.51	0.45
34:AA:2590:U:H2'	34:AA:2590:U:O2	2.16	0.45
34:AA:687:G:H2'	34:AA:688:U:C6	2.51	0.45
34:AA:921:C:H2'	34:AA:922:C:C6	2.52	0.45
34:AA:2020:A:H2'	34:AA:2021:A:C8	2.51	0.45
34:AA:293:U:H2'	34:AA:294:G:C8	2.52	0.45
34:AA:2084:U:C6	34:AA:2084:U:H5''	2.52	0.45
34:AA:1574:C:H2'	34:AA:1575:C:C6	2.52	0.45
1:A:1850:G:H3'	10:X:47:ARG:HH12	1.82	0.45
34:AA:320:C:H2'	34:AA:321:A:C8	2.51	0.45
1:A:1720:G:H2'	1:A:1721:A:C8	2.52	0.45
34:AA:88:A:C2	34:AA:99:A:C4	3.05	0.45
34:AA:1216:C:H2'	34:AA:1217:U:H5'	1.98	0.45
34:AA:1675:C:H4'	34:AA:1737:A:C4	2.51	0.45
41:A2:32:LEU:HD23	41:A2:37:ASN:HD21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A9:39:ARG:HH22	48:A9:42:GLU:CD	2.24	0.45
1:A:520:U:H2'	1:A:521:G:C8	2.52	0.44
30:J:69:TYR:CD1	30:J:96:ALA:HB2	2.51	0.44
34:AA:63:A:H2'	34:AA:64:G:C8	2.52	0.44
1:A:149:A:N1	1:A:161:U:C4	2.85	0.44
18:1:20:ARG:HH12	27:F:60:GLU:CD	2.26	0.44
34:AA:2559:U:H2'	34:AA:2560:C:C6	2.52	0.44
34:AA:2709:U:H2'	34:AA:2710:U:C6	2.52	0.44
1:A:1976:G:H3'	1:A:1977:G:C8	2.52	0.44
1:A:1299:G:C6	1:A:1301:G:C6	3.06	0.44
34:AA:659:U:H2'	34:AA:660:U:C6	2.53	0.44
34:AA:1133:A:C2	34:AA:1163:A:C2	3.05	0.44
34:AA:2506:A:H2'	34:AA:2507:A:C8	2.52	0.44
34:AA:3131:A:C6	34:AA:3133:U:H1'	2.52	0.44
34:AA:3511:C:H2'	34:AA:3512:A:C8	2.52	0.44
1:A:2068:A:H2'	1:A:2069:G:C8	2.53	0.44
34:AA:888:A:H3'	34:AA:889:U:H5''	2.00	0.44
34:AA:1628:U:C5	34:AA:1629:G:C5	3.05	0.44
34:AA:1974:U:H2'	34:AA:1975:A:C8	2.52	0.44
34:AA:2672:U:H2'	34:AA:2673:U:C6	2.53	0.44
1:A:1883:A:C5	1:A:1908:A:C2	3.05	0.44
1:A:1448:U:H2'	1:A:1449:U:H2'	2.00	0.44
34:AA:2138:U:H2'	34:AA:2139:C:C6	2.53	0.44
1:A:458:A:H3'	1:A:459:A:H5''	1.99	0.43
1:A:1293:C:H3'	1:A:1294:A:H2'	2.00	0.43
1:A:1815:U:H2'	1:A:1816:U:C5	2.52	0.43
25:B:30:TYR:CE2	25:B:94:ARG:HA	2.54	0.43
34:AA:1093:G:H2'	34:AA:1094:U:C6	2.53	0.43
53:Af:28:HIS:CD2	53:Af:30:ARG:H	2.36	0.43
34:AA:26:A:N6	34:AA:58:A:H61	2.15	0.43
21:3:13:HIS:CD2	21:3:13:HIS:H	2.37	0.43
34:AA:629:A:C2	34:AA:630:U:C2	3.06	0.43
34:AA:1072:A:H3'	34:AA:1245:G:C8	2.53	0.43
34:AA:1096:G:HO2'	34:AA:1097:A:H8	1.66	0.43
35:AC:32:C:H2'	35:AC:33:C:C6	2.54	0.43
34:AA:1435:G:C5	34:AA:1436:A:C6	3.05	0.43
34:AA:2838:A:C2	34:AA:2917:C:C5	3.07	0.43
34:AA:764:G:H2'	34:AA:765:A:C8	2.54	0.43
34:AA:2981:A:H2'	34:AA:2982:A:C8	2.54	0.43
75:AV:45:CYS:H	75:AV:59:HIS:CD2	2.37	0.43
34:AA:136:U:C4	34:AA:141:A:C2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:75:ILE:HD12	11:G:75:ILE:H	1.84	0.43
34:AA:740:U:H2'	34:AA:741:C:C6	2.53	0.43
34:AA:1263:A:H4'	42:A4:7:HIS:ND1	2.34	0.42
62:AR:33:ARG:HH22	62:AR:72:ASP:CG	2.27	0.42
27:F:73:ASP:CG	27:F:145:ARG:HH22	2.27	0.42
34:AA:344:A:C2	34:AA:345:G:C5	3.07	0.42
34:AA:1572:U:C5	34:AA:1573:C:C5	3.07	0.42
70:AE:353:LEU:H	70:AE:353:LEU:HD23	1.83	0.42
34:AA:276:G:H2'	54:AP:121:TRP:CE2	2.55	0.42
34:AA:899:A:H3'	34:AA:900:G:H5''	2.01	0.42
1:A:1675:G:H2'	1:A:1676:U:C6	2.54	0.42
34:AA:3386:A:H2'	34:AA:3387:U:C6	2.54	0.42
45:A1:11:ILE:HG22	45:A1:82:PRO:HA	2.02	0.42
70:AE:71:GLU:CD	70:AE:71:GLU:H	2.27	0.42
34:AA:1683:A:H2'	34:AA:1684:A:C8	2.54	0.42
46:AN:71:LEU:HD13	73:AU:162:HIS:CD2	2.55	0.42
34:AA:734:A:H2'	34:AA:735:A:C8	2.55	0.42
34:AA:2650:A:H2'	34:AA:2651:A:C8	2.55	0.42
34:AA:2884:G:H2'	34:AA:2885:A:H5'	2.01	0.42
1:A:993:A:H2'	1:A:994:G:C8	2.55	0.42
22:4:71:LEU:HG	22:4:72:THR:H	1.84	0.42
34:AA:2122:U:H2'	34:AA:2123:C:C6	2.55	0.42
34:AA:332:A:H2'	34:AA:333:A:C8	2.55	0.42
34:AA:1739:C:H2'	34:AA:1740:A:C8	2.55	0.42
71:AF:290:TYR:CZ	71:AF:294:HIS:CE1	3.08	0.42
1:A:1922:C:H2'	1:A:1923:U:C6	2.55	0.42
34:AA:136:U:O4	34:AA:141:A:C2	2.73	0.42
34:AA:1540:G:C8	34:AA:1565:G:C2	3.08	0.42
34:AA:2563:A:H2'	34:AA:2564:A:C8	2.54	0.42
1:A:1876:G:H2'	1:A:1877:C:C6	2.55	0.41
34:AA:73:U:C6	37:AL:58:HIS:CE1	3.09	0.41
34:AA:580:A:H2'	34:AA:581:C:C6	2.54	0.41
34:AA:1675:C:H4'	34:AA:1737:A:C5	2.55	0.41
72:AG:15:ASN:H	72:AG:130:HIS:CD2	2.38	0.41
77:AX:110:TYR:CE1	77:AX:114:HIS:CE1	3.08	0.41
1:A:576:C:H41	3:Q:69:ARG:NH2	2.17	0.41
1:A:1846:U:C5	10:X:39:ALA:HB3	2.55	0.41
34:AA:914:G:H2'	34:AA:915:G:C8	2.54	0.41
34:AA:3241:U:H2'	34:AA:3242:U:C6	2.55	0.41
1:A:945:G:C6	1:A:1005:G:C6	3.08	0.41
3:Q:29:TYR:CE2	3:Q:33:HIS:CE1	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AA:1184:A:H2'	34:AA:1185:A:C8	2.56	0.41
35:AC:73:A:C6	35:AC:74:A:H1'	2.54	0.41
70:AE:85:VAL:HB	70:AE:160:HIS:CE1	2.55	0.41
25:B:89:ASP:CG	25:B:220:ARG:HH12	2.27	0.41
34:AA:140:A:C5	34:AA:141:A:H1'	2.56	0.41
34:AA:314:A:C2	34:AA:3143:G:H1'	2.56	0.41
35:AC:101:A:H3'	35:AC:102:U:C6	2.56	0.41
1:A:1008:A:H2'	1:A:1009:A:C8	2.55	0.41
1:A:1304:A:C6	1:A:1852:A:C6	3.08	0.41
34:AA:1063:A:H4'	47:A8:33:ARG:HE	1.86	0.41
34:AA:3486:G:H2'	34:AA:3487:A:C8	2.54	0.41
34:AA:1015:A:C2	34:AA:1032:A:C2	3.08	0.41
36:AB:77:A:C2	36:AB:100:A:C4	3.09	0.41
36:AB:116:U:H2'	36:AB:117:C:C6	2.55	0.41
50:Ab:17:PHE:CG	50:Ab:18:ASN:N	2.87	0.41
1:A:105:A:C8	1:A:366:A:C6	3.09	0.41
1:A:1226:A:C5	1:A:1227:G:H1'	2.56	0.41
35:AC:146:C:H2'	35:AC:147:U:C6	2.56	0.41
1:A:483:A:N6	1:A:518:A:H61	2.19	0.41
1:A:1656:A:H2'	1:A:1657:A:C8	2.56	0.41
1:A:1947:U:H2'	1:A:1948:A:C8	2.56	0.41
3:Q:102:VAL:HG12	3:Q:127:VAL:HG12	2.03	0.41
7:U:36:ALA:HB1	7:U:58:TYR:CE2	2.56	0.41
29:K:7:LEU:HD12	29:K:7:LEU:H	1.86	0.41
34:AA:709:A:H2'	34:AA:710:C:C6	2.55	0.41
34:AA:1031:G:H2'	34:AA:1033:A:C5	2.56	0.41
34:AA:1752:C:H2'	34:AA:1753:U:C6	2.56	0.41
58:AK:13:HIS:CE1	58:AK:119:LEU:H	2.37	0.41
34:AA:1431:A:C2	34:AA:3246:A:C4	3.08	0.41
34:AA:3195:C:C5	34:AA:3212:G:C2	3.09	0.41
1:A:1414:A:H4'	1:A:1415:A:OP1	2.21	0.40
8:V:58:ASP:CG	8:V:85:ARG:HH12	2.30	0.40
34:AA:492:U:H2'	34:AA:493:C:C6	2.56	0.40
34:AA:1212:U:H2'	34:AA:1213:U:C6	2.56	0.40
70:AE:61:ASP:CG	70:AE:62:LYS:H	2.28	0.40
71:AF:107:ILE:HD12	71:AF:107:ILE:H	1.85	0.40
34:AA:60:A:C8	34:AA:335:A:C6	3.10	0.40
34:AA:453:A:C4	34:AA:503:A:C2	3.09	0.40
34:AA:947:U:H2'	34:AA:948:G:C8	2.57	0.40
1:A:262:A:C5	1:A:263:A:H1'	2.57	0.40
1:A:1821:A:H2'	1:A:1822:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AA:606:A:H2'	34:AA:607:A:C8	2.57	0.40
1:A:1188:A:H2'	1:A:1189:A:C8	2.57	0.40
2:7:70:G:C3'	2:7:71:C:H5''	2.52	0.40
34:AA:141:A:C2	34:AA:142:C:N3	2.90	0.40
34:AA:445:A:C2	34:AA:702:U:C5	3.10	0.40
34:AA:1228:A:C6	34:AA:1230:A:C5	3.09	0.40
34:AA:3444:G:H2'	34:AA:3445:C:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	142/144 (99%)	134 (94%)	6 (4%)	2 (1%)	9	40
4	S	126/128 (98%)	107 (85%)	11 (9%)	8 (6%)	1	12
5	T	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
6	M	136/138 (99%)	128 (94%)	6 (4%)	2 (2%)	8	39
7	U	147/149 (99%)	144 (98%)	2 (1%)	1 (1%)	18	56
8	V	142/156 (91%)	134 (94%)	4 (3%)	4 (3%)	4	24
9	E	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
10	X	92/103 (89%)	82 (89%)	6 (6%)	4 (4%)	2	17
11	G	222/224 (99%)	209 (94%)	10 (4%)	3 (1%)	9	40
12	W	91/108 (84%)	87 (96%)	3 (3%)	1 (1%)	11	45
13	R	92/114 (81%)	78 (85%)	10 (11%)	4 (4%)	2	17
14	I	176/189 (93%)	166 (94%)	7 (4%)	3 (2%)	7	36
15	O	77/79 (98%)	70 (91%)	3 (4%)	4 (5%)	1	14
16	Y	152/154 (99%)	141 (93%)	7 (5%)	4 (3%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Z	70/72 (97%)	65 (93%)	4 (6%)	1 (1%)	9	40
18	1	118/120 (98%)	109 (92%)	7 (6%)	2 (2%)	7	36
19	2	35/68 (52%)	32 (91%)	1 (3%)	2 (6%)	1	13
20	C	193/195 (99%)	180 (93%)	11 (6%)	2 (1%)	12	48
21	3	93/95 (98%)	81 (87%)	12 (13%)	0	100	100
22	4	74/76 (97%)	67 (90%)	4 (5%)	3 (4%)	2	17
23	5	54/65 (83%)	52 (96%)	1 (2%)	1 (2%)	6	31
24	6	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
25	B	208/210 (99%)	188 (90%)	16 (8%)	4 (2%)	6	31
26	D	149/209 (71%)	143 (96%)	4 (3%)	2 (1%)	9	41
27	F	255/257 (99%)	244 (96%)	10 (4%)	1 (0%)	30	67
28	H	200/214 (94%)	186 (93%)	13 (6%)	1 (0%)	24	63
29	K	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	7	37
30	J	186/188 (99%)	175 (94%)	7 (4%)	4 (2%)	5	28
31	N	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
32	P	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
33	L	165/214 (77%)	149 (90%)	15 (9%)	1 (1%)	21	59
37	AL	209/211 (99%)	190 (91%)	13 (6%)	6 (3%)	3	23
38	A0	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
39	AO	145/147 (99%)	134 (92%)	8 (6%)	3 (2%)	5	29
40	Ai	93/95 (98%)	84 (90%)	6 (6%)	3 (3%)	3	21
41	A2	96/118 (81%)	92 (96%)	3 (3%)	1 (1%)	12	48
42	A4	64/66 (97%)	56 (88%)	8 (12%)	0	100	100
43	A6	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
44	A7	92/102 (90%)	90 (98%)	2 (2%)	0	100	100
45	A1	136/145 (94%)	131 (96%)	5 (4%)	0	100	100
46	AN	144/146 (99%)	138 (96%)	4 (3%)	2 (1%)	9	40
47	A8	123/125 (98%)	111 (90%)	10 (8%)	2 (2%)	7	37
48	A9	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	3	22
49	Aa	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
50	Ab	91/105 (87%)	86 (94%)	3 (3%)	2 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	Ad	68/76 (90%)	65 (96%)	2 (3%)	1 (2%)	8	39
52	Ae	39/50 (78%)	38 (97%)	1 (3%)	0	100	100
53	Af	49/51 (96%)	44 (90%)	5 (10%)	0	100	100
54	AP	202/204 (99%)	182 (90%)	11 (5%)	9 (4%)	2	16
55	Ah	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
56	AI	203/213 (95%)	188 (93%)	10 (5%)	5 (2%)	4	25
57	Ac	87/89 (98%)	78 (90%)	6 (7%)	3 (3%)	3	20
58	AK	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	24	63
59	AM	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	16	54
60	AS	184/186 (99%)	166 (90%)	13 (7%)	5 (3%)	4	25
61	AQ	185/205 (90%)	169 (91%)	11 (6%)	5 (3%)	4	25
62	AR	244/289 (84%)	219 (90%)	19 (8%)	6 (2%)	4	25
63	AW	149/170 (88%)	137 (92%)	10 (7%)	2 (1%)	9	41
64	AY	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	48
65	AT	179/181 (99%)	174 (97%)	3 (2%)	2 (1%)	11	45
66	AZ	119/121 (98%)	113 (95%)	5 (4%)	1 (1%)	16	54
67	A3	117/119 (98%)	110 (94%)	5 (4%)	2 (2%)	7	36
68	A5	221/223 (99%)	197 (89%)	19 (9%)	5 (2%)	5	27
69	AD	245/247 (99%)	232 (95%)	9 (4%)	4 (2%)	7	37
70	AE	378/380 (100%)	350 (93%)	27 (7%)	1 (0%)	36	72
71	AF	388/390 (100%)	355 (92%)	24 (6%)	9 (2%)	5	27
72	AG	116/159 (73%)	106 (91%)	7 (6%)	3 (3%)	4	25
73	AU	178/180 (99%)	162 (91%)	12 (7%)	4 (2%)	5	28
74	AH	183/185 (99%)	163 (89%)	17 (9%)	3 (2%)	7	37
75	AV	153/155 (99%)	142 (93%)	10 (6%)	1 (1%)	18	56
76	Ag	35/37 (95%)	29 (83%)	5 (14%)	1 (3%)	3	23
77	AX	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
78	AJ	216/244 (88%)	201 (93%)	12 (6%)	3 (1%)	9	40
All	All	10111/10698 (94%)	9380 (93%)	565 (6%)	166 (2%)	10	37

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	41	GLU
8	V	41	VAL
10	X	52	LYS
13	R	42	ILE
14	I	70	HIS
16	Y	55	LYS
25	B	98	THR
28	H	25	LEU
29	K	120	HIS
33	L	29	LEU
39	AO	25	HIS
54	AP	16	SER
54	AP	188	SER
56	AI	47	GLN
57	Ac	42	TYR
57	Ac	80	LYS
60	AS	174	GLU
61	AQ	175	PRO
65	AT	56	VAL
70	AE	196	LEU
71	AF	235	LEU
73	AU	13	ILE
3	Q	8	GLY
3	Q	137	LYS
4	S	20	THR
4	S	101	ILE
8	V	10	GLU
10	X	51	LYS
10	X	90	VAL
12	W	4	VAL
13	R	39	LYS
30	J	112	ILE
37	AL	101	LYS
37	AL	160	ILE
40	Ai	85	LYS
50	Ab	19	SER
54	AP	150	ASN
57	Ac	75	ARG
60	AS	166	VAL
61	AQ	35	ASP
62	AR	44	TYR
62	AR	142	LYS
64	AY	105	LEU

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Mol	Chain	Res	Type
68	A5	229	ALA
71	AF	287	PRO
73	AU	160	ALA
75	AV	14	TYR
78	AJ	45	ILE
78	AJ	66	SER
4	S	88	ARG
11	G	121	GLY
13	R	37	GLY
15	O	15	PRO
17	Z	30	GLY
18	1	5	PHE
22	4	19	LEU
25	B	146	ARG
26	D	29	LEU
29	K	58	SER
30	J	31	SER
37	AL	61	THR
37	AL	130	ASN
37	AL	171	TYR
47	A8	50	ASN
48	A9	94	GLY
54	AP	113	ASN
56	AI	88	PRO
60	AS	184	ALA
61	AQ	131	ILE
62	AR	59	GLN
63	AW	64	ASN
65	AT	129	ASN
67	A3	75	LYS
68	A5	116	ARG
69	AD	29	LEU
71	AF	80	PRO
76	Ag	8	TYR
4	S	51	ASN
7	U	16	LEU
8	V	115	SER
11	G	101	GLN
14	I	174	GLU
16	Y	19	PRO
18	1	96	GLY
19	2	38	HIS

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Mol	Chain	Res	Type
20	C	143	VAL
22	4	18	LYS
22	4	47	HIS
25	B	132	ASN
37	AL	21	VAL
39	AO	64	LEU
41	A2	95	GLN
47	A8	40	CYS
50	Ab	17	PHE
54	AP	72	LYS
56	AI	212	ASN
60	AS	154	ALA
62	AR	89	PRO
62	AR	174	ASN
63	AW	20	VAL
68	A5	100	GLY
68	A5	223	PRO
69	AD	199	VAL
71	AF	115	VAL
71	AF	279	LEU
72	AG	96	PHE
74	AH	11	LEU
74	AH	169	LYS
4	S	24	GLY
4	S	99	HIS
10	X	115	TYR
11	G	80	GLN
13	R	126	SER
15	O	41	PRO
15	O	70	TYR
16	Y	143	LYS
20	C	202	LEU
23	5	4	SER
26	D	162	GLY
30	J	132	SER
39	AO	40	HIS
40	Ai	29	LYS
46	AN	88	LYS
54	AP	94	SER
56	AI	19	VAL
59	AM	114	SER
61	AQ	140	THR

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Mol	Chain	Res	Type
67	A3	84	LYS
68	A5	228	LYS
71	AF	19	VAL
71	AF	144	ILE
71	AF	216	GLY
71	AF	304	ALA
74	AH	86	LYS
8	V	16	GLN
25	B	75	ASN
27	F	133	LYS
48	A9	47	LEU
56	AI	139	THR
61	AQ	94	PHE
72	AG	153	LYS
73	AU	143	VAL
73	AU	166	LEU
78	AJ	248	LYS
6	M	98	VAL
16	Y	110	VAL
46	AN	46	VAL
48	A9	38	VAL
54	AP	56	ILE
66	AZ	70	VAL
19	2	60	THR
54	AP	149	ILE
58	AK	88	PRO
60	AS	82	VAL
69	AD	4	VAL
72	AG	45	PRO
4	S	76	PRO
4	S	100	VAL
30	J	13	PRO
54	AP	79	ILE
15	O	44	PRO
40	Ai	55	PRO
62	AR	152	ILE
69	AD	127	VAL
14	I	71	GLY
51	Ad	68	LEU

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	
3	Q	120/120 (100%)	119 (99%)	1 (1%)	73	79
4	S	114/114 (100%)	111 (97%)	3 (3%)	40	61
5	T	43/43 (100%)	41 (95%)	2 (5%)	23	44
6	M	116/116 (100%)	113 (97%)	3 (3%)	40	61
7	U	132/132 (100%)	130 (98%)	2 (2%)	57	71
8	V	131/140 (94%)	129 (98%)	2 (2%)	57	71
9	E	161/164 (98%)	157 (98%)	4 (2%)	42	62
10	X	88/94 (94%)	88 (100%)	0	100	100
11	G	191/191 (100%)	188 (98%)	3 (2%)	55	69
12	W	86/99 (87%)	86 (100%)	0	100	100
13	R	83/97 (86%)	83 (100%)	0	100	100
14	I	154/160 (96%)	150 (97%)	4 (3%)	40	61
15	O	76/76 (100%)	75 (99%)	1 (1%)	61	73
16	Y	137/137 (100%)	132 (96%)	5 (4%)	31	52
17	Z	60/60 (100%)	60 (100%)	0	100	100
18	1	104/104 (100%)	100 (96%)	4 (4%)	29	50
19	2	35/61 (57%)	35 (100%)	0	100	100
20	C	167/167 (100%)	164 (98%)	3 (2%)	51	67
21	3	87/87 (100%)	87 (100%)	0	100	100
22	4	70/70 (100%)	68 (97%)	2 (3%)	37	57
23	5	47/52 (90%)	46 (98%)	1 (2%)	47	65
24	6	36/36 (100%)	36 (100%)	0	100	100
25	B	195/195 (100%)	192 (98%)	3 (2%)	57	71
26	D	132/177 (75%)	129 (98%)	3 (2%)	44	63
27	F	233/233 (100%)	223 (96%)	10 (4%)	26	47
28	H	182/190 (96%)	179 (98%)	3 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	K	115/115 (100%)	114 (99%)	1 (1%)	70	78
30	J	177/177 (100%)	173 (98%)	4 (2%)	44	63
31	N	91/91 (100%)	90 (99%)	1 (1%)	65	75
32	P	99/99 (100%)	97 (98%)	2 (2%)	48	66
33	L	151/190 (80%)	150 (99%)	1 (1%)	76	81
37	AL	190/190 (100%)	184 (97%)	6 (3%)	34	55
38	A0	53/53 (100%)	52 (98%)	1 (2%)	50	66
39	AO	121/121 (100%)	119 (98%)	2 (2%)	53	68
40	Ai	87/87 (100%)	86 (99%)	1 (1%)	65	75
41	A2	97/109 (89%)	95 (98%)	2 (2%)	47	65
42	A4	60/60 (100%)	59 (98%)	1 (2%)	53	68
43	A6	83/83 (100%)	81 (98%)	2 (2%)	43	63
44	A7	90/96 (94%)	89 (99%)	1 (1%)	65	75
45	A1	127/131 (97%)	125 (98%)	2 (2%)	55	69
46	AN	135/135 (100%)	133 (98%)	2 (2%)	57	71
47	A8	114/114 (100%)	113 (99%)	1 (1%)	70	78
48	A9	90/90 (100%)	85 (94%)	5 (6%)	19	40
49	Aa	89/89 (100%)	89 (100%)	0	100	100
50	Ab	82/92 (89%)	80 (98%)	2 (2%)	43	63
51	Ad	69/73 (94%)	68 (99%)	1 (1%)	59	72
52	Ae	40/47 (85%)	38 (95%)	2 (5%)	22	42
53	Af	45/45 (100%)	44 (98%)	1 (2%)	45	64
54	AP	179/179 (100%)	170 (95%)	9 (5%)	22	42
55	Ah	70/70 (100%)	70 (100%)	0	100	100
56	AI	189/195 (97%)	184 (97%)	5 (3%)	40	61
57	Ac	74/74 (100%)	73 (99%)	1 (1%)	59	72
58	AK	181/181 (100%)	178 (98%)	3 (2%)	53	68
59	AM	106/106 (100%)	105 (99%)	1 (1%)	70	78
60	AS	158/158 (100%)	155 (98%)	3 (2%)	50	66
61	AQ	165/176 (94%)	160 (97%)	5 (3%)	36	57
62	AR	215/250 (86%)	212 (99%)	3 (1%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	AW	128/128 (100%)	123 (96%)	5 (4%)	28	49
64	AY	90/90 (100%)	88 (98%)	2 (2%)	45	64
65	AT	162/162 (100%)	162 (100%)	0	100	100
66	AZ	111/111 (100%)	109 (98%)	2 (2%)	51	67
67	A3	110/110 (100%)	108 (98%)	2 (2%)	51	67
68	A5	201/201 (100%)	199 (99%)	2 (1%)	68	77
69	AD	191/191 (100%)	184 (96%)	7 (4%)	30	51
70	AE	335/335 (100%)	334 (100%)	1 (0%)	86	85
71	AF	336/336 (100%)	329 (98%)	7 (2%)	47	65
72	AG	110/142 (78%)	107 (97%)	3 (3%)	39	60
73	AU	162/162 (100%)	162 (100%)	0	100	100
74	AH	168/168 (100%)	166 (99%)	2 (1%)	63	75
75	AV	140/140 (100%)	137 (98%)	3 (2%)	47	65
76	Ag	34/34 (100%)	33 (97%)	1 (3%)	37	57
77	AX	92/92 (100%)	91 (99%)	1 (1%)	65	75
78	AJ	204/224 (91%)	200 (98%)	4 (2%)	48	66
All	All	9096/9417 (97%)	8924 (98%)	172 (2%)	49	66

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	27	LYS
4	S	18	LEU
4	S	36	LYS
4	S	129	TRP
5	T	18	GLN
5	T	31	LYS
6	M	10	THR
6	M	62	LYS
6	M	64	LEU
7	U	3	ARG
7	U	62	GLN
8	V	16	GLN
8	V	25	LYS
9	E	2	PRO
9	E	37	LYS

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Mol	Chain	Res	Type
9	E	47	TYR
9	E	69	ARG
11	G	189	GLN
11	G	215	LYS
11	G	242	TRP
14	I	25	SER
14	I	62	ARG
14	I	132	VAL
14	I	136	ARG
15	O	75	GLN
16	Y	25	THR
16	Y	29	ILE
16	Y	30	LYS
16	Y	105	LYS
16	Y	119	SER
18	1	6	THR
18	1	48	TYR
18	1	107	ARG
18	1	118	LYS
20	C	12	GLU
20	C	156	VAL
20	C	168	GLU
22	4	32	ASP
22	4	47	HIS
23	5	28	GLN
25	B	68	VAL
25	B	146	ARG
25	B	149	GLN
26	D	107	ARG
26	D	158	LEU
26	D	166	LYS
27	F	17	HIS
27	F	18	TRP
27	F	35	PRO
27	F	59	ASP
27	F	84	VAL
27	F	102	LEU
27	F	103	TYR
27	F	132	ARG
27	F	133	LYS
27	F	249	ILE
28	H	13	GLN

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Mol	Chain	Res	Type
28	H	159	ILE
28	H	197	ARG
29	K	69	ILE
30	J	5	GLN
30	J	67	LYS
30	J	127	LEU
30	J	149	ARG
31	N	64	THR
32	P	68	GLU
32	P	131	ASP
33	L	64	SER
37	AL	51	GLU
37	AL	75	THR
37	AL	91	THR
37	AL	94	ILE
37	AL	106	GLU
37	AL	115	LEU
38	A0	10	THR
39	AO	32	ARG
39	AO	132	VAL
40	Ai	78	LYS
41	A2	5	SER
41	A2	114	ARG
42	A4	32	ARG
43	A6	26	TYR
43	A6	64	MET
44	A7	88	ASN
45	A1	32	GLN
45	A1	135	LYS
46	AN	10	GLU
46	AN	71	LEU
47	A8	41	ARG
48	A9	39	ARG
48	A9	53	GLN
48	A9	66	LYS
48	A9	104	VAL
48	A9	136	TYR
50	Ab	86	THR
50	Ab	89	ARG
51	Ad	38	ILE
52	Ae	8	ARG
52	Ae	42	ARG

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Mol	Chain	Res	Type
53	Af	29	PRO
54	AP	13	LYS
54	AP	31	ARG
54	AP	61	ILE
54	AP	85	LYS
54	AP	124	GLN
54	AP	161	GLU
54	AP	163	ARG
54	AP	190	ARG
54	AP	192	ASN
56	AI	27	LYS
56	AI	88	PRO
56	AI	97	LYS
56	AI	111	ILE
56	AI	159	MET
57	Ac	55	LYS
58	AK	39	ASP
58	AK	116	LYS
58	AK	127	ARG
59	AM	89	ARG
60	AS	91	LEU
60	AS	122	PHE
60	AS	174	GLU
61	AQ	40	LYS
61	AQ	82	LYS
61	AQ	94	PHE
61	AQ	119	PHE
61	AQ	175	PRO
62	AR	44	TYR
62	AR	145	LYS
62	AR	160	ARG
63	AW	16	LYS
63	AW	37	ARG
63	AW	62	LYS
63	AW	97	ASN
63	AW	131	LYS
64	AY	173	ARG
64	AY	177	GLU
66	AZ	51	LYS
66	AZ	101	SER
67	A3	113	PHE
67	A3	119	LEU

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Mol	Chain	Res	Type
68	A5	192	HIS
68	A5	232	HIS
69	AD	34	TYR
69	AD	40	TYR
69	AD	54	ARG
69	AD	67	GLU
69	AD	125	THR
69	AD	238	ILE
69	AD	242	ARG
70	AE	237	ARG
71	AF	6	PRO
71	AF	106	LYS
71	AF	122	TYR
71	AF	266	LYS
71	AF	287	PRO
71	AF	347	ILE
71	AF	386	LYS
72	AG	16	LYS
72	AG	84	LEU
72	AG	125	MET
74	AH	62	VAL
74	AH	167	ARG
75	AV	48	THR
75	AV	68	ILE
75	AV	71	ARG
76	Ag	8	TYR
77	AX	122	VAL
78	AJ	45	ILE
78	AJ	147	LEU
78	AJ	179	LEU
78	AJ	211	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
4	S	71	HIS
4	S	78	GLN
4	S	103	ASN
6	M	9	GLN
7	U	57	ASN
7	U	105	ASN
8	V	16	GLN

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Mol	Chain	Res	Type
8	V	81	ASN
8	V	101	ASN
8	V	107	HIS
9	E	72	GLN
10	X	82	ASN
11	G	80	GLN
11	G	86	HIS
14	I	170	ASN
15	O	50	ASN
17	Z	60	GLN
17	Z	81	GLN
17	Z	82	ASN
18	1	31	ASN
20	C	23	HIS
20	C	113	GLN
20	C	140	ASN
21	3	50	GLN
24	6	38	GLN
25	B	90	HIS
25	B	148	ASN
25	B	200	GLN
25	B	208	GLN
25	B	209	ASN
26	D	22	ASN
27	F	17	HIS
27	F	231	ASN
28	H	71	ASN
28	H	213	ASN
29	K	64	ASN
33	L	21	HIS
33	L	167	ASN
37	AL	19	HIS
37	AL	45	ASN
37	AL	58	HIS
37	AL	203	GLN
38	A0	49	GLN
39	AO	8	ASN
39	AO	113	ASN
41	A2	39	ASN
41	A2	53	ASN
41	A2	56	ASN
42	A4	7	HIS

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Mol	Chain	Res	Type
42	A4	43	GLN
44	A7	29	HIS
48	A9	73	HIS
49	Aa	10	HIS
49	Aa	18	ASN
54	AP	159	HIS
54	AP	192	ASN
56	AI	10	HIS
56	AI	160	ASN
58	AK	30	GLN
58	AK	175	ASN
58	AK	192	GLN
58	AK	194	GLN
59	AM	77	ASN
60	AS	14	HIS
61	AQ	92	HIS
62	AR	94	ASN
62	AR	193	GLN
62	AR	221	HIS
62	AR	243	HIS
63	AW	25	HIS
63	AW	64	ASN
63	AW	147	GLN
66	AZ	18	HIS
66	AZ	113	ASN
67	A3	112	ASN
68	A5	185	HIS
68	A5	248	HIS
69	AD	217	GLN
70	AE	174	HIS
70	AE	179	GLN
70	AE	181	ASN
70	AE	240	HIS
70	AE	253	HIS
70	AE	310	HIS
70	AE	338	ASN
71	AF	17	ASN
71	AF	34	ASN
71	AF	38	GLN
71	AF	223	ASN
71	AF	294	HIS
71	AF	329	ASN

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Mol	Chain	Res	Type
71	AF	353	ASN
71	AF	372	ASN
72	AG	95	ASN
73	AU	58	ASN
73	AU	83	ASN
73	AU	98	ASN
74	AH	40	HIS
75	AV	56	ASN
75	AV	96	HIS
75	AV	103	ASN
78	AJ	130	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1588/1608 (98%)	484 (30%)	100 (6%)
2	7	74/75 (98%)	33 (44%)	5 (6%)
34	AA	3165/3192 (99%)	984 (31%)	189 (5%)
35	AC	148/151 (98%)	49 (33%)	10 (6%)
36	AB	117/118 (99%)	29 (24%)	2 (1%)
All	All	5092/5144 (98%)	1579 (31%)	306 (6%)

All (1579) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	C
1	A	5	U
1	A	17	C
1	A	26	A
1	A	27	U
1	A	34	G
1	A	35	U
1	A	42	G
1	A	45	U
1	A	47	A
1	A	50	C
1	A	57	G
1	A	59	G
1	A	60	A
1	A	61	A

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Mol	Chain	Res	Type
1	A	67	A
1	A	68	U
1	A	71	A
1	A	81	U
1	A	82	G
1	A	84	A
1	A	103	U
1	A	104	U
1	A	106	A
1	A	107	A
1	A	108	A
1	A	113	U
1	A	116	A
1	A	125	G
1	A	128	A
1	A	129	U
1	A	130	U
1	A	138	U
1	A	139	A
1	A	142	G
1	A	143	A
1	A	144	U
1	A	151	G
1	A	157	G
1	A	159	U
1	A	161	U
1	A	164	C
1	A	165	U
1	A	169	A
1	A	182	U
1	A	183	C
1	A	205	A
1	A	206	A
1	A	207	G
1	A	208	U
1	A	209	A
1	A	217	G
1	A	247	G
1	A	250	A
1	A	252	U
1	A	254	U
1	A	255	A

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Mol	Chain	Res	Type
1	A	258	A
1	A	260	A
1	A	262	A
1	A	264	G
1	A	266	A
1	A	267	A
1	A	268	C
1	A	273	A
1	A	292	G
1	A	305	G
1	A	308	U
1	A	320	C
1	A	322	G
1	A	323	C
1	A	326	U
1	A	327	U
1	A	328	G
1	A	330	U
1	A	335	G
1	A	339	A
1	A	342	G
1	A	343	G
1	A	344	C
1	A	345	C
1	A	350	A
1	A	357	U
1	A	358	G
1	A	361	G
1	A	365	A
1	A	366	A
1	A	367	C
1	A	375	U
1	A	379	G
1	A	384	A
1	A	386	U
1	A	396	G
1	A	399	C
1	A	405	A
1	A	406	A
1	A	407	A
1	A	408	U
1	A	409	A

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Mol	Chain	Res	Type
1	A	410	G
1	A	422	A
1	A	424	G
1	A	425	G
1	A	430	C
1	A	431	A
1	A	432	G
1	A	433	C
1	A	434	A
1	A	440	G
1	A	445	U
1	A	446	U
1	A	450	C
1	A	451	A
1	A	454	U
1	A	458	A
1	A	459	A
1	A	466	A
1	A	467	G
1	A	470	A
1	A	483	A
1	A	484	A
1	A	488	U
1	A	494	G
1	A	508	U
1	A	509	U
1	A	515	U
1	A	516	G
1	A	521	G
1	A	526	G
1	A	527	A
1	A	543	A
1	A	545	A
1	A	546	G
1	A	548	A
1	A	549	A
1	A	562	A
1	A	563	A
1	A	564	G
1	A	565	U
1	A	566	C
1	A	568	G

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Mol	Chain	Res	Type
1	A	572	C
1	A	575	G
1	A	578	G
1	A	584	G
1	A	587	A
1	A	588	U
1	A	590	C
1	A	592	A
1	A	601	A
1	A	602	G
1	A	614	A
1	A	615	U
1	A	616	U
1	A	617	G
1	A	618	U
1	A	626	A
1	A	627	A
1	A	629	A
1	A	630	C
1	A	631	G
1	A	642	A
1	A	645	U
1	A	646	U
1	A	648	A
1	A	746	U
1	A	752	U
1	A	753	U
1	A	756	A
1	A	760	C
1	A	790	U
1	A	791	U
1	A	792	U
1	A	793	G
1	A	794	U
1	A	800	U
1	A	801	G
1	A	804	U
1	A	805	A
1	A	806	A
1	A	816	U
1	A	818	C
1	A	819	A

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Mol	Chain	Res	Type
1	A	824	A
1	A	830	U
1	A	831	U
1	A	832	A
1	A	833	A
1	A	834	A
1	A	837	A
1	A	844	G
1	A	845	U
1	A	846	G
1	A	849	U
1	A	852	A
1	A	853	U
1	A	856	U
1	A	857	A
1	A	858	U
1	A	866	A
1	A	869	A
1	A	870	A
1	A	873	A
1	A	874	A
1	A	875	A
1	A	876	U
1	A	877	U
1	A	880	A
1	A	881	C
1	A	882	A
1	A	887	A
1	A	888	A
1	A	896	U
1	A	906	U
1	A	908	U
1	A	915	G
1	A	917	C
1	A	920	A
1	A	921	G
1	A	922	U
1	A	924	A
1	A	927	A
1	A	928	U
1	A	929	U
1	A	931	A

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Mol	Chain	Res	Type
1	A	941	C
1	A	942	U
1	A	945	G
1	A	962	A
1	A	965	U
1	A	966	C
1	A	967	A
1	A	974	A
1	A	978	U
1	A	982	A
1	A	983	G
1	A	984	A
1	A	990	U
1	A	1002	A
1	A	1004	U
1	A	1011	G
1	A	1013	A
1	A	1020	U
1	A	1021	A
1	A	1029	U
1	A	1035	A
1	A	1038	C
1	A	1051	U
1	A	1054	G
1	A	1057	A
1	A	1061	A
1	A	1062	A
1	A	1065	C
1	A	1067	A
1	A	1070	A
1	A	1071	G
1	A	1072	A
1	A	1073	U
1	A	1074	A
1	A	1082	A
1	A	1089	A
1	A	1090	C
1	A	1092	A
1	A	1093	U
1	A	1094	A
1	A	1095	A
1	A	1097	C

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Mol	Chain	Res	Type
1	A	1098	U
1	A	1099	A
1	A	1101	G
1	A	1107	U
1	A	1108	A
1	A	1109	G
1	A	1112	G
1	A	1116	G
1	A	1119	G
1	A	1175	G
1	A	1177	A
1	A	1183	U
1	A	1184	G
1	A	1193	A
1	A	1194	A
1	A	1195	G
1	A	1197	C
1	A	1199	U
1	A	1209	G
1	A	1210	G
1	A	1212	C
1	A	1227	G
1	A	1230	A
1	A	1233	A
1	A	1239	A
1	A	1247	G
1	A	1251	G
1	A	1255	G
1	A	1259	C
1	A	1260	C
1	A	1261	A
1	A	1265	G
1	A	1268	G
1	A	1271	G
1	A	1274	C
1	A	1284	A
1	A	1286	U
1	A	1287	U
1	A	1291	C
1	A	1292	U
1	A	1293	C
1	A	1294	A

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Mol	Chain	Res	Type
1	A	1295	A
1	A	1296	C
1	A	1297	A
1	A	1300	G
1	A	1301	G
1	A	1302	G
1	A	1304	A
1	A	1306	C
1	A	1307	U
1	A	1309	A
1	A	1315	U
1	A	1317	A
1	A	1319	G
1	A	1321	C
1	A	1363	U
1	A	1366	A
1	A	1367	U
1	A	1370	U
1	A	1374	G
1	A	1375	C
1	A	1382	G
1	A	1383	U
1	A	1384	U
1	A	1385	U
1	A	1388	A
1	A	1389	G
1	A	1409	U
1	A	1415	A
1	A	1416	U
1	A	1417	U
1	A	1422	U
1	A	1423	A
1	A	1427	A
1	A	1433	A
1	A	1434	U
1	A	1437	U
1	A	1443	G
1	A	1444	C
1	A	1445	U
1	A	1449	U
1	A	1450	A
1	A	1451	G

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Mol	Chain	Res	Type
1	A	1453	G
1	A	1454	G
1	A	1456	G
1	A	1459	U
1	A	1462	A
1	A	1463	C
1	A	1464	U
1	A	1607	U
1	A	1623	U
1	A	1624	U
1	A	1626	U
1	A	1635	C
1	A	1636	A
1	A	1644	U
1	A	1645	C
1	A	1648	A
1	A	1649	C
1	A	1656	A
1	A	1659	U
1	A	1660	U
1	A	1664	G
1	A	1666	C
1	A	1667	A
1	A	1668	A
1	A	1673	A
1	A	1674	G
1	A	1677	C
1	A	1678	U
1	A	1679	G
1	A	1692	A
1	A	1693	U
1	A	1702	C
1	A	1705	C
1	A	1706	A
1	A	1715	A
1	A	1716	C
1	A	1717	A
1	A	1720	G
1	A	1721	A
1	A	1723	A
1	A	1727	A
1	A	1728	U

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Mol	Chain	Res	Type
1	A	1729	A
1	A	1732	G
1	A	1735	U
1	A	1742	A
1	A	1749	C
1	A	1787	U
1	A	1790	C
1	A	1792	U
1	A	1795	G
1	A	1796	C
1	A	1799	A
1	A	1800	A
1	A	1801	A
1	A	1802	G
1	A	1811	A
1	A	1812	A
1	A	1813	U
1	A	1817	U
1	A	1818	A
1	A	1819	U
1	A	1820	C
1	A	1824	A
1	A	1830	C
1	A	1833	G
1	A	1834	A
1	A	1835	U
1	A	1837	G
1	A	1844	A
1	A	1846	U
1	A	1850	G
1	A	1854	U
1	A	1855	U
1	A	1856	A
1	A	1861	U
1	A	1866	A
1	A	1868	C
1	A	1870	A
1	A	1871	G
1	A	1881	G
1	A	1882	U
1	A	1883	A
1	A	1887	A

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Mol	Chain	Res	Type
1	A	1892	U
1	A	1897	A
1	A	1898	G
1	A	1902	G
1	A	1904	G
1	A	1907	A
1	A	1908	A
1	A	1911	A
1	A	1912	C
1	A	1913	G
1	A	1915	C
1	A	1916	C
1	A	1927	U
1	A	1928	A
1	A	1929	C
1	A	1930	A
1	A	1934	C
1	A	1935	G
1	A	1938	C
1	A	1954	U
1	A	1955	G
1	A	1961	U
1	A	1977	G
1	A	1978	A
1	A	1979	C
1	A	1980	A
1	A	1981	A
1	A	1982	G
1	A	2012	G
1	A	2019	C
1	A	2021	U
1	A	2028	U
1	A	2034	U
1	A	2042	A
1	A	2048	A
1	A	2049	G
1	A	2053	U
1	A	2054	A
1	A	2058	A
1	A	2060	G
1	A	2061	U
1	A	2072	G

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Mol	Chain	Res	Type
1	A	2073	A
1	A	2075	C
1	A	2084	G
1	A	2085	G
1	A	2086	A
1	A	2090	U
2	7	2	G
2	7	4	G
2	7	5	G
2	7	6	G
2	7	8	U
2	7	9	G
2	7	13	C
2	7	15	G
2	7	16	C
2	7	17	C
2	7	19	G
2	7	20	U
2	7	21	A
2	7	24	U
2	7	25	C
2	7	27	U
2	7	28	C
2	7	35	A
2	7	44	A
2	7	45	G
2	7	48	C
2	7	52	G
2	7	53	G
2	7	54	U
2	7	55	U
2	7	56	C
2	7	59	A
2	7	61	C
2	7	62	C
2	7	63	G
2	7	71	C
2	7	72	A
2	7	74	C
34	AA	11	A
34	AA	13	G
34	AA	14	U

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Mol	Chain	Res	Type
34	AA	16	A
34	AA	18	G
34	AA	25	A
34	AA	26	A
34	AA	30	G
34	AA	32	C
34	AA	34	A
34	AA	40	A
34	AA	44	U
34	AA	45	A
34	AA	49	U
34	AA	55	G
34	AA	57	A
34	AA	59	G
34	AA	60	A
34	AA	62	A
34	AA	63	A
34	AA	66	A
34	AA	69	U
34	AA	73	U
34	AA	75	U
34	AA	83	U
34	AA	85	A
34	AA	87	U
34	AA	92	G
34	AA	105	G
34	AA	109	A
34	AA	110	G
34	AA	111	C
34	AA	113	C
34	AA	119	G
34	AA	122	A
34	AA	124	U
34	AA	130	G
34	AA	133	U
34	AA	134	G
34	AA	135	G
34	AA	136	U
34	AA	139	A
34	AA	144	U
34	AA	145	U
34	AA	147	C

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Mol	Chain	Res	Type
34	AA	148	G
34	AA	149	A
34	AA	152	G
34	AA	154	A
34	AA	156	U
34	AA	157	G
34	AA	163	G
34	AA	165	A
34	AA	167	U
34	AA	168	A
34	AA	173	A
34	AA	174	U
34	AA	175	G
34	AA	182	U
34	AA	183	U
34	AA	185	A
34	AA	186	A
34	AA	189	U
34	AA	190	G
34	AA	191	A
34	AA	192	G
34	AA	195	A
34	AA	197	G
34	AA	198	U
34	AA	199	G
34	AA	200	A
34	AA	201	G
34	AA	206	A
34	AA	207	A
34	AA	211	U
34	AA	214	C
34	AA	215	C
34	AA	216	C
34	AA	219	A
34	AA	220	G
34	AA	221	A
34	AA	226	G
34	AA	227	A
34	AA	228	A
34	AA	229	A
34	AA	231	G
34	AA	235	A

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Mol	Chain	Res	Type
34	AA	239	U
34	AA	242	U
34	AA	246	U
34	AA	250	U
34	AA	251	U
34	AA	255	C
34	AA	257	U
34	AA	258	U
34	AA	263	U
34	AA	265	U
34	AA	268	C
34	AA	269	A
34	AA	271	G
34	AA	276	G
34	AA	277	U
34	AA	290	G
34	AA	293	U
34	AA	302	A
34	AA	303	A
34	AA	304	U
34	AA	305	A
34	AA	307	G
34	AA	308	U
34	AA	309	G
34	AA	310	U
34	AA	313	U
34	AA	315	C
34	AA	317	U
34	AA	319	U
34	AA	324	U
34	AA	325	A
34	AA	336	U
34	AA	337	A
34	AA	338	U
34	AA	342	G
34	AA	344	A
34	AA	354	C
34	AA	356	A
34	AA	358	C
34	AA	359	A
34	AA	362	U
34	AA	378	U

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Mol	Chain	Res	Type
34	AA	382	A
34	AA	383	U
34	AA	384	A
34	AA	385	G
34	AA	386	U
34	AA	392	G
34	AA	394	A
34	AA	395	A
34	AA	396	U
34	AA	400	C
34	AA	401	A
34	AA	402	A
34	AA	405	A
34	AA	408	U
34	AA	409	A
34	AA	412	A
34	AA	413	C
34	AA	416	G
34	AA	417	A
34	AA	431	G
34	AA	432	A
34	AA	433	A
34	AA	434	C
34	AA	439	U
34	AA	442	G
34	AA	444	G
34	AA	447	A
34	AA	448	A
34	AA	449	A
34	AA	450	A
34	AA	451	C
34	AA	458	A
34	AA	459	G
34	AA	462	G
34	AA	463	G
34	AA	467	U
34	AA	489	U
34	AA	494	U
34	AA	495	U
34	AA	497	U
34	AA	498	U
34	AA	499	U

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Mol	Chain	Res	Type
34	AA	500	A
34	AA	501	U
34	AA	502	U
34	AA	503	A
34	AA	504	A
34	AA	505	A
34	AA	506	A
34	AA	509	A
34	AA	510	A
34	AA	514	C
34	AA	521	U
34	AA	522	A
34	AA	523	A
34	AA	527	A
34	AA	530	U
34	AA	531	U
34	AA	532	C
34	AA	534	A
34	AA	536	A
34	AA	538	A
34	AA	539	G
34	AA	542	A
34	AA	544	C
34	AA	545	C
34	AA	547	C
34	AA	549	G
34	AA	573	U
34	AA	574	G
34	AA	575	U
34	AA	579	C
34	AA	580	A
34	AA	581	C
34	AA	582	U
34	AA	583	U
34	AA	585	C
34	AA	586	U
34	AA	592	C
34	AA	593	A
34	AA	594	C
34	AA	595	U
34	AA	596	A
34	AA	597	A

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Mol	Chain	Res	Type
34	AA	598	U
34	AA	599	G
34	AA	601	G
34	AA	604	G
34	AA	605	A
34	AA	608	A
34	AA	610	U
34	AA	615	U
34	AA	617	A
34	AA	618	U
34	AA	620	U
34	AA	621	C
34	AA	622	U
34	AA	623	U
34	AA	628	U
34	AA	631	U
34	AA	636	U
34	AA	637	U
34	AA	641	G
34	AA	642	A
34	AA	643	G
34	AA	645	A
34	AA	646	A
34	AA	647	U
34	AA	649	U
34	AA	653	A
34	AA	658	U
34	AA	659	U
34	AA	662	A
34	AA	665	U
34	AA	666	U
34	AA	669	C
34	AA	671	U
34	AA	672	C
34	AA	674	U
34	AA	675	A
34	AA	677	A
34	AA	678	A
34	AA	679	U
34	AA	681	U
34	AA	682	A
34	AA	683	A

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Mol	Chain	Res	Type
34	AA	684	G
34	AA	685	U
34	AA	694	U
34	AA	697	A
34	AA	698	G
34	AA	699	U
34	AA	704	U
34	AA	707	U
34	AA	708	A
34	AA	714	C
34	AA	715	U
34	AA	716	C
34	AA	722	G
34	AA	727	A
34	AA	729	G
34	AA	738	A
34	AA	755	A
34	AA	759	U
34	AA	760	A
34	AA	761	U
34	AA	763	U
34	AA	765	A
34	AA	767	U
34	AA	769	U
34	AA	770	U
34	AA	773	A
34	AA	774	A
34	AA	793	A
34	AA	794	C
34	AA	799	A
34	AA	800	A
34	AA	804	A
34	AA	806	G
34	AA	809	A
34	AA	810	U
34	AA	812	U
34	AA	822	A
34	AA	823	U
34	AA	825	G
34	AA	833	G
34	AA	834	U
34	AA	835	G

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Mol	Chain	Res	Type
34	AA	859	C
34	AA	860	A
34	AA	862	U
34	AA	873	U
34	AA	874	A
34	AA	880	A
34	AA	885	A
34	AA	889	U
34	AA	890	G
34	AA	893	U
34	AA	895	A
34	AA	896	U
34	AA	899	A
34	AA	900	G
34	AA	905	A
34	AA	918	G
34	AA	920	A
34	AA	925	A
34	AA	927	A
34	AA	934	G
34	AA	936	A
34	AA	937	C
34	AA	945	G
34	AA	946	A
34	AA	951	A
34	AA	955	A
34	AA	956	A
34	AA	966	A
34	AA	968	G
34	AA	970	C
34	AA	976	G
34	AA	980	A
34	AA	984	A
34	AA	988	G
34	AA	990	U
34	AA	993	U
34	AA	998	U
34	AA	999	G
34	AA	1013	U
34	AA	1014	C
34	AA	1015	A
34	AA	1016	A

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Mol	Chain	Res	Type
34	AA	1024	U
34	AA	1026	G
34	AA	1027	G
34	AA	1028	G
34	AA	1033	A
34	AA	1035	G
34	AA	1036	A
34	AA	1040	A
34	AA	1041	U
34	AA	1042	C
34	AA	1043	G
34	AA	1052	A
34	AA	1053	U
34	AA	1056	G
34	AA	1063	A
34	AA	1070	A
34	AA	1072	A
34	AA	1073	G
34	AA	1078	C
34	AA	1079	U
34	AA	1086	C
34	AA	1087	G
34	AA	1092	A
34	AA	1097	A
34	AA	1098	U
34	AA	1099	U
34	AA	1101	A
34	AA	1102	U
34	AA	1106	A
34	AA	1109	U
34	AA	1111	A
34	AA	1113	C
34	AA	1114	A
34	AA	1115	G
34	AA	1116	G
34	AA	1121	G
34	AA	1122	A
34	AA	1123	U
34	AA	1124	A
34	AA	1128	A
34	AA	1132	G
34	AA	1136	A

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Mol	Chain	Res	Type
34	AA	1158	G
34	AA	1164	U
34	AA	1168	C
34	AA	1169	A
34	AA	1170	A
34	AA	1172	C
34	AA	1174	C
34	AA	1186	A
34	AA	1187	A
34	AA	1193	G
34	AA	1194	A
34	AA	1196	A
34	AA	1197	U
34	AA	1198	A
34	AA	1199	A
34	AA	1200	C
34	AA	1202	C
34	AA	1203	A
34	AA	1205	U
34	AA	1206	U
34	AA	1207	U
34	AA	1210	A
34	AA	1215	A
34	AA	1217	U
34	AA	1218	C
34	AA	1219	A
34	AA	1223	U
34	AA	1224	A
34	AA	1225	A
34	AA	1226	A
34	AA	1229	A
34	AA	1230	A
34	AA	1231	A
34	AA	1232	U
34	AA	1233	A
34	AA	1234	A
34	AA	1239	A
34	AA	1240	A
34	AA	1244	G
34	AA	1245	G
34	AA	1259	G
34	AA	1263	A

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Mol	Chain	Res	Type
34	AA	1272	U
34	AA	1273	G
34	AA	1281	C
34	AA	1283	C
34	AA	1287	A
34	AA	1288	C
34	AA	1291	U
34	AA	1295	A
34	AA	1299	G
34	AA	1300	G
34	AA	1306	A
34	AA	1309	U
34	AA	1310	A
34	AA	1314	G
34	AA	1320	G
34	AA	1321	A
34	AA	1324	U
34	AA	1325	C
34	AA	1329	U
34	AA	1334	G
34	AA	1337	G
34	AA	1340	G
34	AA	1341	G
34	AA	1344	C
34	AA	1345	A
34	AA	1346	U
34	AA	1418	A
34	AA	1420	C
34	AA	1431	A
34	AA	1433	U
34	AA	1434	G
34	AA	1435	G
34	AA	1436	A
34	AA	1437	U
34	AA	1441	G
34	AA	1444	A
34	AA	1445	A
34	AA	1450	G
34	AA	1451	A
34	AA	1453	U
34	AA	1458	A
34	AA	1460	A

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Mol	Chain	Res	Type
34	AA	1473	A
34	AA	1476	A
34	AA	1480	G
34	AA	1481	A
34	AA	1486	A
34	AA	1498	U
34	AA	1499	U
34	AA	1503	A
34	AA	1504	A
34	AA	1505	U
34	AA	1506	C
34	AA	1524	U
34	AA	1535	G
34	AA	1537	G
34	AA	1539	U
34	AA	1540	G
34	AA	1549	U
34	AA	1550	A
34	AA	1556	G
34	AA	1565	G
34	AA	1567	A
34	AA	1571	C
34	AA	1572	U
34	AA	1575	C
34	AA	1583	G
34	AA	1586	C
34	AA	1592	G
34	AA	1595	A
34	AA	1599	G
34	AA	1603	C
34	AA	1604	U
34	AA	1605	A
34	AA	1606	U
34	AA	1619	U
34	AA	1624	A
34	AA	1626	A
34	AA	1630	A
34	AA	1631	A
34	AA	1632	G
34	AA	1633	U
34	AA	1635	G
34	AA	1636	A

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Mol	Chain	Res	Type
34	AA	1637	G
34	AA	1642	G
34	AA	1643	U
34	AA	1649	G
34	AA	1651	C
34	AA	1657	U
34	AA	1659	A
34	AA	1661	U
34	AA	1668	G
34	AA	1676	C
34	AA	1677	G
34	AA	1685	G
34	AA	1688	A
34	AA	1691	G
34	AA	1693	U
34	AA	1703	U
34	AA	1704	U
34	AA	1705	A
34	AA	1706	A
34	AA	1721	C
34	AA	1725	U
34	AA	1730	A
34	AA	1732	A
34	AA	1736	A
34	AA	1737	A
34	AA	1748	A
34	AA	1750	U
34	AA	1751	C
34	AA	1756	G
34	AA	1761	U
34	AA	1762	A
34	AA	1763	G
34	AA	1766	U
34	AA	1767	U
34	AA	1768	A
34	AA	1769	U
34	AA	1770	G
34	AA	1771	A
34	AA	1774	U
34	AA	1780	G
34	AA	1781	A
34	AA	1782	U

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Mol	Chain	Res	Type
34	AA	1783	G
34	AA	1788	C
34	AA	1797	A
34	AA	1799	A
34	AA	1800	U
34	AA	1801	G
34	AA	1805	U
34	AA	1806	C
34	AA	1812	C
34	AA	1817	G
34	AA	1832	U
34	AA	1842	U
34	AA	1850	U
34	AA	1852	C
34	AA	1855	U
34	AA	1856	U
34	AA	1857	A
34	AA	1871	A
34	AA	1873	U
34	AA	1874	C
34	AA	1881	C
34	AA	1882	U
34	AA	1887	G
34	AA	1888	A
34	AA	1898	U
34	AA	1899	U
34	AA	1900	G
34	AA	1902	A
34	AA	1904	U
34	AA	1905	C
34	AA	1914	A
34	AA	1963	U
34	AA	1964	G
34	AA	1965	U
34	AA	1966	A
34	AA	1969	A
34	AA	1970	A
34	AA	1971	U
34	AA	1976	A
34	AA	1978	U
34	AA	1981	U
34	AA	1990	A

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Mol	Chain	Res	Type
34	AA	1991	U
34	AA	1996	C
34	AA	1997	G
34	AA	1998	A
34	AA	1999	A
34	AA	2000	G
34	AA	2003	G
34	AA	2010	C
34	AA	2016	U
34	AA	2017	U
34	AA	2018	G
34	AA	2019	A
34	AA	2030	G
34	AA	2034	G
34	AA	2080	C
34	AA	2082	C
34	AA	2084	U
34	AA	2090	U
34	AA	2092	G
34	AA	2094	A
34	AA	2096	G
34	AA	2097	A
34	AA	2102	A
34	AA	2106	A
34	AA	2107	C
34	AA	2108	A
34	AA	2109	A
34	AA	2113	C
34	AA	2115	U
34	AA	2117	A
34	AA	2125	A
34	AA	2132	A
34	AA	2136	C
34	AA	2145	A
34	AA	2146	A
34	AA	2147	A
34	AA	2148	U
34	AA	2149	A
34	AA	2160	G
34	AA	2161	G
34	AA	2171	U
34	AA	2174	G

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Mol	Chain	Res	Type
34	AA	2186	C
34	AA	2203	G
34	AA	2218	C
34	AA	2219	A
34	AA	2220	U
34	AA	2221	U
34	AA	2389	G
34	AA	2394	C
34	AA	2395	U
34	AA	2403	G
34	AA	2404	A
34	AA	2409	G
34	AA	2410	A
34	AA	2411	C
34	AA	2414	G
34	AA	2415	G
34	AA	2419	A
34	AA	2424	A
34	AA	2427	G
34	AA	2433	U
34	AA	2434	U
34	AA	2435	A
34	AA	2437	A
34	AA	2438	A
34	AA	2451	A
34	AA	2453	A
34	AA	2463	U
34	AA	2464	G
34	AA	2465	G
34	AA	2477	U
34	AA	2486	U
34	AA	2489	C
34	AA	2500	A
34	AA	2510	U
34	AA	2518	U
34	AA	2521	A
34	AA	2524	C
34	AA	2525	A
34	AA	2536	A
34	AA	2537	A
34	AA	2539	G
34	AA	2542	G

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Mol	Chain	Res	Type
34	AA	2544	G
34	AA	2545	A
34	AA	2548	A
34	AA	2549	A
34	AA	2550	C
34	AA	2552	A
34	AA	2555	A
34	AA	2556	C
34	AA	2562	U
34	AA	2564	A
34	AA	2565	G
34	AA	2566	G
34	AA	2573	A
34	AA	2574	A
34	AA	2575	U
34	AA	2576	G
34	AA	2580	C
34	AA	2581	G
34	AA	2584	A
34	AA	2588	A
34	AA	2591	U
34	AA	2596	A
34	AA	2600	G
34	AA	2602	A
34	AA	2603	U
34	AA	2606	A
34	AA	2608	G
34	AA	2627	U
34	AA	2628	G
34	AA	2629	U
34	AA	2640	U
34	AA	2665	A
34	AA	2666	A
34	AA	2667	C
34	AA	2668	G
34	AA	2671	C
34	AA	2676	C
34	AA	2681	U
34	AA	2684	G
34	AA	2686	G
34	AA	2690	A
34	AA	2694	A

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Mol	Chain	Res	Type
34	AA	2695	A
34	AA	2696	G
34	AA	2697	A
34	AA	2698	C
34	AA	2703	U
34	AA	2704	U
34	AA	2705	G
34	AA	2710	U
34	AA	2711	U
34	AA	2712	A
34	AA	2727	U
34	AA	2728	G
34	AA	2730	G
34	AA	2745	G
34	AA	2803	A
34	AA	2809	A
34	AA	2810	A
34	AA	2811	A
34	AA	2817	U
34	AA	2822	U
34	AA	2823	U
34	AA	2832	A
34	AA	2833	U
34	AA	2835	G
34	AA	2837	G
34	AA	2884	G
34	AA	2886	A
34	AA	2887	U
34	AA	2888	U
34	AA	2928	G
34	AA	2932	A
34	AA	2933	C
34	AA	2945	G
34	AA	2946	G
34	AA	2953	G
34	AA	2967	A
34	AA	2968	U
34	AA	2975	A
34	AA	2980	U
34	AA	2981	A
34	AA	2987	G
34	AA	2990	G

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Mol	Chain	Res	Type
34	AA	2991	U
34	AA	2995	A
34	AA	2996	A
34	AA	3005	C
34	AA	3011	G
34	AA	3013	A
34	AA	3014	C
34	AA	3015	A
34	AA	3018	A
34	AA	3019	A
34	AA	3020	U
34	AA	3028	A
34	AA	3029	G
34	AA	3030	A
34	AA	3033	A
34	AA	3034	A
34	AA	3035	A
34	AA	3042	A
34	AA	3053	G
34	AA	3061	U
34	AA	3068	A
34	AA	3073	G
34	AA	3076	G
34	AA	3079	A
34	AA	3081	C
34	AA	3086	A
34	AA	3087	A
34	AA	3088	G
34	AA	3091	U
34	AA	3092	G
34	AA	3094	C
34	AA	3100	G
34	AA	3108	A
34	AA	3111	U
34	AA	3113	U
34	AA	3116	A
34	AA	3118	A
34	AA	3123	C
34	AA	3124	G
34	AA	3126	A
34	AA	3127	A
34	AA	3130	U

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Mol	Chain	Res	Type
34	AA	3131	A
34	AA	3135	A
34	AA	3138	A
34	AA	3139	C
34	AA	3141	G
34	AA	3146	U
34	AA	3155	G
34	AA	3158	U
34	AA	3159	G
34	AA	3160	A
34	AA	3161	A
34	AA	3162	A
34	AA	3167	A
34	AA	3168	C
34	AA	3169	C
34	AA	3173	G
34	AA	3175	G
34	AA	3176	A
34	AA	3177	U
34	AA	3180	C
34	AA	3193	G
34	AA	3201	C
34	AA	3202	U
34	AA	3204	C
34	AA	3208	C
34	AA	3209	G
34	AA	3212	G
34	AA	3220	U
34	AA	3225	C
34	AA	3229	C
34	AA	3230	G
34	AA	3231	A
34	AA	3235	C
34	AA	3245	U
34	AA	3246	A
34	AA	3248	C
34	AA	3253	G
34	AA	3257	G
34	AA	3258	C
34	AA	3262	A
34	AA	3269	A
34	AA	3277	G

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Mol	Chain	Res	Type
34	AA	3281	G
34	AA	3282	U
34	AA	3287	C
34	AA	3292	A
34	AA	3293	A
34	AA	3294	U
34	AA	3295	A
34	AA	3297	G
34	AA	3301	C
34	AA	3302	G
34	AA	3304	G
34	AA	3305	A
34	AA	3306	G
34	AA	3312	U
34	AA	3313	U
34	AA	3330	A
34	AA	3336	G
34	AA	3338	U
34	AA	3342	C
34	AA	3349	G
34	AA	3351	U
34	AA	3353	A
34	AA	3354	A
34	AA	3358	U
34	AA	3359	A
34	AA	3361	U
34	AA	3362	A
34	AA	3374	U
34	AA	3375	A
34	AA	3377	A
34	AA	3378	C
34	AA	3379	A
34	AA	3380	U
34	AA	3381	A
34	AA	3382	U
34	AA	3383	A
34	AA	3389	G
34	AA	3391	G
34	AA	3398	A
34	AA	3415	A
34	AA	3416	G
34	AA	3418	A

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Mol	Chain	Res	Type
34	AA	3419	U
34	AA	3420	U
34	AA	3421	A
34	AA	3432	A
34	AA	3434	A
34	AA	3435	A
34	AA	3436	U
34	AA	3442	C
34	AA	3443	A
34	AA	3444	G
34	AA	3445	C
34	AA	3459	A
34	AA	3463	G
34	AA	3464	U
34	AA	3468	G
34	AA	3471	A
34	AA	3472	A
34	AA	3476	A
34	AA	3477	A
34	AA	3483	U
34	AA	3488	U
34	AA	3493	G
34	AA	3500	G
34	AA	3507	A
34	AA	3510	C
34	AA	3513	G
34	AA	3515	A
34	AA	3516	A
34	AA	3527	U
34	AA	3530	A
34	AA	3555	U
34	AA	3571	A
34	AA	3573	U
34	AA	3575	U
34	AA	3576	A
34	AA	3578	A
34	AA	3579	A
34	AA	3580	G
34	AA	3581	A
34	AA	3582	G
34	AA	3585	A
34	AA	3586	U

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Mol	Chain	Res	Type
34	AA	3588	A
34	AA	3589	U
34	AA	3590	A
34	AA	3591	U
34	AA	3594	G
34	AA	3597	C
34	AA	3612	U
34	AA	3615	A
34	AA	3618	A
34	AA	3619	U
34	AA	3623	A
34	AA	3624	U
34	AA	3625	C
34	AA	3626	A
34	AA	3627	C
34	AA	3628	C
34	AA	3632	U
34	AA	3658	G
34	AA	3659	C
34	AA	3661	A
34	AA	3662	U
34	AA	3663	A
34	AA	3664	G
34	AA	3665	U
34	AA	3667	C
34	AA	3668	U
34	AA	3669	U
34	AA	3670	U
34	AA	3671	A
34	AA	3677	A
34	AA	3680	A
34	AA	3683	G
34	AA	3689	C
34	AA	3697	G
34	AA	3698	U
34	AA	3707	U
34	AA	3711	U
34	AA	3712	G
34	AA	3716	C
34	AA	3727	A
34	AA	3728	A
34	AA	3732	U

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Mol	Chain	Res	Type
34	AA	3733	G
34	AA	3736	A
34	AA	3737	G
34	AA	3739	A
34	AA	3740	A
34	AA	3752	C
34	AA	3761	G
34	AA	3767	U
34	AA	3768	A
34	AA	3770	C
34	AA	3775	G
34	AA	3778	G
34	AA	3779	U
34	AA	3782	A
34	AA	3783	G
35	AC	5	A
35	AC	6	C
35	AC	25	C
35	AC	36	C
35	AC	38	G
35	AC	39	C
35	AC	43	G
35	AC	50	G
35	AC	53	G
35	AC	55	A
35	AC	57	A
35	AC	63	A
35	AC	64	U
35	AC	65	A
35	AC	66	C
35	AC	67	G
35	AC	68	C
35	AC	73	A
35	AC	75	A
35	AC	80	C
35	AC	90	G
35	AC	92	A
35	AC	94	C
35	AC	98	A
35	AC	99	G
35	AC	100	A
35	AC	101	A

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Mol	Chain	Res	Type
35	AC	102	U
35	AC	107	A
35	AC	108	A
35	AC	109	U
35	AC	111	U
35	AC	112	A
35	AC	114	A
35	AC	115	C
35	AC	116	U
35	AC	117	A
35	AC	119	A
35	AC	122	A
35	AC	123	A
35	AC	135	G
35	AC	137	A
35	AC	138	U
35	AC	139	A
35	AC	140	G
35	AC	142	G
35	AC	145	A
35	AC	146	C
35	AC	149	C
36	AB	3	A
36	AB	7	G
36	AB	10	C
36	AB	13	A
36	AB	16	A
36	AB	18	A
36	AB	22	G
36	AB	25	A
36	AB	26	C
36	AB	27	A
36	AB	28	C
36	AB	33	U
36	AB	38	U
36	AB	48	G
36	AB	51	G
36	AB	53	U
36	AB	54	A
36	AB	63	A
36	AB	64	A
36	AB	69	U

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Mol	Chain	Res	Type
36	AB	71	G
36	AB	74	A
36	AB	84	U
36	AB	85	G
36	AB	89	G
36	AB	93	G
36	AB	97	G
36	AB	100	A
36	AB	110	G

All (306) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1	A
1	A	2	A
1	A	25	C
1	A	44	U
1	A	45	U
1	A	95	A
1	A	103	U
1	A	105	A
1	A	107	A
1	A	156	A
1	A	161	U
1	A	206	A
1	A	246	A
1	A	249	A
1	A	251	U
1	A	326	U
1	A	327	U
1	A	357	U
1	A	358	G
1	A	383	G
1	A	406	A
1	A	408	U
1	A	423	A
1	A	474	A
1	A	525	G
1	A	544	G
1	A	561	C
1	A	577	A
1	A	614	A

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Mol	Chain	Res	Type
1	A	616	U
1	A	745	A
1	A	752	U
1	A	753	U
1	A	789	U
1	A	790	U
1	A	793	G
1	A	804	U
1	A	805	A
1	A	815	G
1	A	818	C
1	A	831	U
1	A	844	G
1	A	872	A
1	A	874	A
1	A	876	U
1	A	879	A
1	A	919	U
1	A	973	G
1	A	981	U
1	A	983	G
1	A	1028	U
1	A	1056	G
1	A	1070	A
1	A	1100	U
1	A	1182	A
1	A	1209	G
1	A	1259	C
1	A	1292	U
1	A	1295	A
1	A	1300	G
1	A	1301	G
1	A	1305	A
1	A	1370	U
1	A	1381	C
1	A	1414	A
1	A	1416	U
1	A	1421	A
1	A	1423	A
1	A	1432	G
1	A	1448	U
1	A	1455	C

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Mol	Chain	Res	Type
1	A	1659	U
1	A	1666	C
1	A	1667	A
1	A	1672	C
1	A	1691	G
1	A	1692	A
1	A	1704	G
1	A	1705	C
1	A	1729	A
1	A	1786	U
1	A	1788	U
1	A	1799	A
1	A	1818	A
1	A	1819	U
1	A	1834	A
1	A	1854	U
1	A	1865	G
1	A	1870	A
1	A	1871	G
1	A	1897	A
1	A	1898	G
1	A	1912	C
1	A	1934	C
1	A	1976	G
1	A	1977	G
1	A	2048	A
1	A	2053	U
1	A	2060	G
1	A	2071	U
2	7	34	C
2	7	44	A
2	7	53	G
2	7	55	U
2	7	73	A
34	AA	10	G
34	AA	25	A
34	AA	43	A
34	AA	61	A
34	AA	62	A
34	AA	65	A
34	AA	121	U
34	AA	122	A

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Mol	Chain	Res	Type
34	AA	124	U
34	AA	138	C
34	AA	149	A
34	AA	162	U
34	AA	181	C
34	AA	205	G
34	AA	215	C
34	AA	218	U
34	AA	228	A
34	AA	257	U
34	AA	270	U
34	AA	289	A
34	AA	315	C
34	AA	337	A
34	AA	353	G
34	AA	416	G
34	AA	432	A
34	AA	497	U
34	AA	500	A
34	AA	501	U
34	AA	504	A
34	AA	505	A
34	AA	579	C
34	AA	580	A
34	AA	581	C
34	AA	594	C
34	AA	595	U
34	AA	596	A
34	AA	597	A
34	AA	607	A
34	AA	620	U
34	AA	621	C
34	AA	641	G
34	AA	645	A
34	AA	650	U
34	AA	652	A
34	AA	667	U
34	AA	674	U
34	AA	681	U
34	AA	683	A
34	AA	697	A
34	AA	698	G

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Mol	Chain	Res	Type
34	AA	703	U
34	AA	715	U
34	AA	721	U
34	AA	764	G
34	AA	768	C
34	AA	769	U
34	AA	803	A
34	AA	809	A
34	AA	811	A
34	AA	821	C
34	AA	859	C
34	AA	889	U
34	AA	899	A
34	AA	904	G
34	AA	935	A
34	AA	965	A
34	AA	998	U
34	AA	1013	U
34	AA	1027	G
34	AA	1035	G
34	AA	1042	C
34	AA	1078	C
34	AA	1098	U
34	AA	1101	A
34	AA	1115	G
34	AA	1186	A
34	AA	1197	U
34	AA	1202	C
34	AA	1204	A
34	AA	1217	U
34	AA	1223	U
34	AA	1224	A
34	AA	1243	G
34	AA	1272	U
34	AA	1319	U
34	AA	1422	A
34	AA	1435	G
34	AA	1457	G
34	AA	1503	A
34	AA	1538	U
34	AA	1539	U
34	AA	1574	C

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Mol	Chain	Res	Type
34	AA	1602	A
34	AA	1603	C
34	AA	1605	A
34	AA	1632	G
34	AA	1642	G
34	AA	1658	G
34	AA	1703	U
34	AA	1705	A
34	AA	1750	U
34	AA	1798	A
34	AA	1805	U
34	AA	1872	A
34	AA	1873	U
34	AA	1881	C
34	AA	1898	U
34	AA	1964	G
34	AA	1989	A
34	AA	1990	A
34	AA	1996	C
34	AA	1999	A
34	AA	2015	C
34	AA	2033	C
34	AA	2096	G
34	AA	2146	A
34	AA	2170	G
34	AA	2193	U
34	AA	2219	A
34	AA	2394	C
34	AA	2409	G
34	AA	2434	U
34	AA	2437	A
34	AA	2523	U
34	AA	2563	A
34	AA	2574	A
34	AA	2665	A
34	AA	2696	G
34	AA	2727	U
34	AA	2810	A
34	AA	2816	U
34	AA	2822	U
34	AA	2883	U
34	AA	2886	A

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Mol	Chain	Res	Type
34	AA	2932	A
34	AA	2966	C
34	AA	3013	A
34	AA	3017	A
34	AA	3018	A
34	AA	3019	A
34	AA	3027	U
34	AA	3034	A
34	AA	3085	A
34	AA	3097	A
34	AA	3129	U
34	AA	3137	U
34	AA	3140	U
34	AA	3158	U
34	AA	3161	A
34	AA	3167	A
34	AA	3195	C
34	AA	3229	C
34	AA	3230	G
34	AA	3245	U
34	AA	3291	U
34	AA	3309	G
34	AA	3337	U
34	AA	3361	U
34	AA	3379	A
34	AA	3381	A
34	AA	3382	U
34	AA	3414	G
34	AA	3419	U
34	AA	3434	A
34	AA	3435	A
34	AA	3476	A
34	AA	3500	G
34	AA	3526	U
34	AA	3575	U
34	AA	3577	A
34	AA	3579	A
34	AA	3584	A
34	AA	3585	A
34	AA	3588	A
34	AA	3590	A
34	AA	3617	A

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Mol	Chain	Res	Type
34	AA	3624	U
34	AA	3627	C
34	AA	3658	G
34	AA	3660	A
34	AA	3663	A
34	AA	3667	C
34	AA	3669	U
34	AA	3670	U
34	AA	3688	G
34	AA	3711	U
34	AA	3732	U
34	AA	3774	A
34	AA	3782	A
35	AC	35	A
35	AC	37	A
35	AC	64	U
35	AC	90	G
35	AC	100	A
35	AC	108	A
35	AC	114	A
35	AC	134	G
35	AC	139	A
35	AC	145	A
36	AB	84	U
36	AB	88	A

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
63	AW	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AW	154:ASN	C	197:UNK	N	36.79

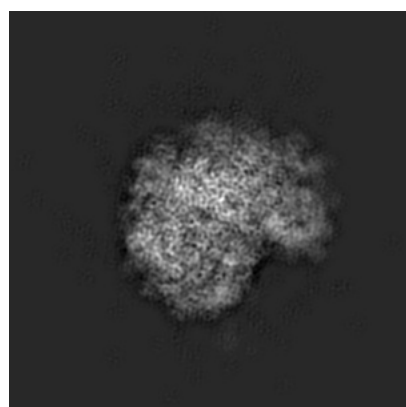
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6452. These allow visual inspection of the internal detail of the map and identification of artifacts.

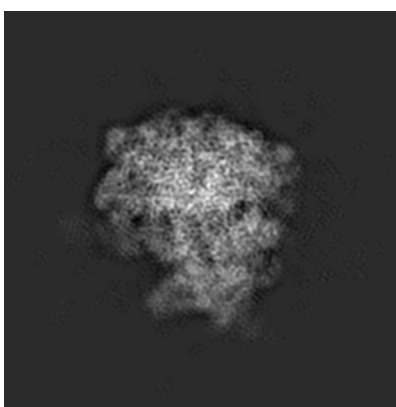
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

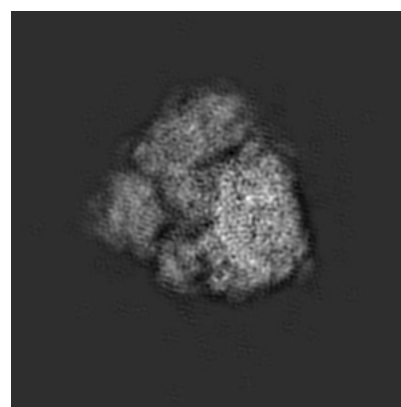
6.1.1 Primary map



X



Y

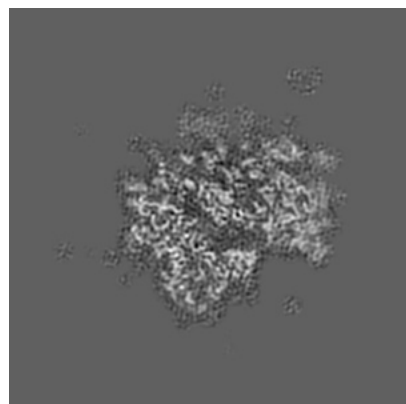


Z

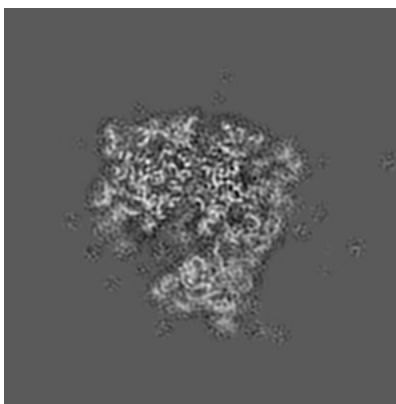
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

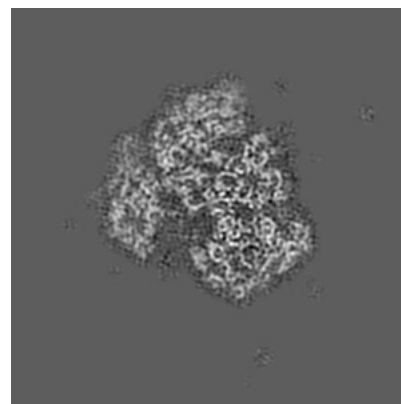
6.2.1 Primary map



X Index: 148



Y Index: 148

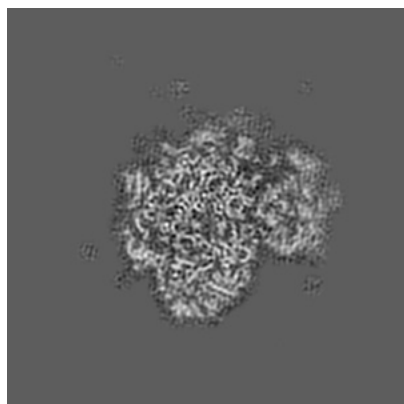


Z Index: 148

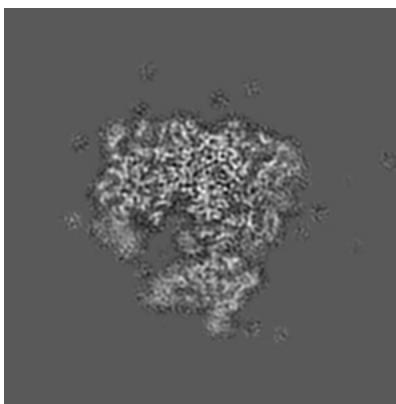
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

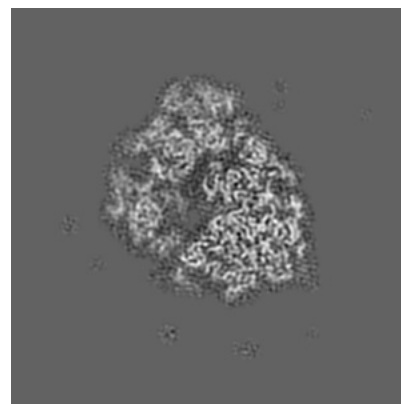
6.3.1 Primary map



X Index: 157



Y Index: 154

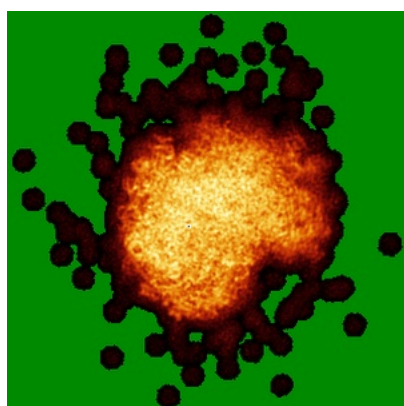


Z Index: 137

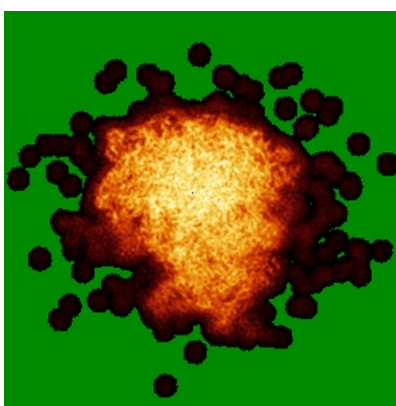
The images above show the largest variance slices of the map in three orthogonal directions.

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

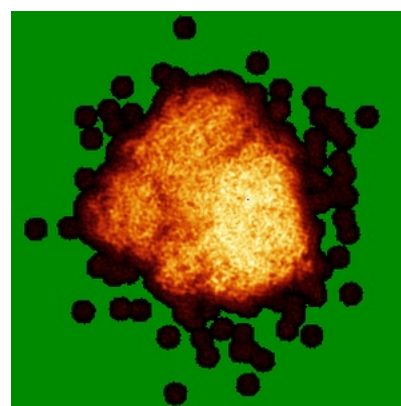
6.4.1 Primary map



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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

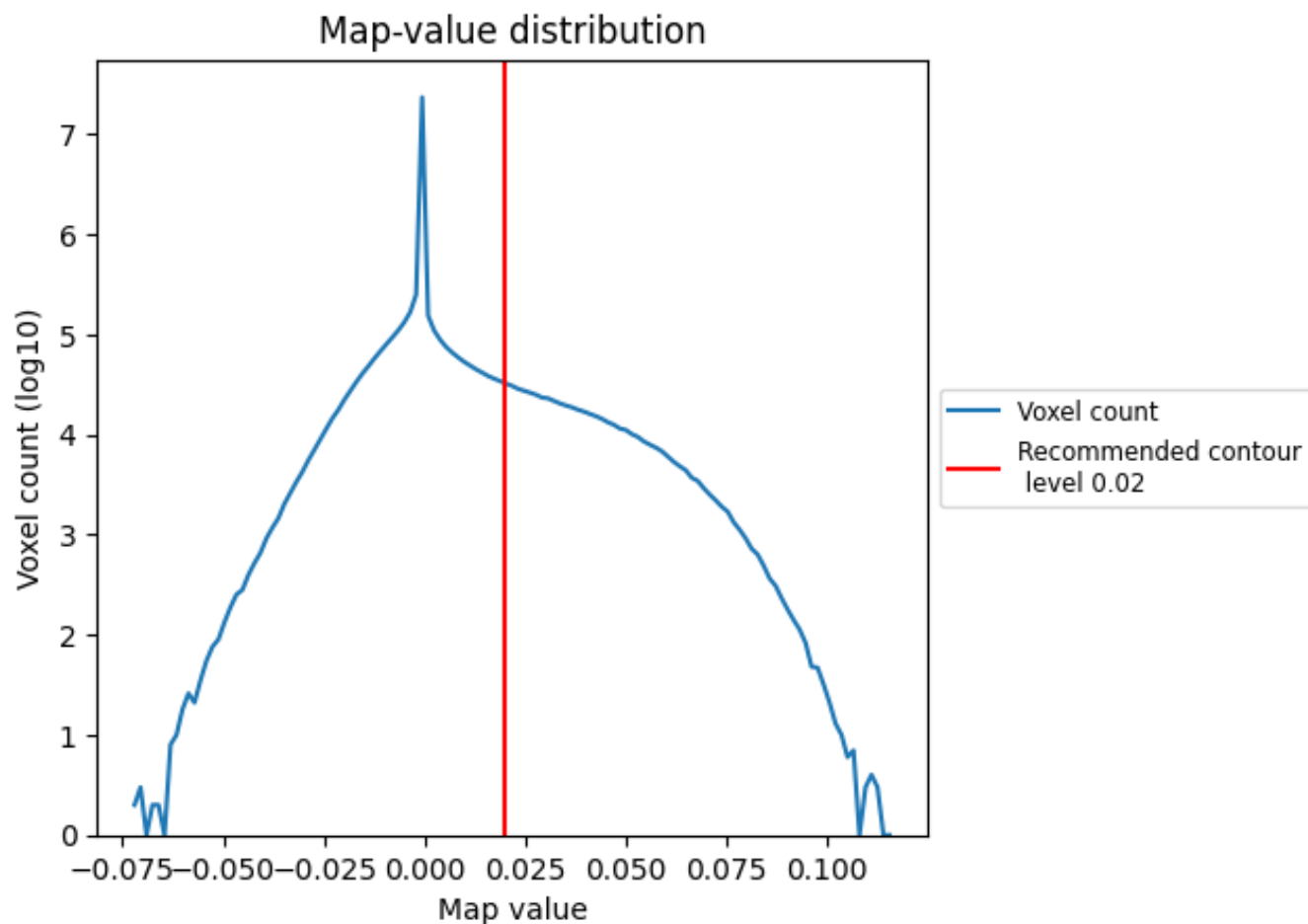
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

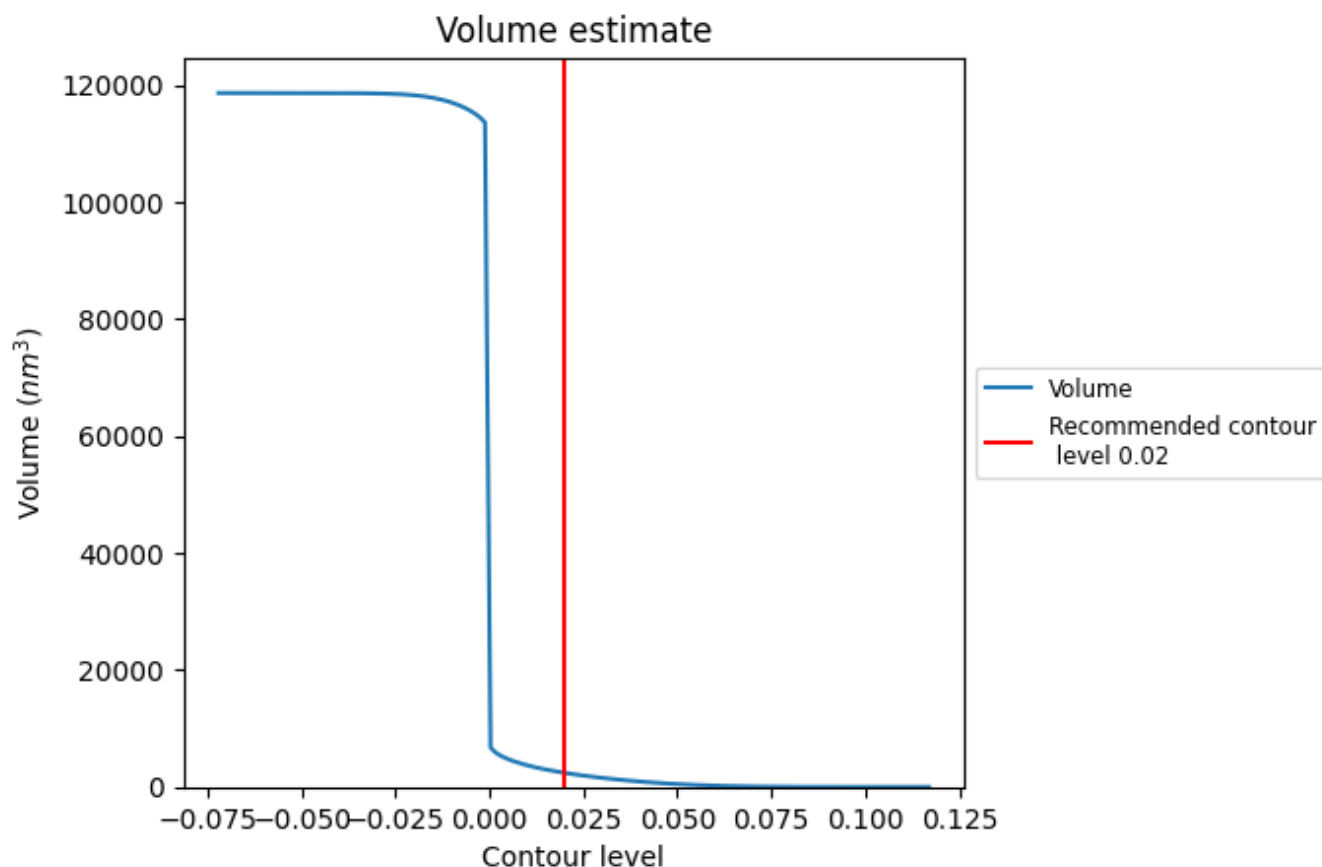
This section contains the results of statistical analysis of the map.

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.

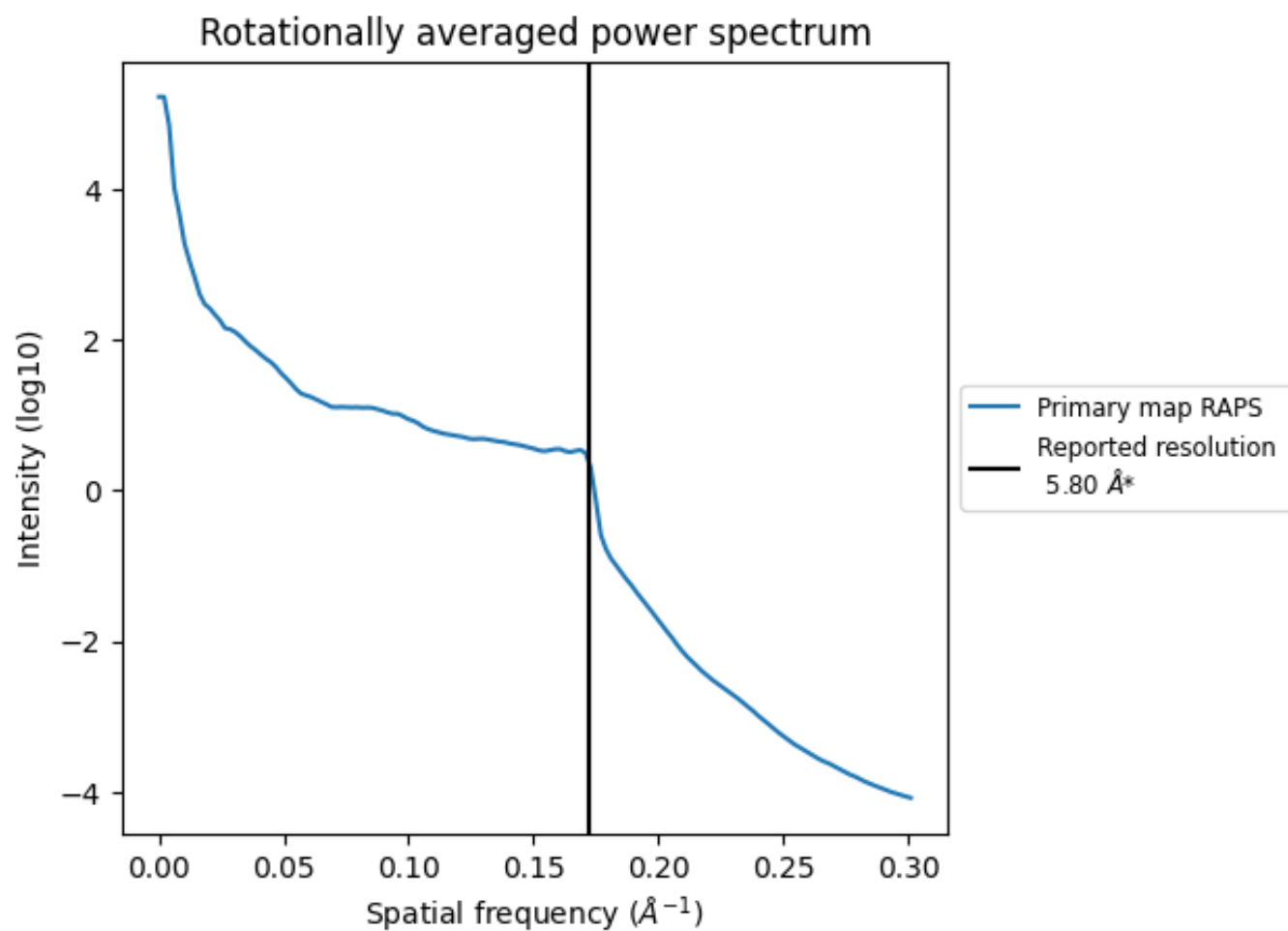
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2413 nm³; this corresponds to an approximate mass of 2180 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 0.172 Å⁻¹

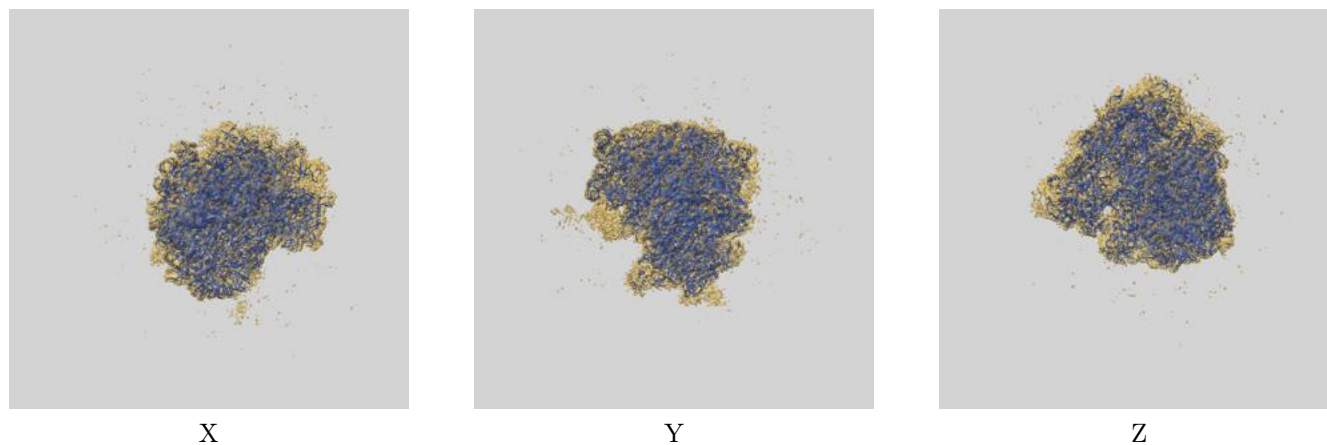
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

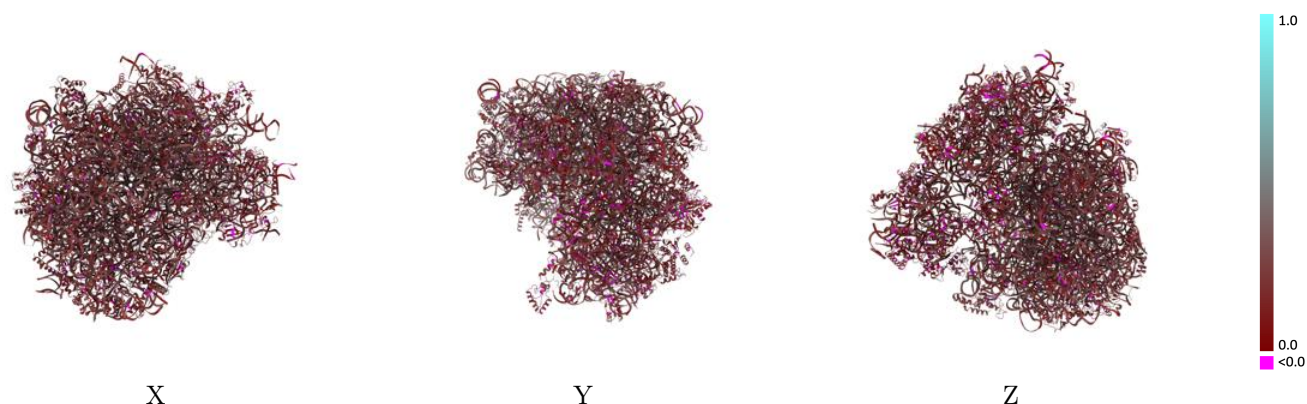
This section contains information regarding the fit between EMDB map EMD-6452 and PDB model 3JBO. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



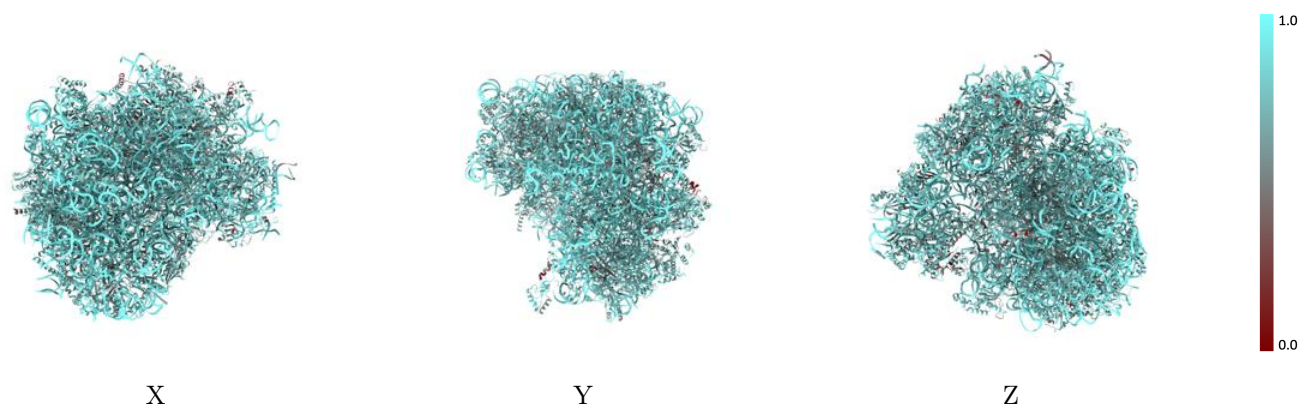
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



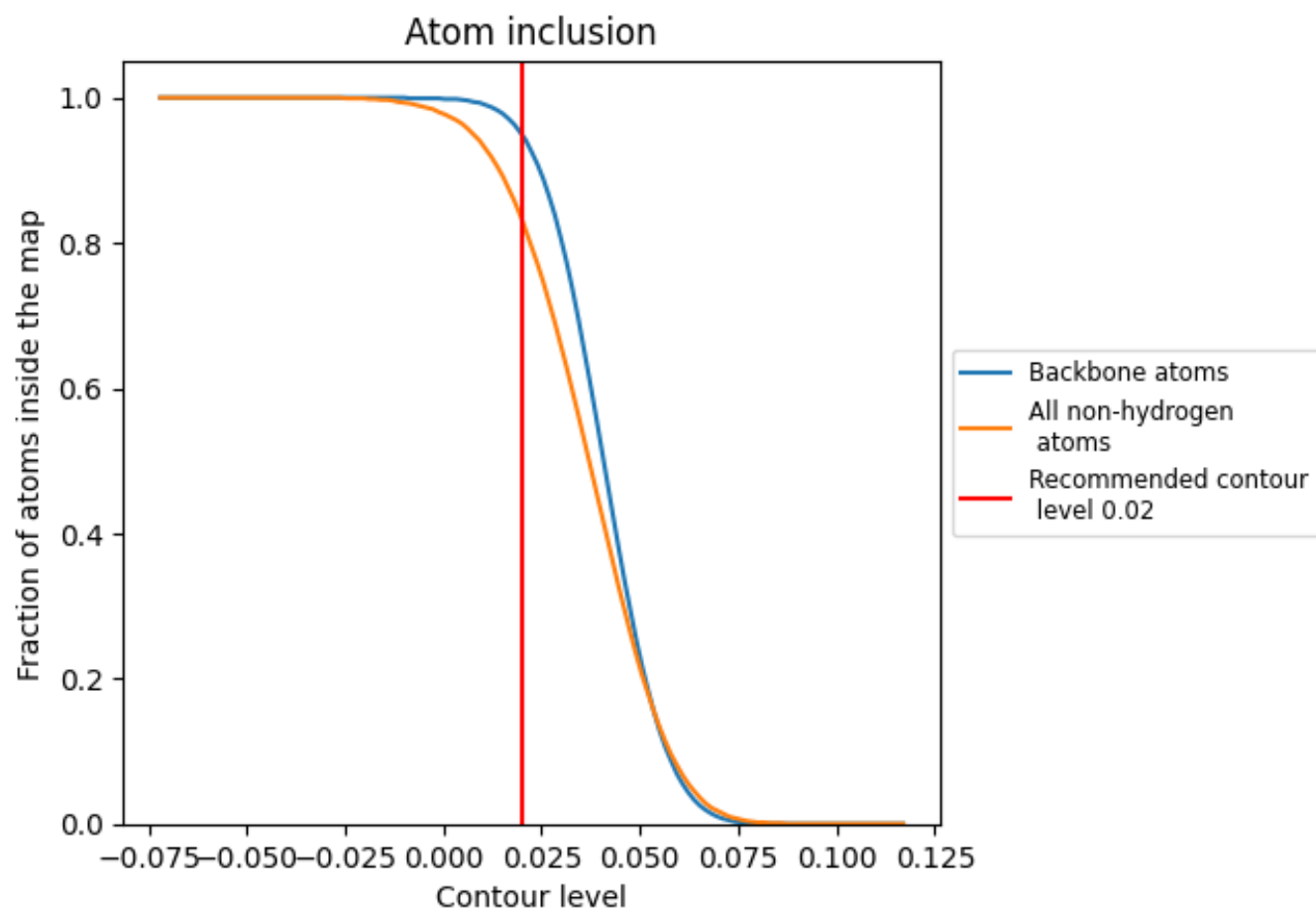
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 83% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.2350
1	 0.7240	 0.1750
2	 0.7350	 0.2180
3	 0.6570	 0.2160
4	 0.7020	 0.2110
5	 0.4790	 0.1990
6	 0.6700	 0.2340
7	 0.7770	 0.2280
A	 0.9220	 0.2420
A0	 0.7200	 0.2300
A1	 0.7180	 0.2170
A2	 0.7690	 0.2350
A3	 0.7210	 0.1910
A4	 0.6860	 0.2280
A5	 0.7050	 0.2010
A6	 0.6820	 0.2190
A7	 0.7110	 0.1910
A8	 0.6500	 0.2200
A9	 0.7000	 0.2040
AA	 0.9290	 0.2660
AB	 0.9700	 0.2630
AC	 0.9480	 0.2660
AD	 0.5990	 0.2000
AE	 0.6930	 0.2120
AF	 0.7100	 0.2030
AG	 0.7160	 0.2170
AH	 0.7420	 0.2140
AI	 0.7470	 0.2030
AJ	 0.7300	 0.2300
AK	 0.6760	 0.1910
AL	 0.7420	 0.2230
AM	 0.6470	 0.2270
AN	 0.7530	 0.2140
AO	 0.6980	 0.2100
AP	 0.6680	 0.1850



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Chain	Atom inclusion	Q-score
AQ	 0.6970	 0.2270
AR	 0.7590	 0.2030
AS	 0.6810	 0.2040
AT	 0.6580	 0.2020
AU	 0.7220	 0.2160
AV	 0.6990	 0.2270
AW	 0.7290	 0.2080
AX	 0.7160	 0.2030
AY	 0.7160	 0.2360
AZ	 0.7600	 0.2110
Aa	 0.6910	 0.2250
Ab	 0.7320	 0.2120
Ac	 0.6590	 0.1940
Ad	 0.7620	 0.2280
Ae	 0.6970	 0.2200
Af	 0.7100	 0.1950
Ag	 0.5760	 0.1850
Ah	 0.6420	 0.1970
Ai	 0.6770	 0.2060
B	 0.6640	 0.1960
C	 0.7410	 0.2030
D	 0.6850	 0.2100
E	 0.7120	 0.1910
F	 0.7300	 0.1900
G	 0.7380	 0.2160
H	 0.7220	 0.1770
I	 0.6440	 0.1850
J	 0.7140	 0.1950
K	 0.6770	 0.1930
L	 0.7160	 0.2060
M	 0.7170	 0.1660
N	 0.7380	 0.1730
O	 0.7770	 0.2150
P	 0.6460	 0.1980
Q	 0.6000	 0.1980
R	 0.8210	 0.2190
S	 0.7550	 0.1920
T	 0.7600	 0.1870
U	 0.6560	 0.1920
V	 0.6900	 0.2190
W	 0.7460	 0.2010
X	 0.7280	 0.2290

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Chain	Atom inclusion	Q-score
Y	0.7860	0.1900
Z	0.7310	0.2160