



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 07:08 AM EST

PDB ID : 6XDR
EMDB ID : EMD-22142
Title : Escherichia coli transcription-translation complex B (TTC-B) containing an
27 nt long mRNA spacer, NusG, and fMet-tRNAs at E-site and P-site
Authors : Molodtsov, V.; Wang, C.; Su, M.; Ebright, R.H.
Deposited on : 2020-06-11
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

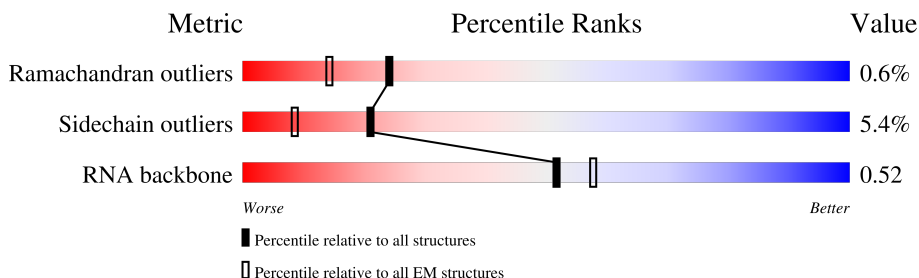
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	103	
2	1	110	
3	2	100	
4	3	104	
5	4	94	
6	5	36	
7	6	36	
8	7	44	

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Mol	Chain	Length	Quality of chain
9	9	165	
10	A	76	
10	B	76	
11	AA	1342	
12	AB	181	
13	AC	329	
13	AD	329	
14	AE	1407	
15	AF	91	
16	C	75	
17	D	1542	
18	E	87	
19	F	71	
20	G	241	
21	H	557	
22	I	233	
23	J	206	
24	K	167	
25	L	135	
26	M	179	
27	N	130	
28	O	130	
29	P	103	
30	Q	129	
31	R	124	

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Mol	Chain	Length	Quality of chain
32	S	101	
33	T	89	
34	U	82	
35	V	84	
36	W	92	
37	X	118	
38	Y	142	
39	Z	121	
40	a	2904	
41	b	85	
42	c	78	
43	d	120	
44	e	63	
45	f	59	
46	g	70	
47	h	273	
48	i	57	
49	j	209	
50	k	55	
51	l	201	
52	m	46	
53	n	179	
54	o	65	
55	p	177	
56	q	38	

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Mol	Chain	Length	Quality of chain
57	r	149	
58	s	142	
59	t	123	
60	u	144	
61	v	136	
62	w	127	
63	x	117	
64	y	115	
65	z	118	

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 276506 atoms, of which 99294 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	94	Total	C	H	N	O	S	0	0
			1557	470	811	140	134	2		

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	3	103	Total	C	H	N	O		0	0
			1632	498	844	148	142			

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	23	Total	C	H	N	O	P	0	0
			732	225	260	87	137	23		

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	27	Total	C	H	N	O	P	0	0
			847	259	305	89	167	27		

- Molecule 8 is a RNA chain called mRNA with 27 nt long spacer.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	34	Total	C	H	N	O	P	0	0
			804	316	97	98	259	34		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 10 is a RNA chain called E-site and P-site tRNA (fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A	76	Total	C	H	N	O	P	0	0
			2446	723	826	295	527	75		
10	B	76	Total	C	H	N	O	P	0	0
			2433	723	813	295	527	75		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

- Molecule 12 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AB	175	Total	C	N	O	S	0	0
			1392	881	249	255	7		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AC	221	Total	C	N	O	S	0	0
			1698	1060	299	333	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	AD	218	Total	C	N	O	S	0	0
			1677	1048	297	326	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AE	1337	Total	C	N	O	S	0	0
			10404	6535	1856	1963	50		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	1384	VAL	MET	conflict	UNP A0A4S1NBU2

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AF	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 16 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	66	Total	C	H	N	O	S	
			1103	344	559	102	97	1	0

- Molecule 17 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	1524	Total	C	H	N	O	P	
			49126	14585	16423	6003	10591	1524	0

- Molecule 18 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	86	Total	C	H	N	O	S	
			1388	414	719	138	114	3	0

- Molecule 19 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	F	70	Total	C	H	N	O	S	0	0
			1218	366	629	125	97	1		

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 21 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 22 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 23 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 24 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 25 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 26 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	M	151	Total	C	H	N	O	S	0	0
			2416	735	1235	227	215	4		

- Molecule 27 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	N	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 28 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	O	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

- Molecule 29 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	P	99	Total	C	H	N	O	S	0	0
			1621	495	831	151	143	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	Q	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

- Molecule 31 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	R	121	Total	C	H	N	O	S	0	0
			1940	580	1001	194	161	4		

- Molecule 32 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	S	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 33 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 34 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 35 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 36 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 37 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 38 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 39 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Z	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 40 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	a	2880	Total	C	H	N	O	P	0	0
			92912	27587	31071	11398	19976	2880		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 41 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	b	76	Total	C	H	N	O	S	0	0
			1181	360	599	117	104	1		

- Molecule 42 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	c	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 43 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	d	120	Total	C	H	N	O	P	0	0
			3870	1144	1301	468	837	120		

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	e	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	f	58	Total	C	H	N	O	S	0	0
			936	281	488	87	78	2		

- Molecule 46 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	g	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

- Molecule 47 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	h	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	j	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	k	52	Total	C	H	N	O	S	0	0
			890	275	464	78	73			

- Molecule 51 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	l	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	m	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 57 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 58 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	s	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 59 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 60 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	u	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 61 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 62 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 63 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	x	116	Total	C	H	N	O		0	0
			1815	552	923	178	162			

- Molecule 64 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	y	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 65 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	z	117	Total	C	H	N	O		0	0
			1967	604	1020	192	151			

- Molecule 66 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
66	7	1	Total	Mg	0
			1	1	

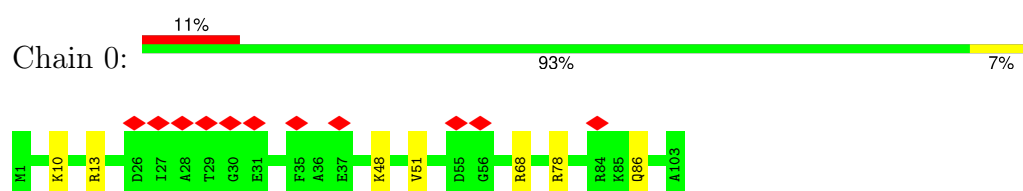
- Molecule 67 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
67	AE	2	Total	Zn	0
			2	2	

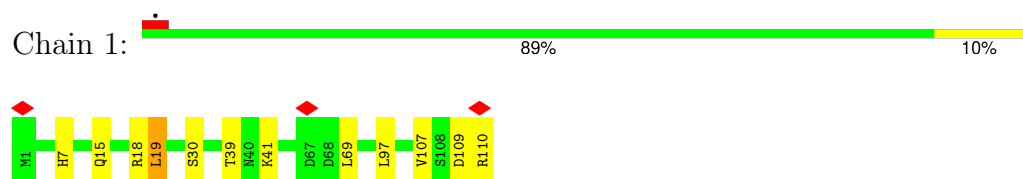
3 Residue-property plots [i](#)

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

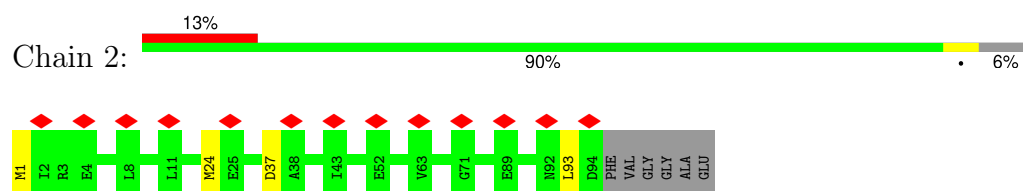
- Molecule 1: 50S ribosomal protein L21



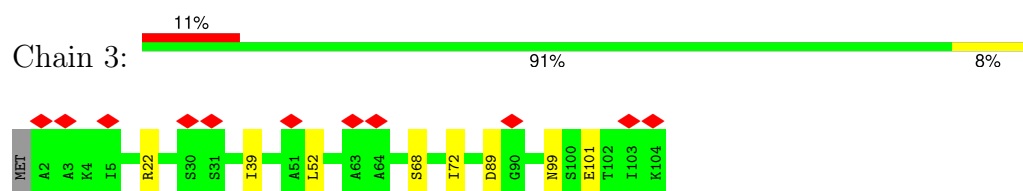
- Molecule 2: 50S ribosomal protein L22



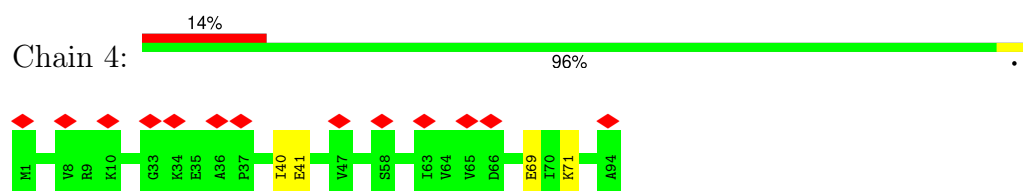
- Molecule 3: 50S ribosomal protein L23

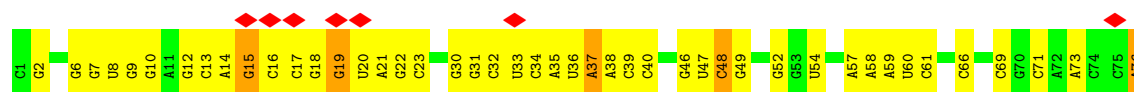


- Molecule 4: 50S ribosomal protein L24

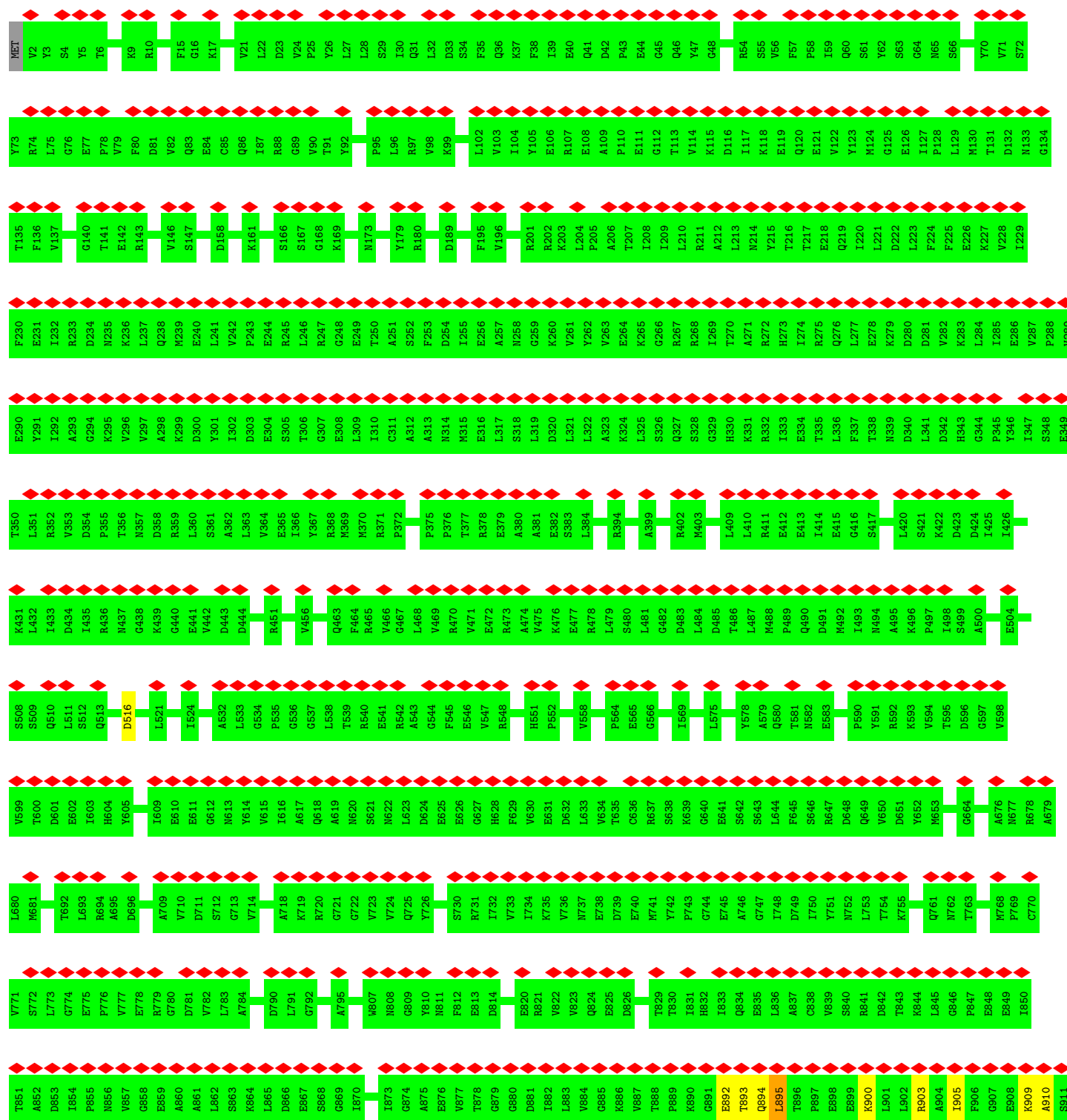


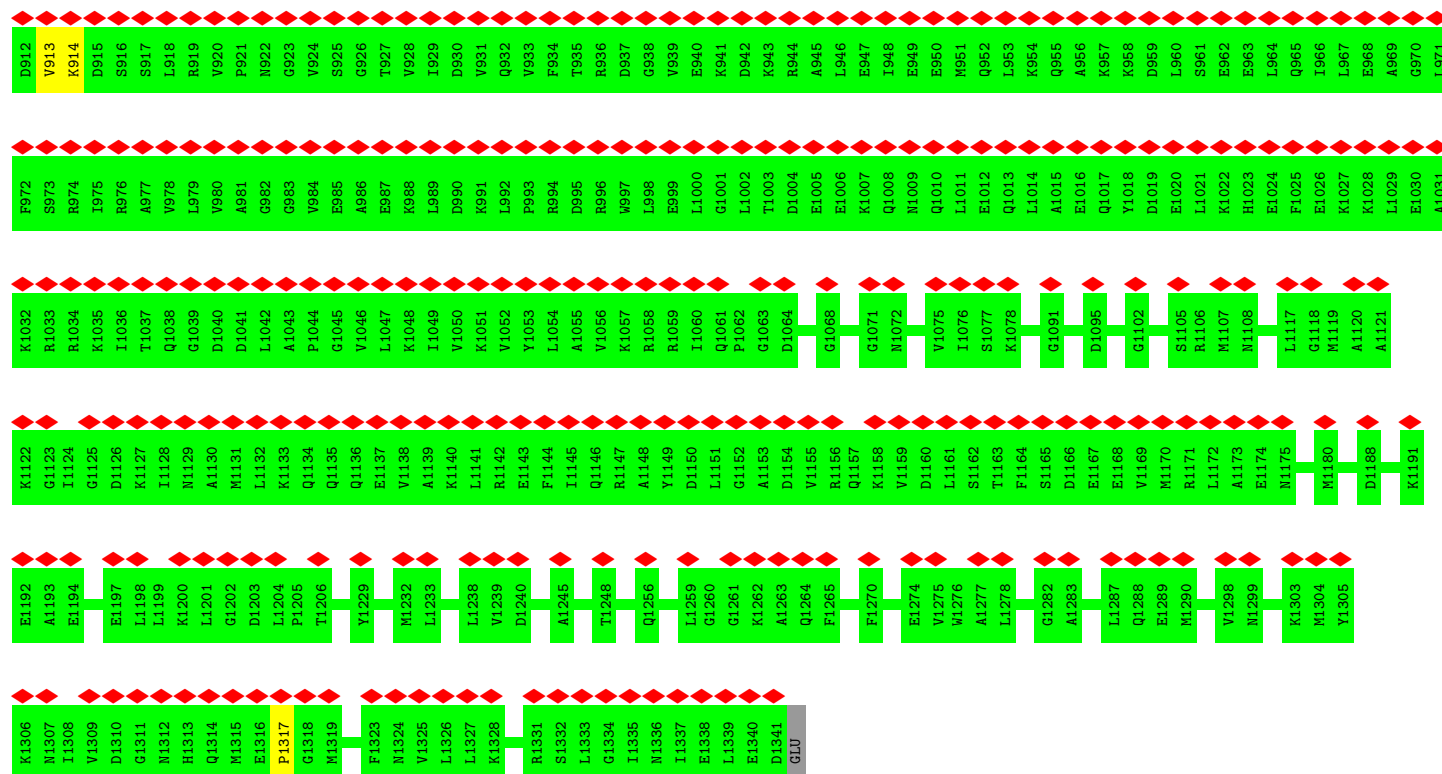
- Molecule 5: 50S ribosomal protein L25



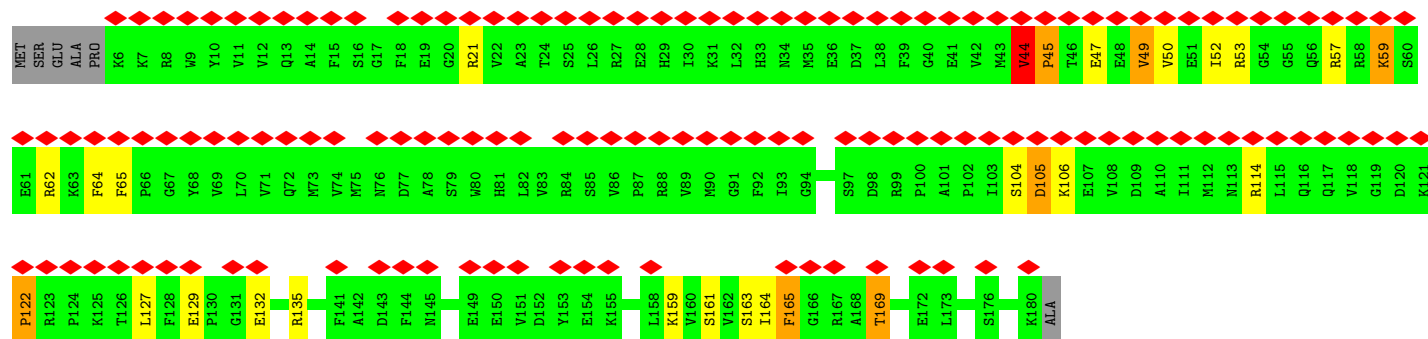
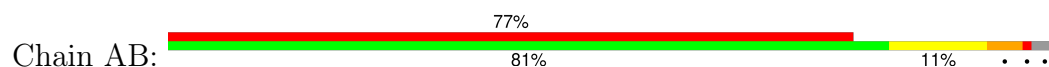


- Molecule 11: DNA-directed RNA polymerase subunit beta

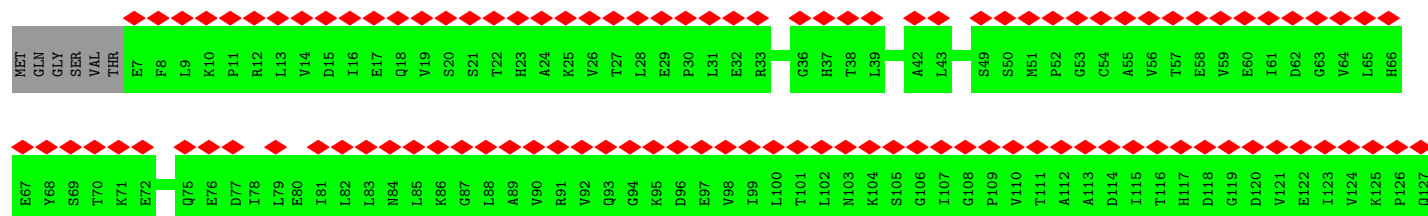


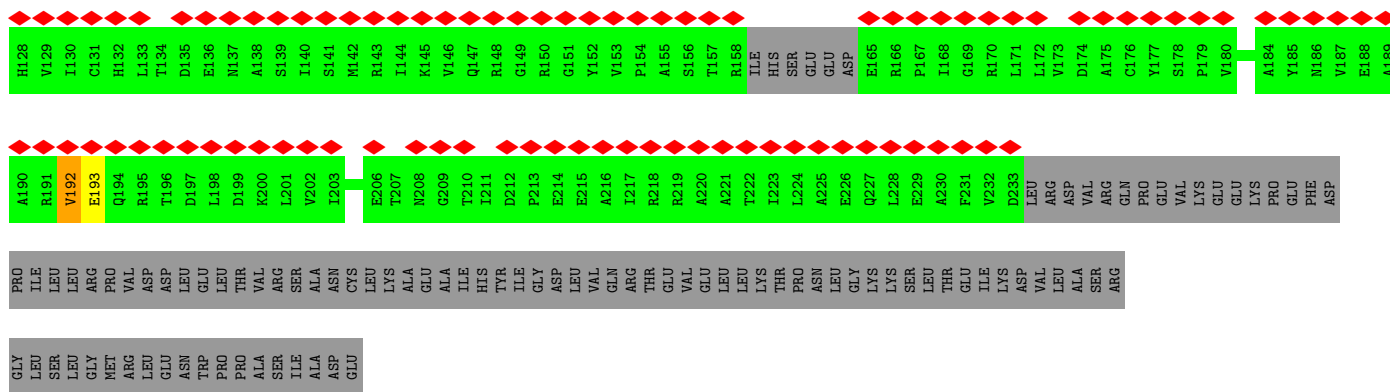


• Molecule 12: Transcription termination/antitermination protein NusG

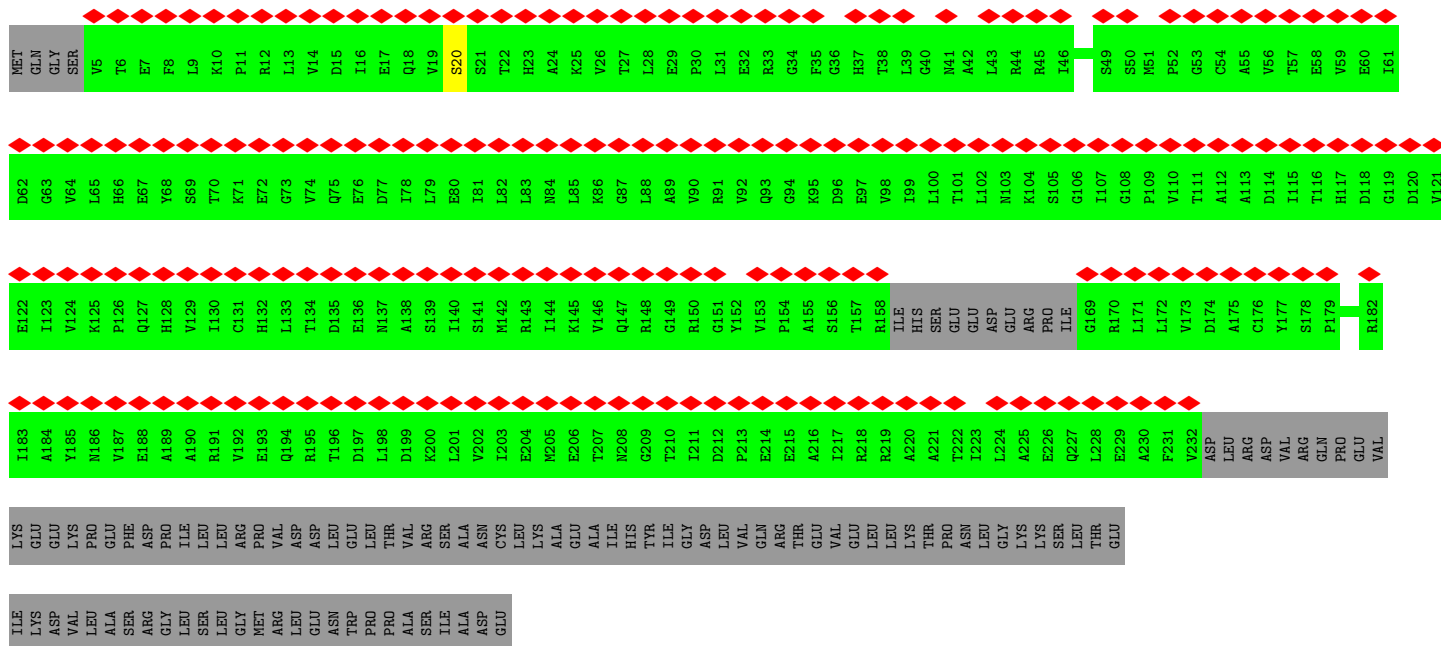


• Molecule 13: DNA-directed RNA polymerase subunit alpha

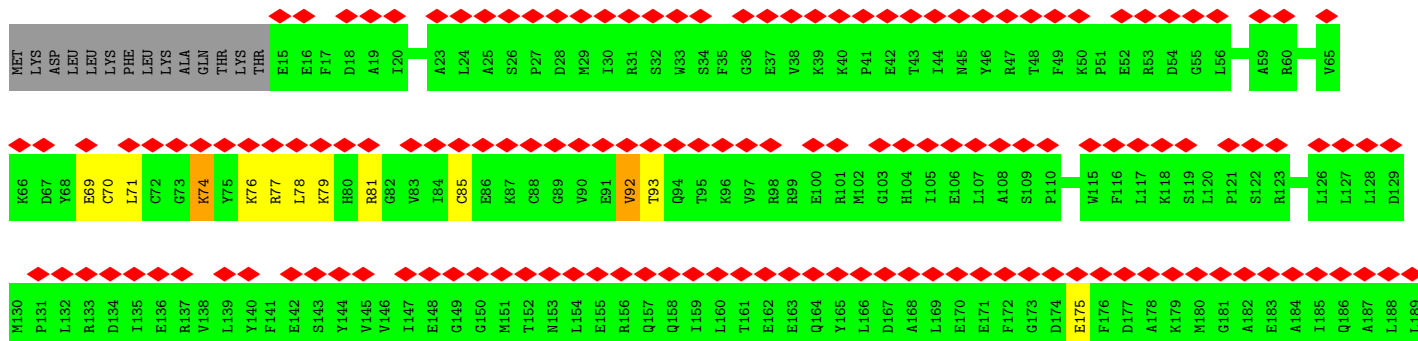




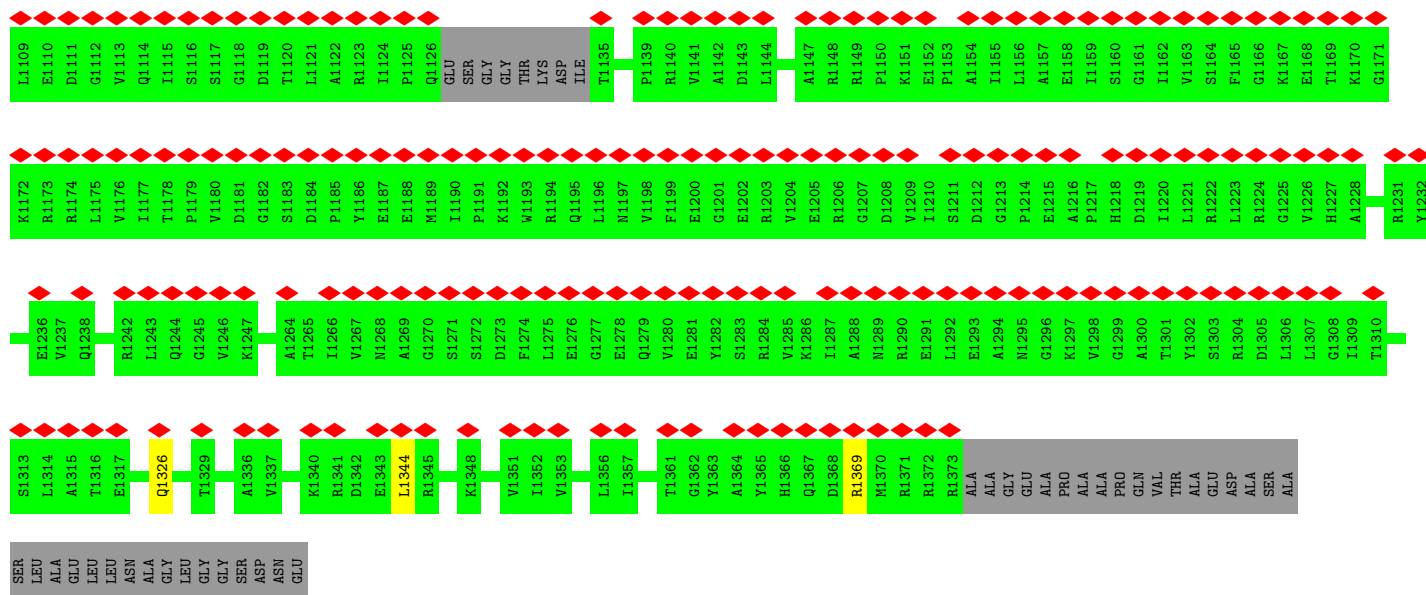
- Molecule 13: DNA-directed RNA polymerase subunit alpha



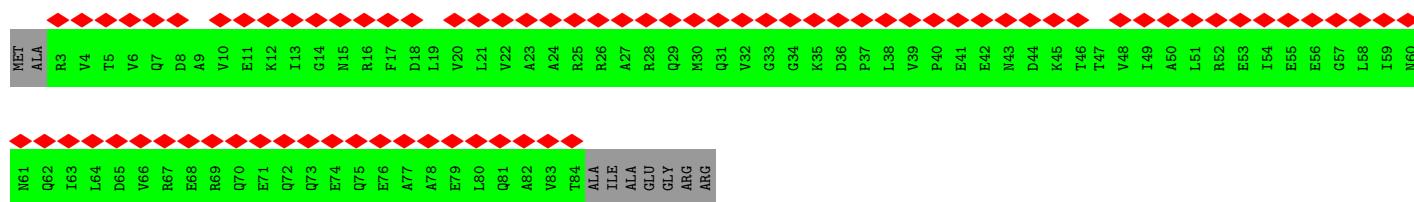
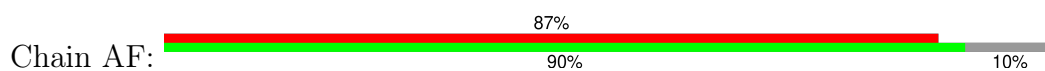
- Molecule 14: DNA-directed RNA polymerase subunit beta'



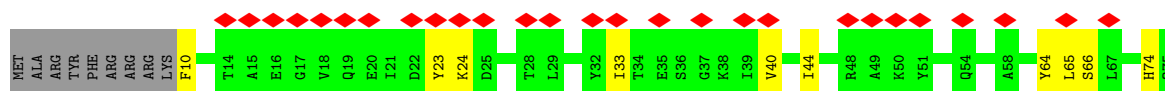
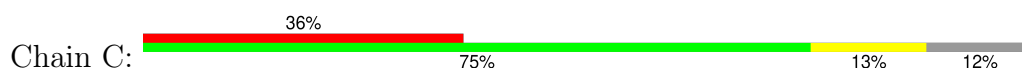
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T1050	R990	L930	L857	D785	T703	A633	K557	L478	E402	L324	P254	S191
D1051	T991	T931	W858	T786	E704	E705	D558	A482	R403	K325	L255	M192
E1052	K992	T932	P859	A787	T705	T706	A559	L483	E404	S326	D256	D193
L1053	E993	R933	R860	L788	V706	I707	N560	M484	E405	L327	G257	L194
T1054	S994	THR	N861	K789	I707	M708	G561	M485	A406	A328	G258	E195
G1055	Y995	PHE	T862	A791	R708	N709	E562	K649	V407	D329	G258	E195
L1056	K996	HIS	L863	T790	E709	D710	L563	S486	V408	K330	R259	Q196
S1057	V997	ILE	L864	N792	R709	D710	L564	T487	V409	I331	F260	E197
P998	P998	GLY	H865	L796	G711	G711	H651	N488	V409	K332	S263	C198
L1059	Y999	ALA	E866	T797	Q712	Q712	E652	N489	D410	G333	D264	E199
V1060	G1000	ALA	Q867	R798	E713	E713	E652	I490	L411	K334	D264	Q200
A1001	A1001	ALA	W868	D802	E714	E714	E654	L491	L412	Q335	D267	L201
V1002	V1002	ALA	C869	D802	K715	K715	S655	S492	D413	D267	D267	R202
L1063	L1003	ALA	D870	D802	Q716	Q716	E656	E497	E414	Y269	L268	E203
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A1012	A1012	N954	D878	T816	A734	A734	L664	D505	A426	R281	R281	T212
K1072	D1012	K955	A879	H817	T736	T736	Q665	L510	P427	L282	L282	K213
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G1014	G1014	S957	C888	G819	I737	I737	Q667	R615	L429	L284	L284	K215
L1074	E1015	I958	D889	T820	R738	R738	F668	D516	H430	D284	D284	K216
P1076	T1016	K959	T890	M821	R744	R744	R622	D516	R431	L285	L285	L217
L1078	A1018	S961	D891	M822	G745	G745	T823	C517	Q435	A286	A286	T218
K1079	N1019	N962	T892	P824	L746	L746	L672	V518	A436	A287	A287	K219
I1080	W1020	V963	H897	V825	W747	W747	V673	N519	V440	P288	P288	R220
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D1082	H1023	D902	R901	E827	K749	K749	A675	K521	L441	I290	I290	K222
A1083	T1024	L903	L902	G828	P750	P750	G676	G522	L442	L291	L291	L223
Q1084	G1084	V967	L903	G829	D751	D751	E677	E523	L443	V292	V292	L224
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D1087	V1027	Q970	Q906	K832	I754	I754	S602	V526	K445	E295	E295	F227
I1028	K1029	Q971	H907	E833	T755	T755	K603	L527	A446	F227	F227	V228
L1088	E1030	K972	I908	P834	E756	E756	M604	T528	Q448	M298	M298	Q229
I1090	V1031	V974	I909	L835	T757	T757	L605	G529	L449	L299	L299	S230
P1091	G1032	I911	N910	R836	F758	F758	L606	P530	L449	G231	G231	G231
G1092	T1033	Q912	K911	D837	I759	I759	T607	L536	P451	V303	V303	N232
L1094	F1034	S977	G912	R838	T760	T760	C608	L541	L452	D304	D304	K233
M1095	V1035	R978	E913	V839	G766	G766	Y609	A542	V453	A305	A305	P234
P1096	R1036	N979	T915	L840	F766	F766	R610	A542	C454	L306	L306	E235
A1097	F1037	T980	Q916	E946	F773	F773	L612	A546	A455	G310	G310	W236
Q1098	T1038	E981	V917	D847	I774	I774	L612	R547	A456	R311	R311	M237
Y1099	D1039	L982	I918	V848	S775	S775	G613	V548	Y457	R312	R312	I238
F1100	M1040	K983	A919	L849	T776	T776	V618	K549	M458	G313	G313	L239
L1101	L1041	L984	R950	K850	H777	H777	I619	V550	A459	R314	R314	T240
P1102	D1042	T985	Q924	P851	G778	G778	Q623	R551	D460	A315	A315	V241
G1103	G1043	D986	G852	G852	A779	A779	Y626	I552	H469	L242	L242	L242
K1104	Q1044	P926	T853	T853	R780	R780	T627	T553	V470	P243	P243	P243
A1105	T1045	Q927	A854	A854	K781	K781	G628	E554	P471	N320	N320	V244
I1106	I1046	T928	D855	D855	L783	L783	F629	Y555	L474	K321	K321	L249
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												P251
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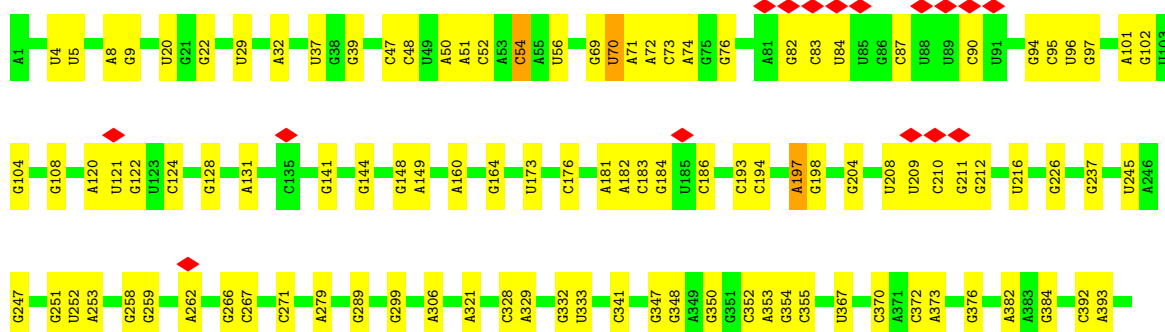
- Molecule 15: DNA-directed RNA polymerase subunit omega

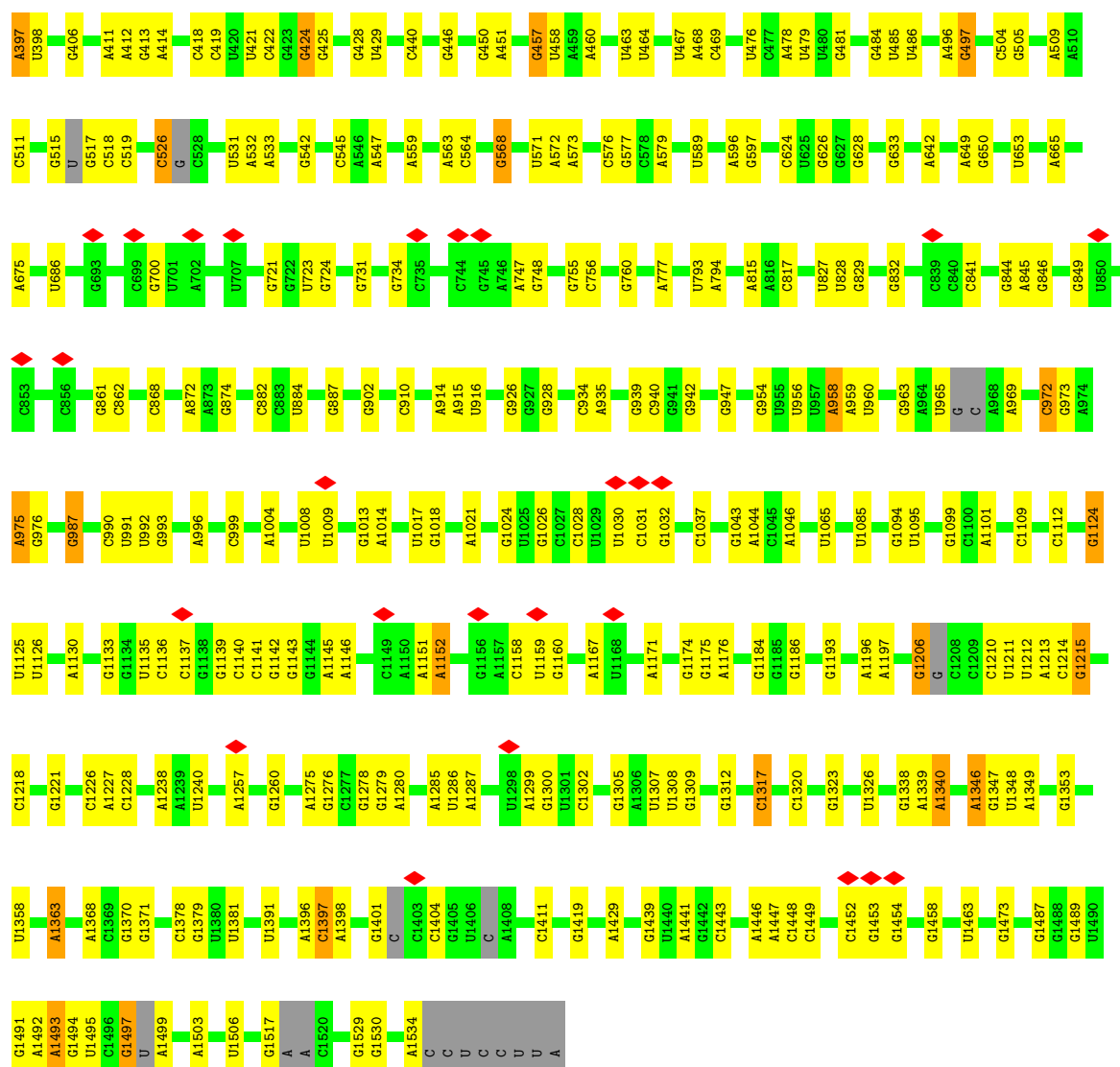


- Molecule 16: 30S ribosomal protein S18

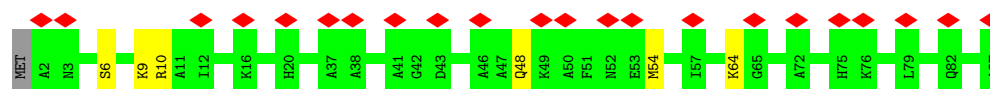


- Molecule 17: 16S rRNA

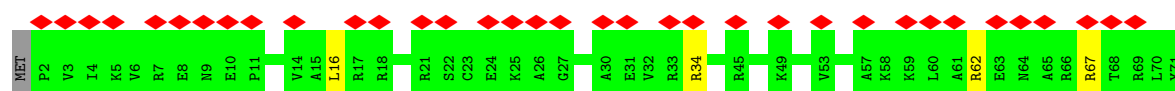
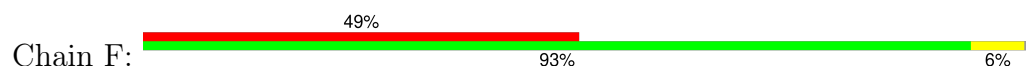




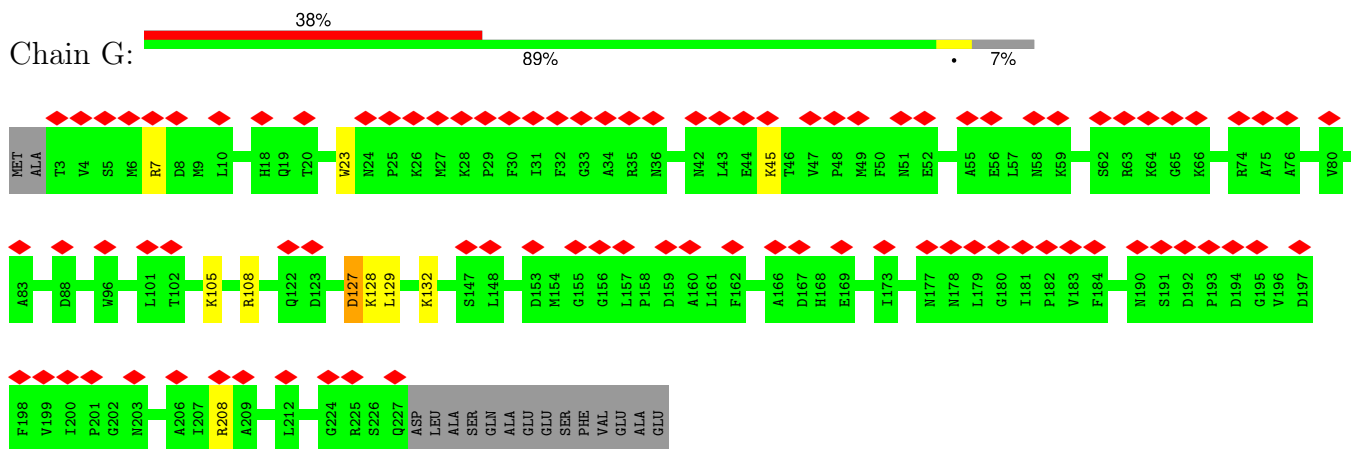
• Molecule 18: 30S ribosomal protein S20



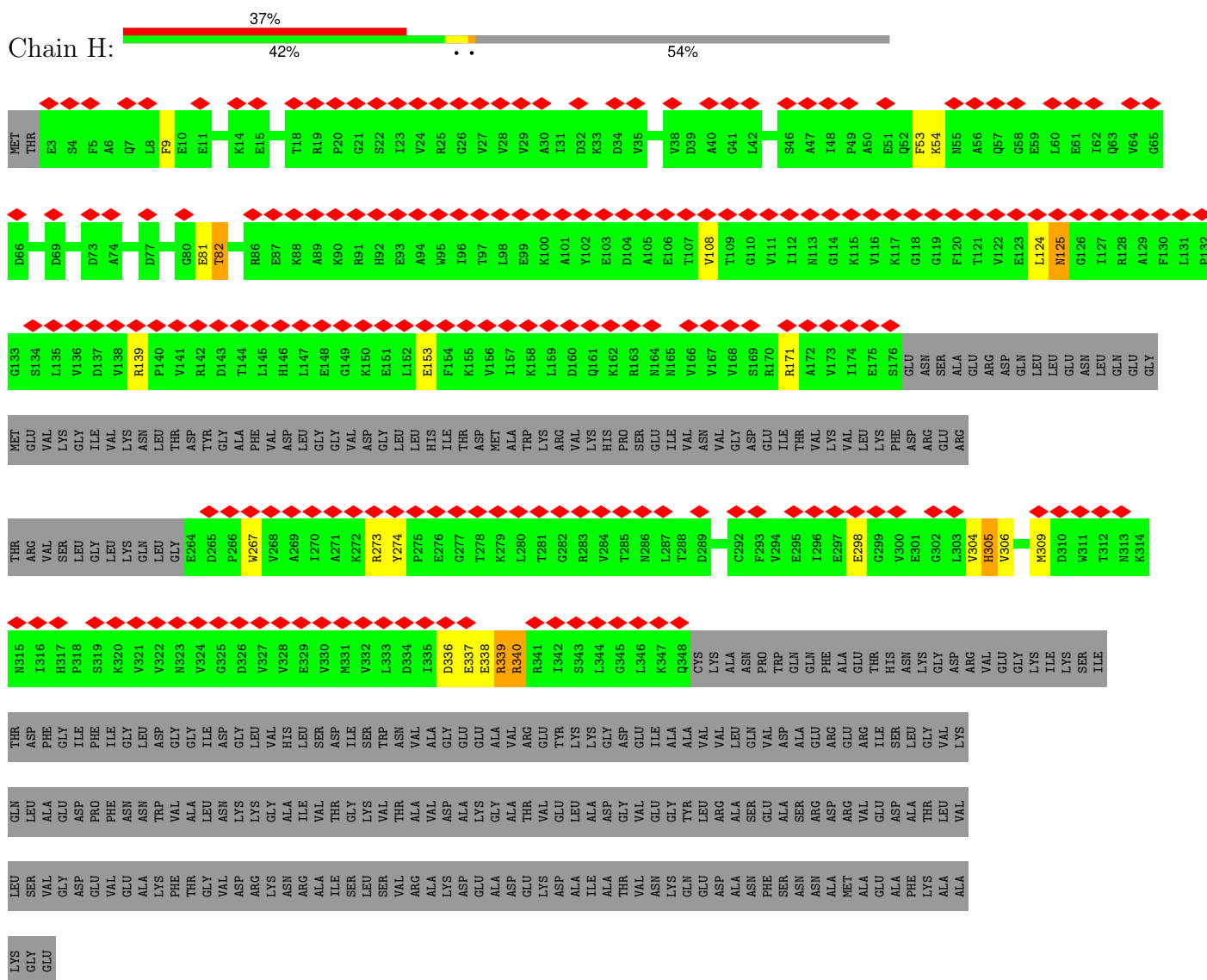
• Molecule 19: 30S ribosomal protein S21



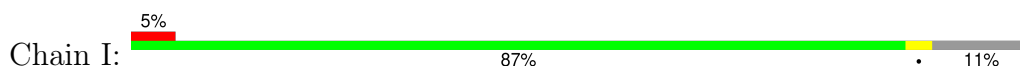
• Molecule 20: 30S ribosomal protein S2

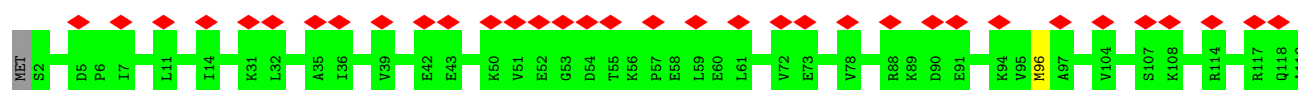


- Molecule 21: 30S ribosomal protein S1



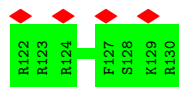
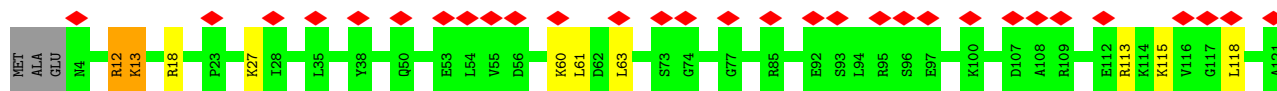
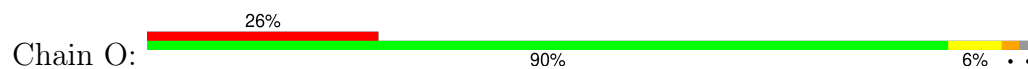
- Molecule 22: 30S ribosomal protein S3



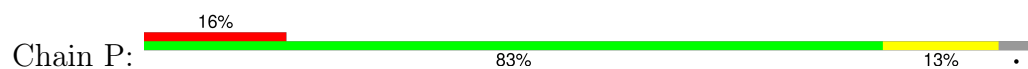




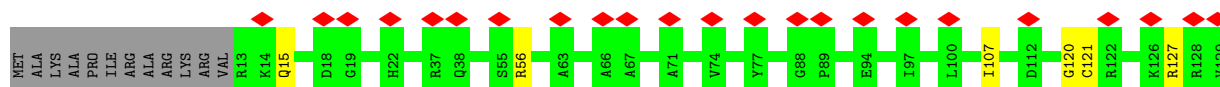
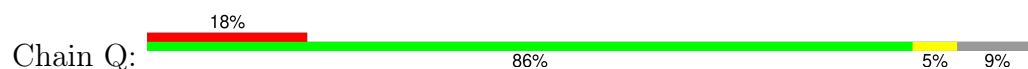
- Molecule 28: 30S ribosomal protein S9



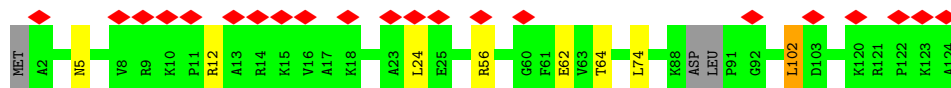
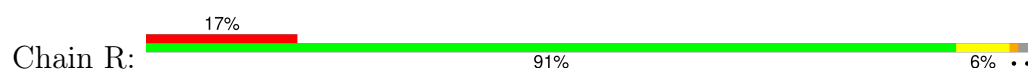
- Molecule 29: 30S ribosomal protein S10



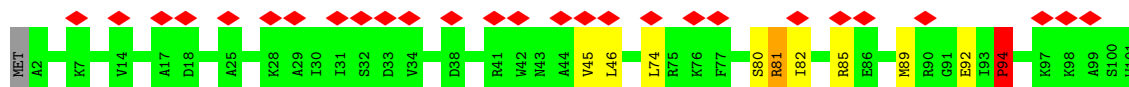
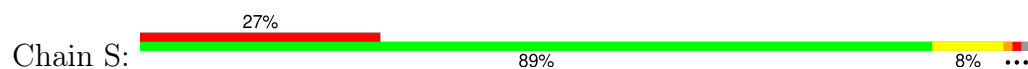
- Molecule 30: 30S ribosomal protein S11



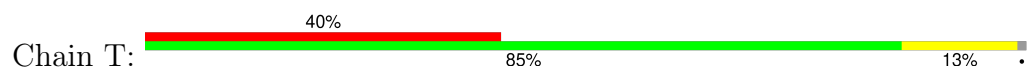
- Molecule 31: 30S ribosomal protein S12

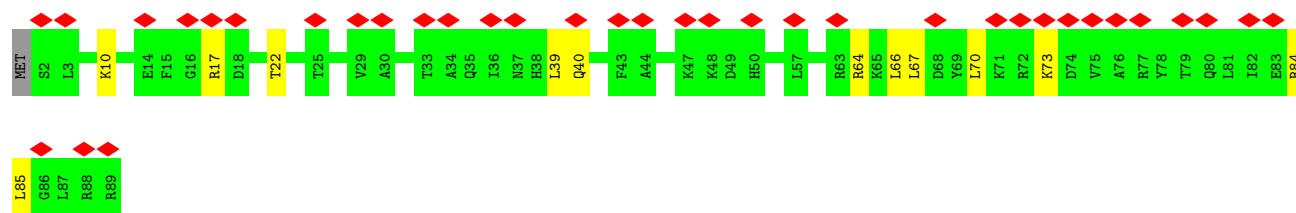


- Molecule 32: 30S ribosomal protein S14

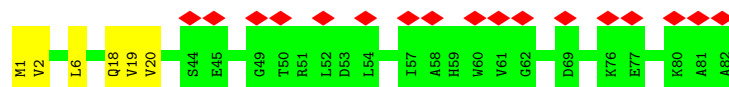


- Molecule 33: 30S ribosomal protein S15

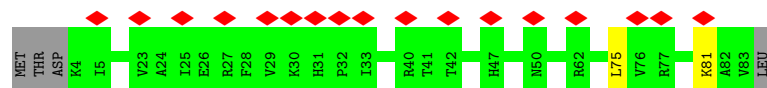




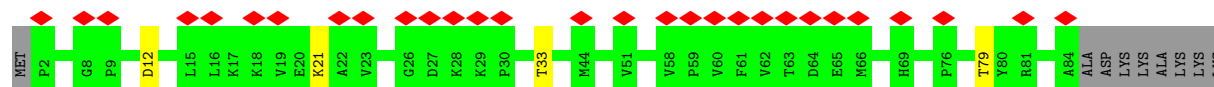
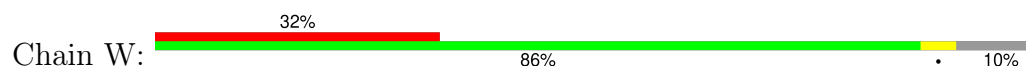
- Molecule 34: 30S ribosomal protein S16



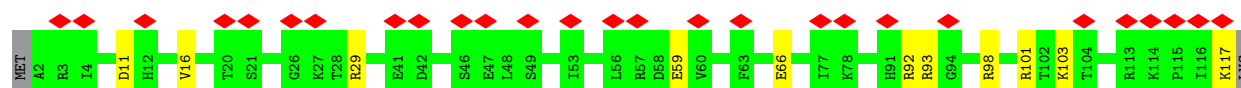
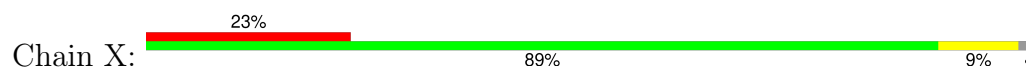
- Molecule 35: 30S ribosomal protein S17



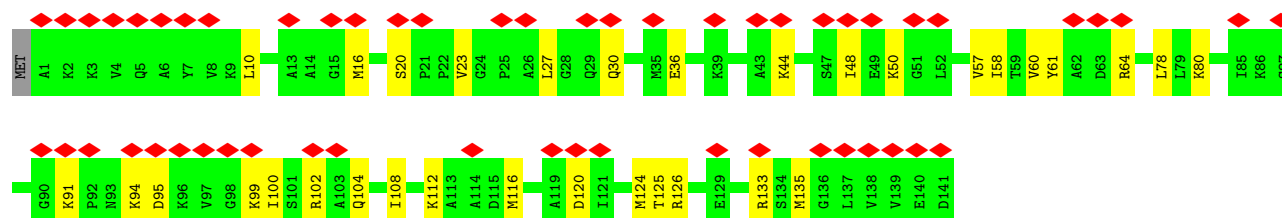
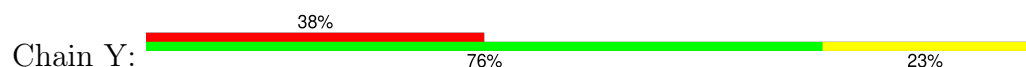
- Molecule 36: 30S ribosomal protein S19



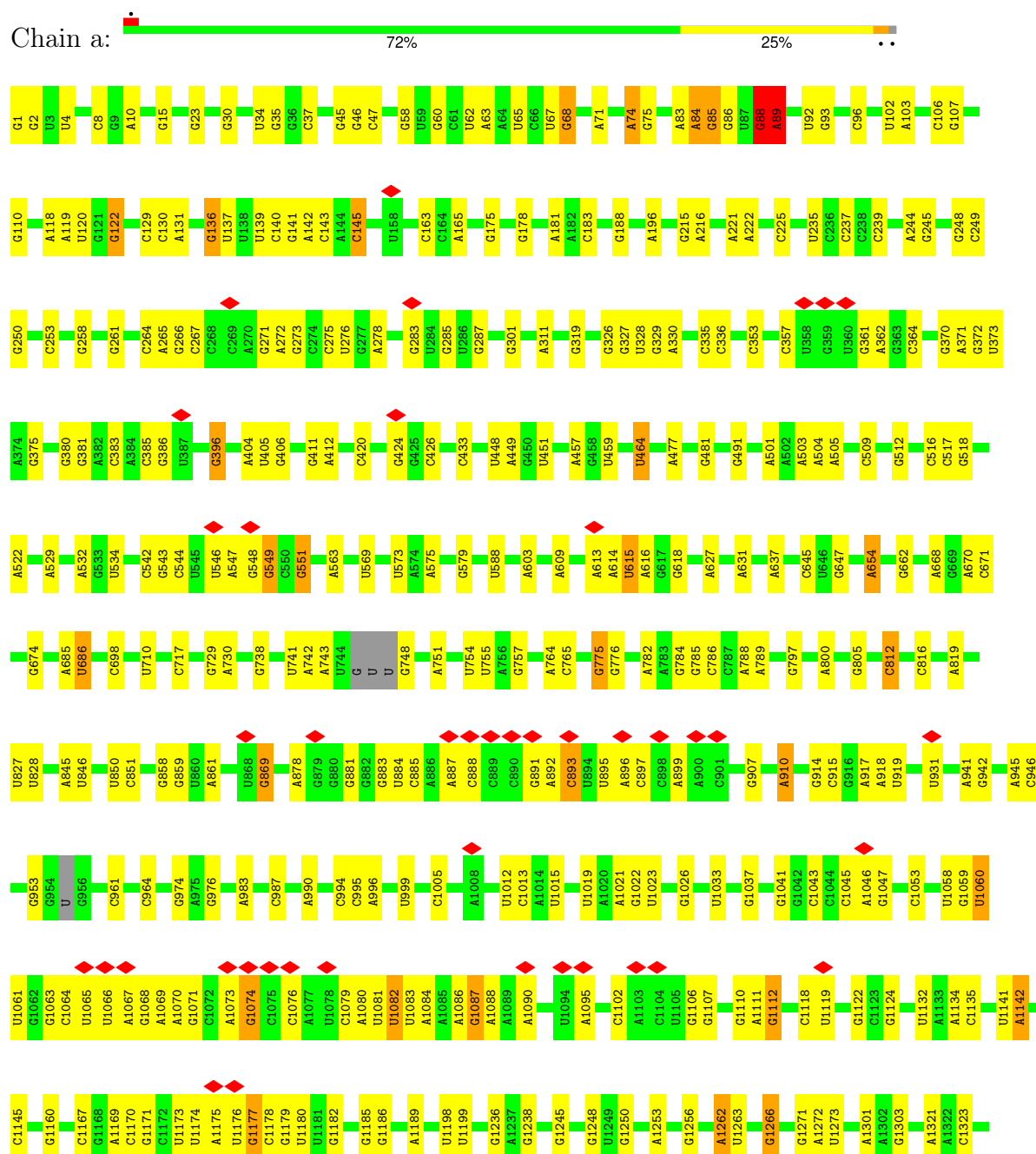
- Molecule 37: 30S ribosomal protein S13

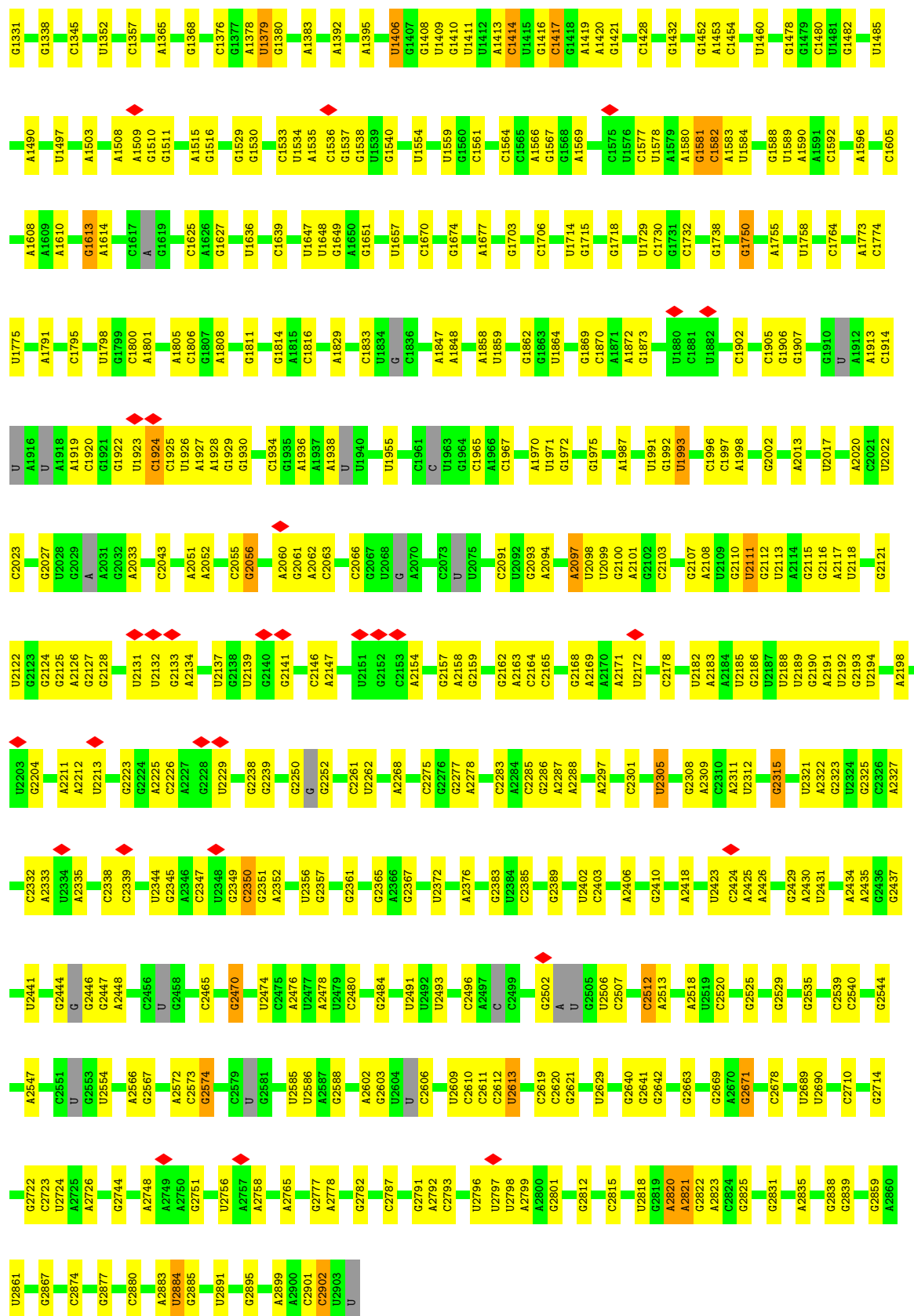


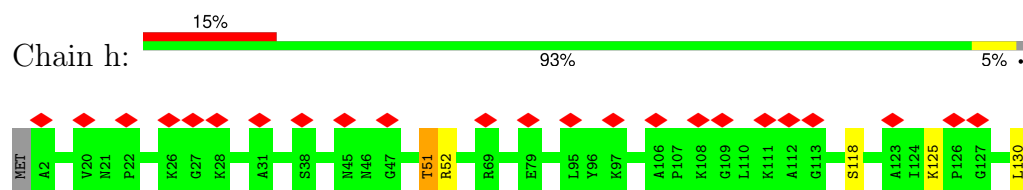
- Molecule 38: 50S ribosomal protein L11

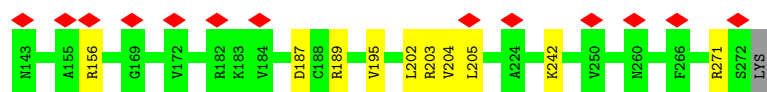


- Molecule 39: 50S ribosomal protein L7/L12

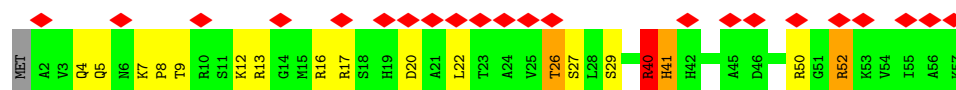
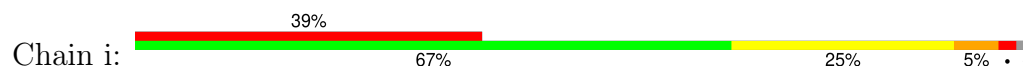




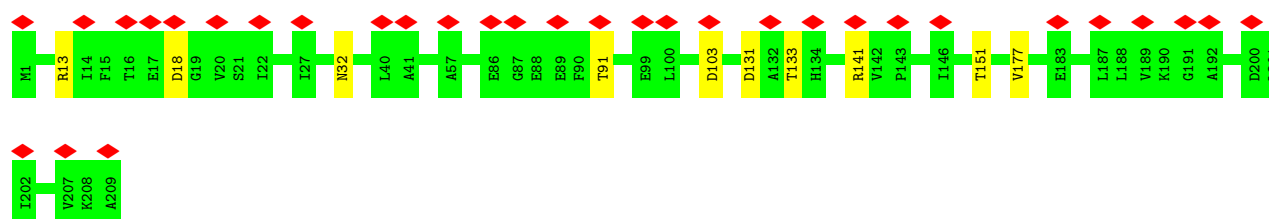
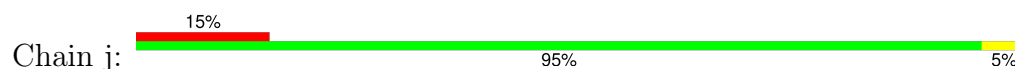




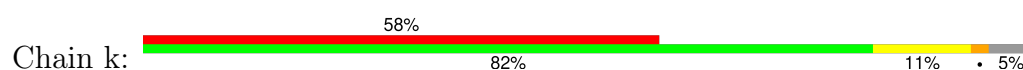
- Molecule 48: 50S ribosomal protein L32



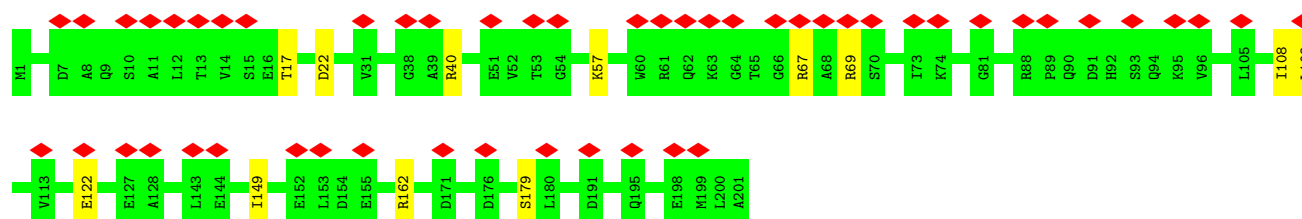
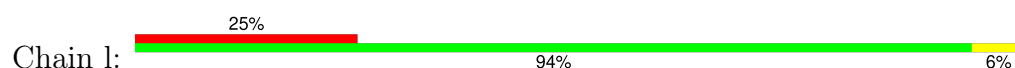
- Molecule 49: 50S ribosomal protein L3



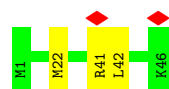
- Molecule 50: 50S ribosomal protein L33



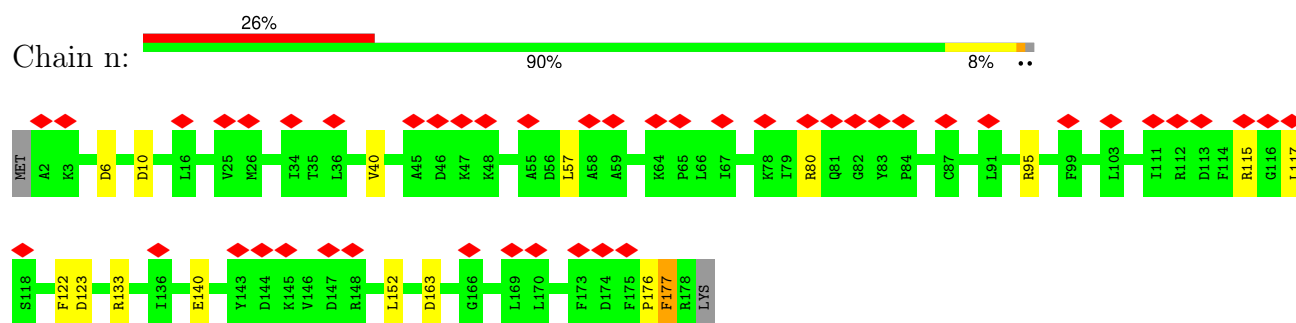
- Molecule 51: 50S ribosomal protein L4



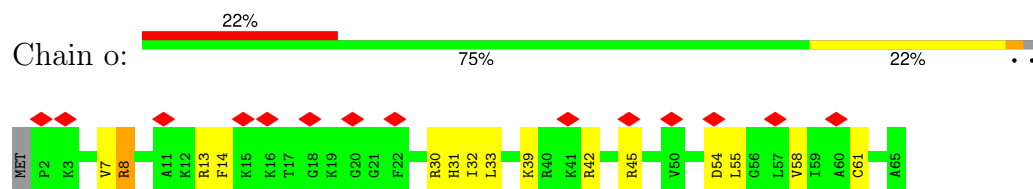
- Molecule 52: 50S ribosomal protein L34



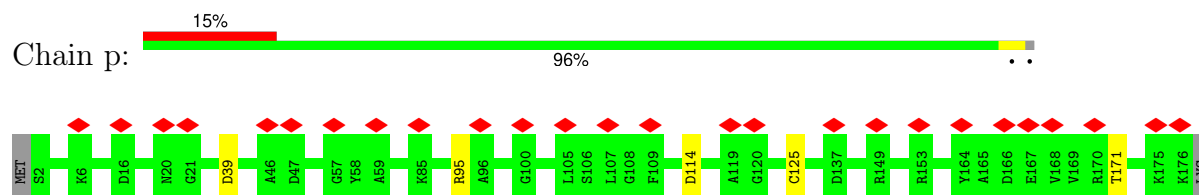
- Molecule 53: 50S ribosomal protein L5



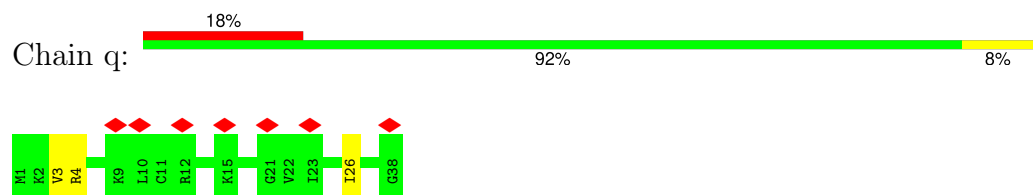
- Molecule 54: 50S ribosomal protein L35



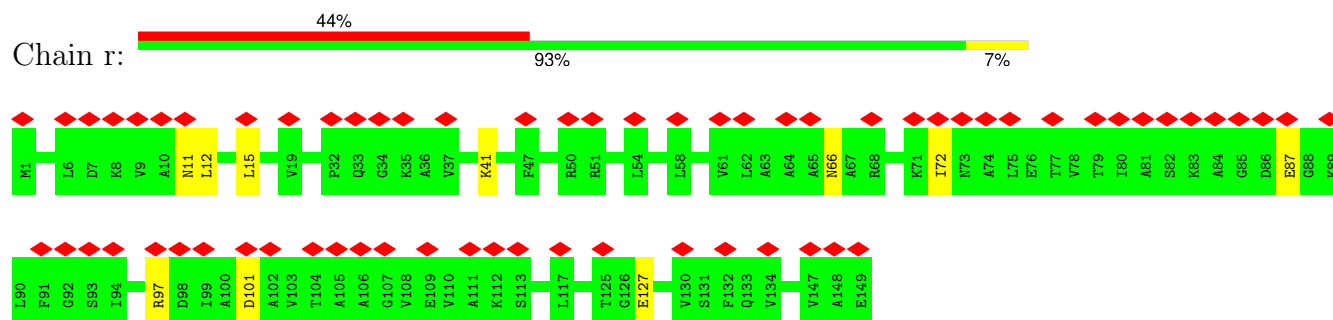
- Molecule 55: 50S ribosomal protein L6



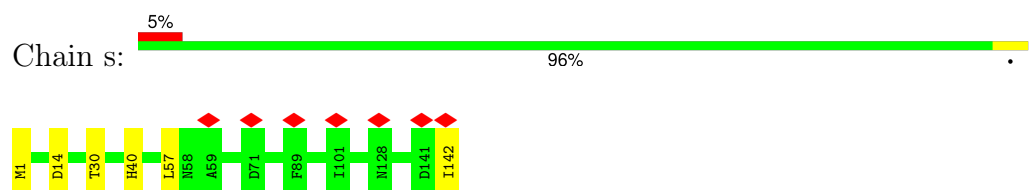
- Molecule 56: 50S ribosomal protein L36



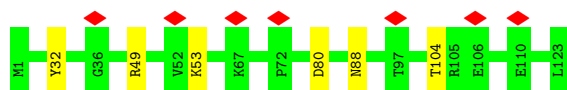
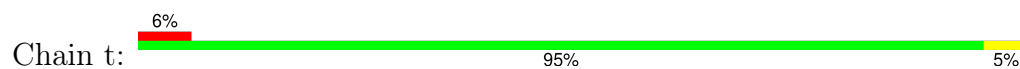
- Molecule 57: 50S ribosomal protein L9



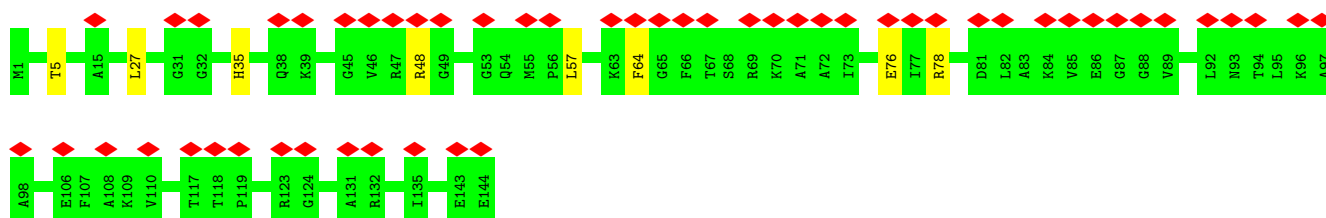
- Molecule 58: 50S ribosomal protein L13



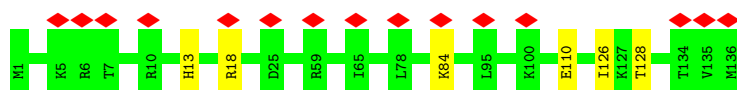
- Molecule 59: 50S ribosomal protein L14



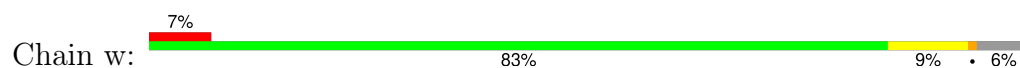
- Molecule 60: 50S ribosomal protein L15



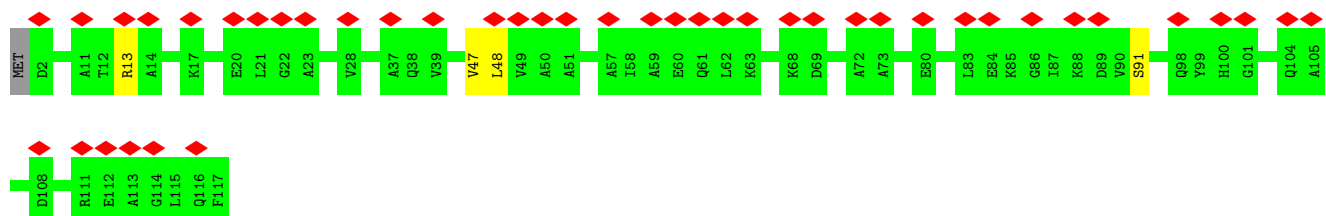
- Molecule 61: 50S ribosomal protein L16



- Molecule 62: 50S ribosomal protein L17

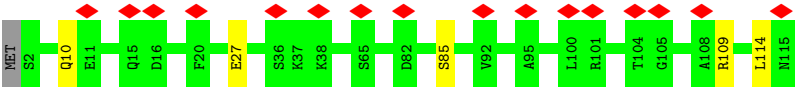


- Molecule 63: 50S ribosomal protein L18

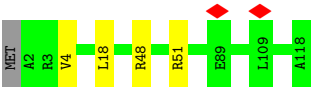


- Molecule 64: 50S ribosomal protein L19





• Molecule 65: 50S ribosomal protein L20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6121	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.046	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00561	Depositor
Map size (\AA)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.44	0/829	0.77	1/1107 (0.1%)
2	1	0.75	2/864 (0.2%)	1.08	6/1156 (0.5%)
3	2	0.41	0/752	0.60	0/1005
4	3	0.35	0/796	0.66	2/1062 (0.2%)
5	4	0.34	0/766	0.53	0/1025
6	5	1.13	6/528 (1.1%)	0.97	1/810 (0.1%)
7	6	1.11	4/603 (0.7%)	0.97	0/926
8	7	0.66	2/783 (0.3%)	1.35	14/1212 (1.2%)
9	9	0.41	0/1131	0.72	1/1524 (0.1%)
10	A	2.15	45/1810 (2.5%)	3.07	88/2821 (3.1%)
10	B	2.15	46/1810 (2.5%)	3.07	89/2821 (3.2%)
11	AA	0.43	0/10736	0.60	1/14487 (0.0%)
12	AB	0.80	3/1421 (0.2%)	0.69	3/1914 (0.2%)
13	AC	0.41	0/1718	0.62	0/2328
13	AD	0.36	0/1696	0.62	0/2298
14	AE	0.41	0/10561	0.63	3/14258 (0.0%)
15	AF	0.33	0/652	0.57	0/879
16	C	1.66	10/553 (1.8%)	1.29	7/743 (0.9%)
17	D	0.71	47/36610 (0.1%)	1.28	300/57091 (0.5%)
18	E	0.64	1/675 (0.1%)	0.65	0/895
19	F	0.41	0/597	0.58	0/792
20	G	0.37	0/1791	0.54	0/2413
21	H	0.58	4/1746 (0.2%)	0.91	5/2382 (0.2%)
22	I	0.35	0/1663	0.54	0/2241
23	J	0.36	0/1665	0.54	1/2227 (0.0%)
24	K	0.82	6/1165 (0.5%)	0.82	7/1568 (0.4%)
25	L	0.70	2/867 (0.2%)	0.76	4/1171 (0.3%)
26	M	0.41	1/1195 (0.1%)	0.61	0/1602
27	N	0.37	0/989	0.55	0/1326
28	O	0.61	1/1034 (0.1%)	1.08	7/1375 (0.5%)
29	P	0.74	3/800 (0.4%)	0.98	8/1082 (0.7%)
30	Q	0.46	1/893 (0.1%)	0.67	4/1205 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	R	0.37	0/952	0.59	0/1274
32	S	0.56	0/817	1.00	6/1088 (0.6%)
33	T	0.42	0/722	0.60	0/964
34	U	0.36	0/659	0.61	0/884
35	V	0.35	0/657	0.54	0/881
36	W	0.38	0/680	0.63	0/915
37	X	0.49	1/909 (0.1%)	0.86	2/1215 (0.2%)
38	Y	0.30	0/1046	0.50	0/1410
39	Z	0.28	0/227	0.46	0/304
40	a	1.08	188/69247 (0.3%)	1.55	922/107985 (0.9%)
41	b	0.46	0/589	0.62	0/779
42	c	0.50	0/635	0.67	1/848 (0.1%)
43	d	0.67	4/2872 (0.1%)	1.13	21/4478 (0.5%)
44	e	0.39	0/502	0.57	0/667
45	f	0.37	0/452	0.58	0/605
46	g	0.48	0/531	0.61	1/709 (0.1%)
47	h	0.41	0/2121	0.62	1/2852 (0.0%)
48	i	1.93	18/450 (4.0%)	2.94	30/599 (5.0%)
49	j	0.53	1/1586 (0.1%)	0.67	3/2134 (0.1%)
50	k	0.59	1/433 (0.2%)	0.88	2/576 (0.3%)
51	l	0.46	0/1571	0.62	2/2113 (0.1%)
52	m	0.53	0/380	0.99	0/498
53	n	0.44	0/1434	0.70	1/1926 (0.1%)
54	o	1.11	8/513 (1.6%)	1.08	6/676 (0.9%)
55	p	0.31	0/1333	0.55	0/1805
56	q	0.46	0/303	0.76	2/397 (0.5%)
57	r	0.32	0/1122	0.55	0/1515
58	s	0.42	0/1152	0.57	0/1551
59	t	0.38	0/955	0.61	0/1279
60	u	0.52	0/1062	0.72	2/1413 (0.1%)
61	v	0.42	0/1093	0.65	0/1460
62	w	0.82	4/964 (0.4%)	1.54	15/1289 (1.2%)
63	x	0.36	0/902	0.58	0/1209
64	y	0.37	0/929	0.75	2/1242 (0.2%)
65	z	0.56	1/960 (0.1%)	0.73	2/1278 (0.2%)
All	All	0.85	410/190459 (0.2%)	1.29	1573/280564 (0.6%)

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
9	9	0	3
10	A	0	2
10	B	0	2
11	AA	0	1
12	AB	0	1
13	AC	0	1
13	AD	0	1
14	AE	0	4
17	D	0	1
21	H	0	5
24	K	0	2
26	M	0	1
28	O	0	1
31	R	0	1
40	a	0	3
48	i	0	1
50	k	0	1
53	n	0	1
60	u	0	1
62	w	0	1
All	All	0	34

All (410) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	1262	A	N1-C2	104.77	2.28	1.34
40	a	88	G	N9-C8	71.95	1.88	1.37
40	a	88	G	N7-C5	64.86	1.78	1.39
40	a	88	G	C8-N7	64.12	1.69	1.30
40	a	88	G	N9-C4	45.00	1.74	1.38
10	B	37	A	C6-N1	-44.87	1.04	1.35
10	A	37	A	C6-N1	-44.80	1.04	1.35
40	a	1262	A	C5-C4	37.24	1.64	1.38
40	a	789	A	N9-C8	30.72	1.62	1.37
40	a	88	G	C5-C4	30.47	1.59	1.38
40	a	1262	A	C5-C6	29.52	1.67	1.41
40	a	1262	A	C6-N1	29.47	1.56	1.35
10	A	37	A	C5-C6	-27.95	1.15	1.41
10	B	37	A	C5-C6	-27.82	1.16	1.41
40	a	88	G	C5'-C4'	25.65	1.82	1.51
40	a	789	A	N7-C5	-23.84	1.25	1.39
40	a	1262	A	N3-C4	23.30	1.48	1.34
10	A	37	A	C8-N7	-19.74	1.17	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	37	A	C8-N7	-19.70	1.17	1.31
17	D	958	A	C6-N6	-19.57	1.18	1.33
17	D	958	A	C5-C4	-19.13	1.25	1.38
40	a	89	A	C5-C4	-18.91	1.25	1.38
10	A	37	A	N9-C8	18.34	1.52	1.37
10	B	37	A	N9-C8	18.28	1.52	1.37
40	a	1262	A	C2-N3	17.79	1.49	1.33
40	a	68	G	P-O5'	17.19	1.76	1.59
10	B	37	A	N1-C2	-17.09	1.19	1.34
10	A	37	A	N1-C2	-17.03	1.19	1.34
16	C	44	ILE	CB-CG2	-16.69	1.01	1.52
16	C	40	VAL	CB-CG1	16.61	1.87	1.52
40	a	74	A	N9-C8	-15.93	1.25	1.37
40	a	336	C	N1-C2	15.67	1.55	1.40
10	B	76	A	N9-C8	-15.57	1.25	1.37
10	A	76	A	N9-C8	-15.54	1.25	1.37
40	a	336	C	C2-N3	-15.41	1.23	1.35
40	a	1262	A	C8-N7	15.37	1.42	1.31
24	K	56	VAL	CB-CG2	15.30	1.84	1.52
40	a	89	A	C5-C6	15.09	1.54	1.41
40	a	2286	G	C6-N1	-15.09	1.28	1.39
40	a	917	A	N9-C4	-15.08	1.28	1.37
40	a	89	A	C5'-C4'	-14.92	1.33	1.51
17	D	958	A	C6-N1	-14.71	1.25	1.35
40	a	88	G	C4'-C3'	-14.54	1.37	1.53
40	a	89	A	N3-C4	-14.41	1.26	1.34
40	a	336	C	N3-C4	-14.30	1.24	1.33
40	a	88	G	C2'-C1'	-14.03	1.38	1.53
10	A	31	G	C8-N7	13.99	1.39	1.30
40	a	2493	U	N1-C6	-13.94	1.25	1.38
40	a	89	A	N7-C5	13.93	1.47	1.39
10	B	31	G	C8-N7	13.90	1.39	1.30
10	A	39	C	N1-C6	13.80	1.45	1.37
12	AB	45	PRO	N-CA	13.73	1.70	1.47
40	a	1262	A	C6-N6	13.70	1.45	1.33
10	B	39	C	N1-C6	13.70	1.45	1.37
40	a	85	G	N7-C5	-13.68	1.31	1.39
40	a	89	A	N9-C4	13.64	1.46	1.37
40	a	89	A	N1-C2	-13.43	1.22	1.34
40	a	88	G	C3'-O3'	-13.31	1.23	1.42
25	L	5	GLU	CB-CG	-13.18	1.27	1.52
16	C	40	VAL	CB-CG2	13.11	1.80	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	68	G	N9-C4	-13.10	1.27	1.38
40	a	917	A	C2-N3	-13.09	1.21	1.33
40	a	1262	A	N9-C4	-13.02	1.30	1.37
16	C	23	TYR	CD2-CE2	-12.95	1.20	1.39
10	A	37	A	C5-C4	-12.93	1.29	1.38
10	A	76	A	C5-C4	-12.90	1.29	1.38
10	B	76	A	C5-C4	-12.89	1.29	1.38
10	B	37	A	C5-C4	-12.88	1.29	1.38
17	D	1493	A	N1-C2	-12.74	1.22	1.34
10	A	38	A	N9-C4	-12.67	1.30	1.37
10	B	38	A	N9-C4	-12.52	1.30	1.37
16	C	24	LYS	CE-NZ	-12.44	1.18	1.49
62	w	96	ARG	CG-CD	12.41	1.82	1.51
40	a	990	A	N9-C4	-12.38	1.30	1.37
40	a	789	A	C1'-N9	12.30	1.67	1.48
10	A	31	G	C6-O6	12.26	1.35	1.24
10	B	31	G	C6-O6	12.23	1.35	1.24
40	a	789	A	C5-C6	-12.23	1.30	1.41
40	a	789	A	N3-C4	-12.07	1.27	1.34
21	H	298	GLU	CB-CG	-11.86	1.29	1.52
17	D	958	A	N1-C2	-11.45	1.24	1.34
17	D	958	A	N7-C5	11.43	1.46	1.39
40	a	654	A	C6-N6	-11.36	1.24	1.33
2	l	39	THR	CB-CG2	-11.33	1.15	1.52
24	K	56	VAL	CB-CG1	-10.96	1.29	1.52
10	A	39	C	N3-C4	-10.92	1.26	1.33
40	a	518	G	P-O5'	10.90	1.70	1.59
40	a	85	G	C8-N7	-10.88	1.24	1.30
10	B	39	C	N3-C4	-10.86	1.26	1.33
10	B	36	U	N1-C6	10.81	1.47	1.38
10	A	36	U	N1-C6	10.77	1.47	1.38
17	D	1309	G	N9-C8	-10.76	1.30	1.37
10	B	39	C	N1-C2	10.63	1.50	1.40
10	B	37	A	C2-N3	10.61	1.43	1.33
40	a	74	A	N7-C5	-10.59	1.32	1.39
10	A	39	C	N1-C2	10.55	1.50	1.40
48	i	41	HIS	CA-CB	10.54	1.77	1.53
40	a	788	A	N9-C4	10.51	1.44	1.37
10	A	37	A	N7-C5	10.50	1.45	1.39
10	A	37	A	C2-N3	10.45	1.43	1.33
40	a	1262	A	N9-C8	10.40	1.46	1.37
40	a	85	G	N9-C8	10.33	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	751	A	N9-C4	-10.30	1.31	1.37
10	B	37	A	N7-C5	10.28	1.45	1.39
48	i	50	ARG	CZ-NH2	-10.28	1.19	1.33
48	i	4	GLN	CD-NE2	10.21	1.58	1.32
10	A	38	A	C8-N7	10.12	1.38	1.31
29	P	55	PRO	N-CA	10.09	1.64	1.47
17	D	104	G	N9-C8	-10.07	1.30	1.37
40	a	89	A	C6-N6	-10.04	1.25	1.33
40	a	789	A	C8-N7	-9.97	1.24	1.31
10	B	38	A	C8-N7	9.97	1.38	1.31
40	a	1141	U	N3-C4	-9.87	1.29	1.38
17	D	675	A	N9-C4	-9.80	1.31	1.37
48	i	13	ARG	CZ-NH1	9.59	1.45	1.33
10	B	31	G	C6-N1	9.53	1.46	1.39
10	A	31	G	C6-N1	9.45	1.46	1.39
48	i	7	LYS	CD-CE	9.39	1.74	1.51
40	a	1262	A	C5'-C4'	9.37	1.62	1.51
40	a	336	C	N1-C6	-9.36	1.31	1.37
40	a	89	A	C3'-C2'	-9.35	1.42	1.52
40	a	1019	U	N3-C4	-9.25	1.30	1.38
40	a	917	A	N3-C4	-9.16	1.29	1.34
40	a	2493	U	C3'-C2'	9.14	1.63	1.52
40	a	89	A	N9-C8	-9.13	1.30	1.37
40	a	2493	U	C2-N3	-9.07	1.31	1.37
40	a	67	U	O3'-P	9.04	1.72	1.61
54	o	7	VAL	CB-CG1	-9.02	1.33	1.52
40	a	68	G	O5'-C5'	8.99	1.58	1.44
40	a	67	U	C3'-O3'	8.95	1.54	1.42
17	D	958	A	C5-C6	-8.92	1.33	1.41
48	i	5	GLN	N-CA	8.89	1.64	1.46
48	i	50	ARG	CB-CG	-8.89	1.28	1.52
40	a	68	G	N9-C8	-8.81	1.31	1.37
40	a	2286	G	C2-N2	-8.78	1.25	1.34
6	5	109	DT	O3'-P	8.75	1.71	1.61
17	D	1317	C	N1-C2	-8.75	1.31	1.40
40	a	85	G	C6-N1	-8.75	1.33	1.39
40	a	336	C	C4-N4	-8.67	1.26	1.33
54	o	39	LYS	CD-CE	-8.66	1.29	1.51
40	a	89	A	P-O5'	8.65	1.68	1.59
40	a	2493	U	C5'-C4'	-8.64	1.41	1.51
40	a	1262	A	C2'-C1'	8.62	1.62	1.53
40	a	516	C	O3'-P	8.59	1.71	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	89	A	C4'-C3'	-8.54	1.43	1.53
40	a	89	A	O4'-C1'	-8.54	1.30	1.41
40	a	68	G	C5-C4	-8.46	1.32	1.38
12	AB	169	THR	C-N	8.45	1.50	1.34
40	a	88	G	C2-N2	-8.44	1.26	1.34
40	a	74	A	C6-N1	-8.34	1.29	1.35
7	6	10	DG	C1'-N9	-8.24	1.35	1.47
48	i	26	THR	CB-CG2	-8.24	1.25	1.52
17	D	563	A	C6-N1	-8.22	1.29	1.35
10	A	37	A	N3-C4	8.20	1.39	1.34
10	B	37	A	N3-C4	8.20	1.39	1.34
40	a	789	A	C2'-C1'	8.16	1.62	1.53
17	D	1493	A	N7-C5	-8.14	1.34	1.39
40	a	2286	G	N1-C2	-8.14	1.31	1.37
40	a	990	A	C2-N3	-8.10	1.26	1.33
17	D	1339	A	N9-C4	-8.09	1.32	1.37
40	a	1262	A	N7-C5	-8.02	1.34	1.39
16	C	10	PHE	CD2-CE2	-8.01	1.23	1.39
40	a	88	G	C4'-O4'	8.00	1.55	1.45
40	a	2493	U	C5-C6	-7.99	1.26	1.34
40	a	1924	C	C2-N3	-7.97	1.29	1.35
40	a	327	G	N1-C2	-7.97	1.31	1.37
17	D	675	A	C2-N3	-7.95	1.26	1.33
40	a	518	G	O5'-C5'	7.93	1.57	1.44
17	D	884	U	N3-C4	-7.91	1.31	1.38
17	D	675	A	N3-C4	-7.87	1.30	1.34
48	i	13	ARG	NE-CZ	7.87	1.43	1.33
40	a	74	A	N3-C4	-7.81	1.30	1.34
40	a	631	A	N9-C4	-7.81	1.33	1.37
40	a	1021	A	C6-N1	-7.80	1.30	1.35
10	B	19	G	C5-C6	-7.79	1.34	1.42
40	a	1924	C	C5-C6	-7.76	1.28	1.34
10	A	19	G	C5-C6	-7.76	1.34	1.42
17	D	872	A	C6-N1	-7.74	1.30	1.35
40	a	1082	U	C4-O4	-7.72	1.17	1.23
10	A	31	G	C2-N3	-7.71	1.26	1.32
40	a	1142	A	C6-N1	-7.70	1.30	1.35
10	B	31	G	N7-C5	7.69	1.43	1.39
48	i	13	ARG	CD-NE	7.69	1.59	1.46
10	A	31	G	N7-C5	7.68	1.43	1.39
10	A	32	C	C4-C5	7.68	1.49	1.43
17	D	1363	A	C6-N1	-7.67	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	31	G	C2-N3	-7.64	1.26	1.32
40	a	2365	G	N9-C8	-7.61	1.32	1.37
17	D	827	U	N3-C4	-7.57	1.31	1.38
40	a	751	A	N3-C4	-7.55	1.30	1.34
40	a	2493	U	P-O5'	-7.52	1.52	1.59
10	B	32	C	C4-C5	7.52	1.49	1.43
40	a	88	G	N3-C4	-7.44	1.30	1.35
40	a	2365	G	N7-C5	7.43	1.43	1.39
29	P	54	SER	C-N	7.33	1.48	1.34
24	K	55	GLU	CB-CG	7.33	1.66	1.52
17	D	958	A	N9-C4	-7.32	1.33	1.37
24	K	56	VAL	CA-C	-7.25	1.34	1.52
17	D	1493	A	C6-N1	-7.24	1.30	1.35
8	7	19	G	C1'-N9	-7.24	1.36	1.46
40	a	2613	U	N3-C4	-7.24	1.31	1.38
6	5	121	DG	C1'-N9	-7.24	1.37	1.47
40	a	2493	U	C2'-C1'	7.23	1.61	1.53
10	B	37	A	C1'-N9	-7.19	1.36	1.46
40	a	2286	G	C5-C4	-7.18	1.33	1.38
40	a	517	C	C4'-C3'	-7.17	1.45	1.53
10	A	39	C	C2-O2	7.17	1.30	1.24
10	A	37	A	C1'-N9	-7.16	1.36	1.46
24	K	55	GLU	CA-CB	-7.16	1.38	1.53
40	a	517	C	O3'-P	-7.13	1.52	1.61
10	B	76	A	C6-N1	7.12	1.40	1.35
2	1	15	GLN	CG-CD	-7.11	1.34	1.51
10	B	39	C	C2-O2	7.09	1.30	1.24
40	a	789	A	C6-N1	-7.09	1.30	1.35
10	A	76	A	C6-N1	7.06	1.40	1.35
17	D	397	A	C6-N1	-7.05	1.30	1.35
40	a	788	A	N3-C4	7.04	1.39	1.34
49	j	133	THR	CB-CG2	-7.01	1.29	1.52
40	a	67	U	C4-O4	-6.99	1.18	1.23
17	D	1358	U	N3-C4	-6.97	1.32	1.38
40	a	89	A	P-OP1	6.97	1.60	1.49
40	a	2365	G	C5-C4	-6.90	1.33	1.38
48	i	7	LYS	CG-CD	6.89	1.75	1.52
40	a	1338	G	N9-C8	-6.88	1.33	1.37
10	A	19	G	C8-N7	-6.88	1.26	1.30
40	a	2192	U	C2-N3	-6.84	1.32	1.37
40	a	918	A	N9-C8	-6.83	1.32	1.37
17	D	1493	A	N3-C4	-6.69	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	2356	U	N1-C2	-6.69	1.32	1.38
18	E	9	LYS	CE-NZ	-6.68	1.32	1.49
6	5	112	DG	C1'-N9	-6.66	1.38	1.47
54	o	58	VAL	CB-CG2	-6.64	1.38	1.52
10	B	19	G	C8-N7	-6.64	1.26	1.30
10	B	76	A	C2-N3	-6.63	1.27	1.33
40	a	674	G	N9-C8	-6.62	1.33	1.37
40	a	68	G	C5-C6	-6.60	1.35	1.42
40	a	2013	A	C6-N6	-6.59	1.28	1.33
10	A	76	A	C2-N3	-6.58	1.27	1.33
48	i	8	PRO	CB-CG	-6.55	1.17	1.50
10	A	37	A	C6-N6	6.54	1.39	1.33
17	D	827	U	C4-O4	-6.53	1.18	1.23
10	B	37	A	C6-N6	6.53	1.39	1.33
54	o	61	CYS	CB-SG	-6.52	1.71	1.82
40	a	1198	U	C2-O2	-6.50	1.16	1.22
6	5	100	DA	C1'-N9	-6.50	1.38	1.47
40	a	68	G	O4'-C1'	-6.48	1.33	1.41
48	i	7	LYS	CE-NZ	-6.47	1.32	1.49
40	a	335	C	N3-C4	-6.46	1.29	1.33
40	a	1262	A	C4'-O4'	6.46	1.53	1.45
43	d	81	G	N9-C4	-6.43	1.32	1.38
40	a	1141	U	C4-C5	-6.42	1.37	1.43
40	a	2493	U	C4'-O4'	6.40	1.53	1.45
48	i	41	HIS	CB-CG	6.40	1.61	1.50
7	6	21	DA	C1'-N9	-6.39	1.38	1.47
40	a	2365	G	C8-N7	-6.39	1.27	1.30
37	X	98	ARG	CZ-NH2	-6.37	1.24	1.33
40	a	2365	G	C2-N2	-6.34	1.28	1.34
17	D	1340	A	N9-C4	-6.32	1.34	1.37
40	a	516	C	C3'-O3'	6.29	1.50	1.42
40	a	459	U	O3'-P	6.27	1.68	1.61
40	a	654	A	C5-C6	-6.26	1.35	1.41
10	A	38	A	C6-N1	6.26	1.40	1.35
40	a	1592	C	N3-C4	6.26	1.38	1.33
40	a	917	A	N7-C5	-6.26	1.35	1.39
10	B	38	A	C6-N1	6.23	1.40	1.35
10	B	31	G	C5-C6	6.20	1.48	1.42
40	a	88	G	O3'-P	-6.20	1.53	1.61
10	B	38	A	C5-C4	6.20	1.43	1.38
40	a	788	A	N9-C8	-6.18	1.32	1.37
10	A	31	G	C5-C6	6.16	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	397	A	C6-N6	-6.16	1.29	1.33
17	D	959	A	N9-C4	-6.16	1.34	1.37
40	a	326	G	C2-N2	-6.16	1.28	1.34
40	a	1021	A	C5-C6	-6.16	1.35	1.41
40	a	85	G	C5-C6	-6.14	1.36	1.42
6	5	116	DG	C1'-N9	-6.13	1.38	1.47
12	AB	44	VAL	C-N	6.12	1.45	1.34
40	a	1142	A	C5-C6	-6.10	1.35	1.41
10	A	38	A	C5-C4	6.09	1.43	1.38
40	a	1019	U	C4-C5	-6.08	1.38	1.43
40	a	2365	G	C6-N1	-6.08	1.35	1.39
50	k	50	LYS	CE-NZ	-6.06	1.33	1.49
30	Q	121	CYS	CB-SG	-6.06	1.72	1.82
40	a	143	C	N3-C4	6.05	1.38	1.33
40	a	2351	G	C6-N1	-6.04	1.35	1.39
40	a	137	U	C2-N3	-6.02	1.33	1.37
62	w	96	ARG	CB-CG	6.01	1.68	1.52
17	D	1363	A	C5-C6	-6.00	1.35	1.41
26	M	32	VAL	CB-CG1	-6.00	1.40	1.52
40	a	464	U	O3'-P	-5.99	1.53	1.61
43	d	80	U	N1-C6	-5.98	1.32	1.38
6	5	115	DA	C1'-N9	-5.97	1.38	1.47
17	D	397	A	C5-C6	-5.97	1.35	1.41
10	B	76	A	N9-C4	-5.96	1.34	1.37
17	D	872	A	C6-N6	-5.96	1.29	1.33
40	a	1141	U	N1-C6	5.96	1.43	1.38
10	A	76	A	N9-C4	-5.95	1.34	1.37
24	K	55	GLU	CA-C	5.95	1.68	1.52
40	a	336	C	C2'-C1'	5.92	1.59	1.53
48	i	4	GLN	C-N	5.92	1.47	1.34
40	a	990	A	N1-C2	5.92	1.39	1.34
40	a	336	C	C5'-C4'	-5.91	1.44	1.51
17	D	37	U	N3-C4	-5.90	1.33	1.38
40	a	2512	C	N1-C6	-5.89	1.33	1.37
17	D	37	U	C4-O4	-5.88	1.19	1.23
17	D	872	A	C5-C6	-5.87	1.35	1.41
10	B	76	A	C1'-N9	-5.86	1.38	1.46
40	a	86	G	C3'-C2'	-5.86	1.46	1.52
10	A	76	A	C1'-N9	-5.85	1.38	1.46
40	a	2815	C	C5-C6	-5.85	1.29	1.34
10	B	76	A	C8-N7	-5.84	1.27	1.31
29	P	55	PRO	N-CD	5.84	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	36	U	C4-C5	5.83	1.48	1.43
10	A	36	U	C4-C5	5.83	1.48	1.43
17	D	1240	U	C2-N3	-5.81	1.33	1.37
40	a	1019	U	C4-O4	-5.81	1.19	1.23
40	a	1199	U	C2-O2	-5.77	1.17	1.22
40	a	2902	C	N3-C4	5.76	1.38	1.33
40	a	2756	U	C4-O4	-5.75	1.19	1.23
7	6	28	DA	C1'-N9	-5.74	1.39	1.47
10	A	76	A	C8-N7	-5.73	1.27	1.31
17	D	1358	U	C4-O4	-5.73	1.19	1.23
40	a	517	C	P-O5'	-5.73	1.54	1.59
40	a	2613	U	C4-O4	-5.71	1.19	1.23
17	D	563	A	C5-C6	-5.71	1.35	1.41
40	a	1262	A	C1'-N9	5.71	1.57	1.48
40	a	89	A	C4'-O4'	-5.71	1.38	1.45
40	a	1805	A	N9-C4	-5.67	1.34	1.37
28	O	115	LYS	CE-NZ	-5.64	1.34	1.49
10	A	30	G	C6-N1	5.63	1.43	1.39
62	w	96	ARG	CZ-NH1	-5.62	1.25	1.33
40	a	1053	C	N3-C4	5.58	1.37	1.33
40	a	861	A	N1-C2	-5.58	1.29	1.34
10	B	30	G	C6-N1	5.57	1.43	1.39
17	D	1317	C	C5-C6	5.57	1.38	1.34
17	D	1339	A	N3-C4	-5.55	1.31	1.34
16	C	64	TYR	CD1-CE1	-5.55	1.31	1.39
10	A	37	A	N9-C4	-5.52	1.34	1.37
40	a	654	A	C5-C4	-5.52	1.34	1.38
40	a	1417	C	N3-C4	5.50	1.37	1.33
40	a	1670	C	C2-O2	-5.50	1.19	1.24
40	a	1927	A	N9-C4	-5.50	1.34	1.37
17	D	397	A	N7-C5	-5.50	1.35	1.39
10	B	37	A	N9-C4	-5.49	1.34	1.37
40	a	670	A	N9-C4	-5.48	1.34	1.37
17	D	884	U	C4-O4	-5.47	1.19	1.23
40	a	142	A	C6-N1	-5.47	1.31	1.35
62	w	100	CYS	N-CA	5.44	1.57	1.46
17	D	1493	A	C6-N6	-5.44	1.29	1.33
43	d	80	U	C2'-O2'	-5.43	1.34	1.41
10	B	37	A	O4'-C1'	-5.40	1.34	1.41
10	A	37	A	O4'-C1'	-5.39	1.34	1.41
7	6	24	DT	C1'-N1	5.35	1.56	1.49
40	a	2017	U	C4-C5	-5.33	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	37	A	C4'-O4'	-5.33	1.38	1.45
48	i	22	LEU	CG-CD1	5.33	1.71	1.51
43	d	80	U	C5-C6	-5.32	1.29	1.34
17	D	563	A	C6-N6	-5.32	1.29	1.33
54	o	14	PHE	CD1-CE1	-5.32	1.28	1.39
40	a	2286	G	C5-C6	5.31	1.47	1.42
40	a	336	C	P-O5'	-5.30	1.54	1.59
54	o	14	PHE	CB-CG	-5.30	1.42	1.51
10	B	37	A	C4'-O4'	-5.29	1.38	1.45
17	D	597	G	N9-C8	-5.29	1.34	1.37
40	a	88	G	C6-N1	-5.29	1.35	1.39
54	o	42	ARG	CB-CG	-5.28	1.38	1.52
10	B	32	C	N1-C6	5.28	1.40	1.37
40	a	2311	A	C5-C4	5.28	1.42	1.38
40	a	68	G	C2'-C1'	-5.27	1.47	1.53
40	a	1019	U	N1-C6	5.27	1.42	1.38
40	a	2365	G	N3-C4	5.26	1.39	1.35
40	a	327	G	C8-N7	5.24	1.34	1.30
40	a	1021	A	C6-N6	-5.24	1.29	1.33
40	a	2613	U	C2-N3	-5.24	1.34	1.37
21	H	267	TRP	CB-CG	-5.23	1.40	1.50
40	a	464	U	P-OP1	-5.23	1.40	1.49
40	a	517	C	N3-C4	-5.22	1.30	1.33
17	D	872	A	N7-C5	-5.22	1.36	1.39
48	i	13	ARG	CZ-NH2	-5.22	1.26	1.33
40	a	2013	A	C6-N1	-5.22	1.31	1.35
40	a	1924	C	C4-N4	5.21	1.38	1.33
40	a	2277	G	N9-C8	-5.21	1.34	1.37
40	a	789	A	C4'-O4'	5.19	1.52	1.45
40	a	743	A	C6-N1	-5.18	1.31	1.35
16	C	23	TYR	CB-CG	-5.18	1.43	1.51
10	A	32	C	N3-C4	-5.18	1.30	1.33
16	C	24	LYS	CG-CD	-5.18	1.34	1.52
25	L	49	TYR	CE1-CZ	5.17	1.45	1.38
16	C	23	TYR	CD1-CE1	-5.14	1.31	1.39
40	a	1798	U	C2-N3	-5.14	1.34	1.37
10	B	76	A	C6-N6	-5.14	1.29	1.33
10	B	30	G	C6-O6	5.13	1.28	1.24
40	a	85	G	P-O5'	5.13	1.64	1.59
48	i	17	ARG	CZ-NH1	-5.13	1.26	1.33
17	D	1346	A	N9-C4	-5.12	1.34	1.37
40	a	1614	A	C2'-C1'	-5.12	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	32	C	N3-C4	-5.12	1.30	1.33
8	7	-12	U	C5-C6	-5.12	1.29	1.34
40	a	579	G	C2'-C1'	-5.12	1.47	1.53
40	a	2311	A	C6-N6	-5.12	1.29	1.33
21	H	340	ARG	CG-CD	-5.11	1.39	1.51
10	A	32	C	N1-C6	5.10	1.40	1.37
10	A	30	G	C6-O6	5.09	1.28	1.24
65	z	4	VAL	CB-CG1	-5.08	1.42	1.52
40	a	92	U	C4-C5	-5.08	1.39	1.43
10	B	30	G	C8-N7	-5.06	1.27	1.30
21	H	339	ARG	CG-CD	-5.06	1.39	1.51
54	o	39	LYS	CE-NZ	-5.03	1.36	1.49
10	A	76	A	C6-N6	-5.02	1.29	1.33
40	a	1454	C	C4-N4	-5.00	1.29	1.33

All (1573) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	336	C	N3-C2-O2	-87.70	60.51	121.90
40	a	789	A	C8-N9-C4	-73.67	76.33	105.80
40	a	1262	A	N9-C4-C5	69.03	133.41	105.80
40	a	1262	A	C8-N9-C4	-65.11	79.76	105.80
17	D	958	A	C5-C6-N1	62.10	148.75	117.70
40	a	336	C	N1-C2-O2	57.19	153.22	118.90
40	a	789	A	N7-C8-N9	53.94	140.77	113.80
40	a	1262	A	N3-C4-N9	-49.47	87.83	127.40
10	B	37	A	N1-C2-N3	-49.38	104.61	129.30
10	A	37	A	N1-C2-N3	-49.20	104.70	129.30
10	B	37	A	N9-C4-C5	-48.27	86.49	105.80
10	A	37	A	N9-C4-C5	-48.16	86.53	105.80
40	a	89	A	C2-N3-C4	44.95	133.07	110.60
10	A	37	A	N1-C6-N6	-44.63	91.82	118.60
10	B	37	A	N1-C6-N6	-44.46	91.92	118.60
40	a	336	C	C6-N1-C2	-43.02	103.09	120.30
40	a	88	G	N7-C8-N9	-41.88	92.16	113.10
40	a	1262	A	N1-C2-N3	-40.54	109.03	129.30
40	a	789	A	C5-N7-C8	-39.04	84.38	103.90
40	a	336	C	C2-N3-C4	-38.36	100.72	119.90
10	B	37	A	C8-N9-C4	37.95	120.98	105.80
10	A	37	A	C8-N9-C4	37.88	120.95	105.80
40	a	1262	A	C4-C5-N7	-37.85	91.77	110.70
40	a	68	G	C8-N9-C4	37.76	121.50	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	336	C	N1-C2-N3	37.53	145.47	119.20
17	D	958	A	C5-C6-N6	-36.91	94.18	123.70
10	B	37	A	C4-C5-C6	-36.42	98.79	117.00
10	A	37	A	C4-C5-C6	-36.25	98.88	117.00
40	a	85	G	C8-N9-C4	-36.07	91.97	106.40
48	i	13	ARG	NE-CZ-NH1	35.95	138.28	120.30
17	D	958	A	C6-N1-C2	-35.56	97.27	118.60
40	a	789	A	C6-C5-N7	-35.37	107.54	132.30
17	D	1317	C	N1-C2-O2	-34.99	97.91	118.90
10	B	37	A	C4-C5-N7	34.48	127.94	110.70
10	A	37	A	C4-C5-N7	34.43	127.92	110.70
62	w	96	ARG	NE-CZ-NH2	33.36	136.98	120.30
40	a	89	A	C5-C6-N1	32.67	134.03	117.70
40	a	1262	A	N7-C8-N9	32.58	130.09	113.80
10	B	37	A	C5-C6-N1	32.51	133.95	117.70
10	A	37	A	C5-C6-N1	32.41	133.90	117.70
40	a	88	G	C5-N7-C8	32.38	120.49	104.30
40	a	89	A	N1-C6-N6	-31.63	99.62	118.60
17	D	958	A	C4-C5-C6	-31.61	101.19	117.00
40	a	336	C	N3-C4-N4	-30.15	96.90	118.00
40	a	86	G	O5'-P-OP2	-29.69	75.08	110.70
40	a	89	A	C6-N1-C2	-29.21	101.07	118.60
17	D	1493	A	N1-C6-N6	-29.15	101.11	118.60
40	a	1141	U	C2-N3-C4	28.02	143.81	127.00
10	A	39	C	C4-C5-C6	27.87	131.33	117.40
10	B	39	C	C4-C5-C6	27.75	131.28	117.40
40	a	789	A	C4-C5-C6	27.68	130.84	117.00
40	a	789	A	N9-C4-C5	27.49	116.80	105.80
40	a	2493	U	C6-N1-C2	27.37	137.42	121.00
40	a	2286	G	N1-C6-O6	-27.36	103.49	119.90
40	a	1141	U	C5-C4-O4	26.44	141.76	125.90
40	a	68	G	N9-C4-C5	-26.00	95.00	105.40
40	a	1019	U	C2-N3-C4	25.95	142.57	127.00
10	A	39	C	C5-C6-N1	-25.80	108.10	121.00
40	a	2613	U	N3-C4-O4	-25.71	101.40	119.40
40	a	85	G	N7-C8-N9	25.70	125.95	113.10
10	B	39	C	C5-C6-N1	-25.70	108.15	121.00
40	a	1262	A	C5-C6-N6	25.68	144.25	123.70
17	D	1317	C	C6-N1-C2	-25.68	110.03	120.30
17	D	37	U	N3-C4-O4	-25.60	101.48	119.40
48	i	50	ARG	NE-CZ-NH1	25.28	132.94	120.30
40	a	1924	C	N3-C4-C5	24.95	131.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	518	G	O5'-P-OP1	24.95	140.64	110.70
17	D	102	G	O5'-P-OP2	-24.77	80.98	110.70
40	a	1019	U	N1-C2-N3	-24.64	100.11	114.90
17	D	827	U	N3-C4-O4	-24.57	102.20	119.40
17	D	884	U	C5-C4-O4	24.51	140.61	125.90
10	A	37	A	N3-C4-N9	24.43	146.95	127.40
10	B	37	A	N3-C4-N9	24.41	146.93	127.40
40	a	1019	U	C5-C4-O4	24.37	140.52	125.90
28	O	113	ARG	NE-CZ-NH1	24.23	132.42	120.30
17	D	1358	U	C5-C4-O4	24.10	140.36	125.90
17	D	827	U	C5-C4-O4	23.94	140.26	125.90
10	B	76	A	C8-N9-C4	23.82	115.33	105.80
10	A	76	A	C8-N9-C4	23.81	115.33	105.80
40	a	1262	A	C5-C6-N1	-23.75	105.82	117.70
40	a	2613	U	C5-C4-O4	23.73	140.14	125.90
40	a	89	A	C6-C5-N7	23.32	148.62	132.30
17	D	1358	U	N3-C4-O4	-22.86	103.39	119.40
40	a	518	G	OP1-P-OP2	-22.77	85.45	119.60
17	D	37	U	C5-C4-O4	22.72	139.53	125.90
10	B	37	A	N7-C8-N9	-22.52	102.54	113.80
40	a	336	C	C2-N1-C1'	22.46	143.51	118.80
10	A	37	A	N7-C8-N9	-22.44	102.58	113.80
40	a	1019	U	N3-C4-O4	-22.21	103.85	119.40
17	D	884	U	N3-C4-O4	-22.20	103.86	119.40
40	a	327	G	C2-N3-C4	21.97	122.89	111.90
40	a	789	A	C4-C5-N7	21.83	121.61	110.70
40	a	1141	U	N3-C4-O4	-21.63	104.26	119.40
40	a	1141	U	N1-C2-N3	-21.51	102.00	114.90
17	D	675	A	N1-C2-N3	21.45	140.03	129.30
40	a	789	A	N1-C6-N6	21.29	131.37	118.60
40	a	1082	U	N3-C4-O4	-21.21	104.55	119.40
40	a	88	G	N3-C4-C5	-20.74	118.23	128.60
40	a	88	G	N1-C2-N3	20.45	136.17	123.90
40	a	67	U	N3-C4-O4	-20.40	105.12	119.40
40	a	85	G	C6-C5-N7	-20.34	118.20	130.40
40	a	88	G	P-O3'-C3'	-19.79	95.95	119.70
40	a	68	G	N3-C4-C5	19.77	138.48	128.60
40	a	89	A	N9-C4-C5	19.76	113.70	105.80
17	D	1493	A	C8-N9-C4	-19.71	97.92	105.80
17	D	958	A	C8-N9-C4	19.68	113.67	105.80
40	a	2493	U	C5-C6-N1	-19.42	112.99	122.70
40	a	917	A	C2-N3-C4	-19.38	100.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	88	G	C8-N9-C4	19.35	114.14	106.40
40	a	2756	U	N3-C4-O4	-19.27	105.91	119.40
40	a	89	A	N3-C4-C5	-19.24	113.33	126.80
17	D	1014	A	O5'-P-OP2	19.08	133.60	110.70
17	D	958	A	N9-C4-C5	-19.04	98.18	105.80
40	a	88	G	OP1-P-O3'	-18.89	63.63	105.20
40	a	336	C	C5-C4-N4	18.87	133.41	120.20
40	a	89	A	C4-C5-N7	-18.82	101.29	110.70
10	A	76	A	N1-C2-N3	-18.70	119.95	129.30
10	B	76	A	N1-C2-N3	-18.64	119.98	129.30
17	D	958	A	C4-C5-N7	18.49	119.94	110.70
40	a	789	A	N1-C2-N3	18.25	138.43	129.30
40	a	2678	C	O5'-P-OP2	-18.19	88.88	110.70
10	A	32	C	C6-N1-C2	18.05	127.52	120.30
17	D	675	A	C2-N3-C4	-18.03	101.58	110.60
62	w	96	ARG	NE-CZ-NH1	-18.02	111.29	120.30
16	C	40	VAL	CG1-CB-CG2	18.00	139.70	110.90
40	a	2286	G	C5-C6-N1	17.84	120.42	111.50
40	a	917	A	C5-C6-N1	-17.84	108.78	117.70
40	a	1262	A	C6-C5-N7	17.83	144.78	132.30
40	a	990	A	C5-C6-N1	-17.80	108.80	117.70
10	B	31	G	C5-N7-C8	-17.73	95.44	104.30
10	B	32	C	C6-N1-C2	17.72	127.39	120.30
10	A	31	G	C5-N7-C8	-17.70	95.45	104.30
17	D	1317	C	N1-C2-N3	17.69	131.59	119.20
40	a	1199	U	N1-C2-O2	-17.64	110.45	122.80
17	D	827	U	N1-C2-N3	-17.44	104.43	114.90
10	A	31	G	C2-N3-C4	17.35	120.58	111.90
40	a	1262	A	N1-C6-N6	-17.33	108.20	118.60
48	i	50	ARG	NE-CZ-NH2	-17.26	111.67	120.30
40	a	917	A	N3-C4-N9	-17.22	113.62	127.40
10	B	31	G	C2-N3-C4	17.21	120.51	111.90
40	a	2493	U	O4'-C1'-N1	17.05	121.84	108.20
40	a	1	G	N1-C6-O6	16.88	130.03	119.90
40	a	1581	G	N1-C6-O6	16.80	129.98	119.90
40	a	2493	U	C6-N1-C1'	-16.78	97.71	121.20
40	a	1262	A	N3-C4-C5	16.73	138.51	126.80
40	a	88	G	C4-C5-N7	-16.70	104.12	110.80
40	a	89	A	O5'-P-OP1	16.64	130.67	110.70
43	d	80	U	C6-N1-C2	16.63	130.98	121.00
40	a	327	G	N3-C4-C5	-16.62	120.29	128.60
10	B	19	G	C5-C6-O6	-16.57	118.66	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	884	U	C2-N3-C4	16.54	136.93	127.00
10	A	19	G	C5-C6-O6	-16.49	118.70	128.60
17	D	1358	U	N1-C2-N3	-16.33	105.10	114.90
40	a	68	G	N7-C8-N9	-16.32	104.94	113.10
17	D	884	U	N1-C2-N3	-16.30	105.12	114.90
17	D	1317	C	N3-C4-C5	-16.26	115.39	121.90
2	1	18	ARG	NE-CZ-NH1	16.18	128.39	120.30
10	B	76	A	C4-C5-C6	-16.13	108.93	117.00
10	A	76	A	C4-C5-C6	-16.13	108.94	117.00
17	D	1371	G	O5'-P-OP2	-16.07	91.24	105.70
40	a	674	G	C8-N9-C4	16.05	112.82	106.40
40	a	2756	U	C5-C4-O4	15.92	135.45	125.90
40	a	631	A	C8-N9-C4	15.81	112.12	105.80
40	a	67	U	C5-C4-O4	15.78	135.37	125.90
40	a	2512	C	C6-N1-C2	15.66	126.56	120.30
40	a	2493	U	O5'-P-OP1	-15.64	91.62	105.70
10	B	76	A	N9-C4-C5	-15.62	99.55	105.80
40	a	1410	G	N1-C6-O6	15.59	129.25	119.90
10	B	19	G	N1-C6-O6	15.53	129.22	119.90
10	A	19	G	N1-C6-O6	15.52	129.21	119.90
10	A	76	A	N9-C4-C5	-15.47	99.61	105.80
40	a	136	G	N1-C6-O6	15.40	129.14	119.90
40	a	551	G	N1-C6-O6	15.39	129.13	119.90
1	0	78	ARG	NE-CZ-NH1	-15.34	112.63	120.30
40	a	990	A	C2-N3-C4	-15.19	103.00	110.60
40	a	89	A	OP1-P-OP2	-15.17	96.84	119.60
10	A	39	C	N1-C2-O2	15.12	127.97	118.90
10	B	39	C	N1-C2-O2	15.11	127.97	118.90
40	a	89	A	O5'-P-OP2	15.02	128.72	110.70
40	a	327	G	N1-C6-O6	-15.02	110.89	119.90
40	a	89	A	C4-C5-C6	-14.95	109.52	117.00
40	a	1019	U	C4-C5-C6	-14.95	110.73	119.70
28	O	18	ARG	NE-CZ-NH2	-14.93	112.83	120.30
40	a	1082	U	C5-C4-O4	14.91	134.84	125.90
40	a	85	G	C4-C5-C6	14.87	127.72	118.80
40	a	85	G	C5-N7-C8	-14.76	96.92	104.30
40	a	2356	U	C6-N1-C2	14.68	129.81	121.00
40	a	336	C	N3-C4-C5	14.68	127.77	121.90
64	y	109	ARG	NE-CZ-NH1	-14.46	113.07	120.30
40	a	68	G	OP1-P-OP2	-14.46	97.92	119.60
10	A	19	G	N9-C4-C5	-14.37	99.65	105.40
17	D	1358	U	C2-N3-C4	14.34	135.61	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	956	U	C6-N1-C2	14.29	129.58	121.00
40	a	654	A	C5-C6-N1	14.29	124.84	117.70
40	a	88	G	C4-C5-C6	14.28	127.37	118.80
40	a	2262	U	O5'-P-OP2	-14.28	92.85	105.70
40	a	68	G	C4-C5-N7	14.27	116.51	110.80
10	B	32	C	N3-C4-C5	14.27	127.61	121.90
40	a	516	C	P-O3'-C3'	14.27	136.82	119.70
10	B	19	G	N9-C4-C5	-14.25	99.70	105.40
10	A	32	C	N3-C4-C5	14.17	127.57	121.90
40	a	74	A	C2-N3-C4	-14.16	103.52	110.60
17	D	597	G	C8-N9-C4	14.16	112.06	106.40
40	a	2350	C	O5'-P-OP2	-14.15	92.97	105.70
40	a	2902	C	C6-N1-C2	14.12	125.95	120.30
40	a	1614	A	C8-N9-C4	14.06	111.42	105.80
40	a	542	C	C6-N1-C2	14.05	125.92	120.30
40	a	2286	G	C6-N1-C2	-13.99	116.71	125.10
17	D	1013	G	OP1-P-O3'	13.96	135.91	105.20
48	i	22	LEU	CB-CG-CD1	13.93	134.68	111.00
2	1	19	LEU	CB-CG-CD2	-13.93	87.33	111.00
17	D	1493	A	C5-C6-N6	13.92	134.84	123.70
37	X	98	ARG	NE-CZ-NH1	13.84	127.22	120.30
17	D	1348	U	OP1-P-O3'	-13.74	74.96	105.20
40	a	1417	C	C6-N1-C2	13.68	125.77	120.30
10	B	37	A	C4-N9-C1'	-13.67	101.69	126.30
10	A	37	A	C4-N9-C1'	-13.67	101.70	126.30
40	a	1141	U	C4-C5-C6	-13.59	111.55	119.70
40	a	2094	A	O5'-P-OP1	-13.59	93.47	105.70
10	B	39	C	N3-C4-C5	-13.58	116.47	121.90
40	a	654	A	N9-C4-C5	-13.57	100.37	105.80
40	a	918	A	C8-N9-C4	13.55	111.22	105.80
40	a	1106	G	N1-C6-O6	13.53	128.02	119.90
40	a	789	A	C5-C6-N1	-13.48	110.96	117.70
40	a	1060	U	C5-C4-O4	-13.47	117.82	125.90
10	A	39	C	N3-C4-C5	-13.42	116.53	121.90
48	i	50	ARG	CG-CD-NE	13.42	139.98	111.80
17	D	1493	A	N9-C4-C5	13.42	111.17	105.80
10	B	19	G	C4-C5-N7	13.35	116.14	110.80
10	A	19	G	C4-C5-N7	13.35	116.14	110.80
40	a	1262	A	C6-N1-C2	13.33	126.60	118.60
40	a	1021	A	N1-C2-N3	-13.33	122.64	129.30
48	i	13	ARG	NH1-CZ-NH2	-13.30	104.77	119.40
40	a	68	G	O5'-P-OP1	13.27	126.63	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	2350	C	O5'-P-OP1	13.26	126.62	110.70
40	a	326	G	C2-N3-C4	-13.12	105.34	111.90
40	a	2188	U	N3-C4-O4	13.11	128.58	119.40
17	D	958	A	C5-N7-C8	-13.10	97.35	103.90
40	a	2815	C	C6-N1-C2	13.07	125.53	120.30
17	D	1317	C	C6-N1-C1'	13.02	136.42	120.80
40	a	89	A	C5-N7-C8	12.99	110.40	103.90
40	a	1053	C	C6-N1-C2	12.93	125.47	120.30
40	a	654	A	C4-C5-N7	12.90	117.15	110.70
40	a	1262	A	C4-C5-C6	12.89	123.44	117.00
40	a	1592	C	C6-N1-C2	12.87	125.45	120.30
48	i	4	GLN	O-C-N	-12.87	102.10	122.70
17	D	1014	A	OP1-P-OP2	-12.83	100.36	119.60
40	a	68	G	C4-N9-C1'	-12.79	109.87	126.50
29	P	55	PRO	CA-N-CD	-12.76	93.64	111.50
40	a	2286	G	N1-C2-N2	-12.75	104.72	116.20
40	a	917	A	N3-C4-C5	12.71	135.69	126.80
17	D	975	A	N1-C6-N6	-12.70	110.98	118.60
40	a	2493	U	C2-N3-C4	-12.68	119.39	127.00
40	a	1060	U	N3-C4-O4	12.65	128.26	119.40
40	a	751	A	C2-N3-C4	-12.63	104.29	110.60
40	a	2188	U	C5-C4-O4	-12.62	118.33	125.90
40	a	85	G	N9-C4-C5	12.57	110.43	105.40
17	D	1493	A	C5-C6-N1	12.56	123.98	117.70
40	a	2493	U	N3-C4-C5	12.54	122.13	114.60
10	B	37	A	C6-N1-C2	12.44	126.07	118.60
40	a	74	A	C5-C6-N1	-12.43	111.48	117.70
40	a	1924	C	C2-N3-C4	-12.40	113.70	119.90
40	a	516	C	OP2-P-O3'	12.39	132.45	105.20
40	a	1087	G	N1-C6-O6	12.35	127.31	119.90
40	a	89	A	C5'-C4'-O4'	-12.31	94.33	109.10
17	D	827	U	C2-N3-C4	12.30	134.38	127.00
40	a	2286	G	C5-C6-O6	12.28	135.97	128.60
10	A	37	A	C6-N1-C2	12.26	125.96	118.60
43	d	81	G	C8-N9-C4	12.25	111.30	106.40
40	a	1266	G	O5'-P-OP2	12.20	125.34	110.70
40	a	1142	A	N9-C4-C5	-12.19	100.92	105.80
40	a	1	G	C6-C5-N7	-12.17	123.10	130.40
40	a	1262	A	C8-N9-C1'	12.14	149.56	127.70
40	a	917	A	N9-C4-C5	12.13	110.65	105.80
17	D	1339	A	C2-N3-C4	-12.08	104.56	110.60
10	B	31	G	C4-C5-N7	12.07	115.63	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	w	98	LEU	CB-CG-CD2	-12.04	90.53	111.00
10	A	31	G	C4-C5-N7	12.04	115.61	110.80
40	a	136	G	C6-C5-N7	-12.02	123.19	130.40
40	a	1581	G	C6-C5-N7	-11.96	123.22	130.40
40	a	68	G	C2-N3-C4	-11.95	105.93	111.90
40	a	2351	G	C4-C5-N7	11.94	115.58	110.80
10	B	19	G	C6-C5-N7	-11.93	123.24	130.40
40	a	2884	U	N3-C4-O4	-11.91	111.06	119.40
10	A	19	G	C6-C5-N7	-11.88	123.27	130.40
40	a	107	G	O5'-P-OP1	-11.86	95.03	105.70
17	D	194	C	C6-N1-C2	11.83	125.03	120.30
40	a	143	C	C6-N1-C2	11.83	125.03	120.30
17	D	563	A	N1-C6-N6	-11.79	111.53	118.60
40	a	551	G	C6-C5-N7	-11.79	123.33	130.40
40	a	2351	G	N9-C4-C5	-11.78	100.69	105.40
64	y	109	ARG	NE-CZ-NH2	11.78	126.19	120.30
40	a	74	A	N1-C2-N3	11.77	135.18	129.30
40	a	86	G	OP1-P-OP2	-11.77	101.95	119.60
40	a	751	A	N1-C2-N3	11.77	135.19	129.30
40	a	1	G	C5-C6-N1	-11.72	105.64	111.50
40	a	615	U	C6-N1-C2	11.72	128.03	121.00
40	a	674	G	N9-C4-C5	-11.72	100.71	105.40
40	a	88	G	C5'-C4'-C3'	11.69	134.71	116.00
40	a	107	G	O5'-P-OP2	11.64	124.67	110.70
10	B	37	A	C5-C6-N6	-11.62	114.41	123.70
10	A	36	U	C5-C4-O4	11.61	132.87	125.90
40	a	1924	C	C6-N1-C2	11.60	124.94	120.30
10	A	37	A	C5-C6-N6	-11.57	114.45	123.70
17	D	675	A	N3-C4-N9	-11.56	118.15	127.40
40	a	654	A	C5-C6-N6	-11.56	114.45	123.70
10	B	76	A	C2-N3-C4	11.55	116.38	110.60
10	B	36	U	C5-C4-O4	11.53	132.82	125.90
40	a	1019	U	N3-C2-O2	11.52	130.26	122.20
10	A	76	A	C2-N3-C4	11.52	116.36	110.60
40	a	869	G	C8-N9-C4	11.52	111.01	106.40
40	a	788	A	N9-C4-C5	-11.50	101.20	105.80
40	a	861	A	N1-C6-N6	-11.49	111.70	118.60
40	a	615	U	C5-C4-O4	-11.48	119.01	125.90
40	a	1581	G	C5-C6-N1	-11.48	105.76	111.50
24	K	78	ASN	N-CA-CB	-11.46	89.98	110.60
17	D	872	A	N1-C6-N6	-11.44	111.74	118.60
40	a	244	A	O5'-P-OP2	-11.41	95.43	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	788	A	C8-N9-C4	11.41	110.37	105.80
62	w	98	LEU	CB-CG-CD1	-11.38	91.66	111.00
40	a	1924	C	C4-C5-C6	-11.36	111.72	117.40
17	D	827	U	C4-C5-C6	-11.34	112.90	119.70
17	D	526	C	C6-N1-C2	11.33	124.83	120.30
40	a	1414	C	C6-N1-C2	11.32	124.83	120.30
48	i	26	THR	CA-CB-CG2	-11.31	96.57	112.40
40	a	2884	U	C5-C4-O4	11.31	132.68	125.90
40	a	88	G	O4'-C1'-N9	-11.27	99.18	108.20
48	i	13	ARG	CD-NE-CZ	11.23	139.33	123.60
40	a	89	A	C5'-C4'-C3'	-11.22	98.04	116.00
43	d	81	G	N3-C4-C5	11.22	134.21	128.60
40	a	551	G	C5-C6-N1	-11.20	105.90	111.50
10	B	39	C	C2-N3-C4	11.16	125.48	119.90
40	a	85	G	C8-N9-C1'	11.16	141.51	127.00
40	a	1614	A	N9-C4-C5	-11.16	101.34	105.80
40	a	2641	G	C8-N9-C4	11.16	110.86	106.40
40	a	74	A	N7-C8-N9	11.16	119.38	113.80
40	a	2261	C	N3-C4-C5	11.14	126.36	121.90
40	a	1262	A	C2-N3-C4	11.12	116.16	110.60
40	a	2312	U	O5'-P-OP1	-11.13	95.69	105.70
40	a	1198	U	N3-C2-O2	-11.10	114.43	122.20
40	a	917	A	N1-C2-N3	11.10	134.85	129.30
48	i	20	ASP	CB-CG-OD1	11.09	128.28	118.30
40	a	789	A	C8-N9-C1'	11.04	147.57	127.70
40	a	1141	U	C5-C6-N1	11.03	128.21	122.70
40	a	327	G	C5-C6-N1	11.02	117.01	111.50
10	A	39	C	C2-N3-C4	11.01	125.41	119.90
40	a	990	A	N3-C4-C5	11.01	134.51	126.80
17	D	476	U	N3-C4-O4	11.01	127.10	119.40
40	a	1142	A	C4-C5-N7	11.01	116.20	110.70
8	7	-12	U	C6-N1-C2	11.00	127.60	121.00
40	a	89	A	O5'-C5'-C4'	10.99	132.59	111.70
40	a	67	U	P-O3'-C3'	10.99	132.88	119.70
40	a	1596	A	N1-C2-N3	10.94	134.77	129.30
40	a	990	A	N3-C4-N9	-10.89	118.69	127.40
40	a	631	A	N9-C4-C5	-10.87	101.45	105.80
40	a	789	A	N9-C1'-C2'	10.82	128.07	114.00
40	a	2815	C	N3-C4-C5	10.79	126.22	121.90
17	D	1493	A	C6-N1-C2	-10.79	112.13	118.60
17	D	1358	U	C4-C5-C6	-10.77	113.24	119.70
40	a	1021	A	C6-N1-C2	10.76	125.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	-12	U	C5-C4-O4	-10.75	119.45	125.90
40	a	544	C	C6-N1-C2	10.75	124.60	120.30
40	a	2822	G	O5'-P-OP1	-10.73	96.05	105.70
40	a	2013	A	N1-C6-N6	-10.71	112.17	118.60
40	a	86	G	O5'-P-OP1	10.70	123.53	110.70
62	w	46	ARG	NE-CZ-NH2	10.68	125.64	120.30
17	D	1363	A	N9-C4-C5	-10.66	101.54	105.80
40	a	1410	G	C6-C5-N7	-10.65	124.01	130.40
17	D	1152	A	O5'-P-OP1	-10.64	96.12	105.70
40	a	88	G	N3-C2-N2	-10.59	112.49	119.90
40	a	1199	U	N3-C2-O2	10.57	129.60	122.20
40	a	1670	C	N1-C2-O2	-10.56	112.56	118.90
40	a	74	A	C4-C5-C6	10.53	122.26	117.00
17	D	397	A	C4-C5-N7	10.52	115.96	110.70
17	D	958	A	N3-C4-N9	10.49	135.79	127.40
37	X	98	ARG	NE-CZ-NH2	-10.49	115.06	120.30
40	a	2	G	N1-C6-O6	10.49	126.19	119.90
48	i	20	ASP	CB-CG-OD2	-10.47	108.88	118.30
40	a	2286	G	N1-C2-N3	10.44	130.17	123.90
40	a	65	U	C2-N3-C4	10.40	133.24	127.00
17	D	97	G	N1-C6-O6	10.38	126.13	119.90
17	D	476	U	C5-C4-O4	-10.38	119.67	125.90
10	B	76	A	N9-C1'-C2'	-10.35	100.54	114.00
10	A	76	A	N9-C1'-C2'	-10.35	100.54	114.00
40	a	136	G	C4-C5-N7	10.34	114.94	110.80
17	D	397	A	N1-C6-N6	-10.34	112.40	118.60
8	7	-12	U	N3-C2-O2	10.32	129.43	122.20
40	a	2815	C	O5'-P-OP2	-10.32	96.41	105.70
40	a	136	G	N9-C4-C5	-10.31	101.28	105.40
17	D	1339	A	C5-C6-N1	-10.31	112.55	117.70
17	D	884	U	C4-C5-C6	-10.29	113.52	119.70
40	a	742	A	N1-C2-N3	10.29	134.45	129.30
40	a	1530	G	N1-C6-O6	10.29	126.08	119.90
40	a	789	A	C2-N3-C4	-10.29	105.46	110.60
40	a	85	G	C5-C6-N1	-10.28	106.36	111.50
21	H	340	ARG	NE-CZ-NH2	10.24	125.42	120.30
17	D	675	A	N9-C4-C5	10.24	109.89	105.80
40	a	1406	U	C2-N3-C4	10.22	133.13	127.00
40	a	336	C	C4-C5-C6	10.20	122.50	117.40
17	D	1112	C	N1-C2-O2	-10.19	112.79	118.90
16	C	24	LYS	CD-CE-NZ	-10.18	88.29	111.70
40	a	789	A	N3-C4-C5	-10.15	119.70	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	396	G	C8-N9-C4	10.14	110.46	106.40
40	a	464	U	O5'-P-OP1	-10.14	96.57	105.70
40	a	2815	C	O4'-C1'-N1	-10.13	100.10	108.20
17	D	1130	A	O5'-P-OP1	10.11	122.83	110.70
40	a	2612	C	C6-N1-C2	10.11	124.34	120.30
2	1	19	LEU	CB-CG-CD1	10.11	128.18	111.00
17	D	1493	A	N7-C8-N9	10.08	118.84	113.80
40	a	2367	G	N1-C6-O6	10.08	125.95	119.90
40	a	2902	C	C2-N1-C1'	-10.07	107.72	118.80
40	a	1021	A	N1-C6-N6	-10.06	112.56	118.60
40	a	2640	G	OP1-P-O3'	-10.06	83.08	105.20
40	a	990	A	C6-N1-C2	10.04	124.62	118.60
40	a	1198	U	C6-N1-C2	-10.02	114.99	121.00
40	a	326	G	N1-C2-N2	-9.99	107.21	116.20
17	D	1363	A	C4-C5-N7	9.99	115.69	110.70
40	a	2286	G	N3-C4-C5	-9.98	123.61	128.60
40	a	2901	C	C6-N1-C2	9.98	124.29	120.30
17	D	1240	U	N3-C4-O4	-9.97	112.42	119.40
40	a	1530	G	C5-C6-O6	-9.96	122.62	128.60
40	a	2512	C	N3-C4-C5	9.96	125.88	121.90
40	a	942	G	N1-C6-O6	-9.95	113.93	119.90
40	a	1021	A	C4-C5-N7	9.94	115.67	110.70
40	a	88	G	C5-C6-N1	-9.91	106.54	111.50
40	a	326	G	C5-C6-N1	-9.90	106.55	111.50
17	D	1348	U	C6-N1-C2	9.90	126.94	121.00
40	a	2365	G	C5-C6-N1	9.88	116.44	111.50
40	a	88	G	C2-N3-C4	-9.85	106.97	111.90
10	B	38	A	C5-N7-C8	-9.83	98.99	103.90
17	D	1317	C	N3-C2-O2	9.81	128.77	121.90
17	D	1493	A	N3-C4-C5	-9.79	119.95	126.80
40	a	1993	U	C6-N1-C2	9.79	126.87	121.00
40	a	1198	U	N1-C2-N3	9.78	120.77	114.90
8	7	-12	U	N1-C2-N3	-9.78	109.03	114.90
10	A	36	U	N3-C4-O4	-9.77	112.56	119.40
10	A	38	A	C5-N7-C8	-9.77	99.02	103.90
40	a	380	G	C8-N9-C4	9.76	110.30	106.40
29	P	55	PRO	N-CA-CB	9.75	115.00	103.30
17	D	1349	A	O5'-P-OP1	9.74	122.39	110.70
40	a	2365	G	N1-C2-N2	-9.73	107.44	116.20
40	a	2493	U	O5'-C5'-C4'	-9.73	93.22	111.70
40	a	85	G	OP2-P-O3'	9.72	126.59	105.20
40	a	1406	U	N3-C4-O4	9.72	126.21	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	36	U	N3-C4-O4	-9.72	112.60	119.40
17	D	597	G	N9-C4-C5	-9.70	101.52	105.40
10	B	19	G	C8-N9-C4	9.69	110.28	106.40
40	a	85	G	O5'-P-OP1	9.68	122.31	110.70
40	a	2351	G	C5-C6-O6	-9.67	122.80	128.60
43	d	81	G	N9-C4-C5	-9.67	101.53	105.40
40	a	327	G	C6-N1-C2	-9.65	119.31	125.10
40	a	273	G	N1-C6-O6	9.63	125.68	119.90
10	A	31	G	C4-C5-C6	-9.62	113.03	118.80
10	A	19	G	C8-N9-C4	9.62	110.25	106.40
40	a	1142	A	C6-N1-C2	9.61	124.37	118.60
43	d	81	G	C2-N3-C4	-9.59	107.10	111.90
17	D	1308	U	OP1-P-O3'	9.59	126.30	105.20
40	a	1086	A	N1-C6-N6	-9.58	112.85	118.60
40	a	918	A	C5-C6-N1	9.58	122.49	117.70
40	a	1106	G	C6-C5-N7	-9.57	124.66	130.40
40	a	1019	U	C5-C6-N1	9.54	127.47	122.70
10	B	31	G	C4-C5-C6	-9.54	113.08	118.80
40	a	2351	G	C5-C6-N1	9.53	116.26	111.50
17	D	1493	A	N1-C2-N3	9.51	134.06	129.30
40	a	2351	G	C8-N9-C4	9.49	110.20	106.40
40	a	917	A	C8-N9-C4	-9.49	102.00	105.80
17	D	1309	G	N7-C8-N9	9.45	117.82	113.10
40	a	851	C	O5'-P-OP1	-9.43	97.21	105.70
40	a	1588	G	N1-C6-O6	9.43	125.56	119.90
40	a	2356	U	N3-C2-O2	9.41	128.79	122.20
10	A	30	G	C2-N3-C4	9.40	116.60	111.90
40	a	551	G	C4-C5-N7	9.37	114.55	110.80
40	a	2613	U	C4-C5-C6	-9.37	114.08	119.70
10	A	76	A	C5-C6-N1	9.36	122.38	117.70
10	B	32	C	N3-C4-N4	-9.36	111.45	118.00
40	a	918	A	N9-C4-C5	-9.36	102.06	105.80
2	1	39	THR	CA-CB-CG2	-9.35	99.31	112.40
40	a	1021	A	N9-C4-C5	-9.31	102.08	105.80
17	D	1309	G	C5-N7-C8	-9.31	99.65	104.30
10	A	31	G	N7-C8-N9	9.30	117.75	113.10
10	A	76	A	N7-C8-N9	-9.30	109.15	113.80
40	a	89	A	N9-C1'-C2'	9.30	126.09	114.00
10	B	31	G	N7-C8-N9	9.29	117.75	113.10
10	A	32	C	N3-C4-N4	-9.27	111.51	118.00
17	D	563	A	C5-C6-N6	9.27	131.11	123.70
10	B	30	G	C2-N3-C4	9.26	116.53	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	326	G	N3-C2-N2	9.26	126.38	119.90
40	a	2493	U	N1-C2-N3	-9.24	109.36	114.90
17	D	1363	A	N1-C6-N6	-9.24	113.06	118.60
40	a	1102	C	C6-N1-C2	9.24	124.00	120.30
40	a	654	A	C8-N9-C4	9.23	109.49	105.80
40	a	755	U	N3-C4-O4	9.23	125.86	119.40
40	a	1082	U	N3-C4-C5	9.23	120.14	114.60
40	a	861	A	N1-C2-N3	9.22	133.91	129.30
40	a	2512	C	C2-N3-C4	-9.22	115.29	119.90
10	B	76	A	C5-C6-N1	9.21	122.30	117.70
10	A	34	C	N1-C2-O2	9.20	124.42	118.90
40	a	1141	U	N3-C2-O2	9.18	128.63	122.20
10	B	76	A	N7-C8-N9	-9.18	109.21	113.80
40	a	518	G	P-O5'-C5'	9.17	135.58	120.90
40	a	92	U	C4-C5-C6	9.17	125.20	119.70
10	A	19	G	N3-C4-N9	9.17	131.50	126.00
40	a	85	G	N1-C2-N3	9.16	129.40	123.90
40	a	85	G	C2-N3-C4	-9.16	107.32	111.90
40	a	2512	C	C5-C6-N1	-9.15	116.42	121.00
40	a	788	A	N9-C1'-C2'	9.15	125.89	114.00
40	a	1141	U	N1-C2-O2	9.14	129.20	122.80
40	a	1581	G	C4-C5-N7	9.13	114.45	110.80
40	a	2286	G	N3-C4-N9	9.13	131.48	126.00
40	a	326	G	N3-C4-C5	9.12	133.16	128.60
17	D	563	A	C4-C5-N7	9.11	115.26	110.70
40	a	2186	G	N1-C6-O6	9.11	125.37	119.90
40	a	1924	C	N3-C4-N4	-9.11	111.62	118.00
40	a	615	U	N3-C2-O2	9.10	128.57	122.20
40	a	1410	G	N9-C4-C5	-9.08	101.77	105.40
40	a	336	C	O5'-P-OP1	-9.07	97.54	105.70
10	B	34	C	N1-C2-O2	9.06	124.34	118.90
10	B	19	G	N3-C4-N9	9.06	131.44	126.00
17	D	1317	C	C4-C5-C6	9.06	121.93	117.40
48	i	22	LEU	CB-CG-CD2	-9.06	95.60	111.00
10	B	40	C	N1-C2-O2	9.04	124.33	118.90
40	a	2493	U	O5'-P-OP2	-9.04	97.57	105.70
17	D	497	G	N1-C6-O6	9.00	125.30	119.90
40	a	88	G	N3-C4-N9	8.98	131.39	126.00
40	a	1775	U	C5-C4-O4	-8.97	120.52	125.90
40	a	1338	G	C5-N7-C8	8.96	108.78	104.30
40	a	2365	G	C6-N1-C2	-8.96	119.72	125.10
40	a	1167	C	C6-N1-C2	8.96	123.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	397	A	N9-C4-C5	-8.96	102.22	105.80
17	D	1125	U	C5-C4-O4	-8.96	120.53	125.90
40	a	136	G	C5-C6-N1	-8.95	107.03	111.50
40	a	2356	U	N1-C2-N3	-8.95	109.53	114.90
40	a	2112	G	OP1-P-OP2	-8.93	106.21	119.60
10	A	40	C	N1-C2-O2	8.91	124.25	118.90
40	a	1592	C	C2-N1-C1'	-8.91	109.00	118.80
17	D	1186	G	C8-N9-C4	8.90	109.96	106.40
40	a	2365	G	C8-N9-C4	8.88	109.95	106.40
40	a	88	G	N1-C6-O6	8.87	125.22	119.90
40	a	2820	A	C8-N9-C4	8.86	109.34	105.80
40	a	1019	U	N1-C2-O2	8.86	129.00	122.80
17	D	563	A	N9-C4-C5	-8.86	102.26	105.80
10	A	76	A	C6-C5-N7	8.85	138.50	132.30
43	d	80	U	N1-C2-N3	-8.83	109.60	114.90
40	a	2192	U	N3-C4-O4	-8.81	113.23	119.40
50	k	14	SER	CB-CA-C	8.80	126.83	110.10
54	o	42	ARG	NE-CZ-NH1	-8.80	115.90	120.30
40	a	1613	G	O5'-P-OP2	-8.80	97.78	105.70
40	a	2620	C	C6-N1-C2	8.79	123.82	120.30
17	D	910	C	O5'-P-OP2	-8.79	97.79	105.70
10	A	37	A	O4'-C1'-N9	-8.78	101.17	108.20
40	a	755	U	C2-N3-C4	8.78	132.26	127.00
10	B	76	A	C6-C5-N7	8.77	138.44	132.30
17	D	956	U	N3-C4-C5	8.77	119.86	114.60
40	a	788	A	C5-C6-N1	8.76	122.08	117.70
40	a	2815	C	C4-C5-C6	-8.75	113.02	117.40
10	B	37	A	O4'-C1'-N9	-8.74	101.20	108.20
40	a	1	G	C4-C5-N7	8.74	114.30	110.80
40	a	1410	G	C4-C5-N7	8.74	114.30	110.80
40	a	2323	G	N1-C6-O6	8.71	125.12	119.90
17	D	397	A	N1-C2-N3	-8.70	124.95	129.30
48	i	52	ARG	NE-CZ-NH1	8.69	124.64	120.30
10	A	32	C	C5-C6-N1	-8.68	116.66	121.00
40	a	74	A	C4-N9-C1'	8.68	141.92	126.30
54	o	45	ARG	NE-CZ-NH1	8.67	124.63	120.30
40	a	2332	C	C6-N1-C2	8.65	123.76	120.30
48	i	17	ARG	NE-CZ-NH1	-8.64	115.98	120.30
40	a	2351	G	N3-C4-N9	8.63	131.18	126.00
62	w	96	ARG	CB-CG-CD	8.62	134.02	111.60
53	n	177	PHE	N-CA-CB	-8.62	95.08	110.60
40	a	869	G	N9-C4-C5	-8.62	101.95	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	742	A	C6-N1-C2	-8.61	113.43	118.60
40	a	2613	U	N1-C2-N3	-8.61	109.74	114.90
40	a	74	A	C5-C6-N6	8.60	130.58	123.70
40	a	542	C	C2-N1-C1'	-8.60	109.34	118.80
40	a	1410	G	C5-C6-N1	-8.60	107.20	111.50
40	a	2017	U	N3-C4-O4	-8.59	113.38	119.40
40	a	2103	C	C6-N1-C2	8.58	123.73	120.30
17	D	1340	A	C8-N9-C4	8.58	109.23	105.80
62	w	100	CYS	CA-CB-SG	8.57	129.43	114.00
48	i	41	HIS	N-CA-CB	8.57	126.03	110.60
10	B	32	C	C5-C6-N1	-8.55	116.72	121.00
40	a	1417	C	N1-C2-O2	-8.54	113.78	118.90
17	D	1363	A	C5-C6-N6	8.53	130.52	123.70
40	a	88	G	N1-C2-N2	-8.52	108.53	116.20
17	D	1368	A	O5'-P-OP1	-8.52	98.03	105.70
17	D	1126	U	C5-C4-O4	-8.51	120.79	125.90
40	a	1581	G	C2-N3-C4	-8.51	107.65	111.90
40	a	2013	A	N9-C4-C5	-8.49	102.40	105.80
40	a	788	A	N3-C4-N9	8.49	134.19	127.40
40	a	1775	U	N3-C4-O4	8.49	125.34	119.40
17	D	73	C	C6-N1-C2	8.49	123.70	120.30
17	D	1125	U	N3-C4-O4	8.49	125.34	119.40
40	a	2365	G	N1-C2-N3	8.47	128.98	123.90
28	O	113	ARG	NH1-CZ-NH2	-8.47	110.08	119.40
10	B	32	C	C4-C5-C6	-8.44	113.18	117.40
40	a	1142	A	N1-C6-N6	-8.44	113.54	118.60
10	A	32	C	C4-C5-C6	-8.43	113.19	117.40
40	a	68	G	N1-C6-O6	8.43	124.96	119.90
40	a	1410	G	C5-C6-O6	-8.43	123.55	128.60
40	a	143	C	N1-C2-O2	-8.42	113.85	118.90
40	a	2350	C	N3-C4-N4	8.42	123.89	118.00
40	a	1406	U	N1-C2-N3	-8.40	109.86	114.90
40	a	551	G	C2-N3-C4	-8.38	107.71	111.90
40	a	65	U	N1-C2-N3	-8.38	109.87	114.90
40	a	1454	C	N3-C4-C5	8.37	125.25	121.90
40	a	615	U	N1-C2-N3	-8.36	109.88	114.90
40	a	1338	G	C8-N9-C4	8.33	109.73	106.40
17	D	872	A	C4-C5-N7	8.32	114.86	110.70
17	D	1309	G	N3-C2-N2	-8.32	114.07	119.90
40	a	1262	A	N9-C1'-C2'	8.32	124.82	114.00
12	AB	45	PRO	CA-N-CD	-8.32	99.85	111.50
40	a	1	G	C6-N1-C2	8.32	130.09	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	1087	G	C6-C5-N7	-8.32	125.41	130.40
17	D	872	A	C5-C6-N6	8.31	130.35	123.70
40	a	1142	A	N1-C2-N3	-8.31	125.15	129.30
40	a	364	C	C6-N1-C2	8.30	123.62	120.30
17	D	956	U	C5-C6-N1	-8.29	118.56	122.70
40	a	1118	C	C6-N1-C2	8.28	123.61	120.30
40	a	1581	G	C6-N1-C2	8.28	130.07	125.10
40	a	615	U	C5-C6-N1	-8.27	118.56	122.70
17	D	987	G	N1-C6-O6	8.27	124.86	119.90
17	D	1348	U	N1-C2-N3	-8.27	109.94	114.90
8	7	-15	U	C6-N1-C2	-8.25	116.05	121.00
17	D	1317	C	C5-C4-N4	8.25	125.98	120.20
10	B	76	A	N3-C4-C5	8.24	132.57	126.80
40	a	137	U	N3-C4-O4	-8.22	113.64	119.40
40	a	89	A	N7-C8-N9	-8.22	109.69	113.80
40	a	1417	C	N3-C2-O2	8.21	127.65	121.90
48	i	4	GLN	CG-CD-OE1	-8.21	105.18	121.60
40	a	85	G	C4-C5-N7	8.19	114.08	110.80
10	A	76	A	N3-C4-C5	8.19	132.53	126.80
40	a	253	C	C6-N1-C2	8.19	123.57	120.30
40	a	327	G	N3-C4-N9	8.19	130.91	126.00
40	a	1106	G	N9-C4-C5	-8.19	102.12	105.40
17	D	1339	A	N3-C4-N9	-8.18	120.85	127.40
40	a	2013	A	C4-C5-N7	8.18	114.79	110.70
14	AE	710	ASP	CB-CG-OD1	8.17	125.65	118.30
10	B	39	C	C6-N1-C1'	-8.17	111.00	120.80
10	A	39	C	C6-N1-C1'	-8.15	111.02	120.80
40	a	1338	G	C4-C5-N7	-8.15	107.54	110.80
40	a	551	G	C6-N1-C2	8.15	129.99	125.10
40	a	2839	G	O5'-P-OP1	-8.12	98.39	105.70
17	D	1363	A	C6-N1-C2	8.11	123.47	118.60
25	L	90	MET	CG-SD-CE	8.10	113.15	100.20
40	a	1581	G	N9-C4-C5	-8.10	102.16	105.40
17	D	958	A	C6-C5-N7	8.09	137.97	132.30
17	D	97	G	C6-C5-N7	-8.09	125.55	130.40
28	O	18	ARG	NH1-CZ-NH2	8.07	128.28	119.40
40	a	517	C	P-O3'-C3'	-8.07	110.02	119.70
40	a	942	G	C5-C6-O6	8.06	133.44	128.60
40	a	1577	C	C6-N1-C2	8.06	123.53	120.30
43	d	79	G	C8-N9-C4	8.06	109.62	106.40
17	D	1349	A	OP1-P-OP2	-8.04	107.53	119.60
40	a	143	C	N3-C2-O2	8.04	127.53	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	2017	U	N3-C4-C5	8.05	119.43	114.60
40	a	2365	G	N1-C6-O6	-8.04	115.08	119.90
48	i	4	GLN	CA-C-N	8.04	134.88	117.20
43	d	80	U	C5-C6-N1	-8.03	118.69	122.70
40	a	85	G	N3-C4-C5	-8.02	124.59	128.60
40	a	990	A	N1-C6-N6	8.02	123.41	118.60
40	a	1199	U	N1-C2-N3	8.02	119.71	114.90
40	a	1037	G	N1-C6-O6	8.00	124.70	119.90
40	a	136	G	C5-C6-O6	-7.97	123.82	128.60
40	a	74	A	C8-N9-C1'	-7.97	113.36	127.70
40	a	67	U	OP1-P-O3'	-7.96	87.68	105.20
17	D	990	C	C6-N1-C2	7.96	123.48	120.30
40	a	2902	C	N1-C2-O2	-7.95	114.13	118.90
17	D	397	A	C5-N7-C8	-7.94	99.93	103.90
40	a	1627	G	N1-C6-O6	7.94	124.67	119.90
40	a	893	C	C2-N3-C4	-7.92	115.94	119.90
40	a	1	G	C2-N3-C4	-7.92	107.94	111.90
40	a	549	G	N1-C6-O6	7.91	124.64	119.90
40	a	250	G	N3-C4-C5	7.90	132.55	128.60
40	a	2192	U	C2-N3-C4	-7.89	122.26	127.00
40	a	1	G	N9-C4-C5	-7.88	102.25	105.40
40	a	2444	G	C5-C6-O6	7.88	133.32	128.60
17	D	975	A	C5-C6-N6	7.87	130.00	123.70
17	D	958	A	N7-C8-N9	-7.86	109.87	113.80
40	a	326	G	N3-C4-N9	-7.86	121.28	126.00
40	a	1657	U	C6-N1-C2	7.85	125.71	121.00
40	a	751	A	N3-C4-N9	-7.85	121.12	127.40
40	a	2820	A	O4'-C1'-N9	-7.85	101.92	108.20
17	D	1339	A	N1-C2-N3	7.85	133.22	129.30
40	a	1263	U	C6-N1-C2	7.83	125.70	121.00
43	d	79	G	N9-C4-C5	-7.83	102.27	105.40
16	C	44	ILE	CG1-CB-CG2	-7.83	94.17	111.40
40	a	615	U	N3-C4-O4	7.83	124.88	119.40
40	a	2056	G	N1-C6-O6	7.83	124.59	119.90
17	D	1368	A	OP2-P-O3'	-7.81	88.01	105.20
8	7	-12	U	C6-N1-C1'	-7.81	110.27	121.20
40	a	542	C	N1-C2-O2	-7.80	114.22	118.90
40	a	2350	C	C5-C4-N4	-7.79	114.75	120.20
40	a	2349	G	OP2-P-O3'	-7.78	88.08	105.20
40	a	1414	C	C2-N1-C1'	-7.77	110.25	118.80
17	D	675	A	C5-C6-N1	-7.77	113.81	117.70
40	a	1142	A	C5-C6-N6	7.77	129.92	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	327	G	N9-C4-C5	7.77	108.51	105.40
40	a	2357	G	O5'-P-OP1	-7.77	98.71	105.70
40	a	1053	C	C2-N1-C1'	-7.76	110.27	118.80
40	a	2619	C	C6-N1-C2	7.75	123.40	120.30
48	i	40	ARG	C-N-CA	7.75	141.07	121.70
40	a	84	A	OP2-P-O3'	-7.75	88.16	105.20
40	a	910	A	C4-C5-C6	-7.75	113.13	117.00
48	i	13	ARG	NE-CZ-NH2	-7.73	116.43	120.30
40	a	327	G	C6-C5-N7	7.71	135.03	130.40
16	C	40	VAL	CA-CB-CG2	-7.71	99.33	110.90
40	a	2902	C	N3-C2-O2	7.70	127.29	121.90
40	a	1021	A	C5-C6-N6	7.69	129.85	123.70
40	a	433	C	C6-N1-C2	7.68	123.37	120.30
17	D	563	A	C6-N1-C2	7.67	123.20	118.60
40	a	551	G	N9-C4-C5	-7.67	102.33	105.40
40	a	1670	C	N1-C2-N3	7.66	124.56	119.20
40	a	1338	G	N7-C8-N9	-7.66	109.27	113.10
17	D	104	G	C2-N3-C4	-7.66	108.07	111.90
40	a	2444	G	N1-C6-O6	-7.66	115.31	119.90
40	a	789	A	C5-C6-N6	-7.65	117.58	123.70
40	a	1357	C	C6-N1-C2	7.64	123.36	120.30
40	a	1106	G	C4-C5-N7	7.63	113.85	110.80
40	a	883	G	C6-N1-C2	-7.63	120.52	125.10
2	1	18	ARG	NE-CZ-NH2	-7.63	116.49	120.30
40	a	84	A	C8-N9-C4	7.62	108.85	105.80
40	a	2	G	C6-C5-N7	-7.62	125.83	130.40
17	D	37	U	C4-C5-C6	-7.61	115.13	119.70
40	a	1142	A	C5-N7-C8	-7.61	100.09	103.90
40	a	2356	U	O4'-C1'-N1	-7.60	102.12	108.20
17	D	884	U	C5-C6-N1	7.60	126.50	122.70
40	a	2017	U	C2-N3-C4	-7.58	122.45	127.00
40	a	2192	U	N3-C2-O2	-7.58	116.89	122.20
40	a	2112	G	C2-N3-C4	-7.58	108.11	111.90
40	a	1421	G	N1-C6-O6	7.57	124.44	119.90
17	D	341	C	C6-N1-C2	7.55	123.32	120.30
40	a	68	G	P-O5'-C5'	7.54	132.96	120.90
43	d	81	G	C4-C5-N7	7.52	113.81	110.80
40	a	2606	C	C6-N1-C2	7.52	123.31	120.30
40	a	326	G	N1-C6-O6	7.51	124.41	119.90
40	a	449	A	O5'-P-OP1	-7.51	98.94	105.70
40	a	1106	G	C5-C6-O6	-7.51	124.09	128.60
40	a	68	G	C4-C5-C6	-7.51	114.30	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	917	A	N7-C8-N9	7.50	117.55	113.80
17	D	568	G	N1-C6-O6	7.50	124.40	119.90
40	a	1975	G	N1-C6-O6	-7.49	115.41	119.90
40	a	686	U	N1-C2-N3	7.47	119.38	114.90
40	a	917	A	C5-C6-N6	7.47	129.68	123.70
17	D	1358	U	N3-C2-O2	7.47	127.43	122.20
17	D	193	C	C6-N1-C2	7.46	123.28	120.30
40	a	1262	A	C5'-C4'-O4'	7.46	118.05	109.10
40	a	2756	U	N1-C2-N3	-7.46	110.42	114.90
17	D	959	A	C2-N3-C4	-7.45	106.88	110.60
10	B	37	A	C5'-C4'-O4'	-7.43	100.18	109.10
17	D	37	U	N1-C2-N3	-7.43	110.44	114.90
10	A	37	A	C5'-C4'-O4'	-7.42	100.19	109.10
17	D	1309	G	C2-N3-C4	-7.42	108.19	111.90
17	D	1126	U	N3-C4-C5	7.42	119.05	114.60
62	w	100	CYS	N-CA-CB	7.42	123.95	110.60
10	B	38	A	C5'-C4'-O4'	7.41	117.99	109.10
40	a	542	C	N3-C2-O2	7.40	127.08	121.90
40	a	2902	C	N3-C4-C5	7.39	124.85	121.90
40	a	788	A	C5-C6-N6	-7.38	117.79	123.70
16	C	66	SER	CA-CB-OG	-7.38	91.27	111.20
10	A	38	A	C5'-C4'-O4'	7.38	117.95	109.10
40	a	1533	C	C6-N1-C2	7.37	123.25	120.30
40	a	88	G	O5'-P-OP1	-7.36	99.07	105.70
10	A	35	A	C2-N3-C4	-7.34	106.93	110.60
17	D	675	A	N3-C4-C5	7.34	131.94	126.80
17	D	958	A	N1-C6-N6	-7.33	114.20	118.60
21	H	339	ARG	NE-CZ-NH2	-7.32	116.64	120.30
40	a	2	G	C5-C6-N1	-7.32	107.84	111.50
40	a	1262	A	C2'-C3'-O3'	7.32	125.60	109.50
40	a	68	G	C5-C6-O6	-7.31	124.21	128.60
40	a	542	C	N3-C4-C5	7.30	124.82	121.90
40	a	1581	G	C5-C6-O6	-7.30	124.22	128.60
40	a	1021	A	C5-N7-C8	-7.29	100.25	103.90
17	D	882	C	C6-N1-C2	7.29	123.21	120.30
17	D	104	G	C5-C6-N1	-7.28	107.86	111.50
40	a	2286	G	N3-C2-N2	7.27	124.99	119.90
40	a	1588	G	C6-C5-N7	-7.26	126.04	130.40
30	Q	121	CYS	CA-CB-SG	-7.25	100.94	114.00
10	A	19	G	C4-N9-C1'	-7.24	117.08	126.50
10	B	19	G	C4-N9-C1'	-7.24	117.09	126.50
17	D	176	C	C6-N1-C2	7.23	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	1348	U	N3-C2-O2	7.23	127.26	122.20
40	a	1106	G	C5-C6-N1	-7.23	107.88	111.50
40	a	88	G	N9-C4-C5	7.22	108.29	105.40
40	a	654	A	C4-C5-C6	-7.20	113.40	117.00
8	7	-15	U	C5-C6-N1	7.19	126.30	122.70
17	D	1368	A	OP1-P-O3'	7.19	121.02	105.20
40	a	237	C	C6-N1-C2	7.19	123.18	120.30
40	a	2620	C	N3-C4-C5	7.19	124.78	121.90
40	a	1417	C	C2-N1-C1'	-7.17	110.91	118.80
29	P	55	PRO	N-CD-CG	7.17	113.95	103.20
10	B	35	A	C2-N3-C4	-7.16	107.02	110.60
40	a	30	G	OP1-P-OP2	7.16	130.34	119.60
10	A	39	C	N3-C2-O2	-7.15	116.89	121.90
17	D	97	G	C5-C6-N1	-7.15	107.92	111.50
40	a	1432	G	N1-C6-O6	-7.15	115.61	119.90
17	D	1349	A	O5'-P-OP2	7.14	119.27	110.70
40	a	2493	U	N1-C2-O2	7.14	127.80	122.80
32	S	81	ARG	N-CA-CB	-7.14	97.75	110.60
17	D	872	A	N9-C4-C5	-7.14	102.94	105.80
43	d	31	C	N1-C2-O2	7.13	123.18	118.90
10	B	39	C	N3-C2-O2	-7.13	116.91	121.90
40	a	1413	A	N1-C2-N3	7.12	132.86	129.30
40	a	788	A	O4'-C1'-N9	7.11	113.89	108.20
40	a	1	G	C5-C6-O6	-7.11	124.34	128.60
32	S	81	ARG	CB-CA-C	7.10	124.60	110.40
10	A	19	G	O4'-C1'-N9	-7.10	102.52	108.20
62	w	96	ARG	NH1-CZ-NH2	-7.10	111.59	119.40
8	7	-11	U	C4-C5-C6	7.09	123.96	119.70
17	D	1363	A	C5-N7-C8	-7.09	100.35	103.90
17	D	563	A	N1-C2-N3	-7.09	125.75	129.30
17	D	104	G	N3-C2-N2	-7.09	114.94	119.90
48	i	40	ARG	NE-CZ-NH2	-7.09	116.76	120.30
17	D	1014	A	O5'-P-OP1	-7.08	99.32	105.70
40	a	68	G	O5'-C5'-C4'	7.08	125.15	111.70
40	a	2815	C	N1-C2-N3	-7.08	114.24	119.20
40	a	2446	G	N1-C6-O6	-7.07	115.66	119.90
40	a	273	G	C6-C5-N7	-7.07	126.16	130.40
10	B	19	G	O4'-C1'-N9	-7.06	102.55	108.20
16	C	65	LEU	CB-CG-CD1	-7.05	99.02	111.00
40	a	1592	C	N3-C2-O2	7.05	126.83	121.90
17	D	418	C	C6-N1-C2	7.05	123.12	120.30
17	D	973	G	O5'-P-OP1	-7.04	99.36	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	958	A	O4'-C1'-N9	-7.04	102.57	108.20
56	q	4	ARG	NE-CZ-NH2	-7.04	116.78	120.30
40	a	542	C	C2-N3-C4	-7.04	116.38	119.90
49	j	141	ARG	NE-CZ-NH1	7.03	123.82	120.30
40	a	137	U	C2-N3-C4	-7.03	122.78	127.00
40	a	37	C	C6-N1-C2	7.03	123.11	120.30
40	a	1592	C	N1-C2-O2	-7.03	114.68	118.90
17	D	526	C	N3-C4-C5	7.02	124.71	121.90
17	D	975	A	N7-C8-N9	7.02	117.31	113.80
40	a	1406	U	N3-C2-O2	7.00	127.10	122.20
40	a	1625	C	C6-N1-C2	7.00	123.10	120.30
40	a	273	G	N9-C4-C5	-6.99	102.60	105.40
40	a	2111	U	OP1-P-O3'	6.99	120.59	105.20
40	a	2350	C	OP1-P-OP2	-6.99	109.11	119.60
40	a	812	C	C4-C5-C6	6.99	120.90	117.40
40	a	2349	G	O5'-P-OP2	-6.99	99.41	105.70
40	a	2756	U	C4-C5-C6	-6.99	115.51	119.70
40	a	910	A	N9-C4-C5	-6.99	103.01	105.80
40	a	1561	C	N1-C2-O2	6.99	123.09	118.90
40	a	1112	G	N1-C6-O6	6.98	124.08	119.90
17	D	104	G	N7-C8-N9	6.97	116.59	113.10
40	a	74	A	C6-C5-N7	-6.97	127.42	132.30
40	a	136	G	C2-N3-C4	-6.97	108.42	111.90
40	a	788	A	N7-C8-N9	-6.97	110.32	113.80
17	D	1309	G	N1-C2-N3	6.96	128.08	123.90
51	l	67	ARG	NE-CZ-NH2	-6.96	116.82	120.30
17	D	1309	G	C4-N9-C1'	6.96	135.54	126.50
40	a	994	C	C6-N1-C2	6.96	123.08	120.30
40	a	89	A	P-O3'-C3'	-6.94	111.37	119.70
40	a	1053	C	N3-C2-O2	6.93	126.75	121.90
40	a	2168	G	C4-C5-N7	6.93	113.57	110.80
40	a	631	A	C4-C5-C6	-6.93	113.54	117.00
10	B	76	A	C5-C6-N6	-6.92	118.17	123.70
9	9	80	THR	N-CA-CB	-6.91	97.17	110.30
40	a	327	G	C4-C5-N7	-6.91	108.04	110.80
40	a	2588	G	N1-C6-O6	6.91	124.05	119.90
54	o	42	ARG	NE-CZ-NH2	6.90	123.75	120.30
48	i	4	GLN	N-CA-CB	-6.88	98.21	110.60
17	D	37	U	N3-C4-C5	6.88	118.73	114.60
17	D	1210	C	C6-N1-C2	6.88	123.05	120.30
28	O	13	LYS	N-CA-CB	-6.88	98.22	110.60
17	D	397	A	C5-C6-N6	6.87	129.20	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	55	GLU	CA-C-O	6.87	134.53	120.10
40	a	1410	G	C6-N1-C2	6.87	129.22	125.10
40	a	1087	G	C5-C6-N1	-6.86	108.07	111.50
10	A	76	A	C5-C6-N6	-6.86	118.22	123.70
17	D	124	C	C6-N1-C2	6.86	123.04	120.30
40	a	92	U	N3-C4-O4	6.85	124.20	119.40
40	a	1266	G	OP1-P-OP2	-6.85	109.32	119.60
40	a	1902	C	C6-N1-C2	6.84	123.03	120.30
40	a	869	G	N3-C4-C5	6.84	132.02	128.60
10	A	34	C	C2-N3-C4	6.83	123.32	119.90
40	a	1413	A	C6-N1-C2	-6.82	114.51	118.60
40	a	2344	U	C2-N3-C4	6.81	131.09	127.00
40	a	2365	G	N9-C4-C5	-6.81	102.68	105.40
8	7	-15	U	C5-C4-O4	6.80	129.98	125.90
17	D	563	A	C5-N7-C8	-6.80	100.50	103.90
17	D	1130	A	OP1-P-OP2	-6.80	109.40	119.60
17	D	1449	C	C6-N1-C2	6.79	123.02	120.30
40	a	1596	A	C6-N1-C2	-6.79	114.52	118.60
40	a	1414	C	C2-N3-C4	-6.78	116.51	119.90
40	a	2574	G	N1-C6-O6	6.77	123.96	119.90
40	a	336	C	C6-N1-C1'	-6.77	112.68	120.80
40	a	1750	G	N1-C6-O6	-6.76	115.85	119.90
62	w	46	ARG	NE-CZ-NH1	-6.76	116.92	120.30
40	a	136	G	C6-N1-C2	6.75	129.15	125.10
48	i	41	HIS	CA-CB-CG	6.75	125.08	113.60
40	a	2902	C	C2-N3-C4	-6.75	116.53	119.90
40	a	1670	C	C2-N3-C4	-6.75	116.53	119.90
17	D	1473	G	N1-C6-O6	-6.74	115.86	119.90
40	a	631	A	N3-C4-C5	6.74	131.52	126.80
17	D	1326	U	N3-C4-O4	6.73	124.11	119.40
40	a	2066	C	N1-C2-O2	6.73	122.94	118.90
40	a	654	A	C5-N7-C8	-6.72	100.54	103.90
8	7	-12	U	O4'-C1'-N1	-6.72	102.82	108.20
40	a	1082	U	C4-C5-C6	-6.72	115.67	119.70
40	a	917	A	C6-N1-C2	6.71	122.63	118.60
10	A	39	C	C6-N1-C2	6.71	122.98	120.30
10	B	39	C	C6-N1-C2	6.70	122.98	120.30
17	D	1240	U	C2-N1-C1'	-6.70	109.66	117.70
48	i	17	ARG	NE-CZ-NH2	6.70	123.65	120.30
40	a	517	C	C4-C5-C6	6.70	120.75	117.40
40	a	137	U	N3-C2-O2	-6.69	117.52	122.20
17	D	1309	G	C8-N9-C1'	-6.69	118.31	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	571	U	N3-C4-O4	-6.68	114.72	119.40
17	D	1439	G	N1-C6-O6	-6.68	115.89	119.90
17	D	884	U	N3-C2-O2	6.68	126.87	122.20
40	a	1924	C	C5-C4-N4	-6.68	115.53	120.20
40	a	789	A	C6-N1-C2	-6.67	114.60	118.60
17	D	1240	U	N3-C4-C5	6.67	118.60	114.60
50	k	14	SER	N-CA-CB	-6.67	100.50	110.50
40	a	2286	G	O4'-C1'-N9	-6.66	102.87	108.20
17	D	1348	U	OP2-P-O3'	6.66	119.85	105.20
40	a	2901	C	C2-N1-C1'	-6.66	111.47	118.80
40	a	686	U	C6-N1-C2	-6.65	117.01	121.00
40	a	1102	C	C2-N1-C1'	-6.65	111.48	118.80
10	A	31	G	C5-C6-O6	-6.64	124.61	128.60
40	a	2671	G	N1-C6-O6	-6.64	115.91	119.90
17	D	419	C	C6-N1-C2	6.64	122.96	120.30
10	B	34	C	C2-N3-C4	6.64	123.22	119.90
40	a	2418	A	C8-N9-C4	6.63	108.45	105.80
40	a	178	G	N1-C6-O6	6.63	123.88	119.90
40	a	258	G	N1-C6-O6	6.63	123.88	119.90
40	a	1087	G	C5-C6-O6	-6.63	124.62	128.60
32	S	85	ARG	CG-CD-NE	6.62	125.71	111.80
40	a	2186	G	C6-C5-N7	-6.62	126.43	130.40
17	D	1411	C	C6-N1-C2	6.62	122.95	120.30
40	a	406	G	N1-C6-O6	6.61	123.87	119.90
17	D	675	A	C8-N9-C4	-6.61	103.16	105.80
10	B	31	G	C5-C6-O6	-6.61	124.64	128.60
17	D	1493	A	C2-N3-C4	6.61	113.90	110.60
40	a	65	U	N3-C4-O4	6.61	124.02	119.40
40	a	850	U	N3-C4-O4	-6.60	114.78	119.40
40	a	2349	G	OP1-P-O3'	6.59	119.71	105.20
17	D	104	G	C4-N9-C1'	6.59	135.07	126.50
40	a	47	C	C6-N1-C2	6.59	122.94	120.30
40	a	1102	C	N1-C2-O2	-6.59	114.95	118.90
40	a	85	G	P-O3'-C3'	6.59	127.60	119.70
40	a	1145	C	C6-N1-C2	6.58	122.93	120.30
40	a	670	A	C8-N9-C4	6.58	108.43	105.80
17	D	872	A	C5-N7-C8	-6.57	100.61	103.90
25	L	49	TYR	CE1-CZ-OH	6.57	137.85	120.10
40	a	2098	U	N3-C4-O4	6.57	124.00	119.40
40	a	2286	G	C8-N9-C4	6.55	109.02	106.40
40	a	2877	G	N1-C6-O6	-6.55	115.97	119.90
40	a	1263	U	OP1-P-OP2	-6.54	109.78	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	497	G	C4-C5-N7	6.54	113.42	110.80
17	D	476	U	N3-C2-O2	6.54	126.78	122.20
40	a	1160	G	N1-C6-O6	6.54	123.82	119.90
17	D	1368	A	OP1-P-OP2	6.53	129.40	119.60
10	A	38	A	O5'-P-OP2	6.53	118.54	110.70
40	a	2480	C	C6-N1-C2	6.53	122.91	120.30
40	a	517	C	P-O5'-C5'	-6.53	110.46	120.90
17	D	1363	A	N1-C2-N3	-6.52	126.04	129.30
10	B	38	A	O5'-P-OP2	6.51	118.52	110.70
40	a	1102	C	N3-C2-O2	6.51	126.46	121.90
40	a	357	C	N1-C2-O2	6.50	122.80	118.90
40	a	2822	G	OP1-P-OP2	6.50	129.35	119.60
40	a	129	C	C6-N1-C2	6.50	122.90	120.30
30	Q	127	ARG	NE-CZ-NH2	-6.49	117.05	120.30
40	a	2344	U	C6-N1-C2	-6.49	117.11	121.00
40	a	2351	G	C6-N1-C2	-6.48	121.21	125.10
40	a	1417	C	N3-C4-C5	6.48	124.49	121.90
8	7	-15	U	C5'-C4'-O4'	-6.47	101.34	109.10
40	a	1331	G	N1-C6-O6	-6.46	116.02	119.90
17	D	450	G	N1-C6-O6	-6.46	116.02	119.90
40	a	987	C	C6-N1-C2	6.46	122.88	120.30
40	a	918	A	N3-C4-N9	6.46	132.56	127.40
40	a	188	G	N1-C6-O6	-6.45	116.03	119.90
40	a	1058	U	N3-C4-O4	6.45	123.91	119.40
40	a	2066	C	N3-C2-O2	-6.45	117.39	121.90
40	a	1414	C	N3-C4-C5	6.44	124.48	121.90
40	a	65	U	N3-C2-O2	6.42	126.70	122.20
40	a	239	C	C6-N1-C2	6.42	122.87	120.30
40	a	2389	G	N1-C6-O6	-6.42	116.05	119.90
40	a	2838	G	C8-N9-C4	6.42	108.97	106.40
40	a	789	A	C5'-C4'-O4'	6.41	116.79	109.10
17	D	1339	A	N3-C4-C5	6.41	131.29	126.80
10	A	76	A	O4'-C1'-N9	6.41	113.33	108.20
10	B	76	A	O4'-C1'-N9	6.40	113.32	108.20
40	a	1417	C	C2-N3-C4	-6.40	116.70	119.90
17	D	56	U	N3-C4-O4	6.39	123.88	119.40
17	D	515	G	N9-C4-C5	-6.39	102.84	105.40
40	a	142	A	C6-N1-C2	6.39	122.44	118.60
40	a	67	U	N1-C2-O2	6.39	127.27	122.80
10	A	33	U	C5-C4-O4	-6.38	122.07	125.90
40	a	328	U	C6-N1-C2	6.38	124.83	121.00
40	a	67	U	O4'-C1'-N1	6.38	113.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	2815	C	O5'-C5'-C4'	6.37	123.81	111.70
40	a	273	G	C4-C5-N7	6.37	113.35	110.80
10	B	33	U	C5-C4-O4	-6.37	122.08	125.90
17	D	1454	G	N1-C6-O6	6.37	123.72	119.90
40	a	1177	G	C5-C6-O6	6.36	132.42	128.60
17	D	975	A	C8-N9-C4	-6.35	103.26	105.80
17	D	497	G	C6-C5-N7	-6.35	126.59	130.40
40	a	2613	U	N3-C4-C5	6.35	118.41	114.60
40	a	2351	G	C6-C5-N7	-6.35	126.59	130.40
40	a	1	G	C4-C5-C6	6.34	122.60	118.80
40	a	883	G	N3-C2-N2	-6.33	115.47	119.90
6	5	109	DT	P-O3'-C3'	6.33	127.29	119.70
17	D	958	A	N9-C1'-C2'	6.33	122.23	114.00
43	d	83	G	O5'-P-OP1	-6.33	100.00	105.70
62	w	98	LEU	N-CA-CB	-6.33	97.75	110.40
17	D	1013	G	OP2-P-O3'	-6.32	91.30	105.20
24	K	55	GLU	N-CA-CB	6.31	121.96	110.60
40	a	385	C	C6-N1-C2	6.31	122.82	120.30
40	a	1530	G	N1-C2-N2	6.31	121.88	116.20
40	a	2831	G	N1-C6-O6	-6.31	116.11	119.90
40	a	1998	A	O5'-P-OP1	-6.30	100.03	105.70
17	D	1112	C	N3-C2-O2	6.30	126.31	121.90
17	D	1218	C	C6-N1-C2	6.30	122.82	120.30
42	c	27	ARG	NE-CZ-NH1	-6.30	117.15	120.30
54	o	13	ARG	NE-CZ-NH2	6.30	123.45	120.30
40	a	2812	G	N1-C6-O6	-6.29	116.12	119.90
40	a	754	U	N3-C2-O2	-6.29	117.80	122.20
56	q	4	ARG	NE-CZ-NH1	6.29	123.44	120.30
17	D	497	G	N9-C4-C5	-6.28	102.89	105.40
17	D	425	G	N1-C6-O6	6.28	123.67	119.90
40	a	464	U	C4'-C3'-O3'	6.28	125.55	113.00
40	a	755	U	N3-C4-C5	-6.28	110.83	114.60
62	w	96	ARG	CD-NE-CZ	6.28	132.39	123.60
40	a	2365	G	C2-N3-C4	-6.27	108.76	111.90
17	D	104	G	C8-N9-C1'	-6.27	118.85	127.00
21	H	125	ASN	N-CA-CB	-6.27	99.32	110.60
40	a	1516	G	N1-C6-O6	6.27	123.66	119.90
40	a	2899	A	C8-N9-C4	6.26	108.31	105.80
17	D	1215	G	N1-C6-O6	6.26	123.66	119.90
17	D	1363	A	C2-N3-C4	-6.26	107.47	110.60
17	D	424	G	N1-C6-O6	6.25	123.65	119.90
10	A	38	A	O4'-C1'-N9	6.25	113.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	o	8	ARG	NE-CZ-NH2	-6.25	117.18	120.30
40	a	1043	C	C6-N1-C2	6.24	122.80	120.30
40	a	2493	U	C5-C4-O4	-6.24	122.15	125.90
17	D	597	G	N7-C8-N9	-6.24	109.98	113.10
40	a	1087	G	C4-C5-N7	6.24	113.30	110.80
40	a	729	G	C5-C6-N1	-6.24	108.38	111.50
40	a	1331	G	C5-C6-O6	6.23	132.34	128.60
40	a	106	C	OP1-P-O3'	6.23	118.90	105.20
43	d	80	U	N3-C4-C5	6.23	118.34	114.60
32	S	85	ARG	CB-CG-CD	6.23	127.79	111.60
24	K	55	GLU	O-C-N	-6.22	112.74	122.70
40	a	2013	A	OP1-P-O3'	-6.21	91.53	105.20
40	a	2641	G	N7-C8-N9	-6.21	109.99	113.10
25	L	49	TYR	OH-CZ-CE2	-6.21	103.33	120.10
40	a	861	A	C5-C6-N6	6.21	128.67	123.70
10	B	39	C	C2-N1-C1'	6.21	125.63	118.80
40	a	2252	G	N9-C1'-C2'	-6.21	105.17	112.00
10	A	38	A	C8-N9-C4	6.21	108.28	105.80
40	a	1996	C	C6-N1-C2	6.21	122.78	120.30
40	a	1588	G	C5-C6-N1	-6.20	108.40	111.50
10	A	39	C	C2-N1-C1'	6.20	125.62	118.80
17	D	972	C	N3-C2-O2	-6.20	117.56	121.90
17	D	1358	U	C5-C6-N1	6.20	125.80	122.70
40	a	335	C	C6-N1-C2	-6.20	117.82	120.30
17	D	862	C	C6-N1-C2	6.19	122.78	120.30
40	a	917	A	C5-N7-C8	-6.18	100.81	103.90
17	D	975	A	N1-C2-N3	6.18	132.39	129.30
40	a	8	C	C6-N1-C2	6.18	122.77	120.30
17	D	102	G	OP1-P-OP2	6.18	128.86	119.60
40	a	812	C	C5-C6-N1	-6.17	117.91	121.00
40	a	86	G	OP2-P-O3'	-6.17	91.62	105.20
40	a	2365	G	N3-C4-N9	6.17	129.70	126.00
40	a	2641	G	N9-C4-C5	-6.17	102.93	105.40
40	a	396	G	N9-C4-C5	-6.17	102.93	105.40
65	z	4	VAL	CA-CB-CG2	-6.17	101.65	110.90
40	a	631	A	N7-C8-N9	-6.16	110.72	113.80
10	B	38	A	O4'-C1'-N9	6.16	113.13	108.20
17	D	571	U	C2-N3-C4	-6.16	123.31	127.00
40	a	301	G	C8-N9-C4	6.15	108.86	106.40
40	a	2367	G	C5-C6-N1	-6.15	108.43	111.50
17	D	457	G	N1-C6-O6	-6.14	116.22	119.90
40	a	1250	G	OP1-P-O3'	6.14	118.71	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	1605	C	C6-N1-C2	6.14	122.76	120.30
40	a	357	C	N3-C2-O2	-6.14	117.60	121.90
17	D	497	G	C5-C6-O6	-6.13	124.92	128.60
40	a	893	C	N3-C2-O2	-6.13	117.61	121.90
40	a	1053	C	N1-C2-O2	-6.13	115.22	118.90
40	a	1564	C	C6-N1-C2	6.13	122.75	120.30
40	a	1538	G	N1-C6-O6	6.13	123.58	119.90
40	a	918	A	C2-N3-C4	6.13	113.67	110.60
24	K	55	GLU	N-CA-C	-6.12	94.48	111.00
40	a	1338	G	N1-C2-N3	6.11	127.57	123.90
2	1	41	LYS	CB-CG-CD	6.11	127.48	111.60
17	D	959	A	N9-C4-C5	-6.11	103.36	105.80
10	B	38	A	C8-N9-C4	6.11	108.24	105.80
40	a	2315	G	C6-N1-C2	-6.10	121.44	125.10
40	a	89	A	O4'-C1'-N9	-6.10	103.32	108.20
40	a	1074	G	N1-C6-O6	6.10	123.56	119.90
40	a	517	C	C5'-C4'-C3'	-6.09	106.25	116.00
40	a	2446	G	C5-C6-O6	6.09	132.25	128.60
32	S	94	PRO	N-CA-C	6.08	127.91	112.10
40	a	85	G	P-O5'-C5'	6.08	130.63	120.90
17	D	756	C	C6-N1-C2	6.08	122.73	120.30
17	D	959	A	N3-C4-C5	6.07	131.05	126.80
17	D	1401	G	C8-N9-C4	6.07	108.83	106.40
10	B	15	G	N1-C2-N2	6.06	121.65	116.20
29	P	31	ARG	NE-CZ-NH1	6.06	123.33	120.30
40	a	551	G	C5-C6-O6	-6.06	124.97	128.60
10	A	15	G	N1-C2-N2	6.06	121.65	116.20
40	a	2895	G	N1-C6-O6	6.05	123.53	119.90
17	D	350	G	N1-C6-O6	-6.05	116.27	119.90
40	a	2356	U	C4-C5-C6	-6.05	116.07	119.70
40	a	741	U	N3-C4-O4	6.05	123.63	119.40
10	A	15	G	N3-C2-N2	-6.04	115.67	119.90
40	a	2367	G	C6-C5-N7	-6.04	126.77	130.40
40	a	654	A	N3-C4-N9	6.04	132.23	127.40
40	a	1639	C	C6-N1-C2	6.04	122.71	120.30
40	a	2539	C	C6-N1-C2	6.03	122.71	120.30
40	a	459	U	P-O3'-C3'	6.03	126.94	119.70
40	a	2285	C	C6-N1-C2	6.03	122.71	120.30
17	D	1339	A	N1-C6-N6	6.03	122.22	118.60
40	a	2352	A	C2-N3-C4	-6.03	107.59	110.60
40	a	1106	G	C6-N1-C2	6.01	128.71	125.10
40	a	2820	A	N9-C4-C5	-6.01	103.39	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	54	C	C6-N1-C2	6.01	122.70	120.30
17	D	101	A	OP1-P-O3'	6.01	118.43	105.20
40	a	2261	C	C6-N1-C2	6.01	122.70	120.30
40	a	85	G	O4'-C1'-N9	6.01	113.01	108.20
40	a	2098	U	C5-C4-O4	-6.00	122.30	125.90
40	a	2782	G	N1-C6-O6	6.00	123.50	119.90
40	a	85	G	O5'-C5'-C4'	6.00	123.09	111.70
10	B	54	U	C2-N3-C4	5.99	130.59	127.00
17	D	73	C	N3-C4-C5	5.99	124.30	121.90
10	B	15	G	N3-C2-N2	-5.98	115.71	119.90
40	a	335	C	N1-C2-O2	5.98	122.49	118.90
40	a	2223	G	N1-C6-O6	-5.98	116.31	119.90
40	a	850	U	C2-N3-C4	-5.98	123.41	127.00
40	a	250	G	C8-N9-C4	5.98	108.79	106.40
17	D	515	G	C8-N9-C4	5.97	108.79	106.40
40	a	2168	G	C5-N7-C8	-5.97	101.32	104.30
14	AE	363	LEU	CA-CB-CG	5.96	129.02	115.30
40	a	1189	A	C8-N9-C4	5.96	108.19	105.80
40	a	2470	G	N1-C6-O6	5.96	123.47	119.90
17	D	1397	C	C6-N1-C2	-5.95	117.92	120.30
10	A	54	U	C2-N3-C4	5.95	130.57	127.00
40	a	2101	A	C5-C6-N1	5.94	120.67	117.70
40	a	2223	G	C5-C6-N1	5.94	114.47	111.50
49	j	133	THR	CA-CB-CG2	-5.94	104.08	112.40
40	a	2311	A	C2-N3-C4	-5.94	107.63	110.60
40	a	910	A	C5-N7-C8	-5.94	100.93	103.90
40	a	1379	U	C5-C4-O4	5.93	129.46	125.90
21	H	339	ARG	NE-CZ-NH1	5.93	123.27	120.30
10	A	31	G	N1-C2-N3	-5.93	120.34	123.90
40	a	2641	G	C4-C5-C6	-5.93	115.25	118.80
40	a	2751	G	N1-C2-N2	5.92	121.53	116.20
16	C	23	TYR	CB-CG-CD2	-5.91	117.45	121.00
17	D	237	G	N1-C6-O6	5.91	123.45	119.90
30	Q	127	ARG	NE-CZ-NH1	5.91	123.26	120.30
17	D	956	U	C2-N3-C4	-5.91	123.45	127.00
32	S	85	ARG	N-CA-CB	5.91	121.24	110.60
40	a	512	G	O4'-C1'-N9	5.91	112.93	108.20
40	a	287	G	N1-C6-O6	-5.91	116.36	119.90
40	a	786	C	C6-N1-C2	5.91	122.66	120.30
17	D	97	G	C4-C5-N7	5.90	113.16	110.80
40	a	1934	C	C6-N1-C2	5.90	122.66	120.30
17	D	397	A	C6-C5-N7	-5.90	128.17	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	2013	A	C5-N7-C8	-5.90	100.95	103.90
17	D	1221	G	N1-C6-O6	-5.90	116.36	119.90
17	D	827	U	N3-C2-O2	5.89	126.32	122.20
40	a	85	G	N3-C2-N2	-5.88	115.78	119.90
40	a	1245	G	C5-C6-O6	5.88	132.13	128.60
40	a	549	G	C6-C5-N7	-5.88	126.87	130.40
10	B	31	G	N1-C2-N3	-5.88	120.37	123.90
40	a	1581	G	C4-C5-C6	5.88	122.33	118.80
40	a	1806	C	C6-N1-C2	5.87	122.65	120.30
17	D	868	C	C6-N1-C2	5.87	122.65	120.30
40	a	751	A	N3-C4-C5	5.87	130.91	126.80
17	D	259	G	N1-C6-O6	-5.86	116.39	119.90
17	D	686	U	O4'-C1'-N1	5.85	112.88	108.20
40	a	729	G	N1-C6-O6	5.85	123.41	119.90
25	L	54	LEU	CA-CB-CG	5.85	128.75	115.30
40	a	816	C	C6-N1-C2	5.84	122.64	120.30
40	a	2168	G	N9-C4-C5	-5.84	103.06	105.40
17	D	568	G	C6-C5-N7	-5.83	126.90	130.40
40	a	2493	U	C5'-C4'-C3'	5.83	125.33	116.00
10	B	39	C	N1-C2-N3	-5.83	115.12	119.20
40	a	143	C	C2-N1-C1'	-5.82	112.39	118.80
40	a	283	G	N1-C6-O6	-5.82	116.41	119.90
40	a	2612	C	N3-C4-C5	5.82	124.23	121.90
40	a	327	G	C5-C6-O6	5.82	132.09	128.60
17	D	73	C	N1-C2-O2	-5.82	115.41	118.90
40	a	2621	G	N1-C6-O6	-5.82	116.41	119.90
10	A	39	C	N1-C2-N3	-5.82	115.13	119.20
40	a	1614	A	C4-C5-C6	-5.82	114.09	117.00
17	D	440	C	C6-N1-C2	5.81	122.62	120.30
40	a	919	U	C6-N1-C2	5.81	124.49	121.00
17	D	987	G	C6-C5-N7	-5.80	126.92	130.40
40	a	2367	G	N9-C4-C5	-5.80	103.08	105.40
17	D	97	G	C6-N1-C2	5.80	128.58	125.10
40	a	1198	U	C2-N1-C1'	5.80	124.66	117.70
40	a	2301	C	C2-N3-C4	-5.80	117.00	119.90
17	D	1126	U	C6-N1-C2	5.79	124.48	121.00
40	a	2344	U	C5-C6-N1	5.79	125.59	122.70
40	a	2323	G	C6-C5-N7	-5.79	126.93	130.40
40	a	1245	G	N1-C6-O6	-5.79	116.43	119.90
40	a	448	U	OP2-P-O3'	5.78	117.92	105.20
28	O	113	ARG	NE-CZ-NH2	-5.78	117.41	120.30
40	a	1406	U	C5-C4-O4	-5.78	122.43	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	i	16	ARG	CG-CD-NE	-5.78	99.67	111.80
40	a	1338	G	C5-C6-O6	5.78	132.07	128.60
10	B	36	U	C2-N3-C4	5.77	130.46	127.00
17	D	1186	G	N9-C1'-C2'	-5.77	105.65	112.00
40	a	2356	U	C5'-C4'-O4'	5.77	116.03	109.10
40	a	89	A	N1-C2-N3	-5.77	126.42	129.30
40	a	1082	U	N1-C2-N3	-5.77	111.44	114.90
40	a	1087	G	C6-N1-C2	5.77	128.56	125.10
43	d	71	C	C6-N1-C2	5.77	122.61	120.30
40	a	74	A	C5-N7-C8	-5.76	101.02	103.90
24	K	55	GLU	CB-CA-C	-5.76	98.88	110.40
17	D	476	U	N1-C2-N3	-5.75	111.45	114.90
40	a	2338	C	C6-N1-C2	5.75	122.60	120.30
40	a	88	G	OP2-P-O3'	5.75	117.85	105.20
17	D	397	A	C6-N1-C2	5.74	122.04	118.60
17	D	1240	U	C6-N1-C2	5.74	124.44	121.00
17	D	1489	G	N1-C6-O6	5.74	123.34	119.90
40	a	2641	G	C5-C6-N1	5.74	114.37	111.50
48	i	4	GLN	CB-CG-CD	5.73	126.49	111.60
10	B	40	C	C2-N3-C4	5.72	122.76	119.90
40	a	1614	A	O5'-P-OP1	-5.71	100.56	105.70
40	a	2186	G	N9-C4-C5	-5.71	103.12	105.40
29	P	9	ARG	NE-CZ-NH2	5.70	123.15	120.30
40	a	2186	G	C4-C5-N7	5.70	113.08	110.80
10	A	36	U	C2-N3-C4	5.70	130.42	127.00
10	A	38	A	C6-C5-N7	-5.70	128.31	132.30
40	a	404	A	P-O3'-C3'	5.70	126.54	119.70
40	a	2437	G	N1-C6-O6	-5.70	116.48	119.90
17	D	1499	A	N9-C1'-C2'	-5.70	105.73	112.00
40	a	670	A	C4-C5-C6	-5.70	114.15	117.00
10	B	38	A	C6-C5-N7	-5.70	128.31	132.30
40	a	893	C	N1-C2-N3	5.70	123.19	119.20
40	a	2321	U	C4-C5-C6	5.69	123.12	119.70
17	D	1363	A	C6-C5-N7	-5.69	128.32	132.30
40	a	1185	G	N1-C6-O6	-5.68	116.49	119.90
43	d	80	U	O5'-P-OP1	-5.68	100.59	105.70
17	D	476	U	C2-N3-C4	5.68	130.41	127.00
40	a	1087	G	N9-C4-C5	-5.67	103.13	105.40
40	a	917	A	O4'-C1'-N9	-5.67	103.67	108.20
40	a	1410	G	C2-N3-C4	-5.67	109.06	111.90
40	a	122	G	N1-C6-O6	5.67	123.30	119.90
40	a	1588	G	C4-C5-N7	5.66	113.07	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	2619	C	N3-C4-C5	5.66	124.17	121.90
40	a	319	G	N1-C6-O6	-5.66	116.50	119.90
40	a	729	G	C2-N3-C4	-5.66	109.07	111.90
40	a	1323	C	N1-C2-O2	5.66	122.30	118.90
17	D	958	A	N1-C2-N3	5.65	132.13	129.30
40	a	1142	A	N3-C4-C5	5.64	130.75	126.80
40	a	1182	G	N1-C6-O6	5.64	123.28	119.90
17	D	504	C	C6-N1-C2	5.64	122.56	120.30
40	a	2188	U	N3-C2-O2	5.64	126.15	122.20
10	A	40	C	C2-N3-C4	5.63	122.72	119.90
40	a	107	G	OP1-P-OP2	-5.63	111.15	119.60
48	i	7	LYS	CG-CD-CE	5.63	128.79	111.90
40	a	551	G	C5-N7-C8	-5.63	101.48	104.30
17	D	972	C	N1-C2-O2	5.63	122.28	118.90
17	D	1493	A	P-O3'-C3'	5.62	126.45	119.70
43	d	21	G	N1-C6-O6	-5.62	116.53	119.90
40	a	67	U	O3'-P-O5'	5.62	114.67	104.00
17	D	987	G	N9-C4-C5	-5.61	103.16	105.40
40	a	85	G	C5'-C4'-O4'	5.61	115.83	109.10
40	a	1588	G	C2-N3-C4	-5.60	109.10	111.90
8	7	-11	U	N3-C2-O2	-5.60	118.28	122.20
17	D	1240	U	C2-N3-C4	-5.59	123.64	127.00
40	a	142	A	N1-C2-N3	-5.59	126.50	129.30
40	a	2066	C	N3-C4-N4	-5.58	114.09	118.00
10	A	33	U	N3-C4-C5	5.58	117.95	114.60
43	d	64	G	N1-C6-O6	-5.58	116.55	119.90
40	a	396	G	N3-C4-C5	5.58	131.39	128.60
40	a	674	G	C4-C5-N7	5.58	113.03	110.80
40	a	2	G	C4-C5-N7	5.57	113.03	110.80
40	a	85	G	N1-C6-O6	5.57	123.24	119.90
40	a	336	C	O5'-C5'-C4'	-5.57	101.11	111.70
17	D	861	G	N1-C6-O6	5.57	123.24	119.90
40	a	130	C	C6-N1-C2	5.57	122.53	120.30
40	a	142	A	N9-C4-C5	-5.56	103.58	105.80
10	A	34	C	N1-C2-N3	-5.56	115.31	119.20
40	a	2642	G	O5'-P-OP1	-5.56	100.70	105.70
40	a	861	A	C6-N1-C2	-5.56	115.27	118.60
40	a	2493	U	C2-N1-C1'	5.55	124.36	117.70
40	a	1614	A	N3-C4-C5	5.54	130.68	126.80
43	d	81	G	N1-C6-O6	5.54	123.22	119.90
40	a	2641	G	N3-C4-C5	5.54	131.37	128.60
40	a	544	C	N3-C4-C5	5.54	124.11	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	1171	G	N1-C6-O6	-5.54	116.58	119.90
40	a	551	G	C4-C5-C6	5.54	122.12	118.80
40	a	579	G	N9-C1'-C2'	5.54	121.20	114.00
10	A	48	C	C2-N1-C1'	5.54	124.89	118.80
40	a	2418	A	OP2-P-O3'	-5.54	93.02	105.20
40	a	2723	C	OP1-P-O3'	-5.53	93.03	105.20
17	D	1458	G	N3-C4-C5	5.53	131.37	128.60
40	a	1627	G	C6-C5-N7	-5.53	127.08	130.40
40	a	2418	A	OP1-P-O3'	5.53	117.37	105.20
10	B	48	C	C2-N1-C1'	5.53	124.88	118.80
40	a	2	G	C6-N1-C2	5.53	128.41	125.10
40	a	918	A	O4'-C1'-N9	5.53	112.62	108.20
10	A	76	A	C5'-C4'-O4'	5.52	115.73	109.10
17	D	197	A	P-O3'-C3'	5.52	126.33	119.70
10	B	34	C	N1-C2-N3	-5.51	115.34	119.20
40	a	755	U	N3-C2-O2	5.51	126.06	122.20
40	a	183	C	C6-N1-C2	5.51	122.50	120.30
40	a	273	G	C5-C6-O6	-5.51	125.29	128.60
40	a	1798	U	C2-N3-C4	-5.51	123.69	127.00
14	AE	709	ARG	C-N-CA	5.51	135.47	121.70
40	a	381	G	O5'-P-OP2	5.50	117.31	110.70
40	a	542	C	C5-C6-N1	-5.50	118.25	121.00
29	P	31	ARG	NE-CZ-NH2	-5.50	117.55	120.30
40	a	674	G	N7-C8-N9	-5.50	110.35	113.10
10	B	76	A	C5'-C4'-O4'	5.50	115.70	109.10
17	D	73	C	C2-N1-C1'	-5.50	112.75	118.80
21	H	340	ARG	NE-CZ-NH1	-5.50	117.55	120.30
40	a	2756	U	C2-N3-C4	5.50	130.30	127.00
12	AB	122	PRO	N-CA-CB	5.49	109.89	103.30
10	B	38	A	N9-C1'-C2'	-5.49	105.96	112.00
40	a	1015	U	N3-C4-O4	5.49	123.24	119.40
40	a	1142	A	C8-N9-C4	5.49	108.00	105.80
10	B	38	A	C4-C5-N7	5.49	113.44	110.70
40	a	1059	G	N1-C6-O6	-5.48	116.61	119.90
40	a	326	G	C6-N1-C2	5.48	128.39	125.10
40	a	2356	U	P-O3'-C3'	5.48	126.28	119.70
17	D	1307	U	OP1-P-O3'	5.48	117.25	105.20
40	a	1454	C	C2-N3-C4	-5.48	117.16	119.90
40	a	964	C	C6-N1-C2	5.47	122.49	120.30
29	P	31	ARG	CG-CD-NE	-5.47	100.31	111.80
10	A	38	A	N9-C1'-C2'	-5.47	105.98	112.00
17	D	1326	U	C5-C4-O4	-5.46	122.62	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	40	C	N3-C2-O2	-5.46	118.08	121.90
17	D	1346	A	C8-N9-C4	5.46	107.98	105.80
40	a	2620	C	C6-N1-C1'	-5.46	114.25	120.80
40	a	698	C	C6-N1-C2	5.46	122.48	120.30
40	a	1338	G	C8-N9-C1'	-5.45	119.92	127.00
17	D	589	U	O5'-P-OP1	-5.45	100.80	105.70
40	a	2112	G	N1-C6-O6	5.44	123.17	119.90
43	d	97	C	C6-N1-C2	5.44	122.48	120.30
17	D	186	C	C6-N1-C2	5.44	122.48	120.30
40	a	143	C	N3-C4-C5	5.44	124.08	121.90
10	A	38	A	C4-C5-N7	5.44	113.42	110.70
46	g	60	PHE	CB-CG-CD1	5.44	124.61	120.80
40	a	188	G	C5-C6-N1	5.44	114.22	111.50
40	a	2821	A	OP1-P-O3'	-5.44	93.24	105.20
10	A	40	C	N3-C2-O2	-5.43	118.10	121.90
40	a	1263	U	N1-C2-N3	-5.43	111.64	114.90
40	a	2815	C	P-O5'-C5'	-5.43	112.21	120.90
17	D	1499	A	C8-N9-C4	5.43	107.97	105.80
17	D	370	C	C6-N1-C2	5.42	122.47	120.30
40	a	2097	A	N9-C4-C5	-5.42	103.63	105.80
40	a	1406	U	N3-C4-C5	-5.42	111.35	114.60
40	a	1480	C	C6-N1-C2	5.42	122.47	120.30
40	a	2710	C	C6-N1-C2	5.42	122.47	120.30
48	i	5	GLN	N-CA-C	5.42	125.63	111.00
40	a	1627	G	C5-C6-N1	-5.42	108.79	111.50
40	a	2815	C	C6-N1-C1'	-5.42	114.30	120.80
17	D	1013	G	P-O3'-C3'	-5.42	113.20	119.70
40	a	751	A	N9-C4-C5	5.42	107.97	105.80
17	D	1348	U	C4-C5-C6	-5.41	116.45	119.70
10	B	33	U	N3-C4-C5	5.41	117.85	114.60
40	a	1588	G	N9-C4-C5	-5.41	103.24	105.40
40	a	1814	G	C8-N9-C4	5.41	108.56	106.40
40	a	2815	C	C5'-C4'-C3'	5.41	124.65	116.00
40	a	2367	G	C4-C5-N7	5.40	112.96	110.80
40	a	1376	C	C6-N1-C2	5.40	122.46	120.30
8	7	-12	U	N3-C4-O4	5.40	123.18	119.40
17	D	1124	G	N1-C6-O6	-5.40	116.66	119.90
40	a	789	A	C4-N9-C1'	5.40	136.01	126.30
17	D	940	C	C6-N1-C2	5.40	122.46	120.30
17	D	104	G	N1-C2-N3	5.39	127.13	123.90
40	a	1177	G	N1-C6-O6	-5.39	116.67	119.90
40	a	2356	U	C5-C6-N1	-5.39	120.00	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	143	C	C2-N3-C4	-5.39	117.21	119.90
40	a	380	G	N7-C8-N9	-5.39	110.41	113.10
40	a	2277	G	N3-C2-N2	-5.38	116.13	119.90
40	a	1086	A	C5-C6-N6	5.37	128.00	123.70
40	a	1250	G	OP2-P-O3'	-5.37	93.39	105.20
17	D	348	G	N1-C6-O6	5.37	123.12	119.90
17	D	827	U	N1-C2-O2	5.37	126.56	122.80
40	a	235	U	N3-C4-O4	5.37	123.16	119.40
17	D	1371	G	OP1-P-OP2	5.36	127.65	119.60
40	a	1037	G	C6-C5-N7	-5.36	127.18	130.40
40	a	662	G	C8-N9-C4	5.36	108.54	106.40
40	a	2351	G	N1-C2-N2	-5.36	111.38	116.20
17	D	252	U	N3-C4-O4	5.36	123.15	119.40
40	a	674	G	C4-C5-C6	-5.36	115.59	118.80
40	a	2357	G	O5'-P-OP2	5.35	117.12	110.70
40	a	654	A	C6-N1-C2	-5.35	115.39	118.60
40	a	671	C	OP1-P-OP2	-5.35	111.58	119.60
62	w	98	LEU	CA-C-O	-5.35	108.87	120.10
40	a	2642	G	P-O5'-C5'	-5.35	112.35	120.90
28	O	113	ARG	CD-NE-CZ	5.34	131.08	123.60
40	a	1993	U	C5-C6-N1	-5.34	120.03	122.70
40	a	1263	U	C5-C6-N1	-5.34	120.03	122.70
17	D	675	A	N7-C8-N9	5.33	116.47	113.80
4	3	22	ARG	NE-CZ-NH1	5.33	122.97	120.30
40	a	2261	C	C5-C4-N4	-5.33	116.47	120.20
40	a	1592	C	C2-N3-C4	-5.33	117.23	119.90
24	K	56	VAL	CA-CB-CG1	5.33	118.89	110.90
40	a	1432	G	C5-C6-O6	5.33	131.80	128.60
40	a	729	G	C6-C5-N7	-5.33	127.20	130.40
10	A	38	A	C2-N3-C4	5.32	113.26	110.60
40	a	327	G	C8-N9-C4	-5.32	104.27	106.40
40	a	1167	C	N3-C4-C5	5.32	124.03	121.90
40	a	45	G	N1-C6-O6	5.31	123.08	119.90
40	a	1592	C	N3-C4-C5	5.31	124.02	121.90
40	a	335	C	C2-N3-C4	5.30	122.55	119.90
17	D	1206	G	C8-N9-C4	5.30	108.52	106.40
17	D	956	U	N1-C2-N3	-5.30	111.72	114.90
47	h	51	THR	CA-CB-CG2	-5.30	104.98	112.40
40	a	1379	U	N3-C4-O4	-5.29	115.70	119.40
40	a	755	U	N1-C2-N3	-5.29	111.73	114.90
40	a	1142	A	C2-N3-C4	-5.29	107.96	110.60
40	a	1774	C	N1-C2-O2	-5.29	115.73	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	928	G	N1-C6-O6	-5.29	116.73	119.90
40	a	2112	G	N9-C4-C5	-5.29	103.28	105.40
40	a	2332	C	C2-N1-C1'	-5.29	112.99	118.80
40	a	1323	C	N3-C4-N4	-5.28	114.30	118.00
40	a	245	G	N1-C6-O6	5.28	123.07	119.90
17	D	1443	C	C6-N1-C2	5.28	122.41	120.30
40	a	1406	U	C5-C6-N1	5.28	125.34	122.70
10	B	38	A	C5-C6-N6	-5.28	119.48	123.70
10	A	37	A	C8-N9-C1'	5.27	137.19	127.70
40	a	2540	C	C6-N1-C2	5.27	122.41	120.30
17	D	457	G	C5-C6-O6	5.27	131.76	128.60
40	a	1485	U	N3-C4-O4	5.27	123.09	119.40
40	a	2792	A	N9-C4-C5	-5.27	103.69	105.80
10	B	37	A	C8-N9-C1'	5.26	137.18	127.70
17	D	987	G	C4-C5-N7	5.26	112.91	110.80
40	a	976	G	N1-C6-O6	5.26	123.06	119.90
40	a	1421	G	C6-C5-N7	-5.26	127.24	130.40
40	a	1112	G	C6-C5-N7	-5.26	127.24	130.40
40	a	1338	G	N1-C6-O6	-5.26	116.74	119.90
40	a	1657	U	N3-C2-O2	5.26	125.88	122.20
51	l	162	ARG	NE-CZ-NH1	-5.26	117.67	120.30
10	A	38	A	C5-C6-N6	-5.26	119.49	123.70
40	a	2493	U	N3-C4-O4	-5.26	115.72	119.40
17	D	1186	G	N9-C4-C5	-5.25	103.30	105.40
40	a	751	A	C5-N7-C8	-5.25	101.27	103.90
40	a	2465	C	OP1-P-O3'	5.25	116.75	105.20
17	D	20	U	C6-N1-C2	5.25	124.15	121.00
40	a	129	C	N3-C4-C5	5.25	124.00	121.90
62	w	99	LYS	C-N-CA	5.25	134.81	121.70
17	D	70	U	N3-C4-O4	5.25	123.07	119.40
17	D	1340	A	N9-C4-C5	-5.24	103.70	105.80
40	a	1636	U	N3-C4-O4	5.24	123.07	119.40
40	a	2192	U	N3-C4-C5	5.24	117.75	114.60
40	a	2367	G	C6-N1-C2	5.24	128.25	125.10
40	a	2056	G	C6-C5-N7	-5.24	127.26	130.40
43	d	80	U	C6-N1-C1'	-5.24	113.87	121.20
17	D	939	G	N1-C6-O6	-5.24	116.76	119.90
40	a	850	U	N3-C4-C5	5.23	117.74	114.60
40	a	1567	G	N3-C4-C5	5.23	131.22	128.60
17	D	8	A	N9-C4-C5	-5.23	103.71	105.80
40	a	2305	U	N3-C4-C5	5.23	117.74	114.60
40	a	88	G	C8-N9-C1'	-5.23	120.21	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	2365	G	C5-N7-C8	-5.22	101.69	104.30
10	B	38	A	C2-N3-C4	5.22	113.21	110.60
40	a	729	G	O4'-C1'-N9	5.22	112.38	108.20
40	a	370	G	O4'-C1'-N9	-5.22	104.02	108.20
40	a	1142	A	C6-C5-N7	-5.22	128.65	132.30
40	a	910	A	C5-C6-N1	5.22	120.31	117.70
40	a	426	C	C6-N1-C2	5.21	122.39	120.30
40	a	2642	G	N3-C4-C5	5.21	131.20	128.60
40	a	2895	G	C6-C5-N7	-5.21	127.28	130.40
17	D	545	C	C6-N1-C2	5.20	122.38	120.30
40	a	2186	G	C5-C6-O6	-5.20	125.48	128.60
40	a	2365	G	N3-C2-N2	5.20	123.54	119.90
49	j	141	ARG	NE-CZ-NH2	-5.20	117.70	120.30
17	D	1463	U	O5'-P-OP2	5.20	116.94	110.70
40	a	2091	C	N3-C4-C5	5.19	123.98	121.90
17	D	333	U	N3-C4-O4	5.19	123.03	119.40
40	a	755	U	C5-C6-N1	5.19	125.30	122.70
40	a	918	A	N7-C8-N9	-5.19	111.21	113.80
12	AB	169	THR	C-N-CD	-5.18	109.20	120.60
40	a	335	C	N3-C2-O2	-5.18	118.27	121.90
40	a	910	A	C4-C5-N7	5.18	113.29	110.70
17	D	947	G	OP1-P-O3'	5.18	116.60	105.20
40	a	869	G	C4-C5-N7	5.18	112.87	110.80
43	d	31	C	N3-C2-O2	-5.18	118.28	121.90
40	a	1795	C	C2-N3-C4	-5.17	117.31	119.90
17	D	1240	U	N3-C2-O2	-5.17	118.58	122.20
40	a	2252	G	C8-N9-C4	5.17	108.47	106.40
17	D	1152	A	OP1-P-OP2	5.17	127.35	119.60
17	D	959	A	C5-N7-C8	-5.17	101.32	103.90
40	a	1414	C	C5-C6-N1	-5.17	118.42	121.00
48	i	5	GLN	C-N-CA	5.17	134.61	121.70
40	a	1561	C	N3-C2-O2	-5.16	118.29	121.90
40	a	2544	G	N1-C6-O6	5.16	123.00	119.90
40	a	2787	C	C6-N1-C2	5.16	122.37	120.30
40	a	2815	C	C5'-C4'-O4'	5.16	115.30	109.10
65	z	48	ARG	NE-CZ-NH1	-5.16	117.72	120.30
17	D	959	A	C4-C5-N7	5.16	113.28	110.70
17	D	1308	U	OP2-P-O3'	-5.16	93.85	105.20
40	a	145	C	O4'-C1'-N1	5.16	112.33	108.20
10	B	38	A	OP2-P-O3'	5.16	116.54	105.20
10	B	36	U	C4-C5-C6	-5.15	116.61	119.70
40	a	518	G	O5'-C5'-C4'	5.15	121.49	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	534	U	O5'-P-OP1	-5.15	101.06	105.70
40	a	175	G	N1-C6-O6	-5.15	116.81	119.90
17	D	1215	G	C6-C5-N7	-5.14	127.31	130.40
40	a	2613	U	C2-N3-C4	5.14	130.09	127.00
40	a	2017	U	C4-C5-C6	-5.14	116.62	119.70
40	a	1511	G	N1-C6-O6	5.14	122.98	119.90
17	D	97	G	N9-C4-C5	-5.14	103.34	105.40
40	a	2496	C	C6-N1-C2	5.14	122.36	120.30
23	J	3	ARG	NE-CZ-NH2	-5.13	117.73	120.30
48	i	8	PRO	CA-N-CD	-5.13	104.32	111.50
17	D	597	G	C4-C5-C6	-5.13	115.72	118.80
4	3	22	ARG	NE-CZ-NH2	-5.13	117.74	120.30
17	D	1240	U	C5-C4-O4	5.13	128.98	125.90
17	D	1439	G	C5-C6-N1	5.12	114.06	111.50
40	a	2640	G	OP2-P-O3'	5.12	116.47	105.20
62	w	97	ILE	CG1-CB-CG2	-5.12	100.13	111.40
40	a	136	G	C4-C5-C6	5.12	121.87	118.80
40	a	2261	C	OP2-P-O3'	5.12	116.47	105.20
40	a	1540	G	N1-C6-O6	5.12	122.97	119.90
17	D	1363	A	N3-C4-C5	5.12	130.38	126.80
40	a	1706	C	C6-N1-C2	5.12	122.35	120.30
17	D	440	C	N3-C4-C5	5.12	123.95	121.90
40	a	990	A	C5-C6-N6	5.12	127.79	123.70
40	a	2356	U	OP2-P-O3'	5.12	116.45	105.20
10	A	38	A	OP2-P-O3'	5.11	116.45	105.20
40	a	88	G	C6-N1-C2	-5.11	122.03	125.10
17	D	1309	G	C5-C6-N1	-5.11	108.94	111.50
30	Q	120	GLY	N-CA-C	5.11	125.88	113.10
40	a	2344	U	C5-C4-O4	5.11	128.97	125.90
40	a	883	G	C5-C6-N1	5.11	114.05	111.50
40	a	2101	A	C6-N1-C2	-5.11	115.54	118.60
40	a	910	A	C8-N9-C4	5.10	107.84	105.80
40	a	1124	G	N1-C6-O6	-5.10	116.84	119.90
40	a	1798	U	N3-C4-O4	-5.10	115.83	119.40
17	D	1497	G	C8-N9-C4	5.10	108.44	106.40
10	B	30	G	N1-C6-O6	-5.09	116.84	119.90
40	a	754	U	C2-N3-C4	-5.09	123.94	127.00
54	o	33	LEU	CB-CG-CD1	5.09	119.66	111.00
17	D	624	C	C6-N1-C2	5.09	122.33	120.30
40	a	748	G	O4'-C1'-N9	5.09	112.27	108.20
17	D	884	U	N1-C2-O2	5.08	126.36	122.80
11	AA	516	ASP	CB-CG-OD2	5.08	122.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	86	G	P-O3'-C3'	-5.08	113.61	119.70
17	D	73	C	N3-C2-O2	5.07	125.45	121.90
17	D	1339	A	N9-C4-C5	5.07	107.83	105.80
10	A	36	U	C4-C5-C6	-5.07	116.66	119.70
40	a	1015	U	C5-C4-O4	-5.06	122.86	125.90
40	a	301	G	P-O3'-C3'	-5.06	113.63	119.70
40	a	1323	C	N3-C2-O2	-5.06	118.36	121.90
40	a	2275	C	C6-N1-C2	-5.06	118.28	120.30
60	u	57	LEU	CB-CG-CD1	5.05	119.59	111.00
40	a	2013	A	C5-C6-N6	5.05	127.74	123.70
17	D	20	U	N3-C4-C5	5.04	117.63	114.60
60	u	64	PHE	CB-CG-CD2	-5.04	117.27	120.80
8	7	-19	U	C5-C4-O4	-5.04	122.87	125.90
40	a	2103	C	C2-N1-C1'	-5.04	113.26	118.80
40	a	2311	A	OP1-P-O3'	5.04	116.29	105.20
40	a	1303	G	N1-C6-O6	5.04	122.92	119.90
29	P	56	HIS	CB-CA-C	5.04	120.47	110.40
40	a	797	G	OP1-P-OP2	5.04	127.15	119.60
40	a	775	G	O4'-C1'-N9	5.03	112.23	108.20
40	a	2574	G	C6-C5-N7	-5.03	127.38	130.40
40	a	137	U	N1-C2-N3	5.03	117.92	114.90
40	a	1058	U	C5-C4-O4	-5.03	122.88	125.90
40	a	1582	C	N1-C2-O2	5.03	121.92	118.90
48	i	4	GLN	CA-CB-CG	-5.03	102.34	113.40
17	D	1307	U	C6-N1-C2	5.03	124.02	121.00
40	a	2137	U	N3-C4-O4	5.03	122.92	119.40
40	a	1581	G	N3-C4-C5	5.02	131.11	128.60
17	D	956	U	C2-N1-C1'	-5.02	111.67	117.70
40	a	544	C	C2-N1-C1'	-5.02	113.28	118.80
40	a	2013	A	OP2-P-O3'	5.02	116.23	105.20
17	D	1240	U	C5-C6-N1	-5.01	120.19	122.70
40	a	674	G	N3-C4-C5	5.01	131.11	128.60
40	a	1798	U	C5-C6-N1	-5.01	120.19	122.70
17	D	915	A	N9-C4-C5	-5.01	103.80	105.80
40	a	788	A	N1-C2-N3	-5.01	126.80	129.30
40	a	2192	U	C5-C4-O4	5.00	128.90	125.90
40	a	1086	A	C4-C5-N7	5.00	113.20	110.70

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	107	GLU	Peptide
9	9	79	PRO	Peptide
9	9	92	ALA	Peptide
10	A	37	A	Sidechain
10	A	76	A	Sidechain
11	AA	910	ALA	Peptide
12	AB	135	ARG	Sidechain
13	AC	192	VAL	Peptide
13	AD	20	SER	Peptide
14	AE	1326	GLN	Peptide
14	AE	1344	LEU	Peptide
14	AE	313	GLY	Peptide
14	AE	416	ILE	Peptide
10	B	37	A	Sidechain
10	B	76	A	Sidechain
17	D	958	A	Sidechain
21	H	124	LEU	Peptide
21	H	274	TYR	Peptide
21	H	53	PHE	Peptide
21	H	81	GLU	Peptide
21	H	82	THR	Peptide
24	K	77	ASN	Peptide
24	K	90	THR	Mainchain
26	M	56	LYS	Mainchain
28	O	12	ARG	Peptide
31	R	102	LEU	Mainchain
40	a	1262	A	Sidechain
40	a	88	G	Sidechain
40	a	89	A	Sidechain
48	i	41	HIS	Mainchain
50	k	14	SER	Mainchain
53	n	176	PRO	Peptide
60	u	35	HIS	Peptide
62	w	98	LEU	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
2	1	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
3	2	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
4	3	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	13	49
5	4	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
9	9	146/165 (88%)	101 (69%)	33 (23%)	12 (8%)	1	10
11	AA	1338/1342 (100%)	1220 (91%)	114 (8%)	4 (0%)	37	72
12	AB	173/181 (96%)	137 (79%)	27 (16%)	9 (5%)	1	15
13	AC	217/329 (66%)	203 (94%)	12 (6%)	2 (1%)	14	51
13	AD	214/329 (65%)	198 (92%)	16 (8%)	0	100	100
14	AE	1331/1407 (95%)	1219 (92%)	109 (8%)	3 (0%)	44	78
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
16	C	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
18	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
19	F	68/71 (96%)	68 (100%)	0	0	100	100
20	G	223/241 (92%)	212 (95%)	10 (4%)	1 (0%)	30	68
21	H	255/557 (46%)	192 (75%)	52 (20%)	11 (4%)	2	17
22	I	206/233 (88%)	197 (96%)	9 (4%)	0	100	100
23	J	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
24	K	154/167 (92%)	144 (94%)	8 (5%)	2 (1%)	10	42
25	L	102/135 (76%)	98 (96%)	3 (3%)	1 (1%)	13	49
26	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	19	56
27	N	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
28	O	125/130 (96%)	116 (93%)	8 (6%)	1 (1%)	16	54
29	P	97/103 (94%)	87 (90%)	10 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	Q	115/129 (89%)	106 (92%)	9 (8%)	0	100	100
31	R	117/124 (94%)	116 (99%)	0	1 (1%)	14	51
32	S	98/101 (97%)	96 (98%)	1 (1%)	1 (1%)	13	49
33	T	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
34	U	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
35	V	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
36	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
37	X	114/118 (97%)	105 (92%)	7 (6%)	2 (2%)	7	34
38	Y	139/142 (98%)	107 (77%)	31 (22%)	1 (1%)	19	56
39	Z	28/121 (23%)	21 (75%)	7 (25%)	0	100	100
41	b	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
42	c	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
44	e	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
45	f	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
46	g	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
47	h	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
48	i	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	6	32
49	j	207/209 (99%)	196 (95%)	11 (5%)	0	100	100
50	k	50/55 (91%)	49 (98%)	0	1 (2%)	6	32
51	l	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
52	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
53	n	175/179 (98%)	164 (94%)	10 (6%)	1 (1%)	22	60
54	o	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	8	38
55	p	173/177 (98%)	163 (94%)	10 (6%)	0	100	100
56	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
57	r	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
58	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
59	t	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
60	u	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
61	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
62	w	117/127 (92%)	107 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	x	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
64	y	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
65	z	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
All	All	9526/10577 (90%)	8823 (93%)	646 (7%)	57 (1%)	24	60

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	88	HIS
9	9	108	VAL
11	AA	913	VAL
12	AB	44	VAL
12	AB	49	VAL
12	AB	122	PRO
12	AB	165	PHE
20	G	127	ASP
21	H	125	ASN
21	H	171	ARG
21	H	309	MET
21	H	340	ARG
24	K	78	ASN
25	L	96	VAL
26	M	56	LYS
28	O	13	LYS
37	X	66	GLU
37	X	103	LYS
48	i	40	ARG
53	n	177	PHE
54	o	32	ILE
9	9	48	ALA
9	9	80	THR
12	AB	50	VAL
12	AB	52	ILE
14	AE	92	VAL
14	AE	175	GLU
21	H	306	VAL
50	k	15	ALA
9	9	93	ALA
9	9	119	PRO
11	AA	893	THR
12	AB	59	LYS

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Mol	Chain	Res	Type
21	H	108	VAL
21	H	153	GLU
9	9	130	PRO
11	AA	895	LEU
12	AB	45	PRO
12	AB	105	ASP
13	AC	193	GLU
31	R	102	LEU
9	9	91	ALA
14	AE	74	LYS
21	H	139	ARG
21	H	305	HIS
24	K	90	THR
4	3	39	ILE
9	9	118	ILE
13	AC	192	VAL
21	H	82	THR
21	H	304	VAL
32	S	94	PRO
38	Y	20	SER
9	9	33	VAL
9	9	129	LEU
9	9	79	PRO
11	AA	1317	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	84/84 (100%)	78 (93%)	6 (7%)	12	32
2	1	93/93 (100%)	85 (91%)	8 (9%)	8	27
3	2	81/84 (96%)	77 (95%)	4 (5%)	21	43
4	3	84/85 (99%)	78 (93%)	6 (7%)	12	32
5	4	78/78 (100%)	74 (95%)	4 (5%)	20	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	9	112/123 (91%)	73 (65%)	39 (35%)	0	1
11	AA	1155/1157 (100%)	1147 (99%)	8 (1%)	81	87
12	AB	150/158 (95%)	127 (85%)	23 (15%)	2	12
13	AC	186/286 (65%)	186 (100%)	0	100	100
13	AD	185/286 (65%)	185 (100%)	0	100	100
14	AE	1122/1168 (96%)	1106 (99%)	16 (1%)	62	76
15	AF	70/75 (93%)	70 (100%)	0	100	100
16	C	57/65 (88%)	55 (96%)	2 (4%)	31	52
18	E	65/66 (98%)	60 (92%)	5 (8%)	10	30
19	F	60/61 (98%)	56 (93%)	4 (7%)	13	34
20	G	187/199 (94%)	177 (95%)	10 (5%)	19	41
21	H	137/461 (30%)	129 (94%)	8 (6%)	17	38
22	I	171/190 (90%)	165 (96%)	6 (4%)	31	52
23	J	172/173 (99%)	165 (96%)	7 (4%)	26	48
24	K	119/126 (94%)	112 (94%)	7 (6%)	16	38
25	L	91/116 (78%)	84 (92%)	7 (8%)	10	30
26	M	124/147 (84%)	115 (93%)	9 (7%)	11	32
27	N	104/105 (99%)	102 (98%)	2 (2%)	52	70
28	O	105/107 (98%)	99 (94%)	6 (6%)	17	39
29	P	86/90 (96%)	78 (91%)	8 (9%)	7	24
30	Q	90/99 (91%)	87 (97%)	3 (3%)	33	54
31	R	101/104 (97%)	94 (93%)	7 (7%)	13	34
32	S	83/84 (99%)	74 (89%)	9 (11%)	5	20
33	T	76/77 (99%)	64 (84%)	12 (16%)	2	11
34	U	65/65 (100%)	59 (91%)	6 (9%)	7	24
35	V	74/78 (95%)	72 (97%)	2 (3%)	40	60
36	W	72/79 (91%)	68 (94%)	4 (6%)	17	40
37	X	94/96 (98%)	86 (92%)	8 (8%)	8	28
38	Y	109/110 (99%)	77 (71%)	32 (29%)	0	2
39	Z	26/85 (31%)	12 (46%)	14 (54%)	0	0
41	b	58/63 (92%)	56 (97%)	2 (3%)	32	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	c	67/68 (98%)	65 (97%)	2 (3%)	36	56
44	e	54/55 (98%)	53 (98%)	1 (2%)	52	70
45	f	48/49 (98%)	46 (96%)	2 (4%)	25	47
46	g	59/62 (95%)	52 (88%)	7 (12%)	4	17
47	h	216/218 (99%)	200 (93%)	16 (7%)	11	31
48	i	47/48 (98%)	40 (85%)	7 (15%)	2	12
49	j	164/164 (100%)	156 (95%)	8 (5%)	21	43
50	k	47/49 (96%)	43 (92%)	4 (8%)	8	28
51	l	165/165 (100%)	155 (94%)	10 (6%)	15	38
52	m	38/38 (100%)	35 (92%)	3 (8%)	10	29
53	n	148/150 (99%)	134 (90%)	14 (10%)	7	23
54	o	51/52 (98%)	46 (90%)	5 (10%)	6	22
55	p	136/138 (99%)	131 (96%)	5 (4%)	29	51
56	q	34/34 (100%)	32 (94%)	2 (6%)	16	38
57	r	114/114 (100%)	104 (91%)	10 (9%)	8	26
58	s	116/116 (100%)	110 (95%)	6 (5%)	19	41
59	t	104/104 (100%)	98 (94%)	6 (6%)	17	38
60	u	103/103 (100%)	98 (95%)	5 (5%)	21	43
61	v	109/109 (100%)	103 (94%)	6 (6%)	18	40
62	w	99/103 (96%)	92 (93%)	7 (7%)	12	32
63	x	86/87 (99%)	82 (95%)	4 (5%)	22	45
64	y	99/100 (99%)	95 (96%)	4 (4%)	27	48
65	z	89/90 (99%)	87 (98%)	2 (2%)	47	66
All	All	7919/8739 (91%)	7489 (95%)	430 (5%)	21	41

All (430) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	LYS
1	0	13	ARG
1	0	48	LYS
1	0	51	VAL
1	0	68	ARG
1	0	86	GLN

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Mol	Chain	Res	Type
2	1	7	HIS
2	1	19	LEU
2	1	30	SER
2	1	69	LEU
2	1	97	LEU
2	1	107	VAL
2	1	109	ASP
2	1	110	ARG
3	2	1	MET
3	2	24	MET
3	2	37	ASP
3	2	93	LEU
4	3	52	LEU
4	3	68	SER
4	3	72	ILE
4	3	89	ASP
4	3	99	ASN
4	3	101	GLU
5	4	40	ILE
5	4	41	GLU
5	4	69	GLU
5	4	71	LYS
9	9	1	MET
9	9	3	LEU
9	9	4	ASN
9	9	5	LEU
9	9	6	GLN
9	9	7	ASP
9	9	14	GLU
9	9	23	LEU
9	9	24	SER
9	9	34	THR
9	9	36	ASP
9	9	37	LYS
9	9	42	ARG
9	9	43	LYS
9	9	52	MET
9	9	56	ARG
9	9	57	ASN
9	9	61	ARG
9	9	69	PHE
9	9	70	GLU

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Mol	Chain	Res	Type
9	9	71	CYS
9	9	72	LEU
9	9	81	LEU
9	9	86	MET
9	9	94	ARG
9	9	96	PHE
9	9	98	GLU
9	9	106	PHE
9	9	107	GLU
9	9	109	LYS
9	9	113	PHE
9	9	117	LEU
9	9	122	GLN
9	9	123	ILE
9	9	125	ARG
9	9	133	GLU
9	9	134	GLU
9	9	138	ARG
9	9	143	MET
11	AA	892	GLU
11	AA	894	GLN
11	AA	895	LEU
11	AA	900	LYS
11	AA	903	ARG
11	AA	905	ILE
11	AA	909	LYS
11	AA	914	LYS
12	AB	21	ARG
12	AB	44	VAL
12	AB	47	GLU
12	AB	49	VAL
12	AB	53	ARG
12	AB	57	ARG
12	AB	59	LYS
12	AB	62	ARG
12	AB	64	PHE
12	AB	65	PHE
12	AB	104	SER
12	AB	105	ASP
12	AB	106	LYS
12	AB	114	ARG
12	AB	127	LEU

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Mol	Chain	Res	Type
12	AB	129	GLU
12	AB	132	GLU
12	AB	159	LYS
12	AB	161	SER
12	AB	163	SER
12	AB	164	ILE
12	AB	165	PHE
12	AB	169	THR
14	AE	69	GLU
14	AE	70	CYS
14	AE	71	LEU
14	AE	74	LYS
14	AE	76	LYS
14	AE	77	ARG
14	AE	78	LEU
14	AE	79	LYS
14	AE	81	ARG
14	AE	85	CYS
14	AE	92	VAL
14	AE	93	THR
14	AE	431	ARG
14	AE	514	THR
14	AE	744	ARG
14	AE	1369	ARG
16	C	33	ILE
16	C	74	HIS
18	E	6	SER
18	E	10	ARG
18	E	48	GLN
18	E	54	MET
18	E	64	LYS
19	F	16	LEU
19	F	34	ARG
19	F	62	ARG
19	F	67	ARG
20	G	7	ARG
20	G	23	TRP
20	G	45	LYS
20	G	105	LYS
20	G	108	ARG
20	G	127	ASP
20	G	128	LYS

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Mol	Chain	Res	Type
20	G	129	LEU
20	G	132	LYS
20	G	208	ARG
21	H	9	PHE
21	H	54	LYS
21	H	273	ARG
21	H	305	HIS
21	H	336	ASP
21	H	337	GLU
21	H	338	GLU
21	H	339	ARG
22	I	14	ILE
22	I	75	ILE
22	I	89	LYS
22	I	164	ARG
22	I	185	ASN
22	I	200	VAL
23	J	47	ARG
23	J	48	LEU
23	J	95	GLU
23	J	104	ARG
23	J	116	GLN
23	J	138	SER
23	J	143	VAL
24	K	10	GLU
24	K	15	LEU
24	K	60	ILE
24	K	114	VAL
24	K	115	LEU
24	K	138	ARG
24	K	162	GLU
25	L	16	GLU
25	L	24	ARG
25	L	38	ARG
25	L	54	LEU
25	L	79	ARG
25	L	86	ARG
25	L	88	MET
26	M	7	ILE
26	M	17	LYS
26	M	21	GLU
26	M	23	LEU

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Mol	Chain	Res	Type
26	M	79	ARG
26	M	91	VAL
26	M	109	ARG
26	M	123	GLU
26	M	146	GLU
27	N	96	MET
27	N	121	LEU
28	O	12	ARG
28	O	27	LYS
28	O	60	LYS
28	O	61	LEU
28	O	63	LEU
28	O	118	LEU
29	P	5	ARG
29	P	17	LEU
29	P	24	GLU
29	P	25	ILE
29	P	27	GLU
29	P	37	ARG
29	P	87	LEU
29	P	90	LEU
30	Q	15	GLN
30	Q	56	ARG
30	Q	107	ILE
31	R	5	ASN
31	R	12	ARG
31	R	24	LEU
31	R	56	ARG
31	R	62	GLU
31	R	64	THR
31	R	74	LEU
32	S	45	VAL
32	S	46	LEU
32	S	74	LEU
32	S	80	SER
32	S	81	ARG
32	S	82	ILE
32	S	89	MET
32	S	92	GLU
32	S	94	PRO
33	T	10	LYS
33	T	17	ARG

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Mol	Chain	Res	Type
33	T	22	THR
33	T	39	LEU
33	T	40	GLN
33	T	64	ARG
33	T	66	LEU
33	T	67	LEU
33	T	70	LEU
33	T	73	LYS
33	T	84	ARG
33	T	85	LEU
34	U	1	MET
34	U	2	VAL
34	U	6	LEU
34	U	18	GLN
34	U	19	VAL
34	U	20	VAL
35	V	75	LEU
35	V	81	LYS
36	W	12	ASP
36	W	21	LYS
36	W	33	THR
36	W	79	THR
37	X	11	ASP
37	X	16	VAL
37	X	29	ARG
37	X	59	GLU
37	X	92	ARG
37	X	93	ARG
37	X	101	ARG
37	X	117	LYS
38	Y	10	LEU
38	Y	16	MET
38	Y	23	VAL
38	Y	27	LEU
38	Y	30	GLN
38	Y	36	GLU
38	Y	44	LYS
38	Y	48	ILE
38	Y	50	LYS
38	Y	57	VAL
38	Y	58	ILE
38	Y	60	VAL

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Mol	Chain	Res	Type
38	Y	61	TYR
38	Y	64	ARG
38	Y	78	LEU
38	Y	80	LYS
38	Y	91	LYS
38	Y	94	LYS
38	Y	95	ASP
38	Y	99	LYS
38	Y	100	ILE
38	Y	102	ARG
38	Y	104	GLN
38	Y	108	ILE
38	Y	112	LYS
38	Y	116	MET
38	Y	120	ASP
38	Y	124	MET
38	Y	125	THR
38	Y	126	ARG
38	Y	133	ARG
38	Y	135	MET
39	Z	1	SER
39	Z	2	ILE
39	Z	4	LYS
39	Z	6	GLN
39	Z	7	ILE
39	Z	8	ILE
39	Z	14	MET
39	Z	15	SER
39	Z	16	VAL
39	Z	23	ILE
39	Z	26	MET
39	Z	28	GLU
39	Z	29	LYS
39	Z	30	PHE
41	b	20	ARG
41	b	70	GLU
42	c	48	THR
42	c	54	LYS
44	e	58	ASN
45	f	3	LYS
45	f	45	ARG
46	g	16	CYS

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Mol	Chain	Res	Type
46	g	36	VAL
46	g	43	PHE
46	g	47	LYS
46	g	56	ARG
46	g	59	ARG
46	g	65	ASN
47	h	51	THR
47	h	52	ARG
47	h	118	SER
47	h	125	LYS
47	h	130	LEU
47	h	141	VAL
47	h	156	ARG
47	h	187	ASP
47	h	189	ARG
47	h	195	VAL
47	h	202	LEU
47	h	203	ARG
47	h	204	VAL
47	h	205	LEU
47	h	242	LYS
47	h	271	ARG
48	i	9	THR
48	i	12	LYS
48	i	26	THR
48	i	27	SER
48	i	29	SER
48	i	40	ARG
48	i	52	ARG
49	j	13	ARG
49	j	18	ASP
49	j	32	ASN
49	j	91	THR
49	j	103	ASP
49	j	131	ASP
49	j	151	THR
49	j	177	VAL
50	k	5	ILE
50	k	17	THR
50	k	24	THR
50	k	26	ASN
51	l	17	THR

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Mol	Chain	Res	Type
51	l	22	ASP
51	l	40	ARG
51	l	57	LYS
51	l	69	ARG
51	l	108	ILE
51	l	109	LEU
51	l	122	GLU
51	l	149	ILE
51	l	179	SER
52	m	22	MET
52	m	41	ARG
52	m	42	LEU
53	n	6	ASP
53	n	10	ASP
53	n	40	VAL
53	n	57	LEU
53	n	80	ARG
53	n	95	ARG
53	n	115	ARG
53	n	117	LEU
53	n	122	PHE
53	n	123	ASP
53	n	133	ARG
53	n	140	GLU
53	n	152	LEU
53	n	163	ASP
54	o	8	ARG
54	o	30	ARG
54	o	31	HIS
54	o	54	ASP
54	o	55	LEU
55	p	39	ASP
55	p	95	ARG
55	p	114	ASP
55	p	125	CYS
55	p	171	THR
56	q	3	VAL
56	q	26	ILE
57	r	11	ASN
57	r	12	LEU
57	r	15	LEU
57	r	41	LYS

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Mol	Chain	Res	Type
57	r	66	ASN
57	r	72	ILE
57	r	87	GLU
57	r	97	ARG
57	r	101	ASP
57	r	127	GLU
58	s	1	MET
58	s	14	ASP
58	s	30	THR
58	s	40	HIS
58	s	57	LEU
58	s	142	ILE
59	t	32	TYR
59	t	49	ARG
59	t	53	LYS
59	t	80	ASP
59	t	88	ASN
59	t	104	THR
60	u	5	THR
60	u	27	LEU
60	u	48	ARG
60	u	76	GLU
60	u	78	ARG
61	v	13	HIS
61	v	18	ARG
61	v	84	LYS
61	v	110	GLU
61	v	126	ILE
61	v	128	THR
62	w	2	ARG
62	w	20	MET
62	w	24	MET
62	w	51	LEU
62	w	63	ARG
62	w	65	LEU
62	w	69	ARG
63	x	13	ARG
63	x	47	VAL
63	x	48	LEU
63	x	91	SER
64	y	10	GLN
64	y	27	GLU

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Mol	Chain	Res	Type
64	y	85	SER
64	y	114	LEU
65	z	18	LEU
65	z	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	78	GLN
11	AA	69	GLN
11	AA	150	HIS
11	AA	314	ASN
11	AA	513	GLN
11	AA	554	HIS
11	AA	580	GLN
11	AA	604	HIS
11	AA	688	GLN
11	AA	1268	GLN
11	AA	1313	HIS
13	AC	147	GLN
13	AD	66	HIS
13	AD	84	ASN
13	AD	117	HIS
13	AD	227	GLN
14	AE	157	GLN
14	AE	450	HIS
14	AE	777	HIS
14	AE	805	GLN
14	AE	910	ASN
14	AE	1108	GLN
14	AE	1326	GLN
14	AE	1367	GLN
15	AF	31	GLN
20	G	18	HIS
21	H	305	HIS
27	N	16	ASN
46	g	6	HIS
47	h	15	HIS
48	i	41	HIS
48	i	42	HIS
49	j	130	GLN
49	j	140	HIS

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Mol	Chain	Res	Type
49	j	148	GLN
51	l	62	GLN
52	m	29	GLN
54	o	43	HIS
58	s	80	HIS
60	u	35	HIS
60	u	104	GLN
61	v	13	HIS
62	w	3	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	7 (9%)
10	B	75/76 (98%)	29 (38%)	6 (8%)
17	D	1515/1542 (98%)	295 (19%)	26 (1%)
40	a	2859/2904 (98%)	534 (18%)	0
43	d	119/120 (99%)	17 (14%)	0
8	7	33/44 (75%)	21 (63%)	3 (9%)
All	All	4676/4762 (98%)	925 (19%)	42 (0%)

All (925) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-18	G
8	7	-17	U
8	7	-16	U
8	7	-15	U
8	7	-14	U
8	7	-13	U
8	7	-12	U
8	7	-11	U
8	7	-10	U
8	7	-9	U
8	7	-8	U
8	7	-7	U
8	7	-6	U
8	7	-5	U
8	7	-4	U
8	7	-3	U
8	7	-2	U

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Mol	Chain	Res	Type
8	7	0	U
8	7	1	U
8	7	12	G
8	7	13	G
10	A	2	G
10	A	6	G
10	A	7	G
10	A	8	U
10	A	10	G
10	A	13	C
10	A	14	A
10	A	15	G
10	A	16	C
10	A	17	C
10	A	18	G
10	A	19	G
10	A	20	U
10	A	21	A
10	A	22	G
10	A	23	C
10	A	46	G
10	A	47	U
10	A	48	C
10	A	49	G
10	A	52	G
10	A	57	A
10	A	58	A
10	A	59	A
10	A	61	C
10	A	66	C
10	A	69	C
10	A	71	C
10	A	73	A
10	B	2	G
10	B	6	G
10	B	7	G
10	B	8	U
10	B	10	G
10	B	13	C
10	B	14	A
10	B	15	G
10	B	16	C

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Mol	Chain	Res	Type
10	B	17	C
10	B	18	G
10	B	19	G
10	B	20	U
10	B	21	A
10	B	22	G
10	B	23	C
10	B	46	G
10	B	47	U
10	B	48	C
10	B	49	G
10	B	52	G
10	B	57	A
10	B	58	A
10	B	59	A
10	B	61	C
10	B	66	C
10	B	69	C
10	B	71	C
10	B	73	A
17	D	4	U
17	D	5	U
17	D	9	G
17	D	22	G
17	D	29	U
17	D	32	A
17	D	39	G
17	D	47	C
17	D	48	C
17	D	50	A
17	D	51	A
17	D	52	C
17	D	54	C
17	D	69	G
17	D	71	A
17	D	72	A
17	D	74	A
17	D	76	G
17	D	82	G
17	D	83	C
17	D	84	U
17	D	87	C

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Mol	Chain	Res	Type
17	D	90	C
17	D	94	G
17	D	95	C
17	D	96	U
17	D	108	G
17	D	120	A
17	D	121	U
17	D	122	G
17	D	128	G
17	D	131	A
17	D	141	G
17	D	144	G
17	D	148	G
17	D	149	A
17	D	160	A
17	D	164	G
17	D	173	U
17	D	181	A
17	D	182	A
17	D	184	G
17	D	197	A
17	D	198	G
17	D	204	G
17	D	208	U
17	D	209	U
17	D	210	C
17	D	211	G
17	D	212	G
17	D	216	U
17	D	226	G
17	D	245	U
17	D	247	G
17	D	251	G
17	D	253	A
17	D	258	G
17	D	262	A
17	D	266	G
17	D	267	C
17	D	271	C
17	D	279	A
17	D	289	G
17	D	299	G

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Mol	Chain	Res	Type
17	D	306	A
17	D	321	A
17	D	328	C
17	D	329	A
17	D	332	G
17	D	347	G
17	D	352	C
17	D	353	A
17	D	354	G
17	D	355	C
17	D	367	U
17	D	372	C
17	D	373	A
17	D	376	G
17	D	382	A
17	D	384	G
17	D	392	C
17	D	393	A
17	D	397	A
17	D	398	U
17	D	406	G
17	D	411	A
17	D	412	A
17	D	413	G
17	D	414	A
17	D	421	U
17	D	422	C
17	D	424	G
17	D	429	U
17	D	446	G
17	D	451	A
17	D	457	G
17	D	458	U
17	D	460	A
17	D	463	U
17	D	464	U
17	D	467	U
17	D	468	A
17	D	469	C
17	D	478	A
17	D	479	U
17	D	481	G

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Mol	Chain	Res	Type
17	D	484	G
17	D	485	U
17	D	486	U
17	D	497	G
17	D	505	G
17	D	509	A
17	D	511	C
17	D	518	C
17	D	519	C
17	D	526	C
17	D	531	U
17	D	532	A
17	D	533	A
17	D	542	G
17	D	547	A
17	D	559	A
17	D	564	C
17	D	568	G
17	D	572	A
17	D	573	A
17	D	576	C
17	D	577	G
17	D	579	A
17	D	596	A
17	D	626	G
17	D	628	G
17	D	633	G
17	D	642	A
17	D	649	A
17	D	650	G
17	D	653	U
17	D	665	A
17	D	700	G
17	D	721	G
17	D	723	U
17	D	724	G
17	D	731	G
17	D	734	G
17	D	747	A
17	D	748	G
17	D	755	G
17	D	760	G

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Mol	Chain	Res	Type
17	D	777	A
17	D	793	U
17	D	794	A
17	D	815	A
17	D	817	C
17	D	828	U
17	D	829	G
17	D	832	G
17	D	841	C
17	D	844	G
17	D	845	A
17	D	846	G
17	D	849	G
17	D	874	G
17	D	887	G
17	D	902	G
17	D	914	A
17	D	916	U
17	D	926	G
17	D	934	C
17	D	935	A
17	D	942	G
17	D	954	G
17	D	960	U
17	D	963	G
17	D	965	U
17	D	969	A
17	D	972	C
17	D	975	A
17	D	976	G
17	D	987	G
17	D	991	U
17	D	992	U
17	D	993	G
17	D	996	A
17	D	999	C
17	D	1004	A
17	D	1008	U
17	D	1009	U
17	D	1017	U
17	D	1018	G
17	D	1021	A

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Mol	Chain	Res	Type
17	D	1024	G
17	D	1026	G
17	D	1028	C
17	D	1030	U
17	D	1031	C
17	D	1032	G
17	D	1037	C
17	D	1043	G
17	D	1044	A
17	D	1046	A
17	D	1065	U
17	D	1085	U
17	D	1094	G
17	D	1095	U
17	D	1099	G
17	D	1101	A
17	D	1124	G
17	D	1133	G
17	D	1135	U
17	D	1136	C
17	D	1137	C
17	D	1139	G
17	D	1140	C
17	D	1141	C
17	D	1142	G
17	D	1143	G
17	D	1145	A
17	D	1146	A
17	D	1151	A
17	D	1152	A
17	D	1158	C
17	D	1159	U
17	D	1160	G
17	D	1167	A
17	D	1171	A
17	D	1174	G
17	D	1175	G
17	D	1176	A
17	D	1184	G
17	D	1193	G
17	D	1196	A
17	D	1197	A

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Mol	Chain	Res	Type
17	D	1206	G
17	D	1211	U
17	D	1212	U
17	D	1213	A
17	D	1214	C
17	D	1215	G
17	D	1226	C
17	D	1227	A
17	D	1228	C
17	D	1238	A
17	D	1257	A
17	D	1260	G
17	D	1275	A
17	D	1276	G
17	D	1278	G
17	D	1279	G
17	D	1280	A
17	D	1285	A
17	D	1286	U
17	D	1287	A
17	D	1299	A
17	D	1300	G
17	D	1302	C
17	D	1305	G
17	D	1312	G
17	D	1317	C
17	D	1320	C
17	D	1323	G
17	D	1338	G
17	D	1340	A
17	D	1346	A
17	D	1347	G
17	D	1353	G
17	D	1363	A
17	D	1370	G
17	D	1378	C
17	D	1379	G
17	D	1381	U
17	D	1391	U
17	D	1396	A
17	D	1397	C
17	D	1398	A

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Mol	Chain	Res	Type
17	D	1404	C
17	D	1419	G
17	D	1429	A
17	D	1441	A
17	D	1446	A
17	D	1447	A
17	D	1448	C
17	D	1452	C
17	D	1453	G
17	D	1487	G
17	D	1492	A
17	D	1493	A
17	D	1494	G
17	D	1495	U
17	D	1497	G
17	D	1503	A
17	D	1506	U
17	D	1517	G
17	D	1529	G
17	D	1530	G
17	D	1534	A
40	a	4	U
40	a	10	A
40	a	15	G
40	a	23	G
40	a	34	U
40	a	35	G
40	a	46	G
40	a	58	G
40	a	60	G
40	a	62	U
40	a	63	A
40	a	68	G
40	a	71	A
40	a	74	A
40	a	75	G
40	a	83	A
40	a	84	A
40	a	85	G
40	a	88	G
40	a	89	A
40	a	93	G

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Mol	Chain	Res	Type
40	a	96	C
40	a	102	U
40	a	103	A
40	a	110	G
40	a	118	A
40	a	119	A
40	a	120	U
40	a	122	G
40	a	131	A
40	a	136	G
40	a	139	U
40	a	140	C
40	a	141	G
40	a	145	C
40	a	163	C
40	a	165	A
40	a	181	A
40	a	196	A
40	a	215	G
40	a	216	A
40	a	221	A
40	a	222	A
40	a	225	C
40	a	248	G
40	a	249	C
40	a	261	G
40	a	264	C
40	a	265	A
40	a	266	G
40	a	267	C
40	a	271	G
40	a	272	A
40	a	275	C
40	a	276	U
40	a	278	A
40	a	285	G
40	a	311	A
40	a	329	G
40	a	330	A
40	a	353	C
40	a	361	G
40	a	362	A

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Mol	Chain	Res	Type
40	a	371	A
40	a	372	G
40	a	373	U
40	a	375	G
40	a	383	C
40	a	386	G
40	a	396	G
40	a	405	U
40	a	411	G
40	a	412	A
40	a	420	C
40	a	424	G
40	a	451	U
40	a	457	A
40	a	464	U
40	a	477	A
40	a	481	G
40	a	491	G
40	a	501	A
40	a	503	A
40	a	504	A
40	a	505	A
40	a	509	C
40	a	522	A
40	a	529	A
40	a	532	A
40	a	543	G
40	a	546	U
40	a	547	A
40	a	548	G
40	a	549	G
40	a	551	G
40	a	563	A
40	a	569	U
40	a	573	U
40	a	575	A
40	a	588	U
40	a	603	A
40	a	609	A
40	a	613	A
40	a	614	A
40	a	615	U

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Mol	Chain	Res	Type
40	a	616	A
40	a	618	G
40	a	627	A
40	a	637	A
40	a	645	C
40	a	647	G
40	a	654	A
40	a	668	A
40	a	685	A
40	a	686	U
40	a	710	U
40	a	717	C
40	a	730	A
40	a	738	G
40	a	757	G
40	a	764	A
40	a	765	C
40	a	775	G
40	a	776	G
40	a	782	A
40	a	784	G
40	a	785	G
40	a	800	A
40	a	805	G
40	a	812	C
40	a	819	A
40	a	827	U
40	a	828	U
40	a	845	A
40	a	846	U
40	a	858	G
40	a	859	G
40	a	869	G
40	a	878	A
40	a	881	G
40	a	884	U
40	a	885	C
40	a	887	A
40	a	888	C
40	a	891	G
40	a	892	A
40	a	893	C

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Mol	Chain	Res	Type
40	a	895	U
40	a	896	A
40	a	897	C
40	a	899	A
40	a	907	G
40	a	910	A
40	a	914	G
40	a	915	C
40	a	931	U
40	a	941	A
40	a	945	A
40	a	946	C
40	a	953	G
40	a	961	C
40	a	974	G
40	a	983	A
40	a	995	C
40	a	996	A
40	a	999	U
40	a	1005	C
40	a	1012	U
40	a	1013	C
40	a	1022	G
40	a	1023	U
40	a	1026	G
40	a	1033	U
40	a	1041	G
40	a	1045	C
40	a	1046	A
40	a	1047	G
40	a	1060	U
40	a	1061	U
40	a	1063	G
40	a	1064	C
40	a	1065	U
40	a	1066	U
40	a	1067	A
40	a	1068	G
40	a	1069	A
40	a	1070	A
40	a	1071	G
40	a	1073	A

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Mol	Chain	Res	Type
40	a	1074	G
40	a	1076	C
40	a	1079	C
40	a	1080	A
40	a	1081	U
40	a	1082	U
40	a	1083	U
40	a	1084	A
40	a	1087	G
40	a	1088	A
40	a	1090	A
40	a	1095	A
40	a	1107	G
40	a	1110	G
40	a	1111	A
40	a	1112	G
40	a	1119	U
40	a	1122	G
40	a	1132	U
40	a	1134	A
40	a	1135	C
40	a	1142	A
40	a	1169	A
40	a	1170	C
40	a	1173	U
40	a	1174	U
40	a	1175	A
40	a	1176	U
40	a	1177	G
40	a	1178	C
40	a	1179	G
40	a	1180	U
40	a	1186	G
40	a	1236	G
40	a	1238	G
40	a	1248	G
40	a	1253	A
40	a	1256	G
40	a	1266	G
40	a	1271	G
40	a	1272	A
40	a	1273	U

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Mol	Chain	Res	Type
40	a	1301	A
40	a	1321	A
40	a	1345	C
40	a	1352	U
40	a	1365	A
40	a	1368	G
40	a	1378	A
40	a	1379	U
40	a	1380	G
40	a	1383	A
40	a	1392	A
40	a	1395	A
40	a	1406	U
40	a	1408	G
40	a	1409	U
40	a	1411	U
40	a	1414	C
40	a	1416	G
40	a	1417	C
40	a	1419	A
40	a	1420	A
40	a	1428	C
40	a	1452	G
40	a	1453	A
40	a	1460	U
40	a	1478	G
40	a	1482	G
40	a	1490	A
40	a	1497	U
40	a	1503	A
40	a	1508	A
40	a	1509	A
40	a	1510	G
40	a	1515	A
40	a	1529	G
40	a	1534	U
40	a	1535	A
40	a	1536	C
40	a	1537	G
40	a	1554	U
40	a	1559	U
40	a	1566	A

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Mol	Chain	Res	Type
40	a	1569	A
40	a	1578	U
40	a	1580	A
40	a	1581	G
40	a	1582	C
40	a	1583	A
40	a	1584	U
40	a	1589	U
40	a	1590	A
40	a	1608	A
40	a	1610	A
40	a	1613	G
40	a	1647	U
40	a	1648	U
40	a	1649	G
40	a	1651	G
40	a	1674	G
40	a	1677	A
40	a	1703	G
40	a	1714	U
40	a	1715	G
40	a	1718	G
40	a	1729	U
40	a	1730	C
40	a	1732	C
40	a	1738	G
40	a	1750	G
40	a	1755	A
40	a	1758	U
40	a	1764	C
40	a	1773	A
40	a	1791	A
40	a	1800	C
40	a	1801	A
40	a	1808	A
40	a	1811	G
40	a	1816	C
40	a	1829	A
40	a	1833	C
40	a	1847	A
40	a	1848	A
40	a	1858	A

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Mol	Chain	Res	Type
40	a	1859	U
40	a	1862	G
40	a	1864	U
40	a	1869	G
40	a	1870	C
40	a	1872	A
40	a	1873	G
40	a	1905	C
40	a	1906	G
40	a	1907	G
40	a	1913	A
40	a	1914	C
40	a	1919	A
40	a	1920	C
40	a	1922	G
40	a	1923	U
40	a	1924	C
40	a	1925	C
40	a	1926	U
40	a	1928	A
40	a	1929	G
40	a	1930	G
40	a	1936	A
40	a	1938	A
40	a	1955	U
40	a	1965	C
40	a	1967	C
40	a	1970	A
40	a	1971	U
40	a	1972	G
40	a	1987	A
40	a	1991	U
40	a	1992	G
40	a	1993	U
40	a	1997	C
40	a	2002	G
40	a	2020	A
40	a	2022	U
40	a	2023	C
40	a	2027	G
40	a	2033	A
40	a	2043	C

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Mol	Chain	Res	Type
40	a	2051	A
40	a	2052	A
40	a	2055	C
40	a	2056	G
40	a	2060	A
40	a	2061	G
40	a	2062	A
40	a	2063	C
40	a	2093	G
40	a	2097	A
40	a	2099	U
40	a	2100	G
40	a	2107	G
40	a	2108	A
40	a	2110	G
40	a	2111	U
40	a	2113	U
40	a	2115	G
40	a	2116	G
40	a	2117	A
40	a	2118	U
40	a	2121	G
40	a	2122	U
40	a	2124	G
40	a	2125	G
40	a	2126	A
40	a	2127	G
40	a	2128	G
40	a	2131	U
40	a	2132	U
40	a	2133	G
40	a	2134	A
40	a	2139	U
40	a	2141	G
40	a	2146	C
40	a	2147	A
40	a	2154	A
40	a	2157	G
40	a	2158	A
40	a	2159	G
40	a	2162	G
40	a	2163	A

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Mol	Chain	Res	Type
40	a	2164	C
40	a	2165	C
40	a	2169	A
40	a	2171	A
40	a	2172	U
40	a	2178	C
40	a	2182	U
40	a	2183	A
40	a	2185	U
40	a	2189	U
40	a	2190	G
40	a	2191	A
40	a	2193	G
40	a	2194	U
40	a	2198	A
40	a	2204	G
40	a	2211	A
40	a	2212	A
40	a	2213	U
40	a	2225	A
40	a	2226	C
40	a	2229	U
40	a	2238	G
40	a	2239	G
40	a	2250	G
40	a	2268	A
40	a	2278	A
40	a	2283	C
40	a	2287	A
40	a	2288	A
40	a	2297	A
40	a	2305	U
40	a	2308	G
40	a	2309	A
40	a	2315	G
40	a	2322	A
40	a	2325	G
40	a	2327	A
40	a	2333	A
40	a	2335	A
40	a	2339	C
40	a	2345	G

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Mol	Chain	Res	Type
40	a	2347	C
40	a	2350	C
40	a	2361	G
40	a	2372	U
40	a	2376	A
40	a	2383	G
40	a	2385	C
40	a	2402	U
40	a	2403	C
40	a	2406	A
40	a	2410	G
40	a	2423	U
40	a	2424	C
40	a	2425	A
40	a	2426	A
40	a	2429	G
40	a	2430	A
40	a	2431	U
40	a	2434	A
40	a	2435	A
40	a	2441	U
40	a	2447	G
40	a	2448	A
40	a	2470	G
40	a	2474	U
40	a	2476	A
40	a	2478	A
40	a	2484	G
40	a	2491	U
40	a	2502	G
40	a	2506	U
40	a	2507	C
40	a	2512	C
40	a	2513	A
40	a	2518	A
40	a	2520	C
40	a	2525	G
40	a	2529	G
40	a	2535	G
40	a	2547	A
40	a	2554	U
40	a	2566	A

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Mol	Chain	Res	Type
40	a	2567	G
40	a	2572	A
40	a	2573	C
40	a	2574	G
40	a	2585	U
40	a	2586	U
40	a	2602	A
40	a	2603	G
40	a	2609	U
40	a	2610	C
40	a	2611	C
40	a	2613	U
40	a	2629	U
40	a	2663	G
40	a	2669	G
40	a	2671	G
40	a	2689	U
40	a	2690	U
40	a	2714	G
40	a	2722	G
40	a	2724	U
40	a	2726	A
40	a	2744	G
40	a	2748	A
40	a	2758	A
40	a	2765	A
40	a	2777	G
40	a	2778	A
40	a	2791	G
40	a	2793	C
40	a	2796	U
40	a	2797	U
40	a	2798	U
40	a	2799	A
40	a	2801	G
40	a	2818	U
40	a	2820	A
40	a	2821	A
40	a	2823	A
40	a	2825	G
40	a	2835	A
40	a	2859	G

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Mol	Chain	Res	Type
40	a	2861	U
40	a	2867	G
40	a	2874	C
40	a	2880	C
40	a	2883	A
40	a	2884	U
40	a	2885	G
40	a	2891	U
40	a	2902	C
43	d	2	G
43	d	9	G
43	d	13	G
43	d	16	G
43	d	17	C
43	d	35	C
43	d	36	C
43	d	45	A
43	d	51	G
43	d	56	G
43	d	64	G
43	d	66	A
43	d	88	C
43	d	89	U
43	d	90	C
43	d	99	A
43	d	109	A

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-17	U
8	7	-11	U
8	7	11	U
10	A	6	G
10	A	7	G
10	A	9	G
10	A	12	G
10	A	22	G
10	A	60	U
10	A	70	G
10	B	6	G
10	B	7	G

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Mol	Chain	Res	Type
10	B	9	G
10	B	12	G
10	B	22	G
10	B	60	U
17	D	70	U
17	D	121	U
17	D	181	A
17	D	183	C
17	D	197	A
17	D	209	U
17	D	328	C
17	D	428	G
17	D	496	A
17	D	517	G
17	D	531	U
17	D	793	U
17	D	991	U
17	D	992	U
17	D	1109	C
17	D	1145	A
17	D	1196	A
17	D	1211	U
17	D	1212	U
17	D	1213	A
17	D	1214	C
17	D	1299	A
17	D	1447	A
17	D	1491	G
17	D	1492	A
17	D	1493	A

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

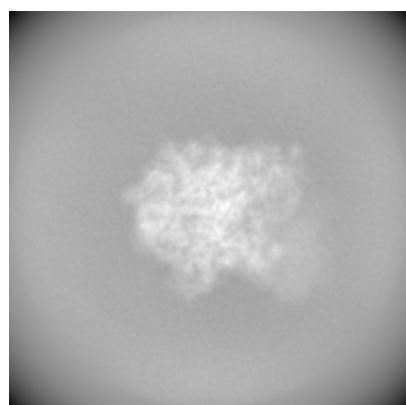
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22142. These allow visual inspection of the internal detail of the map and identification of artifacts.

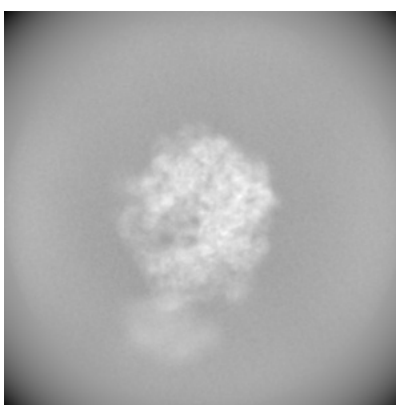
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

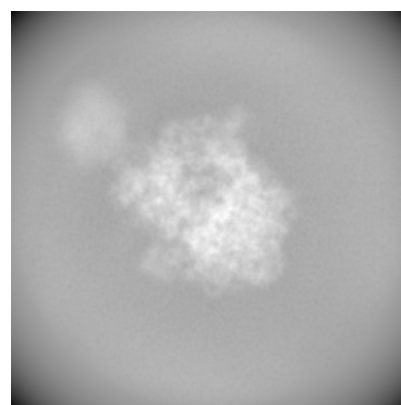
6.1.1 Primary map



X



Y

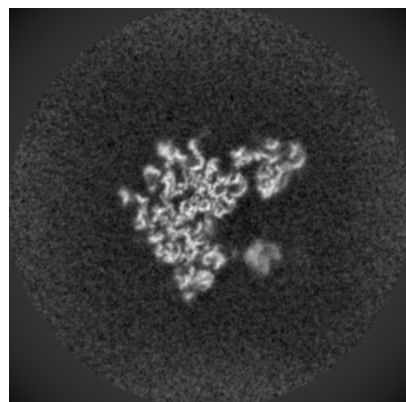


Z

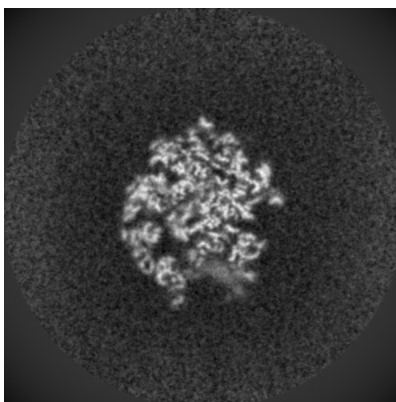
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

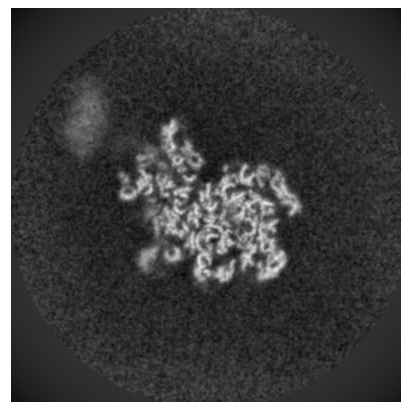
6.2.1 Primary map



X Index: 256



Y Index: 256

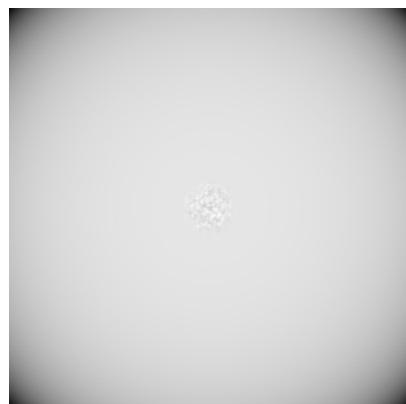


Z Index: 256

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: 0



Y Index: 0

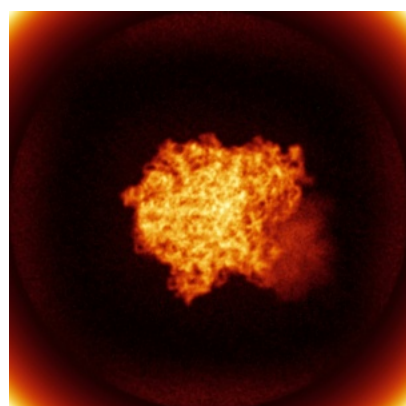


Z Index: 0

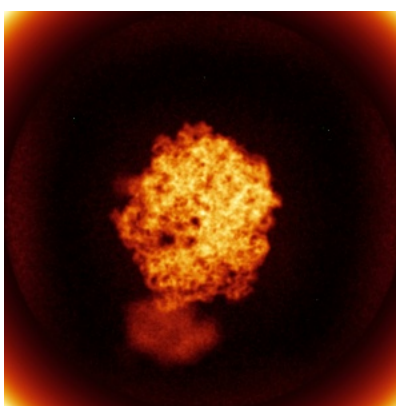
The images above show the largest variance slices of the map in three orthogonal directions.

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

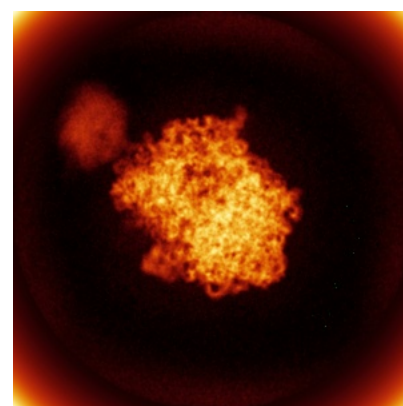
6.4.1 Primary map



X



Y

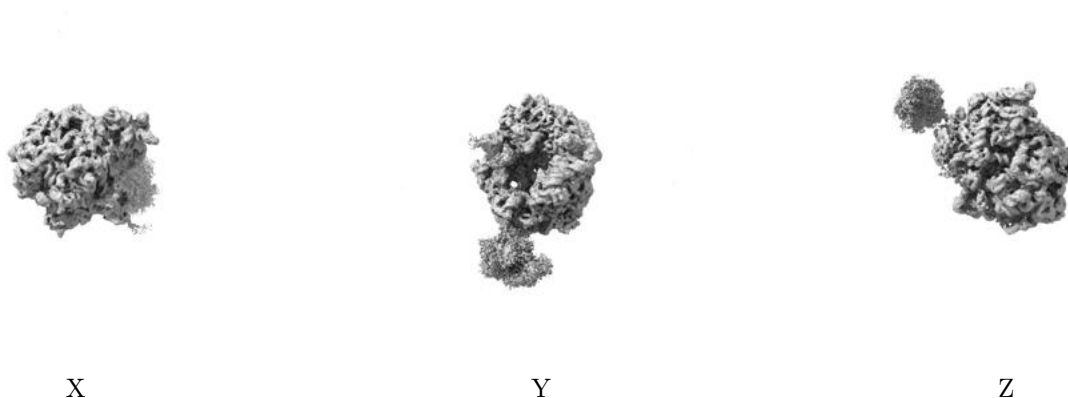


Z

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 0.00561. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

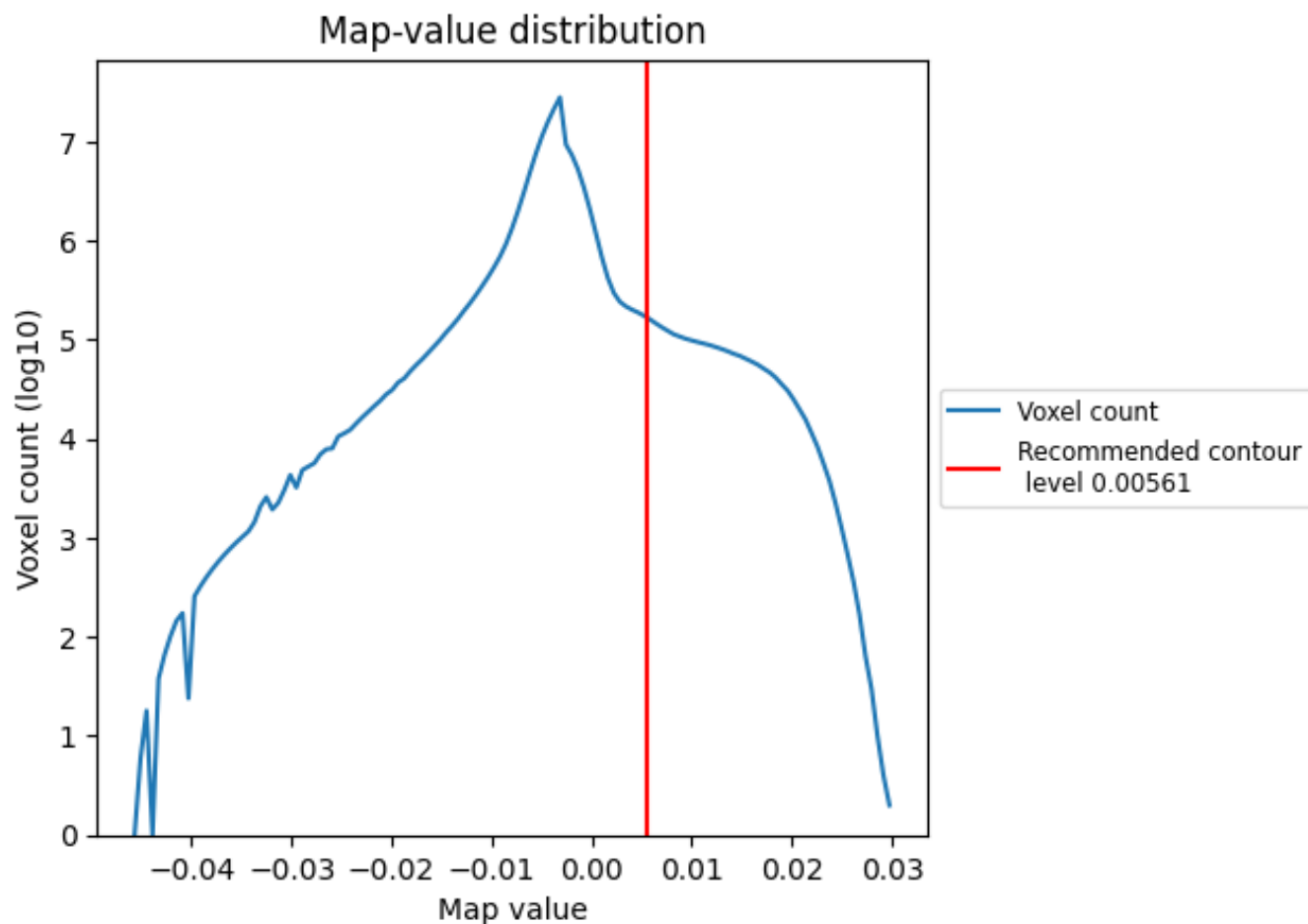
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

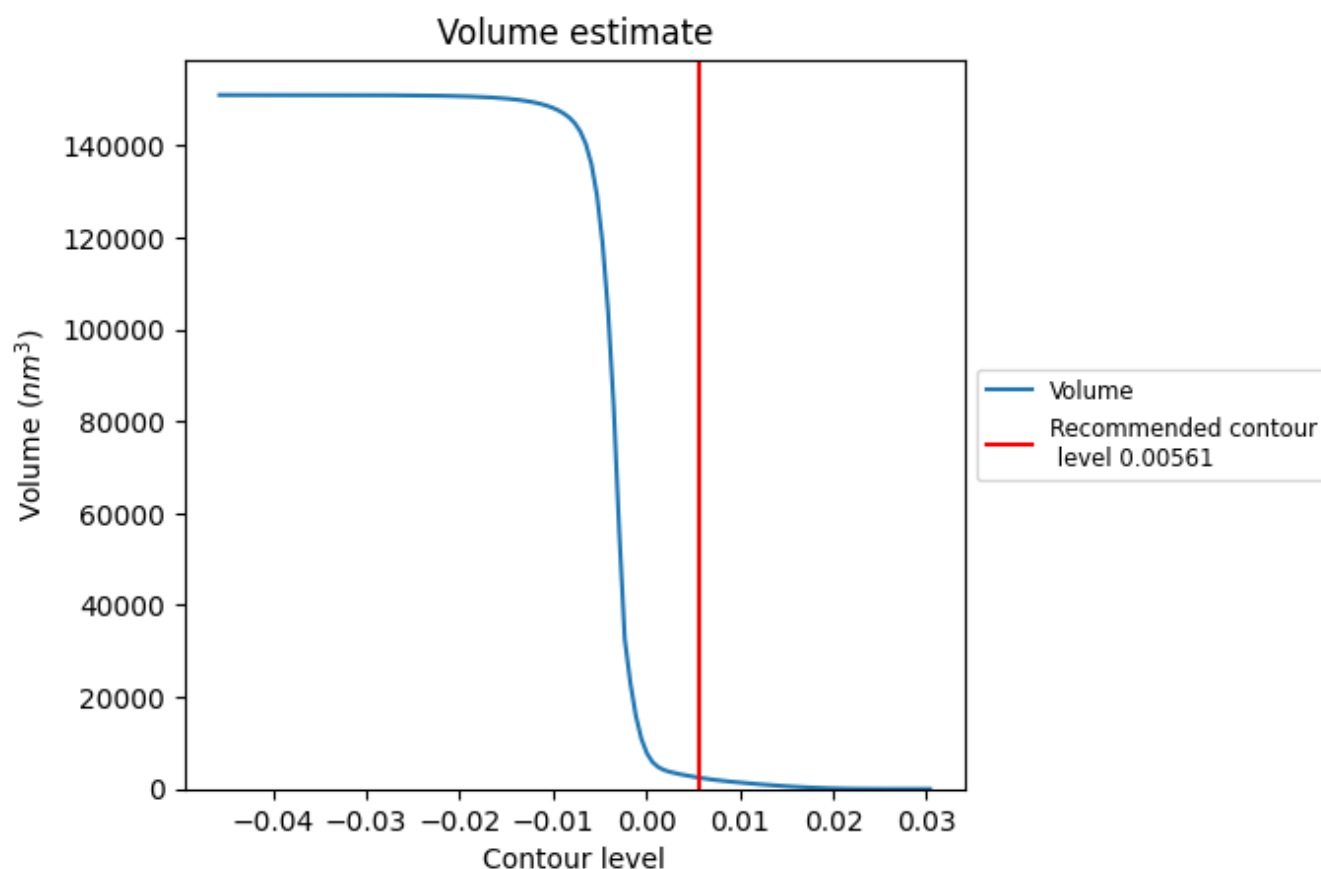
This section contains the results of statistical analysis of the map.

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.

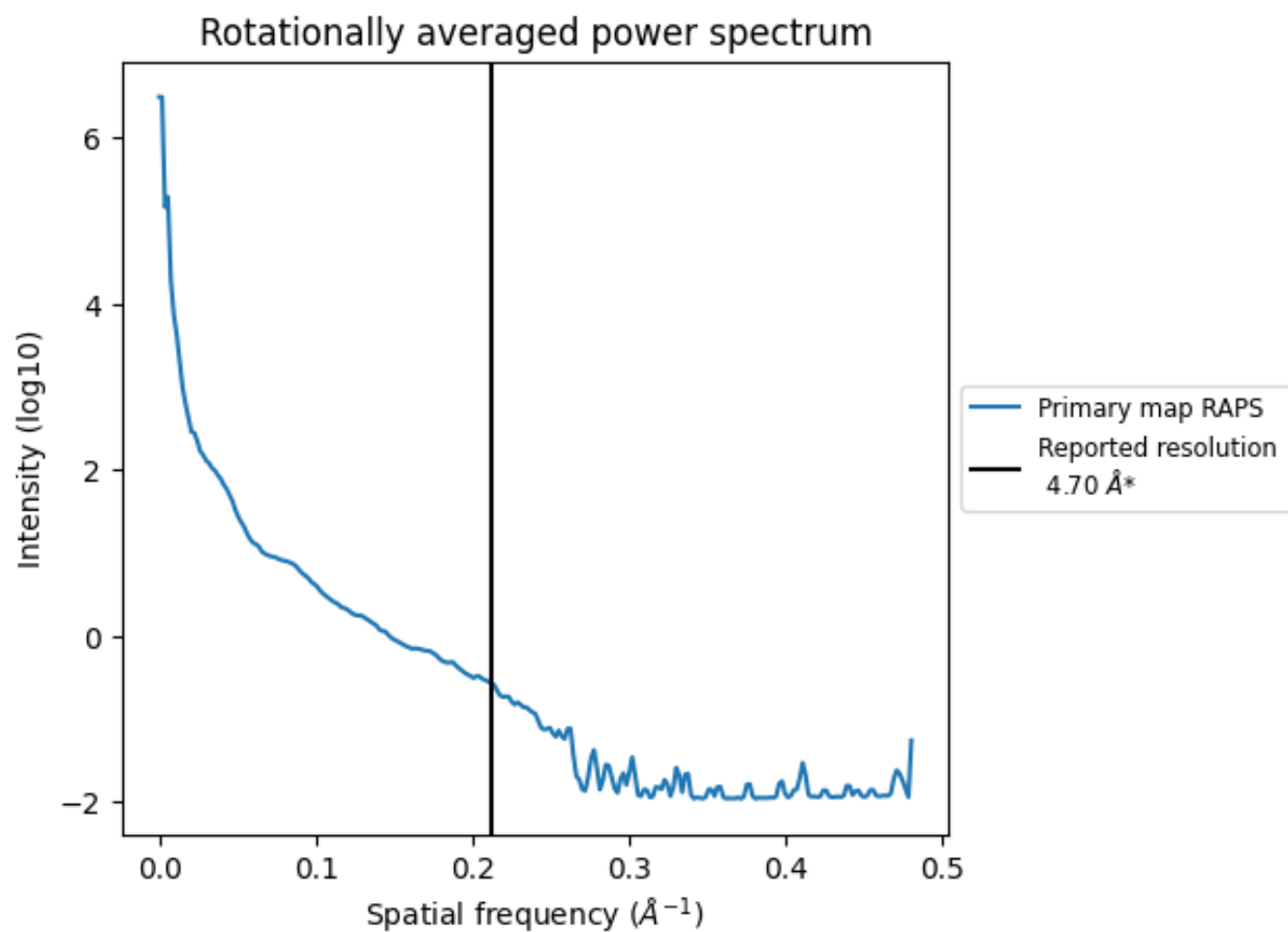
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2463 nm³; this corresponds to an approximate mass of 2225 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 0.213 Å⁻¹

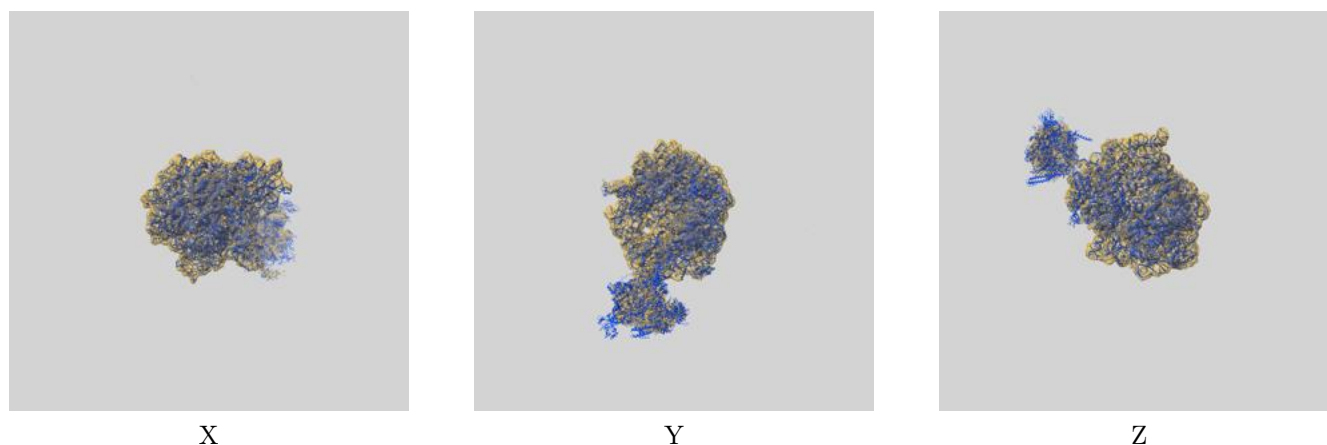
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

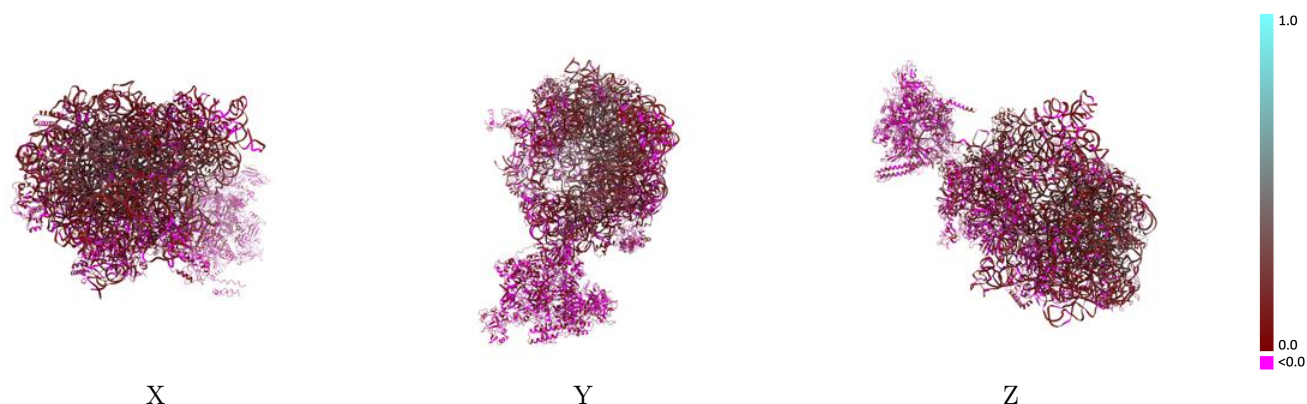
This section contains information regarding the fit between EMDB map EMD-22142 and PDB model 6XDR. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



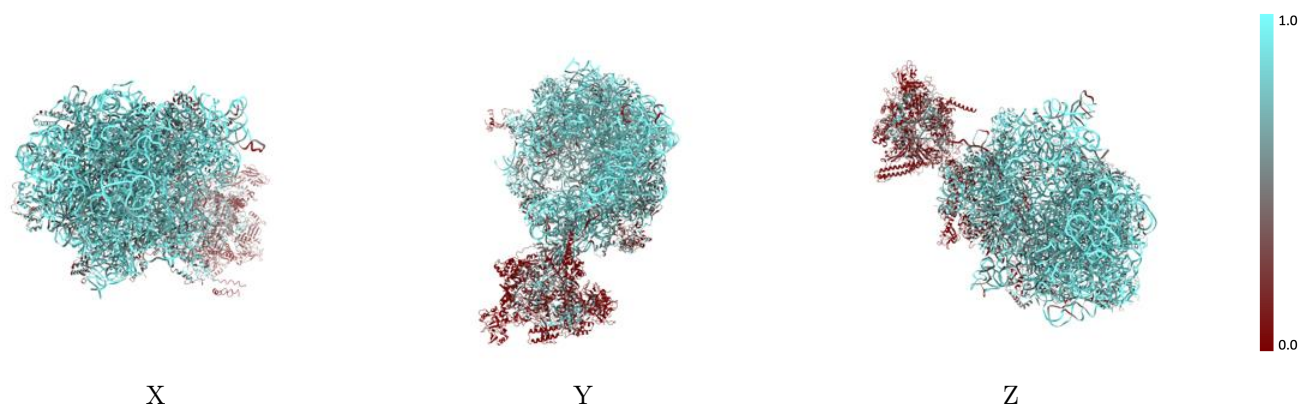
The images above show the 3D surface view of the map at the recommended contour level 0.00561 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



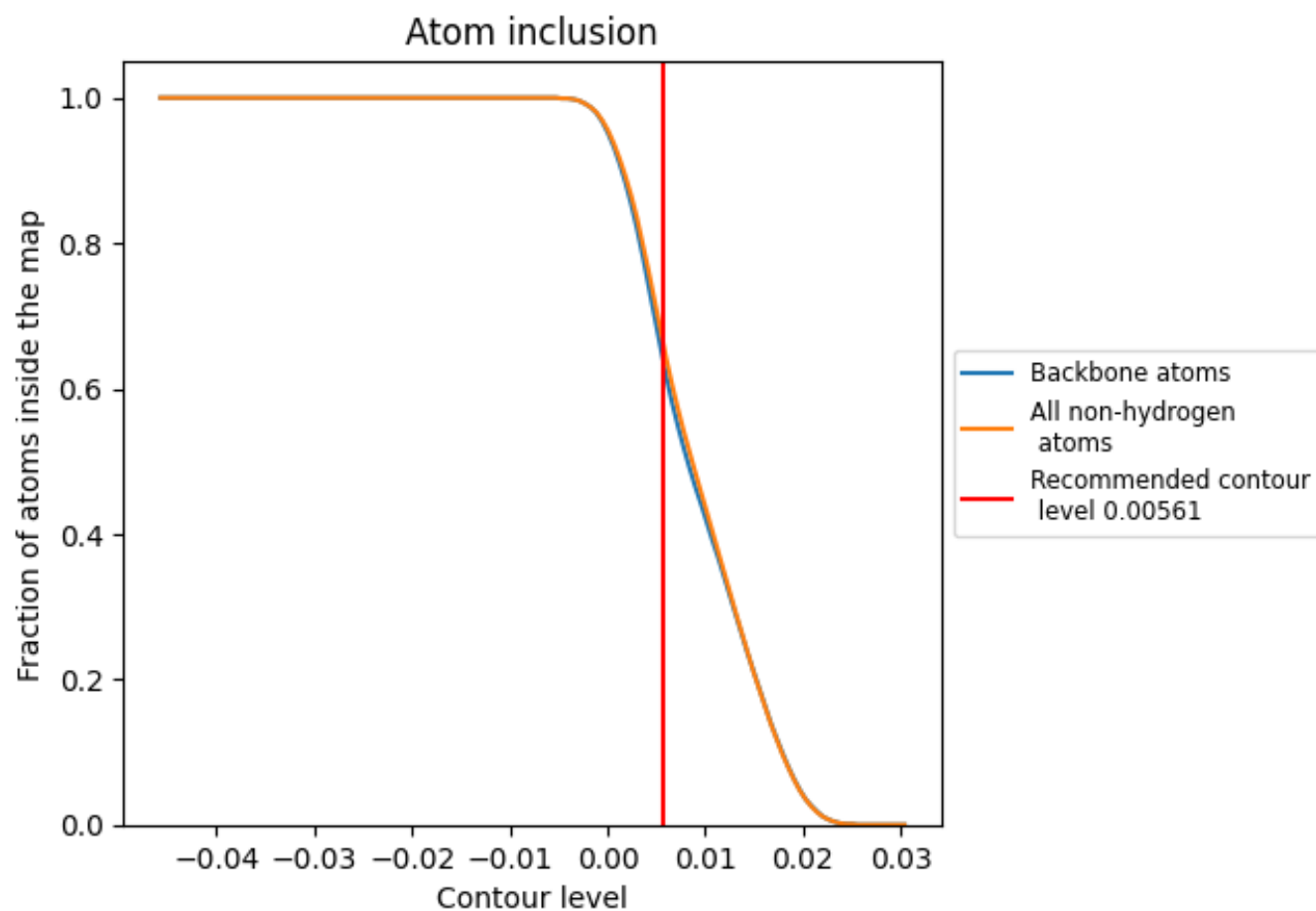
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00561).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 67% 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 (0.00561) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6680	 0.1070
0	 0.7420	 0.1220
1	 0.7890	 0.2450
2	 0.7220	 0.1010
3	 0.7710	 0.1020
4	 0.7560	 0.1040
5	 0.2730	 0.0330
6	 0.4170	 0.0410
7	 0.3970	 0.0630
9	 0.5570	 0.0390
A	 0.7780	 0.1070
AA	 0.2720	 0.0290
AB	 0.1760	 0.0840
AC	 0.1270	 0.0270
AD	 0.0540	 0.0130
AE	 0.2270	 0.0200
AF	 0.0270	 0.0140
B	 0.7760	 0.1310
C	 0.5330	 0.0400
D	 0.8660	 0.1230
E	 0.6710	 0.0850
F	 0.4720	 0.0640
G	 0.5050	 0.0490
H	 0.1990	 0.0420
I	 0.7480	 0.2030
J	 0.7610	 0.1840
K	 0.7430	 0.1450
L	 0.6500	 0.1040
M	 0.5250	 0.0530
N	 0.6290	 0.0660
O	 0.6230	 0.0370
P	 0.6650	 0.1190
Q	 0.6720	 0.0630
R	 0.6570	 0.1250
S	 0.6370	 0.0020



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Chain	Atom inclusion	Q-score
T	 0.5380	 0.0560
U	 0.7100	 0.0890
V	 0.6900	 0.0850
W	 0.6290	 0.0210
X	 0.6570	 0.0940
Y	 0.5290	 0.0530
Z	 0.0440	 0.0440
a	 0.8870	 0.1450
b	 0.6500	 -0.0120
c	 0.6790	 0.1070
d	 0.8570	 0.0770
e	 0.6830	 0.1190
f	 0.7870	 0.1190
g	 0.4250	 0.0960
h	 0.7240	 0.0940
i	 0.5440	 -0.0090
j	 0.7170	 0.1020
k	 0.3590	 0.0070
l	 0.6570	 0.0690
m	 0.7830	 0.1470
n	 0.6420	 0.0630
o	 0.6580	 0.0380
p	 0.7330	 0.1220
q	 0.7300	 0.0820
r	 0.5010	 0.0700
s	 0.8180	 0.1770
t	 0.7420	 0.2010
u	 0.5350	 0.0160
v	 0.7390	 0.1140
w	 0.7870	 0.1490
x	 0.5540	 -0.0010
y	 0.6910	 0.0980
z	 0.8390	 0.1820