



# Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 03:13 PM JST

PDB ID : 5X8P  
EMDB ID : EMD-6709  
Title : Structure of the 70S chloroplast ribosome from spinach  
Authors : Ahmed, T.; Shi, J.; Bhushan, S.  
Deposited on : 2017-03-03  
Resolution : 3.40 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

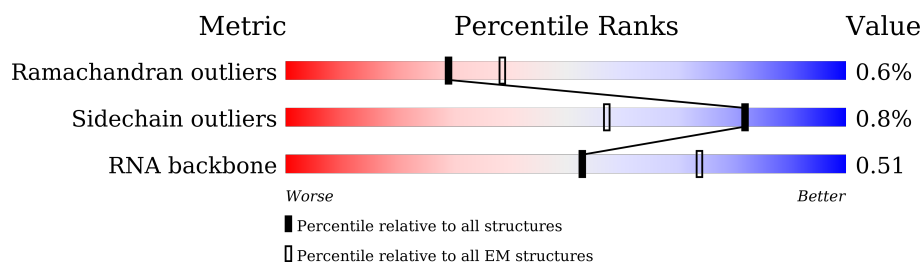
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	56	
2	2	65	
3	3	61	
4	4	73	
5	5	37	
6	6	142	
7	7	116	
8	B	121	

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Mol	Chain	Length	Quality of chain
9	C	271	
10	D	221	
11	E	243	
12	F	220	
13	G	182	
14	H	155	
15	K	197	
16	L	121	
17	M	192	
18	N	135	
19	O	116	
20	P	123	
21	Q	156	
22	R	127	
23	S	201	
24	T	199	
25	U	122	
26	V	145	
27	W	106	
28	X	137	
29	Y	77	
30	Z	109	
31	A	2810	
32	o	94	
33	b	236	

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Mol	Chain	Length	Quality of chain
34	c	218	
35	e	253	
36	f	146	
37	g	155	
38	h	134	
39	i	157	
40	j	122	
41	k	138	
42	l	123	
43	m	126	
44	o	90	
45	p	88	
46	q	108	
47	r	101	
48	s	92	
49	t	108	
50	u	137	
51	y	236	
52	a	1491	
53	w	121	
54	d	201	
55	v	198	
56	n	100	
57	x	47	
58	8	370	

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147126 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	46	Total	C	N	O	0	0
			378	250	70	58		

- Molecule 2 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	51	Total	C	N	O	S	0	0
			415	258	83	70	4		

- Molecule 3 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	57	Total	C	N	O	S	0	0
			445	268	103	71	3		

- Molecule 4 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	69	Total	C	N	O	S	0	0
			563	353	119	90	1		

- Molecule 5 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	37	Total	C	N	O	S	0	0
			304	186	70	44	4		

- Molecule 6 is a protein called protein cL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	49	Total	C	N	O	S	0	0
			422	268	92	57	5		

- Molecule 7 is a protein called protein cL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	46	Total	C	N	O	S	0	0
			368	237	71	59	1		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	117	Total	C	N	O	P	0	0
			2500	1116	452	815	117		

- Molecule 9 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	247	Total	C	N	O	S	0	0
			1904	1181	390	327	6		

- Molecule 10 is a protein called protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	212	Total	C	N	O	S	0	0
			1620	1025	295	289	11		

- Molecule 11 is a protein called 50S ribosomal protein L4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	210	Total	C	N	O	S	0	0
			1655	1052	308	292	3		

- Molecule 12 is a protein called 50S ribosomal protein L5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	175	Total	C	N	O	S	0	0
			1351	862	233	248	8		

- Molecule 13 is a protein called protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	173	Total	C	N	O	S	0	0
			1353	855	249	245	4		

- Molecule 14 is a protein called protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	53	Total	C	N	O	S	0	0
			423	280	74	68	1		

- Molecule 15 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	193	Total	C	N	O	S	0	0
			1568	1000	289	274	5		

- Molecule 16 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	121	Total	C	N	O	S	0	0
			942	588	179	170	5		

- Molecule 17 is a protein called protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	177	Total	C	N	O	S	0	0
			1342	836	264	236	6		

- Molecule 18 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	134	Total	C	N	O	S	0	0
			1067	672	217	173	5		

- Molecule 19 is a protein called protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	116	Total	C	N	O	S	0	0
			944	592	193	155	4		

- Molecule 20 is a protein called protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	120	Total	C	N	O	S	0	0
			947	589	183	170	5		

- Molecule 21 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	118	Total	C	N	O	S	0	0
			953	610	186	156	1		

- Molecule 22 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	115	Total	C	N	O	S	0	0
			996	633	208	153	2		

- Molecule 23 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	147	Total	C	N	O		0	0
			1171	759	202	210			

- Molecule 24 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	144	Total	C	N	O	S	0	0
			1149	731	210	200	8		

- Molecule 25 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	92	Total	C	N	O	S	0	0
			740	477	129	132	2		

- Molecule 26 is a protein called 50S ribosomal protein L24, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	124	Total	C	N	O	S	0	0
			993	624	187	180	2		

- Molecule 27 is a RNA chain called 4.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	102	Total	C	N	O	P	0	0
			2187	977	403	705	102		

- Molecule 28 is a protein called protein L27.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	X	100	Total	C	N	O		
			810	511	159	140	0	0

- Molecule 29 is a protein called protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	74	Total	C	N	O	S		
			605	385	121	98	1	0	0

- Molecule 30 is a protein called protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	90	Total	C	N	O	S		
			754	470	150	131	3	0	0

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A	2809	Total	C	N	O	P		
			60324	26912	11166	19437	2809	0	0

- Molecule 32 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	0	64	Total	C	N	O	S		
			521	330	89	100	2	0	0

- Molecule 33 is a protein called 30S ribosomal protein S2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	227	Total	C	N	O	S		
			1787	1127	326	321	13	0	0

- Molecule 34 is a protein called 30S ribosomal protein S3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	213	Total	C	N	O	S		
			1719	1099	310	304	6	0	0

- Molecule 35 is a protein called 30S ribosomal protein S5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	171	Total	C	N	O	S	0	0
			1292	806	250	230	6		

- Molecule 36 is a protein called 30S ribosomal protein S6 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	111	Total	C	N	O	S	0	0
			886	566	145	171	4		

- Molecule 37 is a protein called 30S ribosomal protein S7, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	149	Total	C	N	O	S	0	0
			1161	723	231	204	3		

- Molecule 38 is a protein called 30S ribosomal protein S8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	134	Total	C	N	O	S	0	0
			1088	684	211	187	6		

- Molecule 39 is a protein called 30S ribosomal protein S9, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	133	Total	C	N	O	S	0	0
			1020	650	191	178	1		

- Molecule 40 is a protein called protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	98	Total	C	N	O	S	0	0
			796	512	142	137	5		

- Molecule 41 is a protein called 30S ribosomal protein S11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	118	Total	C	N	O	S	0	0
			887	549	182	151	5		

- Molecule 42 is a protein called 30S ribosomal protein S12, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	123	Total	C	N	O	S	0	0
			967	604	198	162	3		

- Molecule 43 is a protein called 30S ribosomal protein S13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	110	Total	C	N	O	S	0	0
			898	559	183	153	3		

- Molecule 44 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	62	Total	C	N	O	S	0	0
			525	339	100	85	1		

- Molecule 45 is a protein called 30S ribosomal protein S16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	80	Total	C	N	O	S	0	0
			664	425	123	114	2		

- Molecule 46 is a protein called protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	78	Total	C	N	O	S	0	0
			635	399	124	108	4		

- Molecule 47 is a protein called 30S ribosomal protein S18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	64	Total	C	N	O	S	0	0
			518	326	101	90	1		

- Molecule 48 is a protein called 30S ribosomal protein S19 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	78	Total	C	N	O	S	0	0
			627	403	118	104	2		

- Molecule 49 is a protein called protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	105	Total	C	N	O	S	0	0
			832	514	169	148	1		

- Molecule 50 is a protein called protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	44	Total	C	N	O	S	0	0
			393	238	87	66	2		

- Molecule 51 is a protein called protein plastid pY.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	108	Total	C	N	O	S	0	0
			845	521	164	159	1		

- Molecule 52 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a	1480	Total	C	N	O	P	0	0
			31777	14168	5863	10266	1480		

- Molecule 53 is a protein called protein cS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	84	Total	C	N	O	S	0	0
			689	454	115	118	2		

- Molecule 54 is a protein called 30S ribosomal protein S4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	d	199	Total	C	N	O	S	0	0
			1633	1032	319	278	4		

- Molecule 55 is a protein called protein cS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v	190	Total	C	N	O	S	0	0
			1464	908	255	298	3		

- Molecule 56 is a protein called 30S ribosomal protein S14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	n	99	Total	C	N	O	S	0	0
			819	507	174	135	3		

- Molecule 57 is a protein called protein bTHXc.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	x	37	Total	C	N	O	0	0
			289	179	65	45		

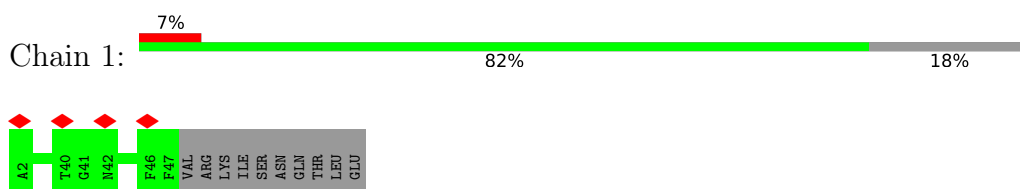
- Molecule 58 is a protein called 30S ribosomal protein S1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	8	154	Total	C	N	O	S	0	0
			1201	744	222	227	8		

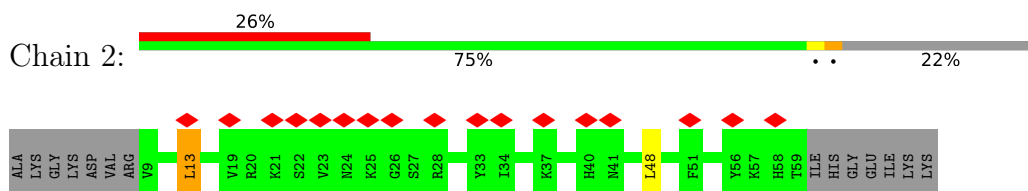
### 3 Residue-property plots [i](#)

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.

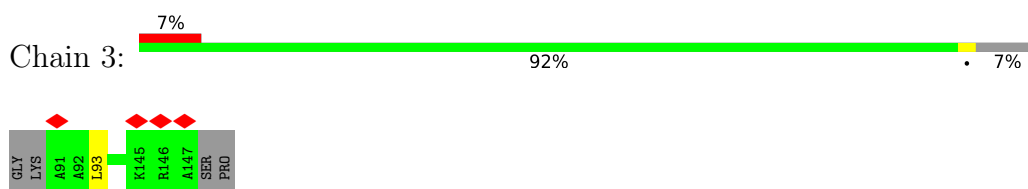
- Molecule 1: 50S ribosomal protein L32, chloroplastic



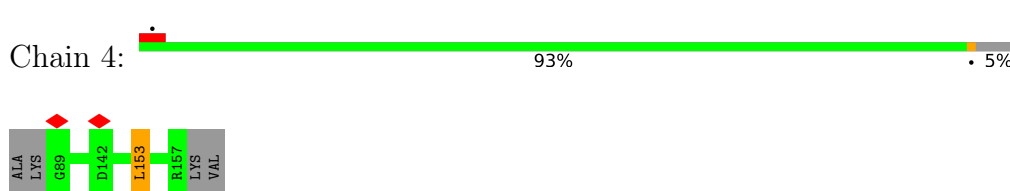
- Molecule 2: 50S ribosomal protein L33, chloroplastic



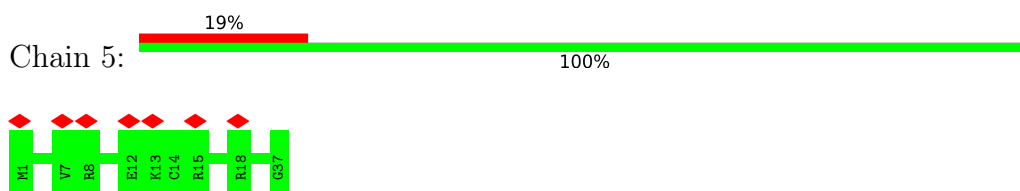
- Molecule 3: 50S ribosomal protein L34, chloroplastic



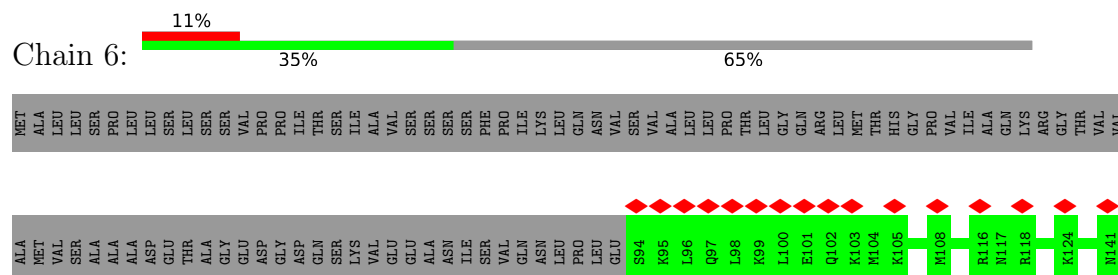
- Molecule 4: 50S ribosomal protein L35, chloroplastic



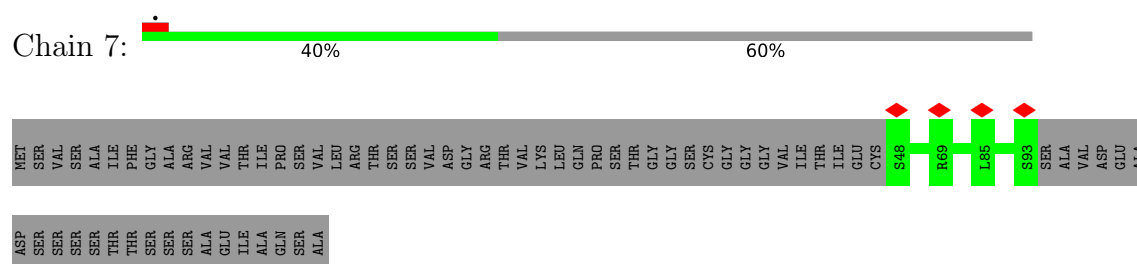
- Molecule 5: 50S ribosomal protein L36, chloroplastic



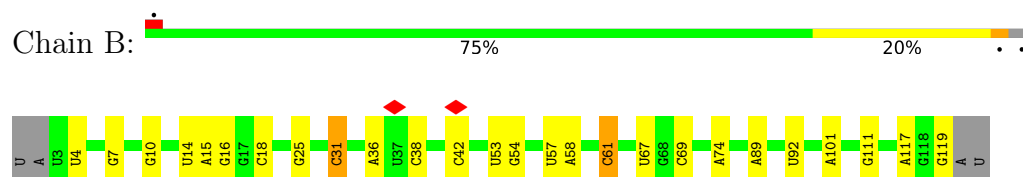
- Molecule 6: protein cL37



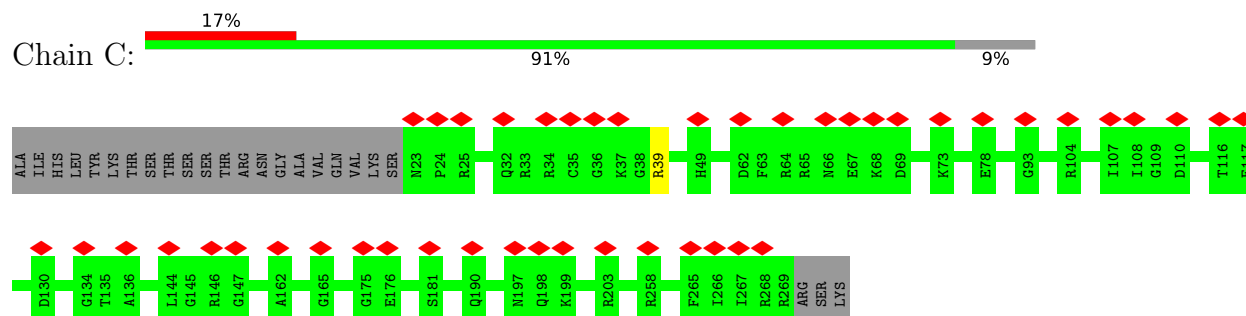
- Molecule 7: protein cL38



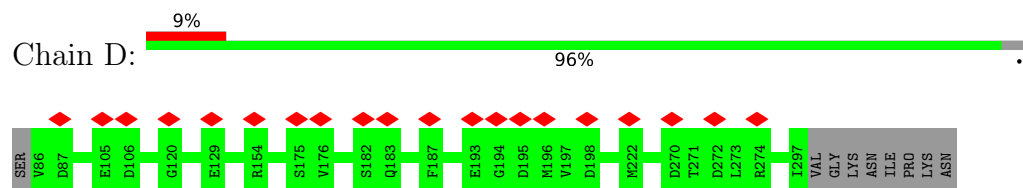
- Molecule 8: 5S rRNA



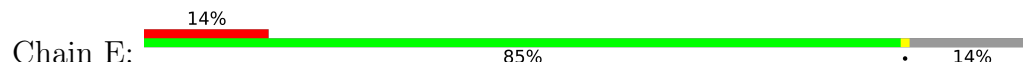
- Molecule 9: 50S ribosomal protein L2, chloroplastic

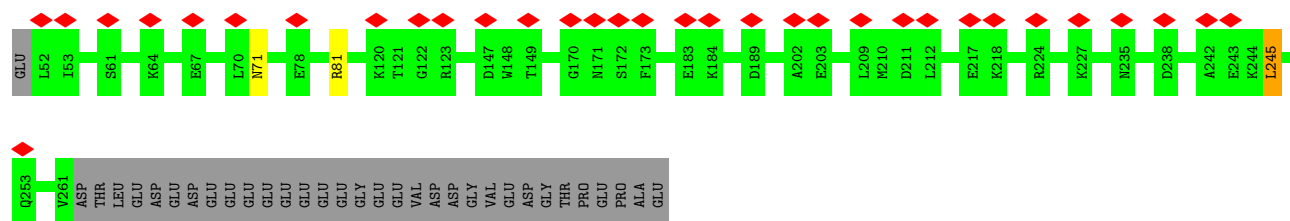


- Molecule 10: protein L3



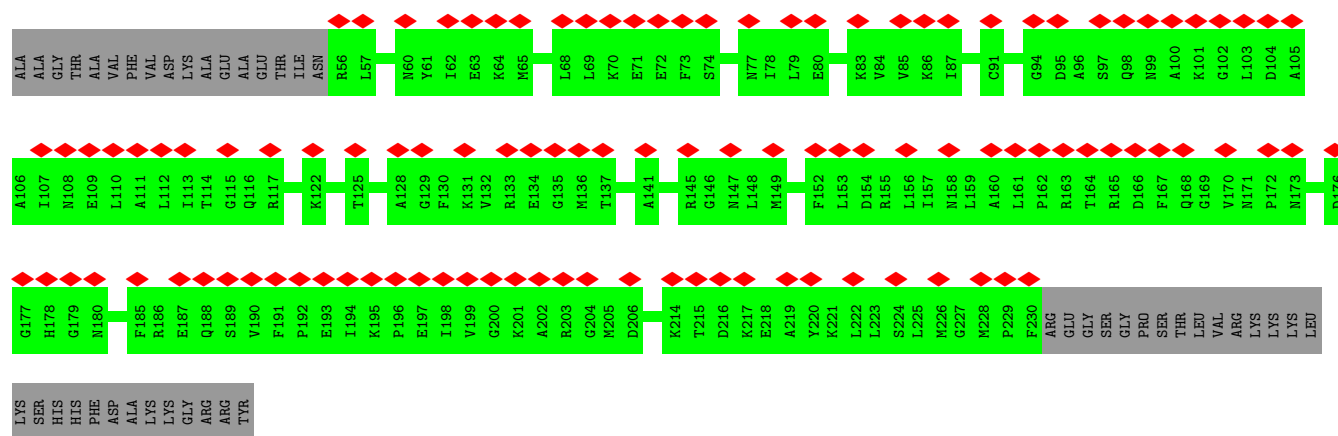
- Molecule 11: 50S ribosomal protein L4, chloroplastic





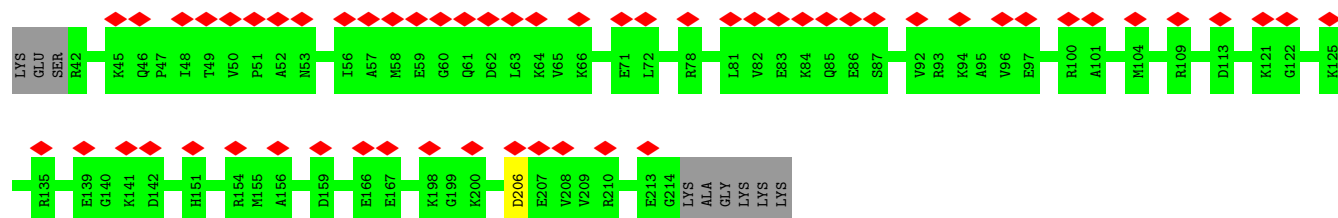
- Molecule 12: 50S ribosomal protein L5, chloroplastic

Chain F:



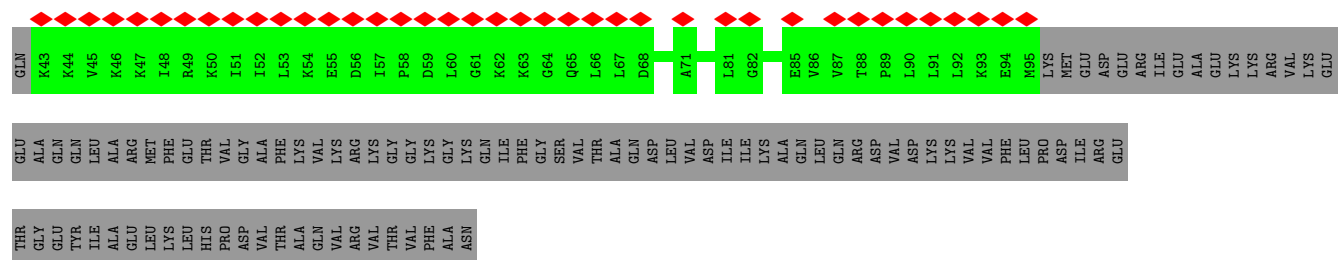
- Molecule 13: protein L6

Chain G:



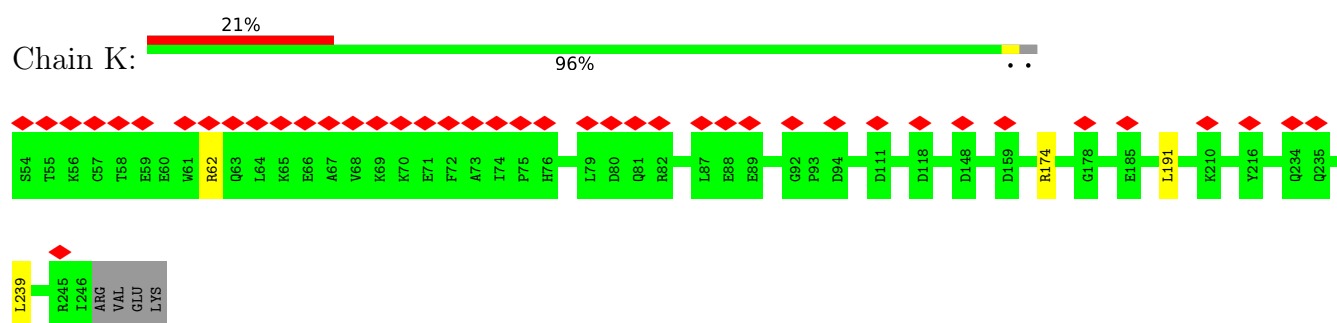
- Molecule 14: protein L9

Chain H:

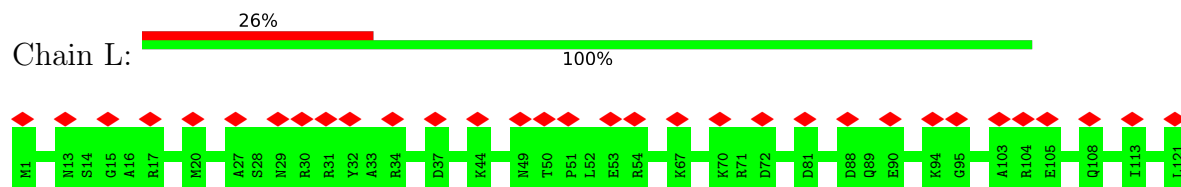


- Molecule 15: 50S ribosomal protein L13, chloroplastic

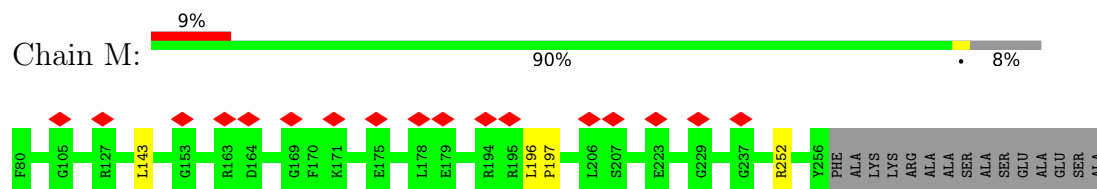




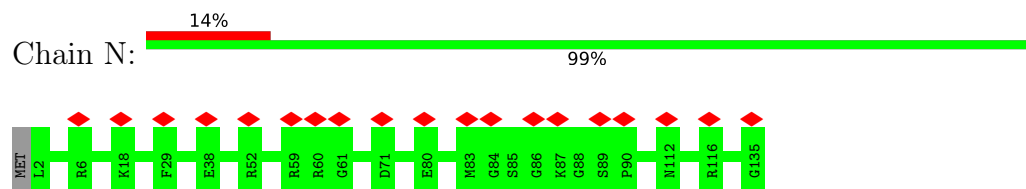
- Molecule 16: 50S ribosomal protein L14, chloroplastic



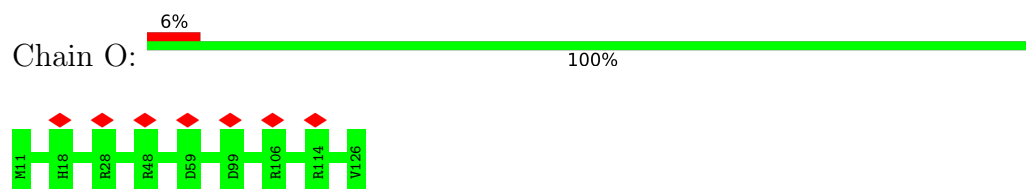
- Molecule 17: protein L15



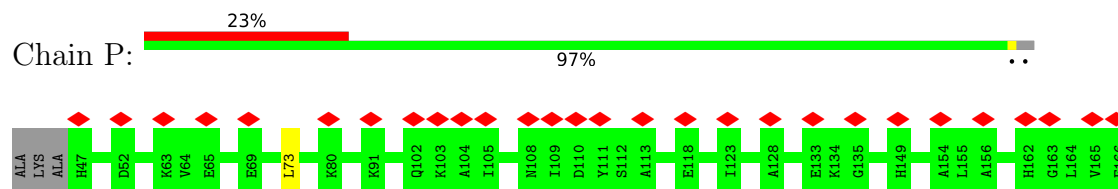
- Molecule 18: 50S ribosomal protein L16, chloroplastic



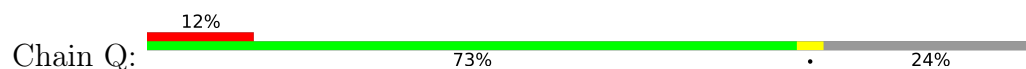
- Molecule 19: protein L17

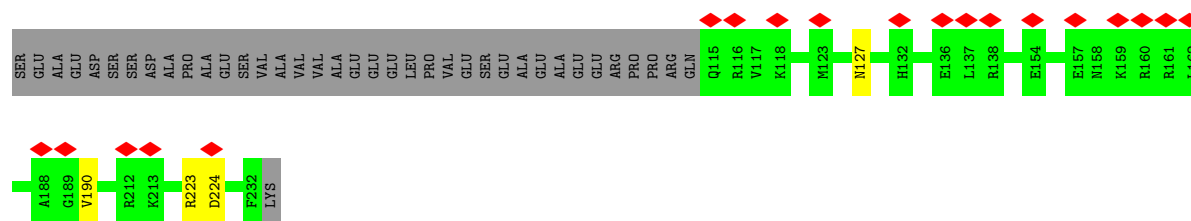


- Molecule 20: protein L18

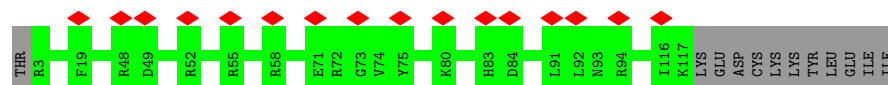


- Molecule 21: 50S ribosomal protein L19, chloroplastic

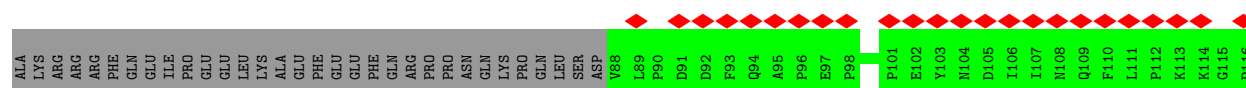
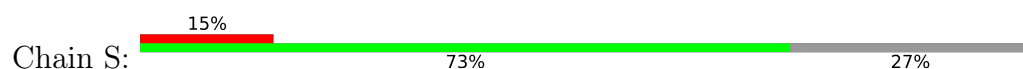




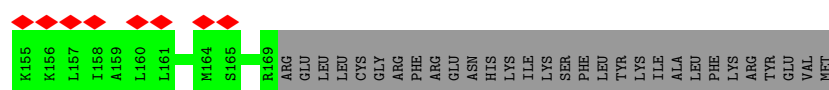
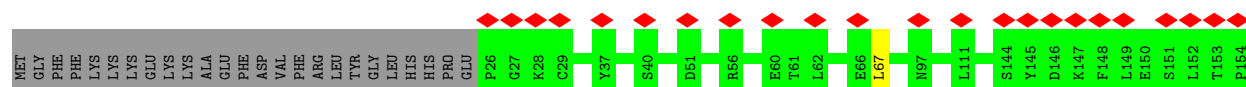
- Molecule 22: 50S ribosomal protein L20, chloroplastic



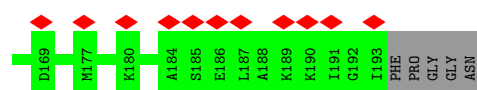
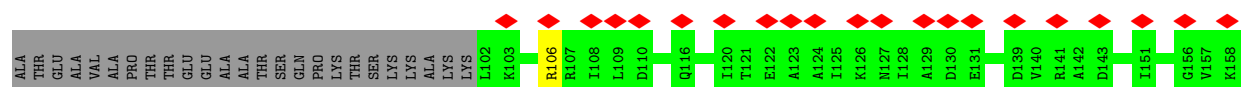
- Molecule 23: 50S ribosomal protein L21, chloroplastic



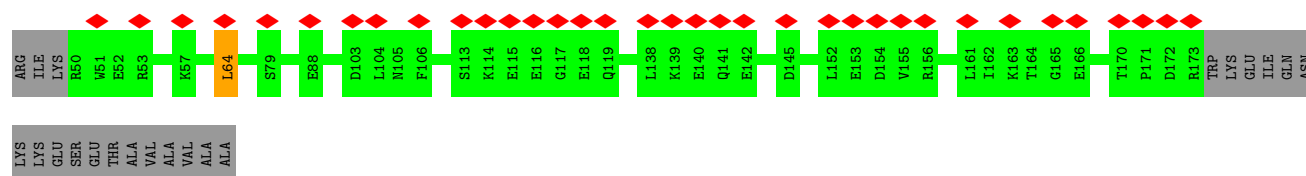
- Molecule 24: 50S ribosomal protein L22, chloroplastic



- Molecule 25: 50S ribosomal protein L23, chloroplastic



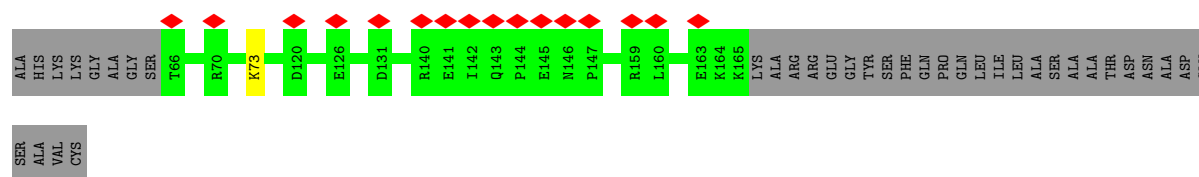
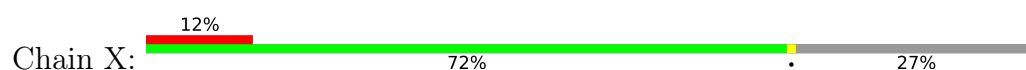
- Molecule 26: 50S ribosomal protein L24, chloroplastic



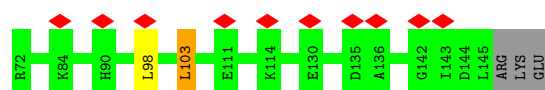
• Molecule 27: 4.8S rRNA



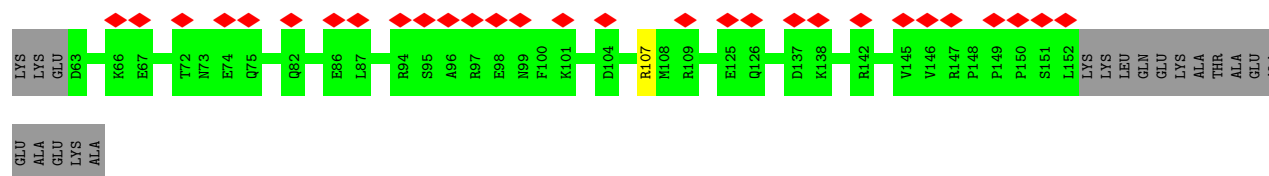
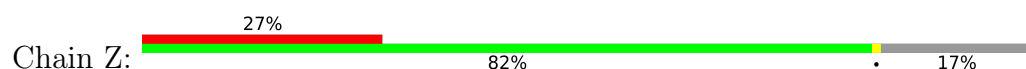
• Molecule 28: protein L27



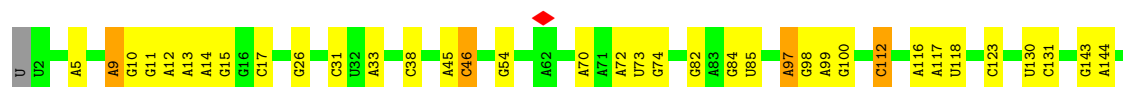
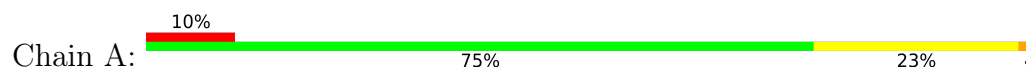
• Molecule 29: protein L28

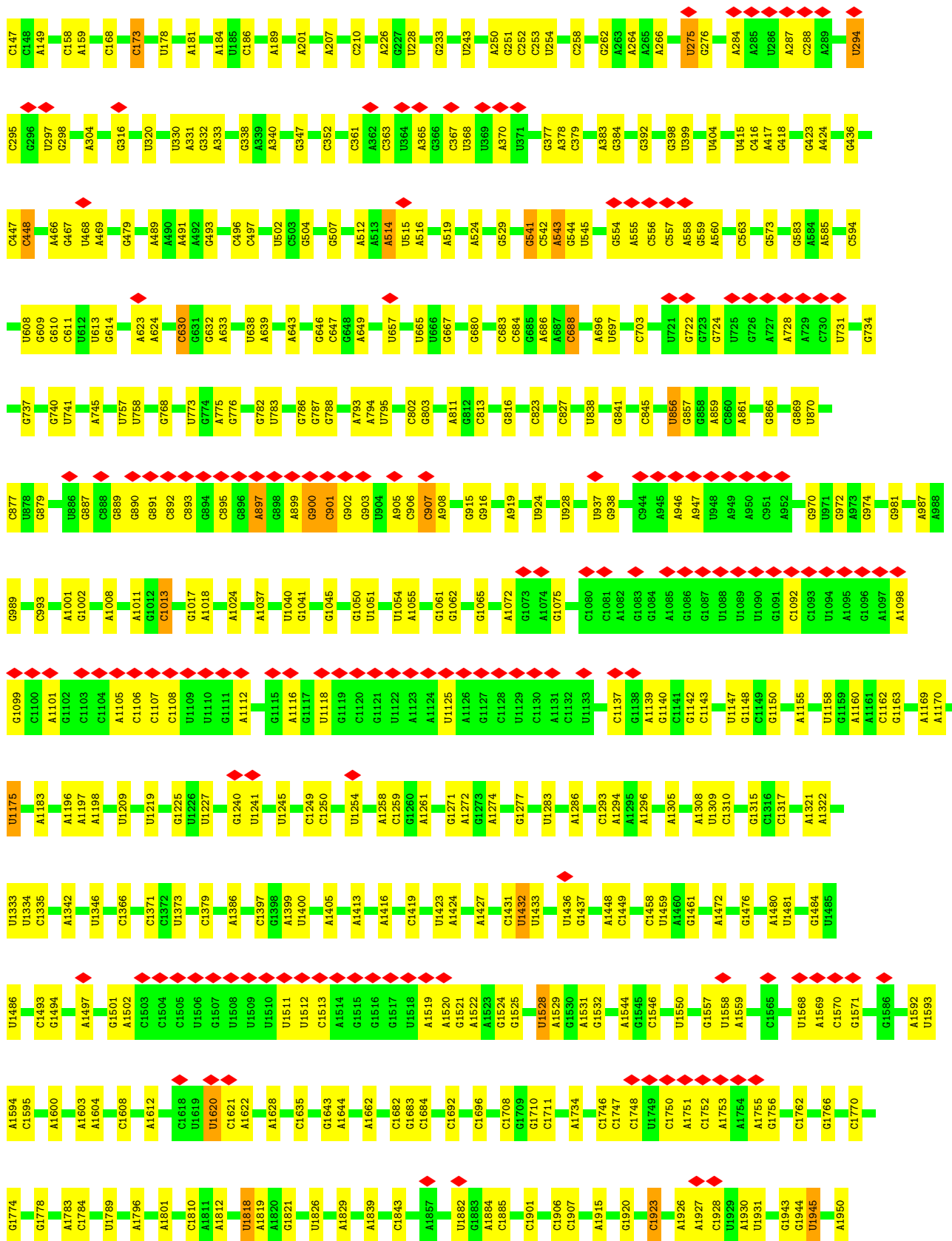


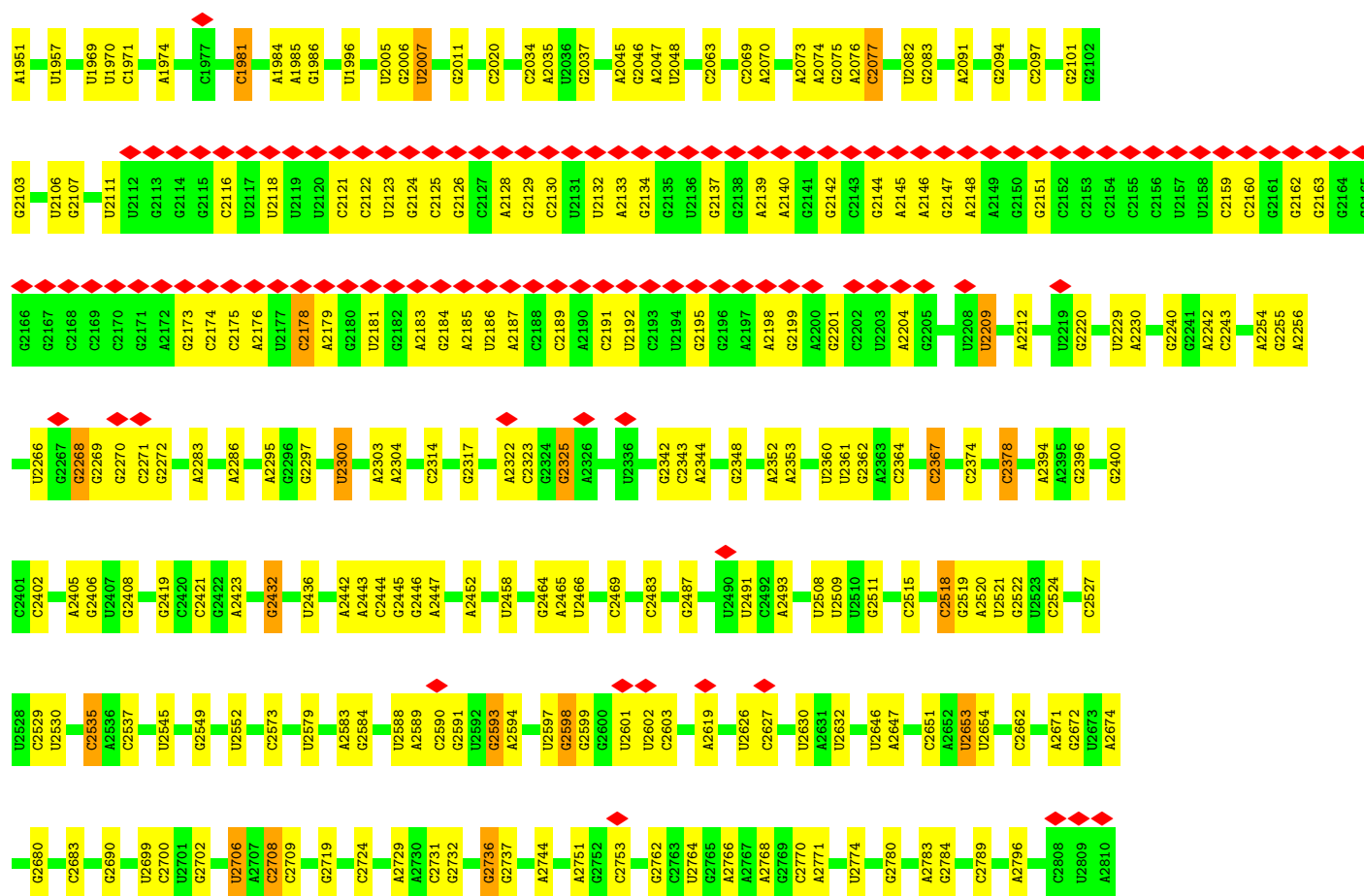
• Molecule 30: protein L29



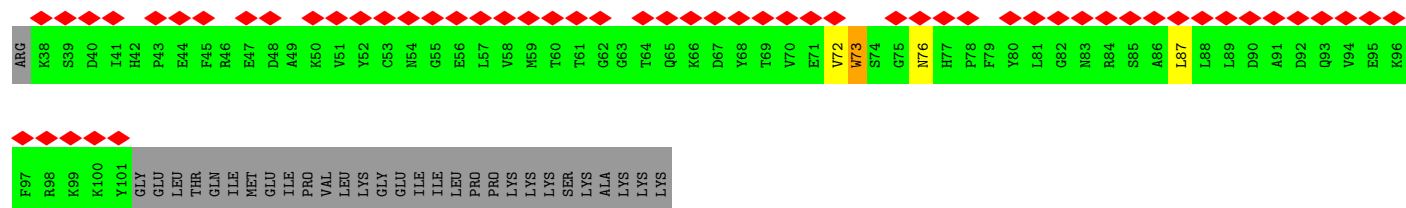
• Molecule 31: 23S rRNA



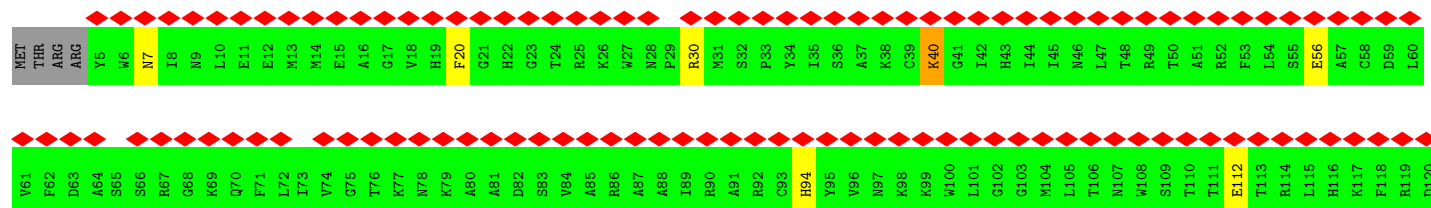
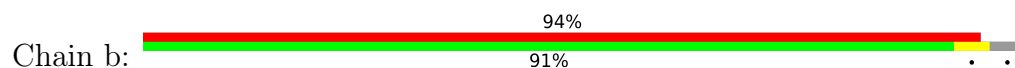


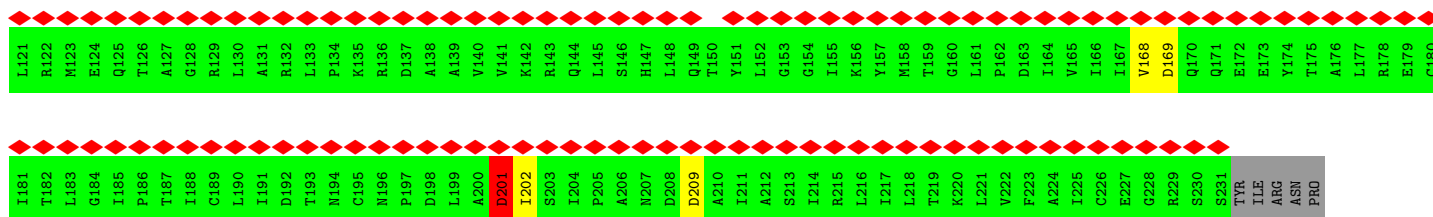


• Molecule 32: 50S ribosomal protein L31



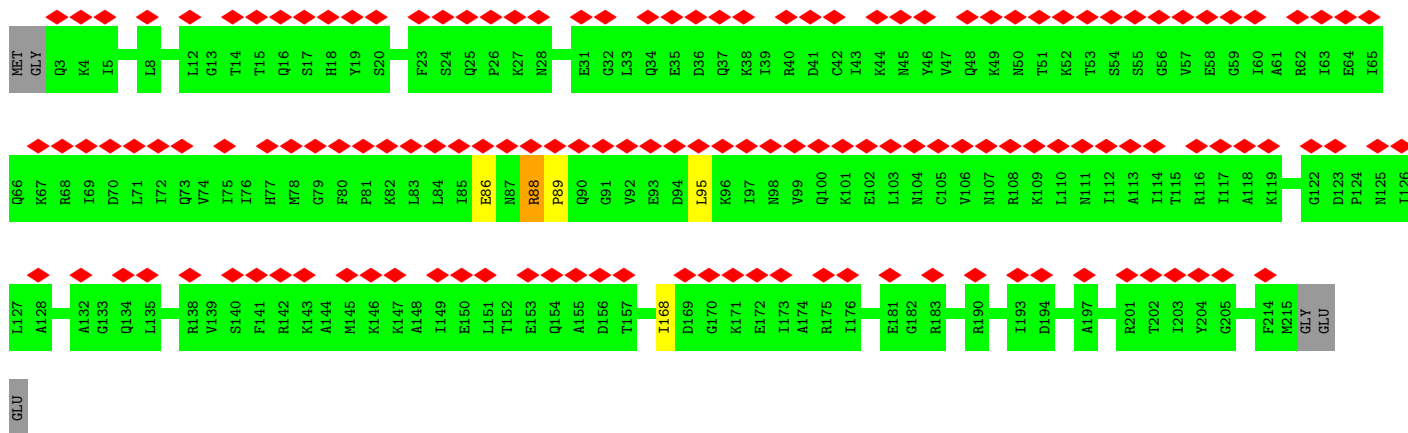
• Molecule 33: 30S ribosomal protein S2, chloroplastic





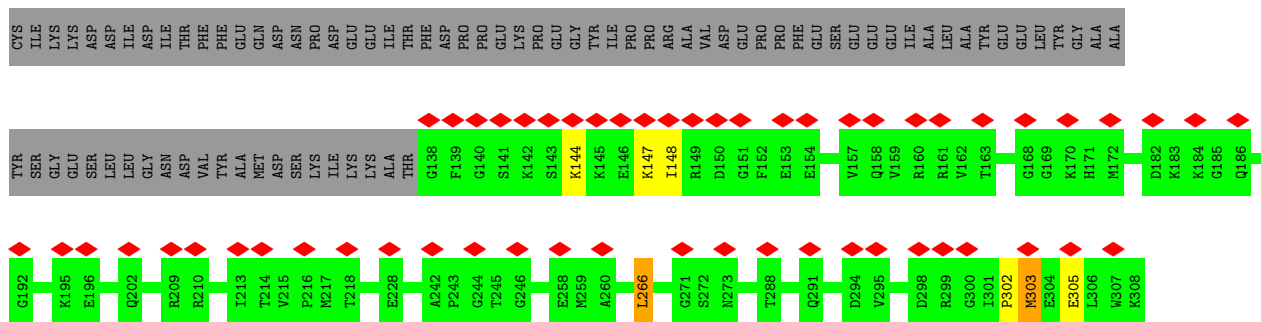
- Molecule 34: 30S ribosomal protein S3, chloroplastic

Chain c:



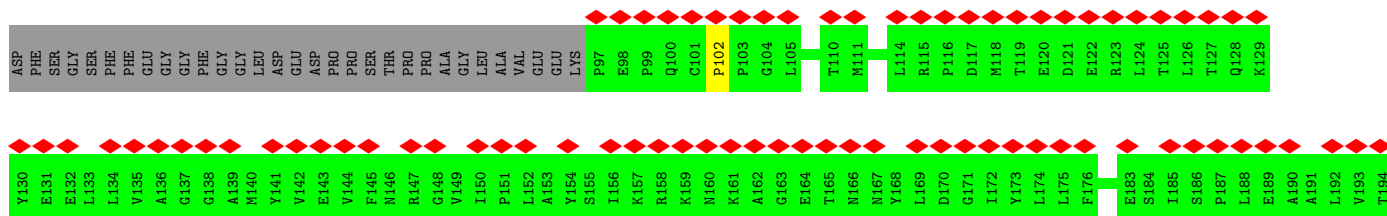
- Molecule 35: 30S ribosomal protein S5, chloroplastic

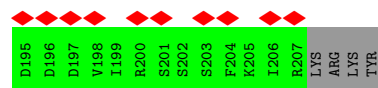
Chain e:



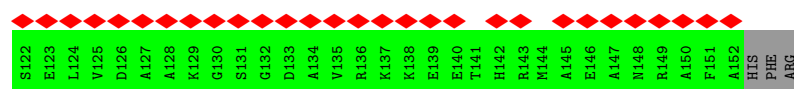
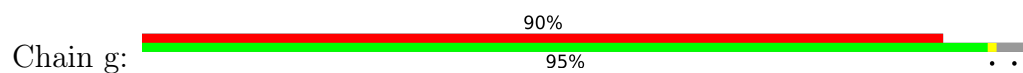
- Molecule 36: 30S ribosomal protein S6 alpha, chloroplastic

Chain f:

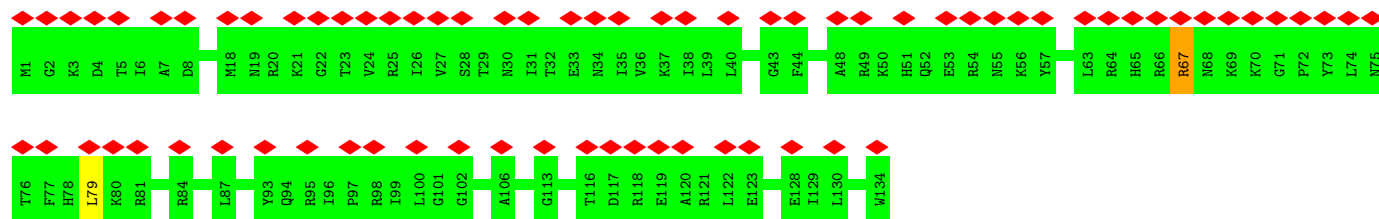




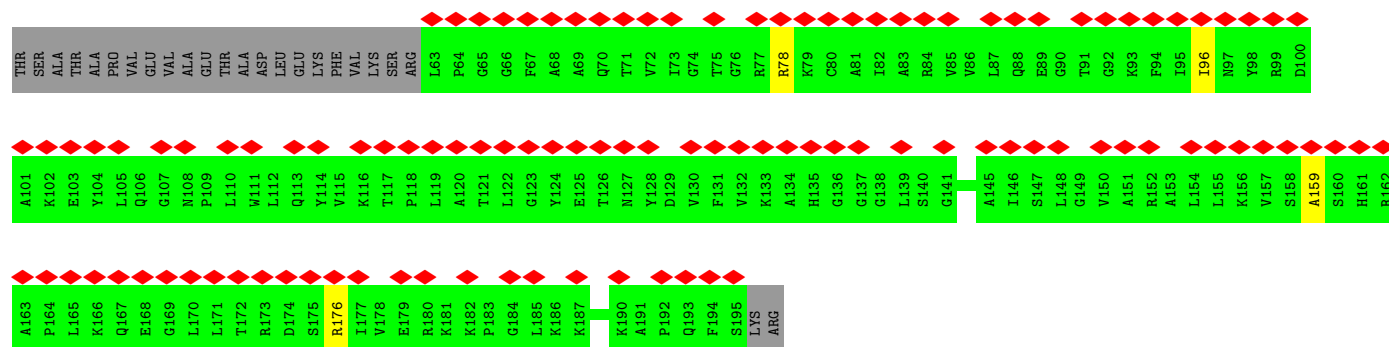
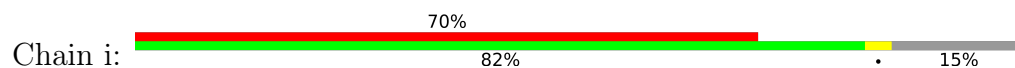
- Molecule 37: 30S ribosomal protein S7, chloroplastic



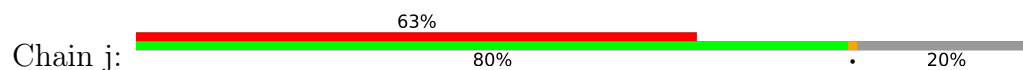
- Molecule 38: 30S ribosomal protein S8, chloroplastic

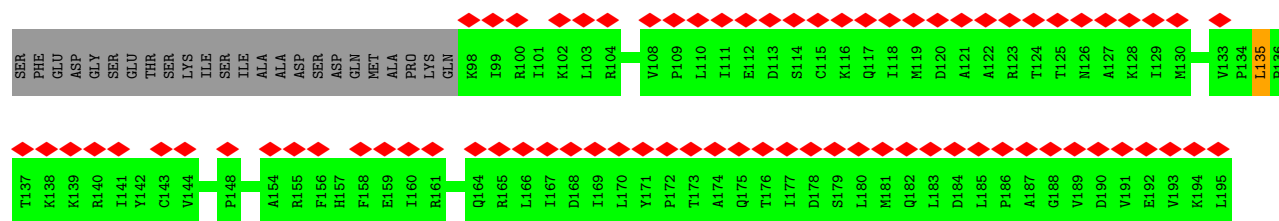


- Molecule 39: 30S ribosomal protein S9, chloroplastic

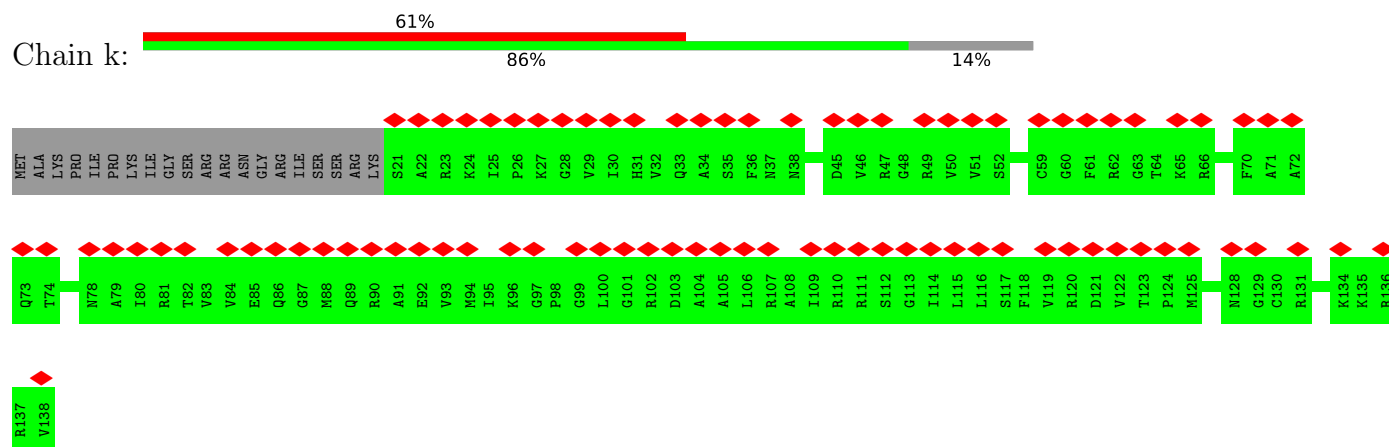


- Molecule 40: protein S10

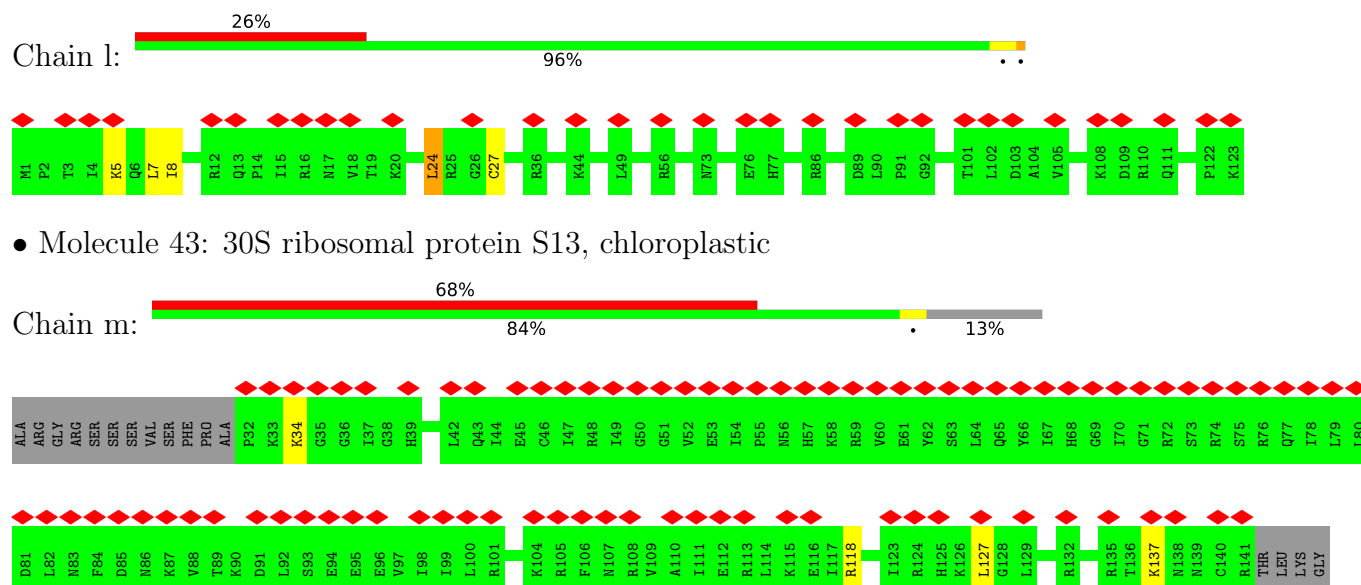




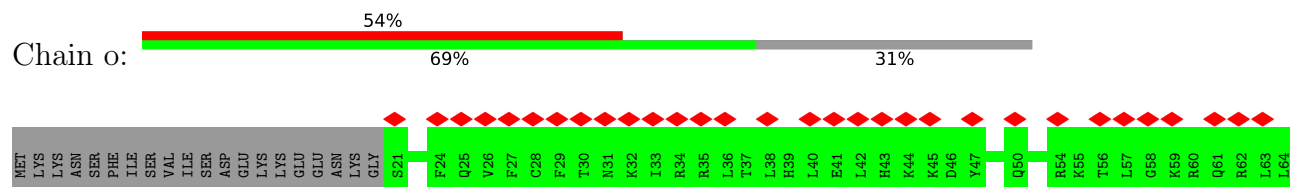
- Molecule 41: 30S ribosomal protein S11, chloroplastic



- Molecule 42: 30S ribosomal protein S12, chloroplastic

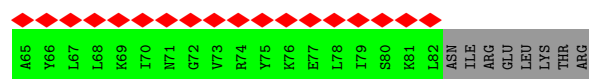


- Molecule 43: 30S ribosomal protein S13, chloroplastic

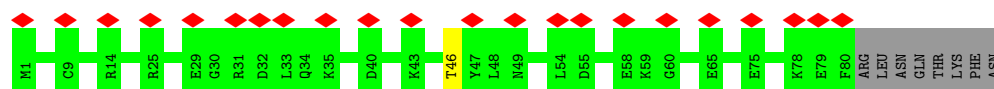
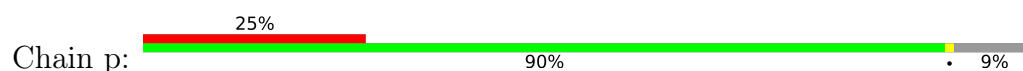


- Molecule 44: 30S ribosomal protein S15, chloroplastic

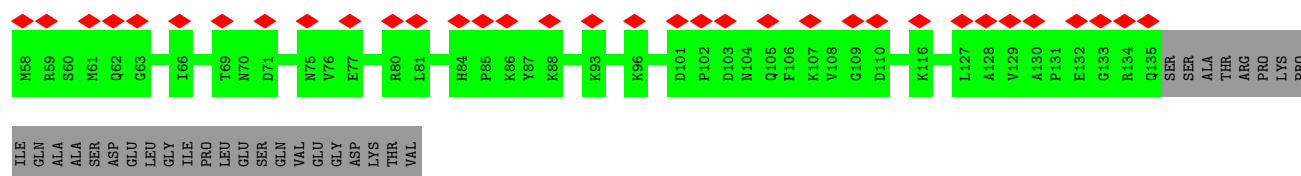




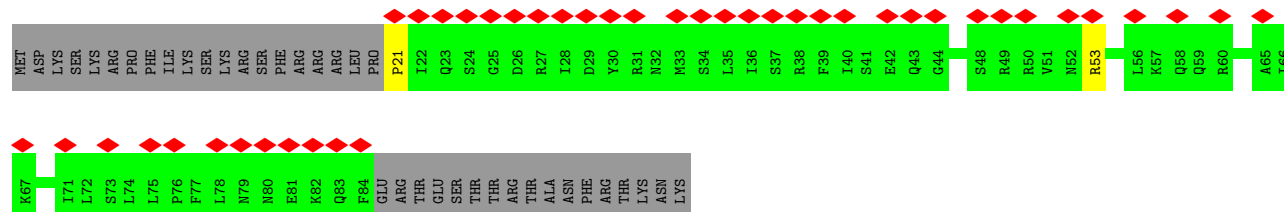
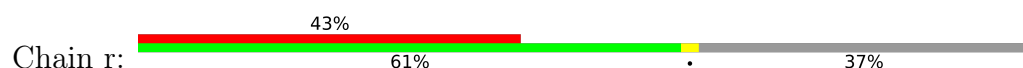
- Molecule 45: 30S ribosomal protein S16, chloroplactic



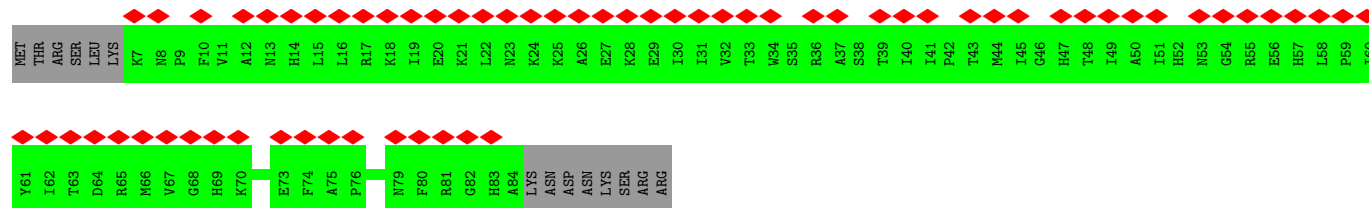
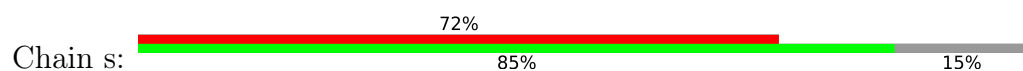
- Molecule 46: protein S17



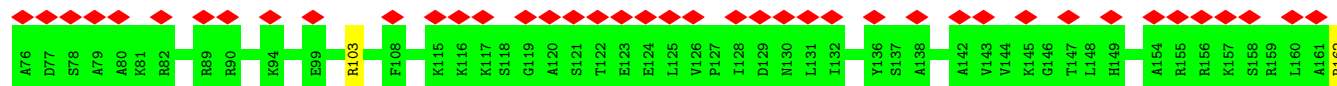
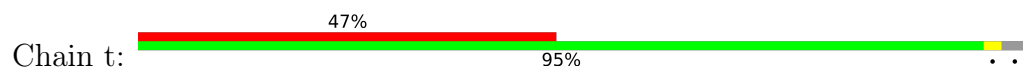
- Molecule 47: 30S ribosomal protein S18, chloroplactic



- Molecule 48: 30S ribosomal protein S19 alpha, chloroplactic



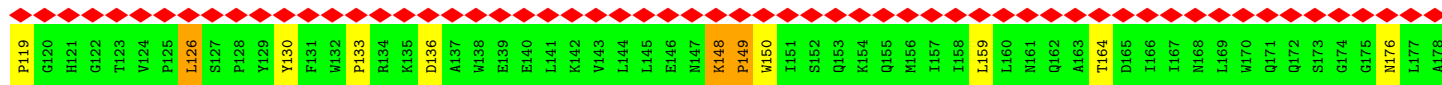
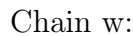
- Molecule 49: protein S20





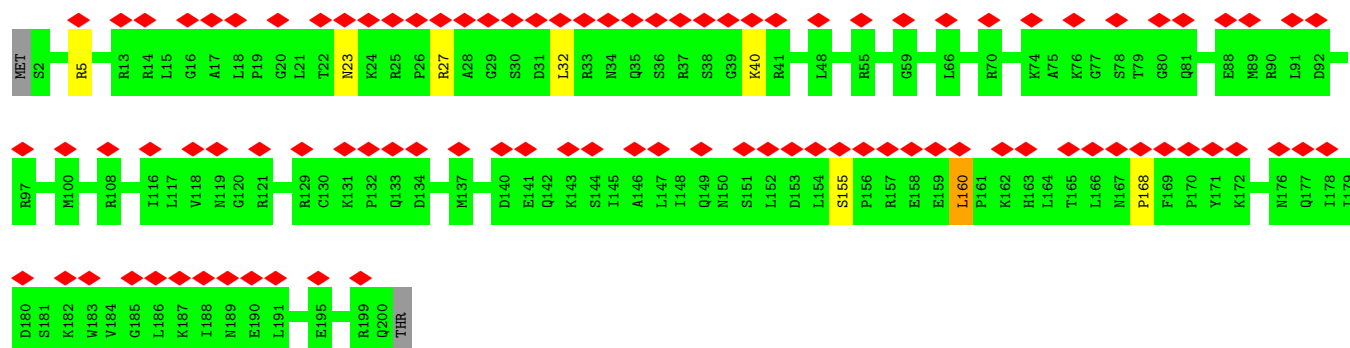


- Molecule 53: protein cS23

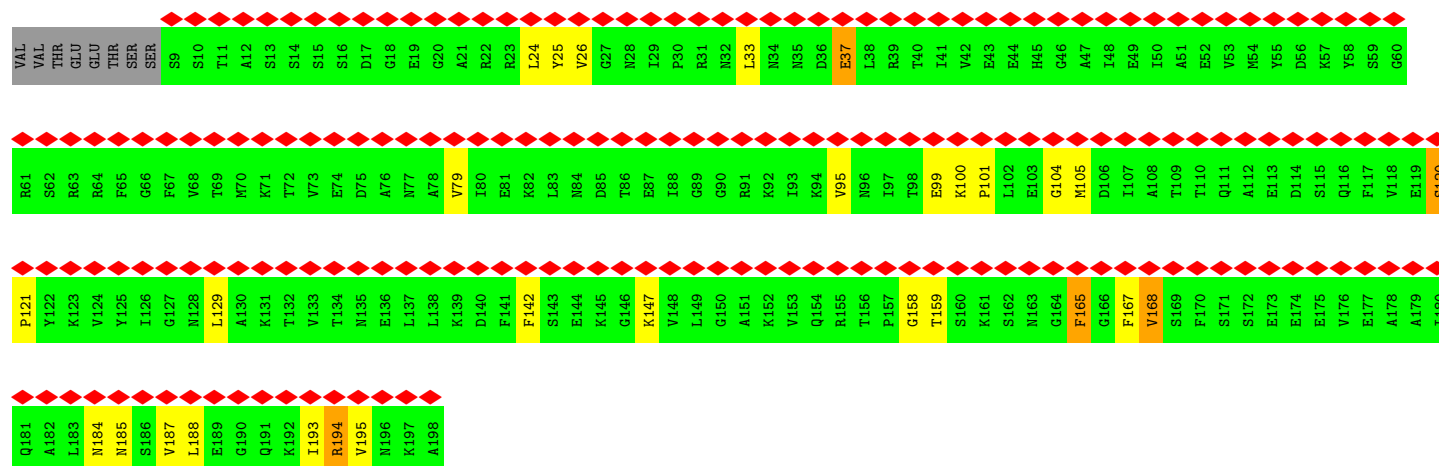
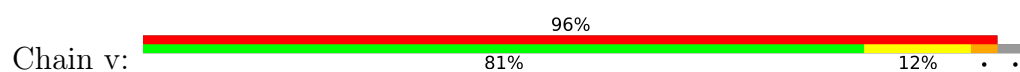




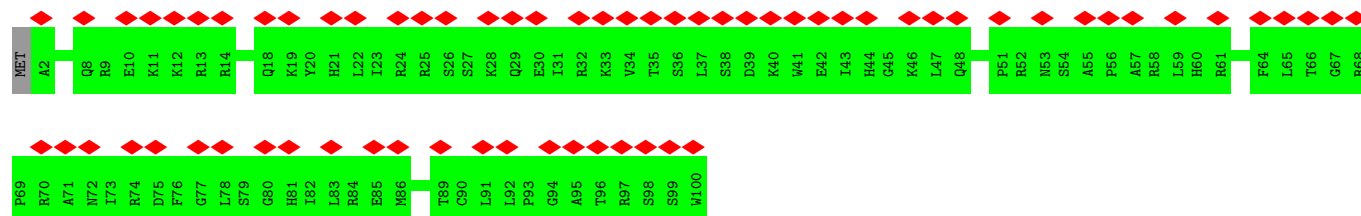
- Molecule 54: 30S ribosomal protein S4, chloroplastic



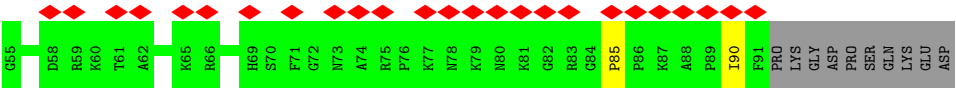
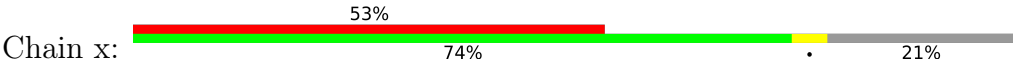
- Molecule 55: protein cS22



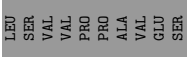
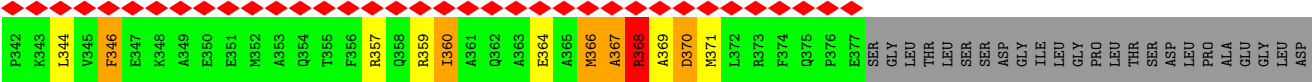
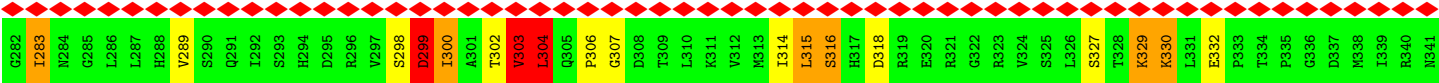
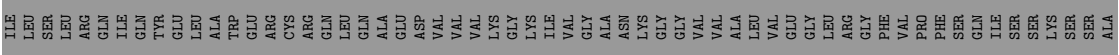
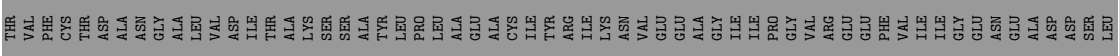
- Molecule 56: 30S ribosomal protein S14, chloroplastic



- Molecule 57: protein bTHXc



• Molecule 58: 30S ribosomal protein S1, chloroplastic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81305	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.5	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	133333	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.475	Depositor
Minimum map value	-0.303	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size ( $\text{\AA}$ )	403.19998, 403.19998, 403.19998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.05, 1.05, 1.05	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.27	0/387	0.51	0/513
2	2	0.32	0/422	0.75	1/564 (0.2%)
3	3	0.27	0/447	0.66	1/588 (0.2%)
4	4	0.31	0/569	0.66	1/752 (0.1%)
5	5	0.30	0/306	0.67	0/403
6	6	0.25	0/425	0.46	0/551
7	7	0.28	0/382	0.54	0/520
8	B	0.31	0/2796	1.05	12/4357 (0.3%)
9	C	0.29	0/1938	0.64	0/2603
10	D	0.31	0/1646	0.65	0/2201
11	E	0.30	0/1687	0.65	1/2271 (0.0%)
12	F	0.28	0/1372	0.61	0/1848
13	G	0.26	0/1374	0.55	1/1849 (0.1%)
14	H	0.26	0/427	0.59	0/568
15	K	0.28	0/1608	0.57	2/2174 (0.1%)
16	L	0.31	0/951	0.59	0/1282
17	M	0.28	0/1361	0.53	0/1806
18	N	0.31	0/1089	0.61	0/1461
19	O	0.28	0/959	0.61	0/1280
20	P	0.26	0/963	0.55	1/1293 (0.1%)
21	Q	0.31	0/967	0.71	2/1300 (0.2%)
22	R	0.33	0/1013	0.61	0/1351
23	S	0.31	0/1199	0.61	0/1633
24	T	0.29	0/1168	0.60	1/1566 (0.1%)
25	U	0.27	0/749	0.58	0/1006
26	V	0.27	0/1006	0.64	1/1343 (0.1%)
27	W	0.35	0/2449	1.07	10/3817 (0.3%)
28	X	0.30	0/825	0.57	0/1099
29	Y	0.28	0/615	0.65	2/819 (0.2%)
30	Z	0.27	0/762	0.57	0/1012
31	A	0.35	1/67572 (0.0%)	1.05	315/105421 (0.3%)
32	0	0.29	0/533	0.66	1/718 (0.1%)
33	b	0.75	8/1819 (0.4%)	0.96	8/2458 (0.3%)
34	c	0.48	0/1746	0.72	1/2348 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	e	0.61	0/1307	0.77	2/1754 (0.1%)
36	f	0.44	0/904	0.69	0/1225
37	g	0.36	0/1175	0.62	0/1574
38	h	0.88	5/1103 (0.5%)	1.69	6/1477 (0.4%)
39	i	0.43	0/1038	0.70	0/1397
40	j	0.51	0/813	0.70	1/1099 (0.1%)
41	k	0.40	0/901	0.63	0/1214
42	l	0.62	0/983	0.80	4/1323 (0.3%)
43	m	0.45	0/909	0.75	2/1209 (0.2%)
44	o	0.42	0/532	0.65	0/707
45	p	0.52	0/674	0.71	0/902
46	q	0.50	0/647	0.64	0/867
47	r	0.49	0/522	0.76	2/697 (0.3%)
48	s	0.44	0/642	0.70	0/866
49	t	0.46	0/842	0.68	0/1127
50	u	1.10	3/396 (0.8%)	0.94	3/518 (0.6%)
51	y	0.45	0/852	0.70	0/1139
52	a	1.13	32/35582 (0.1%)	1.39	473/55510 (0.9%)
53	w	0.80	2/709 (0.3%)	1.23	11/965 (1.1%)
54	d	0.40	0/1661	0.72	2/2230 (0.1%)
55	v	1.49	16/1481 (1.1%)	1.24	13/1991 (0.7%)
56	n	0.37	0/835	0.62	0/1116
57	x	0.55	0/296	0.74	1/390 (0.3%)
58	8	0.87	5/1216 (0.4%)	1.61	28/1631 (1.7%)
All	All	0.65	72/159552 (0.0%)	1.08	909/237703 (0.4%)

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
17	M	0	1
21	Q	0	1
23	S	0	1
32	0	0	1
33	b	0	2
34	c	0	3
35	e	0	1
36	f	0	1
37	g	0	1
39	i	0	2

*Continued on next page...*



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Mol	Chain	#Chirality outliers	#Planarity outliers
40	j	0	1
42	l	0	3
43	m	0	2
50	u	0	1
53	w	0	7
54	d	0	2
55	v	0	15
58	8	0	17
All	All	0	62

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	142	PHE	CE1-CZ	-18.97	1.01	1.37
55	v	142	PHE	CE2-CZ	-17.85	1.03	1.37
55	v	142	PHE	CG-CD2	-15.89	1.15	1.38
38	h	67	ARG	CZ-NH2	-15.34	1.13	1.33
55	v	165	PHE	CE2-CZ	-14.94	1.08	1.37
55	v	142	PHE	CG-CD1	-14.77	1.16	1.38
38	h	67	ARG	CB-CG	-14.59	1.13	1.52
55	v	168	VAL	CB-CG1	-14.33	1.22	1.52
55	v	195	VAL	CB-CG2	-13.41	1.24	1.52
55	v	194	ARG	CG-CD	-12.82	1.19	1.51
50	u	103	PHE	CD1-CE1	-11.76	1.15	1.39
55	v	165	PHE	CG-CD2	-10.85	1.22	1.38
50	u	103	PHE	CD2-CE2	-10.60	1.18	1.39
55	v	26	VAL	CB-CG1	-9.95	1.31	1.52
33	b	7	ASN	CG-ND2	-9.61	1.08	1.32
50	u	103	PHE	CB-CG	-9.12	1.35	1.51
33	b	201	ASP	CB-CG	9.03	1.70	1.51
55	v	142	PHE	CD2-CE2	7.99	1.55	1.39
55	v	142	PHE	CD1-CE1	7.72	1.54	1.39
53	w	149	PRO	CG-CD	-7.71	1.25	1.50
52	a	7	G	C2-N3	-7.63	1.26	1.32
38	h	67	ARG	CZ-NH1	-7.51	1.23	1.33
33	b	209	ASP	CG-OD2	-7.19	1.08	1.25
52	a	4	C	C4-C5	-6.92	1.37	1.43
53	w	164	THR	CB-CG2	-6.82	1.29	1.52
52	a	1081	C	N3-C4	6.76	1.38	1.33
52	a	1087	G	C6-N1	-6.71	1.34	1.39
52	a	900	G	C6-N1	-6.71	1.34	1.39
55	v	193	ILE	CB-CG2	-6.67	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	1480	A	N9-C8	-6.61	1.32	1.37
52	a	147	C	N3-C4	-6.49	1.29	1.33
55	v	79	VAL	CB-CG1	-6.48	1.39	1.52
52	a	4	C	C5-C6	-6.41	1.29	1.34
52	a	786	C	N3-C4	-6.40	1.29	1.33
52	a	107	C	N3-C4	-6.37	1.29	1.33
52	a	150	C	N3-C4	-6.30	1.29	1.33
52	a	881	C	N3-C4	-6.28	1.29	1.33
38	h	67	ARG	CG-CD	-6.17	1.36	1.51
52	a	1441	A	N1-C2	-6.03	1.28	1.34
38	h	67	ARG	CA-CB	-6.02	1.40	1.53
52	a	1482	C	C5-C6	-5.97	1.29	1.34
52	a	7	G	C5-C4	-5.94	1.34	1.38
33	b	20	PHE	CE2-CZ	-5.88	1.26	1.37
58	8	289	VAL	CB-CG1	-5.88	1.40	1.52
52	a	951	C	N3-C4	-5.75	1.29	1.33
52	a	448	G	C6-N1	-5.69	1.35	1.39
52	a	1440	G	N3-C4	-5.68	1.31	1.35
33	b	56	GLU	CD-OE2	-5.66	1.19	1.25
52	a	1029	A	N7-C5	-5.61	1.35	1.39
52	a	450	A	C6-N1	-5.58	1.31	1.35
52	a	1016	A	N9-C4	-5.53	1.34	1.37
58	8	327	SER	CB-OG	-5.53	1.35	1.42
55	v	95	VAL	CB-CG2	-5.50	1.41	1.52
58	8	368	ARG	CB-CG	5.45	1.67	1.52
52	a	74	G	O3'-P	-5.41	1.54	1.61
33	b	40	LYS	CD-CE	-5.40	1.37	1.51
52	a	269	A	N9-C4	-5.40	1.34	1.37
52	a	361	C	N3-C4	-5.38	1.30	1.33
58	8	65	GLU	CB-CG	-5.28	1.42	1.52
52	a	7	G	N3-C4	-5.28	1.31	1.35
31	A	2447	A	N9-C4	5.19	1.41	1.37
52	a	898	A	N7-C5	-5.19	1.36	1.39
33	b	112	GLU	CD-OE2	-5.19	1.20	1.25
52	a	1358	C	C2-O2	-5.14	1.19	1.24
52	a	885	C	N3-C4	-5.13	1.30	1.33
52	a	371	C	N3-C4	-5.12	1.30	1.33
33	b	7	ASN	CB-CG	-5.10	1.39	1.51
52	a	271	A	N7-C5	-5.10	1.36	1.39
55	v	195	VAL	CB-CG1	-5.08	1.42	1.52
52	a	510	G	N9-C4	-5.07	1.33	1.38
58	8	332	GLU	CB-CG	-5.04	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	428	U	C2-N3	-5.03	1.34	1.37

All (909) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	h	67	ARG	NE-CZ-NH1	50.54	145.57	120.30
33	b	201	ASP	CB-CG-OD2	20.66	136.90	118.30
52	a	1440	G	N3-C2-N2	-20.49	105.56	119.90
52	a	7	G	C2-N3-C4	20.20	122.00	111.90
52	a	1441	A	N1-C2-N3	20.05	139.32	129.30
52	a	1439	U	C5-C6-N1	18.99	132.19	122.70
38	h	67	ARG	NH1-CZ-NH2	-16.53	101.21	119.40
52	a	147	C	N1-C2-O2	16.52	128.81	118.90
52	a	976	C	N1-C2-O2	16.12	128.57	118.90
52	a	150	C	N1-C2-O2	16.09	128.55	118.90
52	a	1488	C	C5-C6-N1	15.36	128.68	121.00
38	h	67	ARG	NE-CZ-NH2	-15.35	112.62	120.30
52	a	4	C	C6-N1-C2	-15.01	114.30	120.30
52	a	1480	A	N7-C8-N9	14.64	121.12	113.80
52	a	881	C	N1-C2-O2	14.50	127.60	118.90
38	h	67	ARG	CD-NE-CZ	14.42	143.78	123.60
52	a	786	C	N1-C2-O2	14.14	127.38	118.90
52	a	1077	C	N1-C2-O2	13.21	126.83	118.90
52	a	1445	C	C5-C6-N1	13.13	127.56	121.00
52	a	1487	C	C5-C6-N1	12.95	127.48	121.00
52	a	1485	C	C5-C6-N1	12.60	127.30	121.00
38	h	67	ARG	CB-CG-CD	12.09	143.04	111.60
52	a	1195	G	N1-C6-O6	11.53	126.82	119.90
52	a	147	C	N3-C2-O2	-11.49	113.86	121.90
52	a	107	C	N1-C2-O2	11.48	125.79	118.90
52	a	1440	G	N1-C2-N2	11.43	126.49	116.20
52	a	1195	G	C5-C6-O6	-11.39	121.77	128.60
52	a	1486	U	C5-C6-N1	11.28	128.34	122.70
52	a	1488	C	C6-N1-C2	-11.22	115.81	120.30
52	a	976	C	N3-C4-N4	11.18	125.82	118.00
31	A	2077	C	N1-C2-O2	11.07	125.54	118.90
52	a	1238	C	N3-C2-O2	-10.94	114.24	121.90
33	b	209	ASP	CB-CG-OD1	10.94	128.14	118.30
52	a	147	C	C2-N3-C4	10.88	125.34	119.90
52	a	976	C	N3-C2-O2	-10.87	114.29	121.90
52	a	951	C	N1-C2-O2	10.85	125.41	118.90
58	8	304	LEU	CA-CB-CG	10.83	140.21	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	8	344	LEU	CB-CG-CD2	-10.83	92.59	111.00
52	a	1445	C	C6-N1-C2	-10.81	115.97	120.30
55	v	142	PHE	CB-CG-CD1	10.79	128.35	120.80
52	a	1087	G	N3-C2-N2	10.70	127.39	119.90
52	a	4	C	C5-C6-N1	10.68	126.34	121.00
31	A	2077	C	C2-N1-C1'	10.66	130.53	118.80
52	a	147	C	N3-C4-N4	10.57	125.40	118.00
52	a	881	C	N3-C2-O2	-10.50	114.55	121.90
52	a	1484	C	C5-C6-N1	10.49	126.25	121.00
52	a	786	C	N3-C4-N4	10.43	125.30	118.00
52	a	1441	A	C2-N3-C4	-10.41	105.39	110.60
52	a	976	C	C2-N3-C4	10.39	125.09	119.90
52	a	786	C	N3-C2-O2	-10.37	114.64	121.90
52	a	150	C	N3-C2-O2	-10.30	114.69	121.90
52	a	1480	A	C5-N7-C8	-10.22	98.79	103.90
52	a	1090	U	N3-C2-O2	-10.22	115.05	122.20
52	a	1256	U	C2-N3-C4	10.16	133.09	127.00
53	w	103	PHE	CB-CG-CD2	-10.12	113.71	120.80
52	a	1441	A	C6-N1-C2	-10.10	112.54	118.60
52	a	1440	G	C6-N1-C2	-10.06	119.06	125.10
52	a	150	C	C2-N3-C4	10.06	124.93	119.90
58	8	318	ASP	CB-CG-OD1	9.99	127.29	118.30
52	a	7	G	N3-C4-C5	-9.96	123.62	128.60
31	A	1747	C	N3-C2-O2	-9.95	114.94	121.90
52	a	285	C	N1-C2-O2	9.95	124.87	118.90
52	a	983	G	N1-C6-O6	-9.94	113.93	119.90
52	a	83	C	N1-C2-O2	9.92	124.85	118.90
52	a	448	G	N1-C6-O6	9.90	125.84	119.90
52	a	1116	U	N1-C2-O2	9.88	129.72	122.80
31	A	2314	C	C2-N1-C1'	9.82	129.60	118.80
52	a	1081	C	N1-C2-O2	-9.66	113.11	118.90
52	a	1480	A	C8-N9-C4	-9.59	101.96	105.80
52	a	786	C	C2-N3-C4	9.56	124.68	119.90
52	a	1439	U	C6-N1-C2	-9.55	115.27	121.00
31	A	2314	C	N1-C2-O2	9.54	124.62	118.90
58	8	72	MET	N-CA-C	-9.53	85.27	111.00
52	a	147	C	N3-C4-C5	-9.48	118.11	121.90
52	a	786	C	N3-C4-C5	-9.41	118.13	121.90
52	a	1090	U	N1-C2-O2	9.37	129.36	122.80
52	a	794	C	N1-C2-O2	9.37	124.52	118.90
31	A	2662	C	N1-C2-O2	9.35	124.51	118.90
55	v	194	ARG	NE-CZ-NH2	-9.34	115.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	881	C	N3-C4-N4	9.29	124.50	118.00
52	a	1487	C	C6-N1-C2	-9.21	116.61	120.30
52	a	572	C	N1-C2-O2	9.21	124.43	118.90
31	A	2077	C	C6-N1-C2	-9.17	116.63	120.30
52	a	255	C	N1-C2-O2	9.15	124.39	118.90
53	w	103	PHE	CB-CG-CD1	9.15	127.20	120.80
52	a	107	C	N3-C2-O2	-9.13	115.51	121.90
52	a	976	C	N3-C4-C5	-9.11	118.26	121.90
31	A	2077	C	N3-C2-O2	-9.10	115.53	121.90
52	a	1116	U	N3-C2-O2	-9.10	115.83	122.20
52	a	285	C	N3-C2-O2	-9.04	115.58	121.90
52	a	951	C	N3-C2-O2	-9.02	115.58	121.90
52	a	948	C	C5-C6-N1	9.01	125.51	121.00
52	a	885	C	N1-C2-O2	8.95	124.27	118.90
52	a	142	G	N1-C6-O6	-8.94	114.54	119.90
52	a	1374	C	C6-N1-C2	-8.91	116.73	120.30
31	A	2268	G	C4-N9-C1'	8.90	138.07	126.50
52	a	1238	C	N1-C2-O2	8.89	124.23	118.90
52	a	1485	C	C6-N1-C2	-8.85	116.76	120.30
31	A	294	U	N1-C2-O2	8.85	128.99	122.80
31	A	1334	U	C2-N1-C1'	8.84	128.31	117.70
52	a	1166	C	O5'-P-OP1	-8.75	97.83	105.70
58	8	73	GLU	N-CA-C	-8.74	87.39	111.00
31	A	2314	C	C6-N1-C2	-8.71	116.81	120.30
52	a	1439	U	C4-C5-C6	-8.71	114.48	119.70
33	b	201	ASP	OD1-CG-OD2	-8.70	106.77	123.30
52	a	948	C	C6-N1-C2	-8.69	116.83	120.30
33	b	201	ASP	CB-CG-OD1	-8.68	110.49	118.30
55	v	165	PHE	CB-CG-CD1	8.68	126.88	120.80
31	A	1334	U	N1-C2-O2	8.67	128.87	122.80
31	A	897	A	C5-C6-N6	-8.67	116.76	123.70
31	A	900	G	N7-C8-N9	8.66	117.43	113.10
52	a	1077	C	C2-N3-C4	8.63	124.22	119.90
35	e	266	LEU	CA-CB-CG	8.60	135.08	115.30
52	a	301	C	N1-C2-O2	8.58	124.05	118.90
31	A	46	C	N1-C2-O2	8.55	124.03	118.90
52	a	150	C	N3-C4-N4	8.54	123.98	118.00
52	a	786	C	C6-N1-C2	-8.53	116.89	120.30
52	a	1081	C	C5-C4-N4	-8.53	114.23	120.20
52	a	1003	C	N1-C2-O2	8.49	124.00	118.90
52	a	1077	C	N3-C2-O2	-8.49	115.95	121.90
8	B	61	C	N1-C2-O2	8.48	123.99	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	2662	C	C2-N1-C1'	8.47	128.12	118.80
52	a	1003	C	N3-C2-O2	-8.47	115.97	121.90
52	a	1481	U	C5-C6-N1	8.47	126.94	122.70
52	a	797	G	N1-C6-O6	-8.41	114.86	119.90
33	b	40	LYS	CD-CE-NZ	-8.39	92.39	111.70
58	8	304	LEU	CB-CG-CD1	8.38	125.25	111.00
52	a	987	G	N1-C6-O6	-8.38	114.87	119.90
52	a	1081	C	C2-N3-C4	-8.38	115.71	119.90
31	A	1784	C	N3-C2-O2	-8.32	116.08	121.90
31	A	2709	C	N3-C2-O2	-8.32	116.08	121.90
31	A	294	U	N3-C2-O2	-8.30	116.39	122.20
31	A	1923	C	N3-C2-O2	-8.27	116.11	121.90
52	a	159	C	N1-C2-O2	8.26	123.86	118.90
31	A	899	A	N7-C8-N9	8.25	117.92	113.80
52	a	1358	C	C6-N1-C2	-8.24	117.00	120.30
52	a	1488	C	C4-C5-C6	-8.17	113.32	117.40
31	A	1843	C	N3-C2-O2	-8.16	116.19	121.90
55	v	142	PHE	CD1-CG-CD2	-8.14	107.71	118.30
29	Y	103	LEU	CA-CB-CG	8.12	133.98	115.30
31	A	1334	U	N3-C2-O2	-8.11	116.52	122.20
58	8	315	LEU	CB-CG-CD1	8.11	124.79	111.00
52	a	1244	C	N1-C2-O2	8.11	123.76	118.90
58	8	299	ASP	N-CA-C	-8.11	89.11	111.00
52	a	1225	C	N1-C2-O2	8.09	123.76	118.90
58	8	367	ALA	N-CA-CB	8.09	121.43	110.10
31	A	1283	U	N3-C2-O2	-8.08	116.54	122.20
52	a	881	C	C6-N1-C2	-8.06	117.08	120.30
31	A	1970	U	N1-C2-O2	8.05	128.44	122.80
21	Q	224	ASP	CB-CG-OD1	8.04	125.53	118.30
31	A	294	U	C2-N1-C1'	8.03	127.33	117.70
52	a	1440	G	C8-N9-C4	-8.00	103.20	106.40
52	a	7	G	N1-C2-N3	-8.00	119.10	123.90
52	a	1244	C	N3-C2-O2	-7.99	116.31	121.90
31	A	1970	U	N3-C2-O2	-7.97	116.62	122.20
53	w	148	LYS	C-N-CD	-7.95	103.10	120.60
52	a	881	C	C2-N3-C4	7.90	123.85	119.90
58	8	368	ARG	CB-CG-CD	7.89	132.11	111.60
31	A	112	C	N1-C2-O2	7.88	123.63	118.90
31	A	2268	G	C8-N9-C1'	-7.84	116.81	127.00
52	a	794	C	C2-N1-C1'	7.82	127.41	118.80
52	a	4	C	N3-C4-C5	-7.80	118.78	121.90
52	a	84	C	N1-C2-O2	7.79	123.58	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	2314	C	N3-C2-O2	-7.70	116.51	121.90
52	a	1106	C	C2-N1-C1'	7.70	127.27	118.80
52	a	1484	C	C6-N1-C2	-7.67	117.23	120.30
52	a	987	G	N3-C2-N2	-7.67	114.53	119.90
52	a	139	G	N1-C6-O6	-7.63	115.32	119.90
52	a	1116	U	C2-N1-C1'	7.63	126.86	117.70
58	8	360	ILE	N-CA-C	-7.62	90.42	111.00
31	A	1784	C	N1-C2-O2	7.61	123.46	118.90
31	A	1818	U	C2-N1-C1'	7.61	126.83	117.70
8	B	69	C	N1-C2-O2	7.60	123.46	118.90
31	A	448	C	N1-C2-O2	7.58	123.45	118.90
52	a	1258	C	N1-C2-O2	7.58	123.45	118.90
52	a	361	C	N1-C2-O2	7.58	123.45	118.90
52	a	1163	G	N1-C6-O6	7.57	124.44	119.90
58	8	279	ASP	CB-CG-OD1	7.57	125.11	118.30
31	A	1013	C	N1-C2-O2	7.56	123.44	118.90
52	a	881	C	C2-N1-C1'	7.55	127.10	118.80
52	a	1077	C	C2-N1-C1'	7.54	127.10	118.80
52	a	1087	G	N1-C2-N2	-7.53	109.43	116.20
52	a	147	C	C6-N1-C2	-7.50	117.30	120.30
58	8	73	GLU	CB-CA-C	7.46	125.33	110.40
31	A	2683	C	N1-C2-O2	7.45	123.37	118.90
31	A	168	C	N1-C2-O2	7.44	123.36	118.90
52	a	1095	C	N1-C2-O2	7.42	123.35	118.90
52	a	150	C	N3-C4-C5	-7.41	118.94	121.90
54	d	32	LEU	CA-CB-CG	7.41	132.34	115.30
52	a	794	C	N3-C2-O2	-7.40	116.72	121.90
52	a	1089	U	C5-C6-N1	7.40	126.40	122.70
31	A	1107	C	N1-C2-O2	7.40	123.34	118.90
31	A	38	C	N1-C2-O2	7.38	123.33	118.90
58	8	62	ASP	CB-CG-OD2	-7.37	111.66	118.30
52	a	1453	G	N1-C6-O6	7.37	124.32	119.90
52	a	959	C	N1-C2-O2	7.36	123.31	118.90
52	a	1158	C	N1-C2-O2	7.33	123.30	118.90
52	a	1272	C	N1-C2-O2	7.33	123.30	118.90
4	4	153	LEU	CA-CB-CG	7.32	132.13	115.30
31	A	2662	C	N3-C2-O2	-7.31	116.78	121.90
52	a	7	G	C5-C6-N1	7.31	115.15	111.50
52	a	295	G	C8-N9-C4	-7.30	103.48	106.40
26	V	64	LEU	CA-CB-CG	7.30	132.10	115.30
31	A	46	C	C6-N1-C2	-7.29	117.38	120.30
52	a	881	C	N3-C4-C5	-7.29	118.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	572	C	N3-C2-O2	-7.28	116.81	121.90
52	a	951	C	C6-N1-C2	-7.27	117.39	120.30
52	a	1003	C	C6-N1-C2	-7.27	117.39	120.30
52	a	139	G	N3-C2-N2	-7.26	114.82	119.90
52	a	951	C	N3-C4-N4	7.26	123.08	118.00
52	a	1003	C	C2-N1-C1'	7.25	126.78	118.80
52	a	1077	C	C6-N1-C2	-7.23	117.41	120.30
52	a	1077	C	N3-C4-N4	7.23	123.06	118.00
52	a	910	U	N3-C2-O2	-7.22	117.15	122.20
52	a	1358	C	N3-C2-O2	-7.22	116.85	121.90
52	a	885	C	N3-C2-O2	-7.21	116.85	121.90
52	a	794	C	C6-N1-C2	-7.21	117.42	120.30
52	a	1083	U	C5-C6-N1	7.21	126.30	122.70
31	A	1283	U	N1-C2-O2	7.21	127.84	122.80
31	A	2121	C	N1-C2-O2	7.21	123.22	118.90
52	a	951	C	N3-C4-C5	-7.20	119.02	121.90
52	a	1120	C	N3-C2-O2	-7.19	116.86	121.90
31	A	1432	U	N3-C2-O2	-7.19	117.17	122.20
52	a	951	C	C2-N3-C4	7.19	123.49	119.90
31	A	2314	C	C5-C6-N1	7.18	124.59	121.00
31	A	2077	C	C5-C6-N1	7.17	124.59	121.00
31	A	1595	C	N1-C2-O2	7.16	123.20	118.90
52	a	1290	C	N1-C2-O2	7.15	123.19	118.90
31	A	1459	U	N1-C2-O2	7.15	127.80	122.80
50	u	98	ARG	NE-CZ-NH1	-7.14	116.73	120.30
52	a	361	C	C6-N1-C2	-7.13	117.45	120.30
52	a	428	U	N3-C2-O2	-7.13	117.21	122.20
58	8	357	ARG	NE-CZ-NH1	-7.13	116.74	120.30
52	a	434	U	C2-N1-C1'	7.11	126.24	117.70
52	a	670	A	C2-N3-C4	7.11	114.16	110.60
55	v	165	PHE	CZ-CE2-CD2	7.11	128.63	120.10
31	A	1432	U	C2-N1-C1'	7.10	126.22	117.70
52	a	1030	G	N1-C6-O6	7.09	124.15	119.90
52	a	976	C	C6-N1-C2	-7.08	117.47	120.30
31	A	112	C	C2-N1-C1'	7.07	126.58	118.80
52	a	83	C	N3-C2-O2	-7.05	116.96	121.90
31	A	900	G	C8-N9-C4	-7.05	103.58	106.40
31	A	1432	U	N1-C2-O2	7.04	127.73	122.80
31	A	2268	G	N3-C4-N9	7.04	130.22	126.00
58	8	70	ALA	N-CA-CB	7.01	119.92	110.10
52	a	1485	C	C4-C5-C6	-7.00	113.90	117.40
52	a	1087	G	C6-N1-C2	7.00	129.30	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1335	C	C2-N1-C1'	7.00	126.50	118.80
52	a	877	G	C6-C5-N7	-6.99	126.20	130.40
58	8	318	ASP	CB-CG-OD2	-6.99	112.01	118.30
52	a	1445	C	C4-C5-C6	-6.99	113.91	117.40
31	A	2518	C	C6-N1-C2	-6.98	117.51	120.30
52	a	84	C	N3-C2-O2	-6.98	117.02	121.90
31	A	1818	U	N1-C2-O2	6.97	127.68	122.80
33	b	201	ASP	N-CA-CB	6.97	123.14	110.60
31	A	688	C	C2-N1-C1'	6.96	126.45	118.80
31	A	2209	U	N3-C2-O2	-6.96	117.33	122.20
31	A	2268	G	N3-C4-C5	-6.96	125.12	128.60
52	a	1328	G	N1-C6-O6	-6.96	115.73	119.90
52	a	223	U	N1-C2-O2	6.95	127.66	122.80
11	E	245	LEU	CA-CB-CG	6.95	131.27	115.30
31	A	46	C	N3-C2-O2	-6.95	117.04	121.90
31	A	1419	C	N1-C2-O2	6.89	123.03	118.90
31	A	2706	U	N1-C2-O2	6.89	127.62	122.80
52	a	1150	U	N3-C2-O2	-6.89	117.38	122.20
31	A	2116	C	N1-C2-O2	6.86	123.02	118.90
52	a	561	C	N1-C2-O2	6.86	123.02	118.90
31	A	2709	C	C6-N1-C2	-6.86	117.56	120.30
52	a	938	G	N1-C6-O6	6.86	124.02	119.90
31	A	630	C	N1-C2-O2	6.86	123.01	118.90
31	A	900	G	C5-N7-C8	-6.85	100.87	104.30
52	a	55	C	N3-C2-O2	-6.85	117.11	121.90
58	8	283	ILE	CG1-CB-CG2	-6.83	96.37	111.40
31	A	2209	U	N1-C2-O2	6.83	127.58	122.80
31	A	901	C	N1-C2-O2	6.82	122.99	118.90
52	a	491	U	N3-C2-O2	-6.82	117.43	122.20
52	a	55	C	N1-C2-O2	6.82	122.99	118.90
31	A	897	A	C4-C5-N7	6.81	114.11	110.70
31	A	2209	U	C2-N1-C1'	6.81	125.87	117.70
52	a	1150	U	N1-C2-O2	6.80	127.56	122.80
52	a	511	A	C2-N3-C4	6.80	114.00	110.60
31	A	897	A	N1-C6-N6	6.80	122.68	118.60
52	a	301	C	N3-C2-O2	-6.79	117.15	121.90
52	a	1440	G	N7-C8-N9	6.79	116.49	113.10
31	A	31	C	N1-C2-O2	6.79	122.97	118.90
54	d	160	LEU	CA-CB-CG	6.78	130.89	115.30
58	8	316	SER	C-N-CA	6.78	138.64	121.70
31	A	1620	U	N1-C2-O2	6.78	127.54	122.80
52	a	1120	C	N1-C2-O2	6.78	122.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	223	U	C2-N1-C1'	6.77	125.82	117.70
31	A	38	C	N3-C2-O2	-6.76	117.17	121.90
55	v	165	PHE	CB-CG-CD2	-6.75	116.07	120.80
52	a	1092	G	N1-C6-O6	-6.75	115.85	119.90
52	a	1440	G	N1-C2-N3	6.74	127.94	123.90
52	a	1172	G	N3-C4-N9	-6.74	121.96	126.00
31	A	1528	U	N1-C2-O2	6.72	127.51	122.80
31	A	2378	C	N1-C2-O2	6.72	122.93	118.90
52	a	243	C	N1-C2-O2	6.71	122.93	118.90
52	a	784	U	N3-C2-O2	-6.71	117.50	122.20
52	a	890	G	N3-C2-N2	-6.69	115.22	119.90
52	a	150	C	C6-N1-C2	-6.69	117.62	120.30
53	w	133	PRO	CA-N-CD	-6.68	102.15	111.50
52	a	255	C	N3-C4-N4	6.67	122.67	118.00
31	A	2077	C	C6-N1-C1'	-6.66	112.81	120.80
31	A	2706	U	N3-C2-O2	-6.66	117.54	122.20
31	A	1818	U	C5-C6-N1	6.65	126.03	122.70
52	a	558	U	N3-C2-O2	-6.65	117.54	122.20
52	a	1334	G	N1-C6-O6	-6.65	115.91	119.90
52	a	448	G	C5-C6-O6	-6.65	124.61	128.60
52	a	255	C	N3-C2-O2	-6.65	117.25	121.90
52	a	3	U	C5-C6-N1	6.64	126.02	122.70
8	B	61	C	N3-C2-O2	-6.64	117.25	121.90
31	A	1397	C	N1-C2-O2	6.63	122.88	118.90
52	a	1440	G	C5-C6-O6	-6.63	124.62	128.60
52	a	1149	A	C8-N9-C4	6.62	108.45	105.80
31	A	2483	C	N1-C2-O2	6.60	122.86	118.90
31	A	877	C	N1-C2-O2	6.60	122.86	118.90
52	a	1029	A	C6-C5-N7	-6.58	127.69	132.30
52	a	83	C	C6-N1-C2	-6.58	117.67	120.30
52	a	285	C	C6-N1-C2	-6.56	117.68	120.30
52	a	150	C	C2-N1-C1'	6.56	126.01	118.80
31	A	1528	U	N3-C2-O2	-6.55	117.61	122.20
52	a	511	A	N1-C6-N6	-6.55	114.67	118.60
2	2	13	LEU	CA-CB-CG	6.55	130.37	115.30
8	B	61	C	C2-N1-C1'	6.54	126.00	118.80
52	a	90	C	C6-N1-C2	-6.54	117.69	120.30
31	A	928	U	N1-C2-O2	6.53	127.37	122.80
27	W	33	A	P-O3'-C3'	6.53	127.53	119.70
31	A	1459	U	N3-C2-O2	-6.53	117.63	122.20
31	A	2121	C	C2-N1-C1'	6.51	125.96	118.80
31	A	1620	U	N3-C2-O2	-6.51	117.65	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	1087	G	C5-C6-O6	6.51	132.50	128.60
52	a	976	C	C5-C4-N4	-6.50	115.65	120.20
52	a	958	U	N1-C2-O2	6.49	127.34	122.80
52	a	1254	A	N7-C8-N9	6.48	117.04	113.80
52	a	571	C	N1-C2-O2	6.48	122.79	118.90
52	a	1058	C	N3-C2-O2	-6.48	117.37	121.90
31	A	363	C	N1-C2-O2	6.47	122.78	118.90
34	c	95	LEU	CA-CB-CG	6.46	130.16	115.30
52	a	407	C	C6-N1-C2	-6.46	117.72	120.30
31	A	46	C	C2-N1-C1'	6.45	125.89	118.80
31	A	2447	A	C2-N3-C4	6.44	113.82	110.60
52	a	1487	C	C4-C5-C6	-6.44	114.18	117.40
31	A	168	C	N3-C2-O2	-6.43	117.40	121.90
31	A	901	C	C2-N1-C1'	6.43	125.88	118.80
52	a	1311	C	N3-C2-O2	-6.43	117.40	121.90
52	a	1254	A	C8-N9-C4	-6.43	103.23	105.80
52	a	1029	A	C4-C5-N7	6.43	113.91	110.70
52	a	1077	C	N3-C4-C5	-6.43	119.33	121.90
52	a	1348	C	N1-C2-O2	-6.42	115.05	118.90
52	a	784	U	C2-N1-C1'	6.41	125.40	117.70
52	a	411	U	N1-C2-O2	6.41	127.29	122.80
52	a	1081	C	C5-C6-N1	6.41	124.20	121.00
8	B	69	C	N3-C2-O2	-6.39	117.42	121.90
52	a	59	C	C6-N1-C2	-6.39	117.74	120.30
52	a	828	C	O5'-P-OP1	-6.39	99.95	105.70
31	A	899	A	C8-N9-C4	-6.39	103.25	105.80
52	a	407	C	N1-C2-O2	6.38	122.73	118.90
52	a	1120	C	C6-N1-C2	-6.38	117.75	120.30
52	a	560	C	N1-C2-O2	6.38	122.73	118.90
52	a	890	G	N1-C6-O6	-6.38	116.07	119.90
52	a	682	C	C5-C6-N1	6.38	124.19	121.00
31	A	1013	C	N3-C2-O2	-6.37	117.44	121.90
52	a	371	C	N1-C2-O2	6.37	122.72	118.90
31	A	1528	U	C2-N1-C1'	6.37	125.34	117.70
31	A	2598	G	C4-C5-N7	6.37	113.35	110.80
58	8	329	LYS	CD-CE-NZ	6.36	126.33	111.70
52	a	1078	C	C2-N1-C1'	6.35	125.79	118.80
31	A	783	U	N1-C2-O2	6.35	127.24	122.80
52	a	361	C	N3-C2-O2	-6.34	117.46	121.90
52	a	959	C	N3-C2-O2	-6.34	117.46	121.90
31	A	897	A	N9-C4-C5	-6.33	103.27	105.80
53	w	112	LEU	CB-CG-CD1	-6.33	100.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1335	C	C6-N1-C2	-6.33	117.77	120.30
27	W	32	C	P-O3'-C3'	6.32	127.29	119.70
52	a	1149	A	N9-C4-C5	-6.32	103.27	105.80
31	A	253	C	C2-N1-C1'	6.31	125.75	118.80
52	a	1302	C	C6-N1-C2	-6.30	117.78	120.30
52	a	434	U	N3-C2-O2	-6.30	117.79	122.20
52	a	1374	C	C5-C6-N1	6.30	124.15	121.00
52	a	784	U	N1-C2-O2	6.30	127.21	122.80
38	h	67	ARG	N-CA-CB	-6.30	99.27	110.60
31	A	31	C	C2-N1-C1'	6.29	125.72	118.80
52	a	1353	C	N1-C2-O2	6.29	122.67	118.90
31	A	1250	C	C5-C6-N1	6.27	124.13	121.00
31	A	112	C	N3-C2-O2	-6.27	117.51	121.90
52	a	811	C	N1-C2-O2	6.25	122.65	118.90
52	a	318	G	N1-C6-O6	6.24	123.64	119.90
31	A	448	C	N3-C2-O2	-6.23	117.54	121.90
52	a	794	C	C5-C6-N1	6.23	124.11	121.00
52	a	243	C	N3-C2-O2	-6.22	117.55	121.90
52	a	97	G	N1-C6-O6	-6.22	116.17	119.90
52	a	4	C	N3-C4-N4	6.21	122.35	118.00
31	A	1335	C	C5-C6-N1	6.20	124.10	121.00
31	A	2097	C	N1-C2-O2	6.20	122.62	118.90
52	a	83	C	C2-N3-C4	6.20	123.00	119.90
58	8	69	ASN	N-CA-C	6.20	127.73	111.00
52	a	1360	C	C6-N1-C2	-6.19	117.83	120.30
31	A	38	C	C6-N1-C2	-6.18	117.83	120.30
52	a	755	U	C2-N3-C4	6.18	130.71	127.00
52	a	912	G	N1-C6-O6	-6.17	116.19	119.90
52	a	1077	C	C5-C6-N1	6.17	124.09	121.00
52	a	223	U	N3-C2-O2	-6.17	117.88	122.20
52	a	808	U	N3-C2-O2	-6.17	117.88	122.20
31	A	1108	C	N3-C2-O2	-6.17	117.58	121.90
52	a	1029	A	N1-C6-N6	6.16	122.30	118.60
31	A	2700	C	N1-C2-O2	6.16	122.60	118.90
42	l	7	LEU	CA-CB-CG	6.16	129.47	115.30
52	a	159	C	N3-C2-O2	-6.15	117.59	121.90
52	a	407	C	C5-C6-N1	6.15	124.08	121.00
55	v	142	PHE	CZ-CE2-CD2	6.14	127.47	120.10
31	A	856	U	N3-C2-O2	-6.12	117.91	122.20
52	a	1459	C	N1-C2-O2	6.12	122.57	118.90
52	a	448	G	C6-C5-N7	-6.12	126.73	130.40
52	a	1258	C	N3-C2-O2	-6.12	117.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	2683	C	N3-C2-O2	-6.11	117.62	121.90
58	8	367	ALA	C-N-CA	6.11	136.97	121.70
31	A	2469	C	N1-C2-O2	6.11	122.56	118.90
52	a	434	U	N1-C2-O2	6.11	127.08	122.80
52	a	958	U	N3-C2-O2	-6.11	117.92	122.20
52	a	1158	C	N3-C2-O2	-6.10	117.63	121.90
52	a	1195	G	C6-C5-N7	-6.09	126.75	130.40
52	a	1057	G	C4-N9-C1'	6.09	134.41	126.50
33	b	201	ASP	CA-CB-CG	6.08	126.79	113.40
52	a	698	C	C6-N1-C2	-6.08	117.87	120.30
52	a	1058	C	N1-C2-O2	6.08	122.55	118.90
52	a	1024	C	C5-C6-N1	6.08	124.04	121.00
31	A	1907	C	N1-C2-O2	6.07	122.54	118.90
52	a	411	U	N3-C2-O2	-6.07	117.95	122.20
53	w	126	LEU	CB-CG-CD2	-6.07	100.68	111.00
52	a	1482	C	C6-N1-C2	-6.07	117.87	120.30
31	A	2314	C	C6-N1-C1'	-6.05	113.53	120.80
15	K	239	LEU	CA-CB-CG	6.05	129.21	115.30
42	l	7	LEU	CB-CG-CD2	-6.05	100.72	111.00
31	A	448	C	C2-N1-C1'	6.05	125.45	118.80
52	a	1332	C	N1-C2-O2	6.03	122.52	118.90
52	a	571	C	C6-N1-C2	-6.02	117.89	120.30
52	a	1444	U	C5-C6-N1	6.01	125.71	122.70
31	A	2724	C	N1-C2-O2	6.01	122.51	118.90
31	A	1620	U	C2-N1-C1'	6.01	124.91	117.70
52	a	910	U	N1-C2-N3	6.01	118.50	114.90
52	a	817	C	N1-C2-O2	6.01	122.50	118.90
52	a	1035	U	N3-C2-O2	-6.01	118.00	122.20
47	r	53	ARG	CA-CB-CG	-6.00	100.19	113.40
8	B	69	C	C6-N1-C2	-6.00	117.90	120.30
31	A	253	C	C6-N1-C2	-6.00	117.90	120.30
31	A	38	C	C2-N1-C1'	6.00	125.40	118.80
52	a	591	C	C6-N1-C2	-5.98	117.91	120.30
31	A	186	C	N1-C2-O2	5.98	122.49	118.90
31	A	1013	C	C2-N1-C1'	5.98	125.38	118.80
31	A	173	C	N1-C2-O2	5.98	122.49	118.90
27	W	100	C	N1-C2-O2	5.97	122.48	118.90
52	a	1304	G	N3-C2-N2	5.97	124.08	119.90
52	a	1172	G	C6-C5-N7	5.96	133.97	130.40
52	a	190	C	N1-C2-O2	5.96	122.47	118.90
47	r	21	PRO	N-CA-CB	5.95	110.44	103.30
31	A	1209	U	N1-C2-O2	5.95	126.97	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	921	C	C6-N1-C2	-5.95	117.92	120.30
52	a	1225	C	N3-C2-O2	-5.94	117.74	121.90
31	A	1309	U	N3-C2-O2	-5.93	118.05	122.20
31	A	1142	G	C4-N9-C1'	5.93	134.21	126.50
52	a	1484	C	C4-C5-C6	-5.92	114.44	117.40
31	A	46	C	C5-C6-N1	5.92	123.96	121.00
52	a	282	C	C6-N1-C2	-5.92	117.93	120.30
52	a	313	C	N3-C4-C5	5.92	124.27	121.90
20	P	73	LEU	CA-CB-CG	5.92	128.91	115.30
52	a	571	C	N3-C4-N4	5.92	122.14	118.00
52	a	682	C	C6-N1-C2	-5.92	117.93	120.30
52	a	698	C	C5-C6-N1	5.91	123.96	121.00
52	a	83	C	C2-N1-C1'	5.91	125.30	118.80
31	A	1142	G	N3-C4-C5	-5.91	125.65	128.60
31	A	2789	C	N1-C2-O2	5.91	122.44	118.90
52	a	877	G	C4-C5-N7	5.90	113.16	110.80
31	A	856	U	N1-C2-O2	5.90	126.93	122.80
52	a	564	G	N1-C6-O6	-5.90	116.36	119.90
31	A	2662	C	C6-N1-C1'	-5.89	113.73	120.80
31	A	1770	C	N1-C2-O2	5.89	122.43	118.90
52	a	932	A	C4-N9-C1'	5.89	136.90	126.30
31	A	243	U	N1-C2-O2	5.88	126.92	122.80
52	a	1290	C	N3-C2-O2	-5.88	117.78	121.90
50	u	98	ARG	CA-CB-CG	5.88	126.34	113.40
52	a	484	C	N1-C2-O2	5.88	122.43	118.90
52	a	1296	U	N3-C2-O2	-5.88	118.08	122.20
13	G	206	ASP	CB-CG-OD1	5.88	123.59	118.30
31	A	243	U	N3-C2-O2	-5.88	118.08	122.20
31	A	1748	C	N3-C2-O2	-5.88	117.79	121.90
31	A	2598	G	C5-N7-C8	-5.87	101.36	104.30
55	v	142	PHE	CD1-CE1-CZ	5.86	127.14	120.10
27	W	29	U	P-O3'-C3'	5.86	126.73	119.70
31	A	112	C	C6-N1-C2	-5.86	117.96	120.30
31	A	2654	U	C2-N1-C1'	5.85	124.72	117.70
52	a	107	C	N3-C4-N4	5.85	122.10	118.00
3	3	93	LEU	CA-CB-CG	5.85	128.75	115.30
31	A	9	A	C2-N3-C4	5.84	113.52	110.60
31	A	2706	U	C2-N1-C1'	5.84	124.71	117.70
31	A	1219	U	N3-C2-O2	-5.84	118.11	122.20
31	A	2654	U	N1-C2-O2	5.84	126.89	122.80
33	b	202	ILE	CG1-CB-CG2	-5.84	98.56	111.40
52	a	452	C	C6-N1-C2	-5.84	117.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	178	U	N3-C2-O2	-5.83	118.11	122.20
52	a	450	A	N1-C2-N3	-5.83	126.39	129.30
52	a	848	C	N1-C2-O2	5.83	122.40	118.90
52	a	1172	G	C4-N9-C1'	-5.83	118.92	126.50
31	A	1747	C	C6-N1-C2	-5.82	117.97	120.30
31	A	2491	U	C2-N1-C1'	5.82	124.69	117.70
42	l	24	LEU	CA-CB-CG	5.81	128.66	115.30
31	A	514	A	P-O3'-C3'	5.81	126.67	119.70
52	a	459	C	N1-C2-O2	-5.80	115.42	118.90
52	a	702	C	C2-N1-C1'	5.80	125.18	118.80
31	A	1419	C	N3-C2-O2	-5.79	117.84	121.90
8	B	31	C	N1-C2-O2	5.79	122.37	118.90
31	A	1107	C	C2-N1-C1'	5.79	125.17	118.80
52	a	204	C	C2-N1-C1'	5.79	125.16	118.80
31	A	647	C	C6-N1-C2	-5.78	117.99	120.30
31	A	186	C	N3-C2-O2	-5.78	117.86	121.90
31	A	1784	C	C6-N1-C2	-5.77	117.99	120.30
8	B	7	G	O4'-C1'-N9	5.77	112.82	108.20
52	a	1441	A	N1-C6-N6	-5.77	115.14	118.60
52	a	304	C	N1-C2-O2	5.76	122.36	118.90
52	a	1030	G	C5-C6-O6	-5.76	125.15	128.60
31	A	2653	U	N1-C2-O2	5.75	126.83	122.80
52	a	371	C	C6-N1-C2	-5.75	118.00	120.30
31	A	2121	C	N3-C2-O2	-5.75	117.87	121.90
52	a	293	C	C6-N1-C2	-5.75	118.00	120.30
31	A	1923	C	N1-C2-O2	5.74	122.35	118.90
31	A	2588	U	N1-C2-O2	5.74	126.82	122.80
52	a	137	C	N1-C2-O2	5.74	122.34	118.90
52	a	523	G	N3-C4-N9	-5.74	122.56	126.00
31	A	2007	U	N3-C2-O2	-5.73	118.19	122.20
52	a	374	C	N3-C4-C5	5.73	124.19	121.90
52	a	1172	G	C8-N9-C1'	5.73	134.45	127.00
52	a	1026	G	C6-C5-N7	-5.73	126.96	130.40
52	a	1440	G	N9-C4-C5	5.72	107.69	105.40
31	A	1595	C	C2-N1-C1'	5.72	125.09	118.80
52	a	558	U	N1-C2-O2	5.72	126.81	122.80
52	a	142	G	C5-C6-O6	5.72	132.03	128.60
31	A	210	C	N1-C2-O2	5.71	122.33	118.90
31	A	1334	U	C6-N1-C1'	-5.71	113.21	121.20
31	A	928	U	N3-C2-O2	-5.71	118.20	122.20
31	A	1746	C	N1-C2-O2	5.71	122.32	118.90
31	A	254	U	N3-C2-O2	-5.71	118.21	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	24	C	C5-C6-N1	5.70	123.85	121.00
27	W	74	C	C6-N1-C2	-5.70	118.02	120.30
52	a	797	G	N3-C2-N2	-5.70	115.91	119.90
52	a	71	G	N1-C6-O6	-5.69	116.48	119.90
52	a	1029	A	N9-C4-C5	-5.69	103.53	105.80
31	A	1945	U	N1-C2-O2	5.68	126.78	122.80
52	a	496	G	C6-C5-N7	-5.68	126.99	130.40
31	A	1595	C	N3-C2-O2	-5.68	117.92	121.90
31	A	2111	U	C2-N1-C1'	5.68	124.51	117.70
52	a	1374	C	N1-C2-O2	5.68	122.31	118.90
52	a	411	U	C2-N1-C1'	5.68	124.51	117.70
31	A	2708	C	N1-C2-O2	5.67	122.30	118.90
31	A	1692	C	C6-N1-C2	-5.66	118.03	120.30
52	a	685	U	C5-C6-N1	5.66	125.53	122.70
52	a	1095	C	N3-C2-O2	-5.66	117.94	121.90
55	v	167	PHE	CB-CG-CD2	-5.66	116.83	120.80
58	8	330	LYS	N-CA-CB	5.66	120.79	110.60
31	A	2178	C	N1-C2-O2	5.66	122.29	118.90
31	A	2573	C	N1-C2-O2	5.65	122.29	118.90
31	A	794	A	C2-N3-C4	5.64	113.42	110.60
31	A	367	C	OP1-P-O3'	5.64	117.61	105.20
31	A	1459	U	C2-N1-C1'	5.64	124.47	117.70
31	A	1945	U	C2-N1-C1'	5.64	124.47	117.70
31	A	367	C	P-O3'-C3'	5.63	126.46	119.70
31	A	541	G	C4-N9-C1'	5.63	133.83	126.50
31	A	1923	C	C6-N1-C2	-5.63	118.05	120.30
52	a	410	U	N3-C2-O2	-5.63	118.26	122.20
52	a	1453	G	C5-C6-O6	-5.63	125.22	128.60
31	A	1843	C	C2-N3-C4	-5.63	117.09	119.90
52	a	410	U	N1-C2-O2	5.63	126.74	122.80
52	a	1459	C	C6-N1-C2	-5.63	118.05	120.30
31	A	594	C	C5-C6-N1	5.62	123.81	121.00
52	a	299	C	N1-C2-O2	5.62	122.27	118.90
31	A	210	C	C6-N1-C2	-5.61	118.06	120.30
52	a	765	C	N1-C2-O2	5.61	122.27	118.90
52	a	559	C	N1-C2-O2	5.61	122.27	118.90
31	A	688	C	C6-N1-C2	-5.60	118.06	120.30
31	A	2683	C	C2-N1-C1'	5.60	124.96	118.80
52	a	19	C	C6-N1-C2	-5.59	118.06	120.30
52	a	1446	G	C4-N9-C1'	5.59	133.76	126.50
58	8	280	ILE	CB-CA-C	5.58	122.77	111.60
52	a	976	C	C5-C6-N1	5.58	123.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1142	G	N3-C4-N9	5.58	129.35	126.00
31	A	1981	C	N1-C2-O2	5.58	122.25	118.90
58	8	300	ILE	N-CA-C	-5.58	95.94	111.00
52	a	371	C	N3-C4-N4	5.57	121.90	118.00
52	a	808	U	N1-C2-O2	5.57	126.70	122.80
31	A	2325	G	N3-C4-N9	5.57	129.34	126.00
32	0	87	LEU	CA-CB-CG	5.56	128.09	115.30
52	a	1172	G	N1-C6-O6	-5.56	116.56	119.90
52	a	1374	C	N3-C2-O2	-5.56	118.01	121.90
58	8	73	GLU	CA-CB-CG	5.56	125.63	113.40
8	B	38	C	N1-C2-O2	5.55	122.23	118.90
31	A	683	C	N1-C2-O2	5.55	122.23	118.90
31	A	1317	C	C6-N1-C2	-5.55	118.08	120.30
31	A	594	C	C6-N1-C2	-5.55	118.08	120.30
8	B	69	C	C2-N1-C1'	5.55	124.90	118.80
52	a	131	G	N1-C6-O6	-5.54	116.57	119.90
31	A	448	C	C6-N1-C2	-5.54	118.08	120.30
52	a	1081	C	N3-C4-N4	5.54	121.88	118.00
52	a	1438	G	C8-N9-C4	-5.54	104.18	106.40
52	a	637	C	N1-C2-O2	5.54	122.22	118.90
52	a	1087	G	C2-N3-C4	-5.54	109.13	111.90
31	A	897	A	C5-C6-N1	5.53	120.47	117.70
40	j	135	LEU	CA-CB-CG	5.53	128.02	115.30
52	a	909	U	C2-N1-C1'	5.53	124.33	117.70
31	A	2378	C	N3-C2-O2	-5.53	118.03	121.90
52	a	1358	C	N1-C2-O2	5.52	122.21	118.90
31	A	2421	C	N1-C2-O2	5.52	122.21	118.90
52	a	462	U	C5-C6-N1	5.52	125.46	122.70
31	A	1818	U	N3-C2-O2	-5.52	118.34	122.20
27	W	10	C	N1-C2-O2	5.52	122.21	118.90
27	W	22	A	OP1-P-O3'	5.52	117.34	105.20
31	A	2789	C	N3-C2-O2	-5.52	118.04	121.90
52	a	1058	C	C6-N1-C2	-5.51	118.09	120.30
31	A	2325	G	N3-C4-C5	-5.51	125.85	128.60
31	A	496	C	N1-C2-O2	5.51	122.20	118.90
31	A	1945	U	N3-C2-O2	-5.50	118.35	122.20
52	a	1238	C	C2-N3-C4	-5.50	117.15	119.90
52	a	7	G	N9-C4-C5	5.50	107.60	105.40
31	A	1397	C	N3-C2-O2	-5.50	118.05	121.90
52	a	1005	U	C2-N3-C4	5.49	130.30	127.00
52	a	1330	U	N1-C2-O2	5.49	126.64	122.80
31	A	688	C	N1-C2-O2	5.49	122.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1906	C	N1-C2-O2	5.49	122.19	118.90
52	a	900	G	N3-C2-N2	5.48	123.74	119.90
52	a	1106	C	N1-C2-O2	5.48	122.19	118.90
52	a	484	C	C2-N1-C1'	5.47	124.82	118.80
52	a	1296	U	N1-C2-O2	5.47	126.63	122.80
52	a	285	C	N3-C4-N4	5.47	121.83	118.00
52	a	912	G	C5-C6-O6	5.47	131.88	128.60
31	A	688	C	N3-C2-O2	-5.46	118.08	121.90
31	A	2774	U	C5-C4-O4	5.46	129.18	125.90
52	a	1442	A	N7-C8-N9	5.46	116.53	113.80
31	A	813	C	N1-C2-O2	5.45	122.17	118.90
31	A	2300	U	C2-N1-C1'	5.45	124.24	117.70
52	a	83	C	C5-C6-N1	5.45	123.73	121.00
52	a	910	U	C2-N3-C4	-5.45	123.73	127.00
31	A	1137	C	N1-C2-O2	5.45	122.17	118.90
52	a	152	G	C4-C5-N7	5.44	112.98	110.80
52	a	779	C	C6-N1-C2	-5.44	118.12	120.30
52	a	962	G	N1-C6-O6	-5.44	116.63	119.90
52	a	1290	C	N3-C4-C5	-5.44	119.72	121.90
52	a	454	G	C6-C5-N7	-5.44	127.14	130.40
31	A	2325	G	C4-N9-C1'	5.43	133.56	126.50
52	a	121	C	C2-N1-C1'	5.43	124.77	118.80
53	w	164	THR	CA-CB-CG2	-5.43	104.80	112.40
31	A	178	U	N1-C2-O2	5.43	126.60	122.80
52	a	932	A	C8-N9-C1'	-5.43	117.93	127.70
31	A	2097	C	N3-C2-O2	-5.43	118.10	121.90
52	a	986	C	C6-N1-C2	-5.42	118.13	120.30
52	a	1486	U	C6-N1-C2	-5.42	117.75	121.00
52	a	1352	C	C6-N1-C2	-5.42	118.13	120.30
52	a	147	C	C5-C4-N4	-5.42	116.41	120.20
24	T	67	LEU	CA-CB-CG	5.42	127.76	115.30
52	a	342	G	N3-C2-N2	-5.42	116.11	119.90
31	A	630	C	C2-N1-C1'	5.41	124.75	118.80
31	A	2300	U	C5-C6-N1	5.41	125.41	122.70
31	A	870	U	N1-C2-O2	5.41	126.59	122.80
31	A	1309	U	N1-C2-O2	5.41	126.59	122.80
31	A	856	U	C2-N1-C1'	5.41	124.19	117.70
52	a	1256	U	N3-C4-C5	-5.41	111.36	114.60
52	a	1331	C	N1-C2-O2	5.41	122.14	118.90
31	A	2020	C	N1-C2-O2	5.40	122.14	118.90
35	e	303	MET	CB-CG-SD	5.40	128.59	112.40
55	v	129	LEU	CA-CB-CG	5.40	127.71	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1604	A	N1-C6-N6	5.39	121.84	118.60
31	A	2535	C	N1-C2-O2	5.39	122.14	118.90
52	a	209	G	N1-C6-O6	-5.39	116.66	119.90
52	a	493	C	N3-C4-C5	5.39	124.06	121.90
31	A	186	C	C6-N1-C2	-5.39	118.14	120.30
31	A	2545	U	N1-C2-O2	5.39	126.57	122.80
52	a	1226	U	N1-C2-O2	5.39	126.58	122.80
31	A	1309	U	C2-N1-C1'	5.39	124.17	117.70
52	a	1439	U	C5-C4-O4	-5.39	122.67	125.90
31	A	1283	U	C2-N1-C1'	5.38	124.16	117.70
52	a	566	C	N1-C2-O2	5.38	122.13	118.90
52	a	1087	G	C5-C6-N1	-5.38	108.81	111.50
31	A	2378	C	C6-N1-C2	-5.38	118.15	120.30
31	A	2662	C	C6-N1-C2	-5.38	118.15	120.30
31	A	2699	U	N3-C2-O2	-5.37	118.44	122.20
52	a	784	U	C6-N1-C2	-5.37	117.78	121.00
52	a	850	A	N1-C6-N6	5.37	121.82	118.60
52	a	134	C	C6-N1-C2	-5.37	118.15	120.30
8	B	18	C	N1-C2-O2	5.37	122.12	118.90
31	A	1335	C	N1-C2-O2	5.37	122.12	118.90
52	a	670	A	N3-C4-N9	5.37	131.69	127.40
31	A	703	C	N1-C2-O2	5.36	122.12	118.90
31	A	2007	U	N1-C2-O2	5.36	126.55	122.80
31	A	2653	U	N3-C2-O2	-5.36	118.45	122.20
52	a	1353	C	C6-N1-C2	-5.36	118.16	120.30
31	A	496	C	C5-C6-N1	5.35	123.68	121.00
31	A	2530	U	N3-C2-O2	-5.34	118.46	122.20
52	a	472	G	N3-C2-N2	5.34	123.64	119.90
31	A	2303	A	O4'-C1'-N9	-5.34	103.93	108.20
31	A	2360	U	N1-C2-O2	5.34	126.54	122.80
31	A	907	C	N1-C2-O2	5.34	122.10	118.90
31	A	1175	U	N1-C2-O2	5.33	126.53	122.80
31	A	2737	G	N1-C6-O6	-5.33	116.70	119.90
52	a	1106	C	N3-C2-O2	-5.33	118.17	121.90
31	A	2116	C	N3-C2-O2	-5.33	118.17	121.90
31	A	877	C	N3-C2-O2	-5.33	118.17	121.90
52	a	295	G	N7-C8-N9	5.33	115.77	113.10
52	a	139	G	C5-C6-N1	5.33	114.16	111.50
52	a	784	U	C5-C6-N1	5.33	125.36	122.70
31	A	1209	U	C5-C6-N1	5.33	125.36	122.70
8	B	31	C	C2-N1-C1'	5.32	124.66	118.80
31	A	1397	C	C2-N1-C1'	5.32	124.66	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	1029	A	C5-N7-C8	-5.32	101.24	103.90
52	a	1150	U	C2-N1-C1'	5.32	124.09	117.70
52	a	1238	C	C2-N1-C1'	5.32	124.65	118.80
52	a	1353	C	N3-C2-O2	-5.32	118.18	121.90
52	a	255	C	C5-C4-N4	-5.32	116.48	120.20
31	A	363	C	C2-N1-C1'	5.32	124.65	118.80
52	a	301	C	C6-N1-C2	-5.31	118.17	120.30
31	A	1843	C	N1-C2-N3	5.31	122.92	119.20
52	a	1195	G	N3-C4-N9	5.31	129.19	126.00
52	a	246	G	C4-N9-C1'	5.31	133.40	126.50
31	A	1419	C	C2-N1-C1'	5.31	124.64	118.80
52	a	881	C	C5-C4-N4	-5.31	116.48	120.20
52	a	1106	C	C6-N1-C1'	-5.31	114.43	120.80
52	a	1035	U	N1-C2-O2	5.30	126.51	122.80
31	A	2483	C	N3-C2-O2	-5.30	118.19	121.90
52	a	987	G	C5-C6-O6	5.30	131.78	128.60
21	Q	223	ARG	C-N-CA	5.30	134.94	121.70
31	A	899	A	C5-N7-C8	-5.30	101.25	103.90
53	w	159	LEU	CB-CG-CD1	-5.30	102.00	111.00
31	A	2529	C	C6-N1-C2	-5.29	118.18	120.30
31	A	2708	C	C6-N1-C2	-5.29	118.18	120.30
31	A	1696	C	N1-C2-O2	5.29	122.07	118.90
31	A	2491	U	N1-C2-O2	5.28	126.50	122.80
52	a	1211	C	N1-C2-O2	5.28	122.07	118.90
31	A	1550	U	N1-C2-O2	5.27	126.49	122.80
31	A	2530	U	C2-N1-C1'	5.27	124.02	117.70
53	w	136	ASP	CB-CG-OD2	-5.27	113.56	118.30
52	a	938	G	C5-C6-O6	-5.26	125.44	128.60
58	8	303	VAL	N-CA-C	5.26	125.21	111.00
52	a	229	A	N1-C2-N3	-5.26	126.67	129.30
52	a	90	C	C2-N1-C1'	5.26	124.59	118.80
31	A	630	C	N3-C2-O2	-5.26	118.22	121.90
52	a	800	C	C2-N1-C1'	5.25	124.58	118.80
31	A	972	G	C4-N9-C1'	5.25	133.32	126.50
52	a	139	G	N1-C2-N2	5.25	120.92	116.20
52	a	1295	G	C2-N3-C4	-5.25	109.28	111.90
31	A	563	C	N1-C2-O2	5.24	122.05	118.90
52	a	239	U	N3-C2-O2	-5.24	118.53	122.20
52	a	566	C	C6-N1-C2	-5.24	118.20	120.30
31	A	294	U	C5-C6-N1	5.24	125.32	122.70
31	A	1595	C	C6-N1-C2	-5.24	118.20	120.30
31	A	228	U	N1-C2-O2	5.24	126.47	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	2737	G	C5-C6-O6	5.24	131.74	128.60
52	a	1256	U	N1-C2-N3	-5.24	111.76	114.90
52	a	727	C	N1-C2-O2	5.24	122.04	118.90
52	a	1057	G	C8-N9-C1'	-5.24	120.19	127.00
52	a	204	C	C6-N1-C2	-5.24	118.21	120.30
52	a	336	U	C2-N1-C1'	5.24	123.98	117.70
52	a	912	G	N9-C4-C5	5.24	107.49	105.40
31	A	2683	C	C6-N1-C2	-5.23	118.21	120.30
52	a	444	A	O4'-C1'-N9	5.23	112.38	108.20
52	a	987	G	N1-C2-N2	5.23	120.91	116.20
31	A	541	G	N3-C4-N9	5.23	129.14	126.00
31	A	2654	U	N3-C2-O2	-5.23	118.54	122.20
27	W	29	U	OP2-P-O3'	5.22	116.69	105.20
31	A	2651	C	N1-C2-O2	5.22	122.03	118.90
52	a	523	G	N3-C4-C5	5.22	131.21	128.60
31	A	2300	U	N3-C2-O2	-5.22	118.55	122.20
52	a	361	C	N3-C4-N4	5.22	121.66	118.00
52	a	1290	C	N3-C4-N4	5.22	121.66	118.00
52	a	1446	G	N3-C4-N9	5.22	129.13	126.00
52	a	1099	G	O4'-C1'-N9	5.22	112.38	108.20
31	A	173	C	N3-C2-O2	-5.22	118.25	121.90
52	a	299	C	N3-C2-O2	-5.22	118.25	121.90
52	a	786	C	C5-C4-N4	-5.22	116.55	120.20
31	A	1107	C	N3-C2-O2	-5.22	118.25	121.90
52	a	493	C	C2-N3-C4	-5.22	117.29	119.90
31	A	1901	C	N1-C2-O2	5.21	122.03	118.90
31	A	1907	C	N3-C2-O2	-5.21	118.25	121.90
52	a	88	G	C8-N9-C1'	-5.21	120.22	127.00
52	a	1446	G	C8-N9-C1'	-5.21	120.22	127.00
52	a	909	U	N1-C2-O2	5.21	126.45	122.80
52	a	1334	G	C5-C6-N1	5.21	114.11	111.50
31	A	684	C	C2-N3-C4	-5.21	117.30	119.90
27	W	74	C	C5-C6-N1	5.20	123.60	121.00
31	A	541	G	N3-C4-C5	-5.20	126.00	128.60
52	a	560	C	N3-C2-O2	-5.20	118.26	121.90
52	a	1348	C	C2-N3-C4	-5.20	117.30	119.90
31	A	2699	U	N1-C2-O2	5.20	126.44	122.80
52	a	523	G	N1-C6-O6	5.20	123.02	119.90
52	a	572	C	N3-C4-N4	5.19	121.63	118.00
52	a	933	C	C6-N1-C2	-5.19	118.22	120.30
31	A	2270	G	N3-C4-N9	5.19	129.11	126.00
50	u	103	PHE	CB-CG-CD2	-5.19	117.17	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	372	C	C6-N1-C2	-5.19	118.23	120.30
31	A	404	U	N1-C2-O2	5.18	126.43	122.80
31	A	1092	C	N1-C2-O2	5.18	122.01	118.90
52	a	1234	A	C2-N3-C4	5.18	113.19	110.60
31	A	2447	A	N3-C4-N9	5.18	131.54	127.40
52	a	806	U	N3-C2-O2	-5.18	118.58	122.20
31	A	1604	A	N7-C8-N9	5.17	116.39	113.80
31	A	2593	G	N3-C2-N2	5.17	123.52	119.90
52	a	131	G	C5-C6-N1	5.17	114.09	111.50
52	a	470	C	N1-C2-O2	5.17	122.00	118.90
52	a	568	C	N3-C2-O2	-5.17	118.28	121.90
52	a	702	C	N1-C2-O2	5.17	122.00	118.90
52	a	1453	G	N3-C2-N2	5.16	123.52	119.90
52	a	1017	G	C4-N9-C1'	5.16	133.21	126.50
31	A	1175	U	N3-C2-O2	-5.16	118.59	122.20
52	a	1458	C	C6-N1-C2	-5.16	118.24	120.30
31	A	2121	C	C6-N1-C2	-5.15	118.24	120.30
52	a	1459	C	N3-C4-N4	5.15	121.61	118.00
57	x	85	PRO	C-N-CD	5.15	139.22	128.40
31	A	2367	C	N1-C2-O2	5.15	121.99	118.90
52	a	287	C	N3-C2-O2	-5.15	118.30	121.90
52	a	83	C	N3-C4-C5	-5.14	119.84	121.90
55	v	25	TYR	CB-CG-CD1	5.14	124.09	121.00
31	A	1419	C	C6-N1-C2	-5.14	118.24	120.30
31	A	2360	U	C2-N1-C1'	5.14	123.87	117.70
31	A	703	C	N3-C2-O2	-5.13	118.31	121.90
52	a	190	C	N3-C2-O2	-5.13	118.31	121.90
52	a	1095	C	C2-N1-C1'	5.13	124.44	118.80
52	a	1272	C	N3-C2-O2	-5.13	118.31	121.90
43	m	127	LEU	CA-CB-CG	-5.13	103.50	115.30
52	a	255	C	C6-N1-C2	-5.13	118.25	120.30
52	a	406	U	C5-C6-N1	5.12	125.26	122.70
52	a	1353	C	C5-C6-N1	5.12	123.56	121.00
31	A	1219	U	C6-N1-C2	-5.12	117.93	121.00
52	a	453	G	C4-N9-C1'	5.12	133.16	126.50
31	A	258	C	N3-C2-O2	-5.12	118.31	121.90
52	a	496	G	C4-C5-N7	5.12	112.85	110.80
31	A	845	C	C6-N1-C2	-5.12	118.25	120.30
31	A	275	U	C2-N1-C1'	5.12	123.84	117.70
31	A	112	C	C5-C6-N1	5.12	123.56	121.00
31	A	210	C	N3-C2-O2	-5.11	118.32	121.90
52	a	800	C	C6-N1-C2	-5.11	118.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	797	G	C5-C6-O6	5.11	131.67	128.60
52	a	1244	C	C6-N1-C2	-5.11	118.25	120.30
52	a	83	C	N3-C4-N4	5.11	121.58	118.00
58	8	346	PHE	CB-CG-CD1	-5.11	117.22	120.80
15	K	191	LEU	CA-CB-CG	5.11	127.04	115.30
31	A	258	C	N1-C2-O2	5.11	121.96	118.90
52	a	1163	G	C5-C6-O6	-5.11	125.54	128.60
31	A	543	A	C2-N3-C4	5.10	113.15	110.60
31	A	2432	G	C4-N9-C1'	5.10	133.13	126.50
31	A	1546	C	N1-C2-O2	5.09	121.96	118.90
52	a	295	G	O5'-P-OP2	-5.09	101.12	105.70
52	a	1185	C	C6-N1-C2	-5.09	118.26	120.30
31	A	683	C	C6-N1-C2	-5.08	118.27	120.30
52	a	529	G	C4-C5-N7	5.08	112.83	110.80
52	a	911	C	C6-N1-C2	-5.08	118.27	120.30
31	A	1317	C	N3-C2-O2	-5.08	118.34	121.90
52	a	293	C	C5-C6-N1	5.08	123.54	121.00
52	a	1486	U	C4-C5-C6	-5.08	116.65	119.70
31	A	2243	C	N1-C2-O2	5.08	121.94	118.90
52	a	1332	C	C6-N1-C2	-5.07	118.27	120.30
52	a	35	C	C5-C6-N1	5.07	123.54	121.00
52	a	88	G	N1-C6-O6	5.07	122.94	119.90
52	a	293	C	N3-C2-O2	-5.07	118.35	121.90
52	a	1081	C	N1-C2-N3	5.07	122.75	119.20
31	A	288	C	N1-C2-O2	5.06	121.94	118.90
52	a	1438	G	N1-C6-O6	-5.06	116.86	119.90
31	A	363	C	N3-C2-O2	-5.06	118.36	121.90
31	A	2736	G	N1-C6-O6	-5.06	116.86	119.90
52	a	271	A	N7-C8-N9	5.06	116.33	113.80
52	a	493	C	N3-C4-N4	-5.06	114.46	118.00
52	a	88	G	C6-C5-N7	-5.06	127.36	130.40
52	a	394	G	N3-C4-N9	5.06	129.03	126.00
31	A	502	U	N1-C2-O2	5.05	126.34	122.80
31	A	2518	C	C5-C4-N4	5.05	123.74	120.20
52	a	90	C	C5-C6-N1	5.05	123.53	121.00
31	A	17	C	C6-N1-C2	-5.05	118.28	120.30
31	A	1550	U	N3-C2-O2	-5.05	118.67	122.20
31	A	1770	C	N3-C2-O2	-5.05	118.37	121.90
52	a	1106	C	C6-N1-C2	-5.05	118.28	120.30
42	l	5	LYS	CD-CE-NZ	-5.05	100.09	111.70
31	A	1971	C	N1-C2-O2	5.05	121.93	118.90
29	Y	98	LEU	CA-CB-CG	5.04	126.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	w	136	ASP	N-CA-CB	-5.04	101.52	110.60
31	A	2724	C	C2-N1-C1'	5.04	124.34	118.80
52	a	1318	C	C6-N1-C2	-5.04	118.29	120.30
31	A	97	A	P-O3'-C3'	5.03	125.74	119.70
31	A	827	C	N1-C2-O2	5.03	121.92	118.90
31	A	2300	U	N1-C2-O2	5.03	126.32	122.80
52	a	983	G	C5-C6-N1	5.03	114.02	111.50
31	A	1789	U	C2-N1-C1'	5.03	123.74	117.70
31	A	2063	C	C2-N1-C1'	5.03	124.33	118.80
52	a	806	U	N1-C2-O2	5.03	126.32	122.80
52	a	1092	G	N3-C2-N2	-5.03	116.38	119.90
31	A	253	C	C5-C6-N1	5.03	123.51	121.00
53	w	149	PRO	N-CA-C	5.03	125.17	112.10
52	a	150	C	C5-C6-N1	5.02	123.51	121.00
52	a	1304	G	N3-C4-N9	5.02	129.01	126.00
31	A	1608	C	N1-C2-O2	5.02	121.91	118.90
52	a	881	C	C5-C6-N1	5.02	123.51	121.00
55	v	99	GLU	CA-CB-CG	-5.02	102.36	113.40
31	A	2527	C	N1-C2-O2	5.02	121.91	118.90
52	a	999	G	N1-C6-O6	5.02	122.91	119.90
27	W	100	C	C6-N1-C2	-5.02	118.29	120.30
55	v	37	GLU	CG-CD-OE1	5.02	128.33	118.30
31	A	2469	C	N3-C2-O2	-5.01	118.39	121.90
31	A	1249	C	C6-N1-C2	-5.01	118.30	120.30
31	A	497	C	N1-C2-O2	5.01	121.91	118.90
31	A	1747	C	N1-C2-O2	5.01	121.91	118.90
43	m	118	ARG	NE-CZ-NH1	5.01	122.81	120.30
52	a	423	A	C2-N3-C4	5.01	113.11	110.60
52	a	1189	G	N1-C6-O6	-5.01	116.89	119.90
31	A	496	C	C6-N1-C2	-5.01	118.30	120.30
31	A	1013	C	C6-N1-C2	-5.01	118.30	120.30
52	a	1029	A	C5-C6-N6	-5.00	119.70	123.70

There are no chirality outliers.

All (62) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	0	73	TRP	Peptide
58	8	273	PRO	Peptide
58	8	277	PHE	Peptide
58	8	298	SER	Peptide
58	8	299	ASP	Peptide

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Mol	Chain	Res	Type	Group
58	8	302	THR	Peptide
58	8	303	VAL	Peptide
58	8	304	LEU	Peptide
58	8	315	LEU	Peptide
58	8	329	LYS	Peptide
58	8	346	PHE	Sidechain
58	8	359	ARG	Peptide
58	8	366	MET	Mainchain
58	8	369	ALA	Peptide
58	8	370	ASP	Peptide
58	8	69	ASN	Peptide
58	8	71	PRO	Peptide
58	8	72	MET	Peptide
17	M	143	LEU	Peptide
21	Q	190	VAL	Peptide
23	S	174	THR	Peptide
33	b	168	VAL	Peptide
33	b	201	ASP	Sidechain
34	c	168	ILE	Peptide
34	c	86	GLU	Peptide
34	c	88	ARG	Peptide
54	d	155	SER	Peptide
54	d	23	ASN	Peptide
35	e	147	LYS	Peptide
36	f	102	PRO	Peptide
37	g	8	GLU	Peptide
39	i	78	ARG	Peptide
39	i	96	ILE	Peptide
40	j	135	LEU	Peptide
42	l	24	LEU	Peptide
42	l	27	CYS	Peptide
42	l	8	ILE	Peptide
43	m	137	LYS	Peptide
43	m	34	LYS	Peptide
50	u	103	PHE	Sidechain
55	v	100	LYS	Peptide
55	v	101	PRO	Peptide
55	v	104	GLY	Peptide
55	v	120	SER	Mainchain
55	v	147	LYS	Peptide
55	v	158	GLY	Peptide
55	v	159	THR	Peptide

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Mol	Chain	Res	Type	Group
55	v	165	PHE	Sidechain
55	v	168	VAL	Peptide
55	v	184	ASN	Peptide
55	v	185	ASN	Peptide
55	v	187	VAL	Peptide
55	v	188	LEU	Peptide
55	v	194	ARG	Sidechain
55	v	33	LEU	Peptide
53	w	108	LYS	Peptide
53	w	110	ILE	Peptide
53	w	126	LEU	Peptide
53	w	130	TYR	Peptide
53	w	148	LYS	Peptide
53	w	176	ASN	Peptide
53	w	98	ARG	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	44/56 (79%)	40 (91%)	4 (9%)	0	100	100
2	2	49/65 (75%)	39 (80%)	10 (20%)	0	100	100
3	3	55/61 (90%)	49 (89%)	6 (11%)	0	100	100
4	4	67/73 (92%)	59 (88%)	8 (12%)	0	100	100
5	5	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
6	6	47/142 (33%)	46 (98%)	1 (2%)	0	100	100
7	7	44/116 (38%)	41 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	C	245/271 (90%)	213 (87%)	32 (13%)	0	100	100
10	D	210/221 (95%)	188 (90%)	22 (10%)	0	100	100
11	E	208/243 (86%)	180 (86%)	28 (14%)	0	100	100
12	F	173/220 (79%)	161 (93%)	12 (7%)	0	100	100
13	G	171/182 (94%)	161 (94%)	10 (6%)	0	100	100
14	H	51/155 (33%)	47 (92%)	4 (8%)	0	100	100
15	K	191/197 (97%)	178 (93%)	13 (7%)	0	100	100
16	L	119/121 (98%)	104 (87%)	15 (13%)	0	100	100
17	M	175/192 (91%)	163 (93%)	11 (6%)	1 (1%)	25	57
18	N	132/135 (98%)	111 (84%)	21 (16%)	0	100	100
19	O	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
20	P	118/123 (96%)	116 (98%)	2 (2%)	0	100	100
21	Q	116/156 (74%)	100 (86%)	16 (14%)	0	100	100
22	R	113/127 (89%)	105 (93%)	8 (7%)	0	100	100
23	S	145/201 (72%)	118 (81%)	27 (19%)	0	100	100
24	T	142/199 (71%)	125 (88%)	17 (12%)	0	100	100
25	U	90/122 (74%)	86 (96%)	4 (4%)	0	100	100
26	V	122/145 (84%)	109 (89%)	13 (11%)	0	100	100
28	X	98/137 (72%)	87 (89%)	11 (11%)	0	100	100
29	Y	72/77 (94%)	66 (92%)	6 (8%)	0	100	100
30	Z	88/109 (81%)	87 (99%)	1 (1%)	0	100	100
32	o	62/94 (66%)	54 (87%)	6 (10%)	2 (3%)	4	22
33	b	225/236 (95%)	195 (87%)	29 (13%)	1 (0%)	34	67
34	c	211/218 (97%)	181 (86%)	28 (13%)	2 (1%)	17	49
35	e	169/253 (67%)	150 (89%)	17 (10%)	2 (1%)	13	41
36	f	109/146 (75%)	85 (78%)	24 (22%)	0	100	100
37	g	147/155 (95%)	130 (88%)	16 (11%)	1 (1%)	22	55
38	h	132/134 (98%)	116 (88%)	16 (12%)	0	100	100
39	i	131/157 (83%)	107 (82%)	23 (18%)	1 (1%)	19	51
40	j	96/122 (79%)	83 (86%)	13 (14%)	0	100	100
41	k	116/138 (84%)	104 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	l	121/123 (98%)	100 (83%)	21 (17%)	0	100	100
43	m	108/126 (86%)	90 (83%)	18 (17%)	0	100	100
44	o	60/90 (67%)	59 (98%)	1 (2%)	0	100	100
45	p	78/88 (89%)	61 (78%)	17 (22%)	0	100	100
46	q	76/108 (70%)	64 (84%)	12 (16%)	0	100	100
47	r	62/101 (61%)	58 (94%)	4 (6%)	0	100	100
48	s	76/92 (83%)	61 (80%)	15 (20%)	0	100	100
49	t	103/108 (95%)	93 (90%)	10 (10%)	0	100	100
50	u	42/137 (31%)	39 (93%)	3 (7%)	0	100	100
51	y	106/236 (45%)	96 (91%)	10 (9%)	0	100	100
53	w	82/121 (68%)	79 (96%)	0	3 (4%)	3	20
54	d	197/201 (98%)	173 (88%)	22 (11%)	2 (1%)	15	46
55	v	188/198 (95%)	171 (91%)	14 (7%)	3 (2%)	9	34
56	n	97/100 (97%)	90 (93%)	7 (7%)	0	100	100
57	x	35/47 (74%)	30 (86%)	4 (11%)	1 (3%)	4	24
58	8	150/370 (40%)	116 (77%)	18 (12%)	16 (11%)	0	3
All	All	6213/7898 (79%)	5499 (88%)	679 (11%)	35 (1%)	29	57

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	0	72	VAL
35	e	148	ILE
53	w	149	PRO
55	v	105	MET
58	8	72	MET
58	8	73	GLU
58	8	299	ASP
58	8	300	ILE
58	8	303	VAL
58	8	316	SER
58	8	330	LYS
58	8	366	MET
58	8	367	ALA
58	8	370	ASP
58	8	371	MET

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Mol	Chain	Res	Type
34	c	89	PRO
54	d	5	ARG
55	v	121	PRO
58	8	360	ILE
58	8	368	ARG
17	M	197	PRO
33	b	169	ASP
39	i	159	ALA
53	w	150	TRP
34	c	88	ARG
35	e	302	PRO
57	x	90	ILE
58	8	306	PRO
58	8	364	GLU
37	g	9	GLU
32	0	73	TRP
54	d	168	PRO
55	v	120	SER
53	w	119	PRO
58	8	307	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	39/49 (80%)	39 (100%)	0	100	100
2	2	48/59 (81%)	46 (96%)	2 (4%)	30	59
3	3	47/50 (94%)	47 (100%)	0	100	100
4	4	59/62 (95%)	58 (98%)	1 (2%)	60	80
5	5	34/34 (100%)	34 (100%)	0	100	100
6	6	46/124 (37%)	46 (100%)	0	100	100
7	7	40/96 (42%)	40 (100%)	0	100	100
9	C	195/216 (90%)	194 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	D	174/182 (96%)	174 (100%)	0	100	100
11	E	176/205 (86%)	173 (98%)	3 (2%)	60	80
12	F	148/183 (81%)	148 (100%)	0	100	100
13	G	147/154 (96%)	147 (100%)	0	100	100
14	H	47/134 (35%)	47 (100%)	0	100	100
15	K	167/171 (98%)	165 (99%)	2 (1%)	71	85
16	L	101/101 (100%)	101 (100%)	0	100	100
17	M	135/144 (94%)	133 (98%)	2 (2%)	65	82
18	N	107/108 (99%)	107 (100%)	0	100	100
19	O	96/96 (100%)	96 (100%)	0	100	100
20	P	99/100 (99%)	99 (100%)	0	100	100
21	Q	104/135 (77%)	103 (99%)	1 (1%)	76	88
22	R	102/114 (90%)	102 (100%)	0	100	100
23	S	129/174 (74%)	129 (100%)	0	100	100
24	T	126/176 (72%)	126 (100%)	0	100	100
25	U	81/103 (79%)	80 (99%)	1 (1%)	71	85
26	V	112/129 (87%)	111 (99%)	1 (1%)	78	90
28	X	85/111 (77%)	84 (99%)	1 (1%)	71	85
29	Y	64/67 (96%)	63 (98%)	1 (2%)	62	81
30	Z	83/97 (86%)	82 (99%)	1 (1%)	71	85
32	o	56/83 (68%)	55 (98%)	1 (2%)	59	79
33	b	192/201 (96%)	188 (98%)	4 (2%)	53	76
34	c	185/188 (98%)	185 (100%)	0	100	100
35	e	132/203 (65%)	128 (97%)	4 (3%)	41	68
36	f	98/125 (78%)	98 (100%)	0	100	100
37	g	120/126 (95%)	120 (100%)	0	100	100
38	h	117/117 (100%)	115 (98%)	2 (2%)	60	80
39	i	103/123 (84%)	102 (99%)	1 (1%)	76	88
40	j	90/110 (82%)	90 (100%)	0	100	100
41	k	92/109 (84%)	92 (100%)	0	100	100
42	l	106/106 (100%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	m	97/109 (89%)	97 (100%)	0	100	100
44	o	58/85 (68%)	58 (100%)	0	100	100
45	p	71/79 (90%)	70 (99%)	1 (1%)	67	83
46	q	70/95 (74%)	70 (100%)	0	100	100
47	r	56/96 (58%)	56 (100%)	0	100	100
48	s	67/81 (83%)	67 (100%)	0	100	100
49	t	86/89 (97%)	84 (98%)	2 (2%)	50	74
50	u	40/118 (34%)	40 (100%)	0	100	100
51	y	97/213 (46%)	94 (97%)	3 (3%)	40	68
53	w	75/109 (69%)	74 (99%)	1 (1%)	69	84
54	d	178/180 (99%)	175 (98%)	3 (2%)	60	80
55	v	160/168 (95%)	158 (99%)	2 (1%)	69	84
56	n	89/90 (99%)	89 (100%)	0	100	100
57	x	28/37 (76%)	28 (100%)	0	100	100
58	8	129/310 (42%)	125 (97%)	4 (3%)	40	68
All	All	5383/6724 (80%)	5338 (99%)	45 (1%)	82	91

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	13	LEU
2	2	48	LEU
4	4	153	LEU
9	C	39	ARG
11	E	71	ASN
11	E	81	ARG
11	E	245	LEU
15	K	62	ARG
15	K	174	ARG
17	M	196	LEU
17	M	252	ARG
21	Q	127	ASN
25	U	106	ARG
26	V	64	LEU
28	X	73	LYS
29	Y	103	LEU
30	Z	107	ARG

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Mol	Chain	Res	Type
32	0	76	ASN
33	b	30	ARG
33	b	40	LYS
33	b	94	HIS
33	b	201	ASP
35	e	144	LYS
35	e	266	LEU
35	e	303	MET
35	e	305	GLU
38	h	67	ARG
38	h	79	LEU
39	i	176	ARG
45	p	46	THR
49	t	103	ARG
49	t	162	ARG
51	y	91	ARG
51	y	119	ARG
51	y	159	LEU
53	w	103	PHE
54	d	27	ARG
54	d	40	LYS
54	d	160	LEU
55	v	24	LEU
55	v	37	GLU
58	8	283	ILE
58	8	304	LEU
58	8	314	ILE
58	8	368	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	58	HIS
4	4	95	HIS
4	4	118	GLN
4	4	145	ASN
9	C	54	HIS
9	C	84	ASN
10	D	167	HIS
10	D	209	GLN
11	E	71	ASN
11	E	118	GLN

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Mol	Chain	Res	Type
11	E	153	ASN
11	E	222	ASN
12	F	60	ASN
12	F	77	ASN
12	F	116	GLN
13	G	103	GLN
15	K	97	ASN
15	K	139	ASN
16	L	3	GLN
16	L	73	ASN
16	L	82	ASN
17	M	161	ASN
18	N	13	HIS
19	O	37	GLN
20	P	81	HIS
21	Q	127	ASN
22	R	28	HIS
22	R	77	ASN
22	R	99	GLN
23	S	145	GLN
23	S	212	HIS
23	S	214	GLN
24	T	52	GLN
24	T	106	ASN
26	V	130	HIS
32	0	76	ASN
34	c	18	HIS
34	c	34	GLN
34	c	187	GLN
35	e	225	HIS
35	e	264	ASN
38	h	19	ASN
38	h	51	HIS
38	h	68	ASN
39	i	127	ASN
39	i	161	HIS
40	j	126	ASN
40	j	149	HIS
40	j	151	HIS
41	k	127	HIS
41	k	128	ASN
42	l	77	HIS

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Mol	Chain	Res	Type
43	m	56	ASN
43	m	65	GLN
43	m	83	ASN
43	m	125	HIS
47	r	59	GLN
47	r	83	GLN
48	s	23	ASN
50	u	124	ASN
51	y	165	GLN
53	w	155	GLN
53	w	162	GLN
53	w	172	GLN
54	d	57	HIS
54	d	112	ASN
54	d	115	HIS
54	d	142	GLN
55	v	45	HIS
55	v	96	ASN
55	v	163	ASN
55	v	196	ASN
58	8	58	GLN
58	8	269	GLN
58	8	294	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	W	101/106 (95%)	30 (29%)	4 (3%)
31	A	2808/2810 (99%)	596 (21%)	4 (0%)
52	a	1477/1491 (99%)	310 (20%)	0
8	B	116/121 (95%)	21 (18%)	1 (0%)
All	All	4502/4528 (99%)	957 (21%)	9 (0%)

All (957) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	B	4	U
8	B	10	G
8	B	14	U
8	B	15	A
8	B	16	G

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Mol	Chain	Res	Type
8	B	25	G
8	B	31	C
8	B	36	A
8	B	42	C
8	B	53	U
8	B	54	G
8	B	58	A
8	B	61	C
8	B	67	U
8	B	74	A
8	B	89	A
8	B	92	U
8	B	101	A
8	B	111	G
8	B	117	A
8	B	119	G
27	W	16	G
27	W	17	A
27	W	22	A
27	W	23	G
27	W	28	U
27	W	29	U
27	W	30	A
27	W	31	U
27	W	32	C
27	W	33	A
27	W	34	U
27	W	35	U
27	W	36	A
27	W	37	C
27	W	38	G
27	W	39	A
27	W	48	A
27	W	53	G
27	W	64	A
27	W	65	U
27	W	71	C
27	W	76	G
27	W	77	A
27	W	83	C
27	W	84	C
27	W	88	C

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Mol	Chain	Res	Type
27	W	90	G
27	W	95	A
27	W	97	A
27	W	98	G
31	A	9	A
31	A	10	G
31	A	11	G
31	A	12	A
31	A	13	A
31	A	14	A
31	A	15	G
31	A	26	G
31	A	33	A
31	A	45	A
31	A	46	C
31	A	54	G
31	A	70	A
31	A	72	A
31	A	73	U
31	A	74	G
31	A	82	G
31	A	84	G
31	A	85	U
31	A	98	G
31	A	99	A
31	A	100	G
31	A	112	C
31	A	116	A
31	A	117	A
31	A	118	U
31	A	123	C
31	A	130	U
31	A	131	C
31	A	143	G
31	A	144	A
31	A	147	C
31	A	149	A
31	A	158	C
31	A	159	A
31	A	173	C
31	A	181	A
31	A	184	A

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Mol	Chain	Res	Type
31	A	189	A
31	A	201	A
31	A	207	A
31	A	226	A
31	A	233	G
31	A	250	A
31	A	251	G
31	A	252	C
31	A	262	G
31	A	264	A
31	A	266	A
31	A	275	U
31	A	276	G
31	A	284	A
31	A	287	A
31	A	294	U
31	A	295	C
31	A	297	U
31	A	298	G
31	A	304	A
31	A	316	G
31	A	320	U
31	A	330	U
31	A	331	A
31	A	332	G
31	A	333	A
31	A	338	G
31	A	340	A
31	A	347	G
31	A	352	C
31	A	361	C
31	A	365	A
31	A	368	U
31	A	370	A
31	A	377	G
31	A	378	A
31	A	379	C
31	A	383	A
31	A	384	G
31	A	392	G
31	A	398	G
31	A	399	U

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Mol	Chain	Res	Type
31	A	415	U
31	A	416	C
31	A	417	A
31	A	418	G
31	A	423	G
31	A	424	A
31	A	436	G
31	A	447	C
31	A	448	C
31	A	466	A
31	A	467	G
31	A	468	U
31	A	469	A
31	A	479	G
31	A	489	A
31	A	491	A
31	A	493	G
31	A	504	G
31	A	507	G
31	A	512	A
31	A	515	U
31	A	516	A
31	A	519	A
31	A	524	A
31	A	529	G
31	A	541	G
31	A	542	C
31	A	543	A
31	A	544	G
31	A	545	U
31	A	554	G
31	A	555	A
31	A	557	C
31	A	558	A
31	A	559	G
31	A	560	A
31	A	573	G
31	A	583	G
31	A	585	A
31	A	608	U
31	A	609	G
31	A	610	G

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Mol	Chain	Res	Type
31	A	611	C
31	A	613	U
31	A	614	G
31	A	623	A
31	A	624	A
31	A	630	C
31	A	632	G
31	A	633	A
31	A	638	U
31	A	639	A
31	A	643	A
31	A	646	G
31	A	649	A
31	A	657	U
31	A	665	U
31	A	667	G
31	A	680	G
31	A	686	A
31	A	688	C
31	A	696	A
31	A	697	U
31	A	722	G
31	A	724	G
31	A	728	A
31	A	731	U
31	A	734	G
31	A	737	G
31	A	740	G
31	A	741	U
31	A	745	A
31	A	757	U
31	A	758	U
31	A	768	G
31	A	773	U
31	A	775	A
31	A	776	G
31	A	782	G
31	A	786	G
31	A	787	G
31	A	788	G
31	A	793	A
31	A	795	U

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Mol	Chain	Res	Type
31	A	802	C
31	A	803	G
31	A	811	A
31	A	816	G
31	A	823	C
31	A	838	U
31	A	841	G
31	A	856	U
31	A	857	G
31	A	859	A
31	A	861	A
31	A	866	G
31	A	869	G
31	A	879	G
31	A	887	G
31	A	889	G
31	A	890	G
31	A	891	G
31	A	892	C
31	A	893	C
31	A	895	C
31	A	897	A
31	A	900	G
31	A	901	C
31	A	902	G
31	A	903	G
31	A	905	A
31	A	906	C
31	A	907	C
31	A	908	A
31	A	915	G
31	A	916	G
31	A	919	A
31	A	924	U
31	A	937	U
31	A	938	G
31	A	946	A
31	A	947	A
31	A	970	G
31	A	974	G
31	A	981	G
31	A	987	A

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Mol	Chain	Res	Type
31	A	989	G
31	A	993	C
31	A	1001	A
31	A	1002	G
31	A	1008	A
31	A	1011	A
31	A	1013	C
31	A	1017	G
31	A	1018	A
31	A	1024	A
31	A	1037	A
31	A	1040	U
31	A	1041	G
31	A	1045	G
31	A	1050	G
31	A	1051	U
31	A	1054	U
31	A	1055	A
31	A	1061	G
31	A	1062	G
31	A	1065	G
31	A	1072	A
31	A	1075	G
31	A	1098	A
31	A	1099	G
31	A	1101	A
31	A	1105	A
31	A	1106	C
31	A	1112	A
31	A	1116	A
31	A	1118	U
31	A	1125	U
31	A	1139	A
31	A	1140	G
31	A	1143	C
31	A	1147	U
31	A	1148	G
31	A	1150	G
31	A	1155	A
31	A	1158	U
31	A	1160	A
31	A	1162	C

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Mol	Chain	Res	Type
31	A	1163	G
31	A	1169	A
31	A	1170	A
31	A	1175	U
31	A	1183	A
31	A	1196	A
31	A	1197	A
31	A	1198	A
31	A	1225	G
31	A	1227	U
31	A	1240	G
31	A	1241	U
31	A	1245	U
31	A	1254	U
31	A	1258	A
31	A	1259	C
31	A	1261	A
31	A	1271	G
31	A	1272	A
31	A	1274	A
31	A	1277	G
31	A	1286	A
31	A	1293	C
31	A	1294	A
31	A	1296	A
31	A	1305	A
31	A	1308	A
31	A	1310	C
31	A	1315	G
31	A	1321	A
31	A	1322	A
31	A	1333	U
31	A	1342	A
31	A	1346	U
31	A	1366	C
31	A	1371	C
31	A	1373	U
31	A	1379	C
31	A	1386	A
31	A	1399	A
31	A	1400	U
31	A	1405	A

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Mol	Chain	Res	Type
31	A	1413	A
31	A	1416	A
31	A	1423	U
31	A	1424	A
31	A	1427	A
31	A	1431	C
31	A	1432	U
31	A	1433	U
31	A	1436	U
31	A	1437	G
31	A	1448	A
31	A	1449	C
31	A	1458	C
31	A	1461	G
31	A	1472	A
31	A	1476	G
31	A	1480	A
31	A	1481	U
31	A	1484	G
31	A	1486	U
31	A	1493	C
31	A	1494	G
31	A	1497	A
31	A	1501	G
31	A	1502	A
31	A	1511	U
31	A	1512	U
31	A	1513	C
31	A	1519	A
31	A	1520	A
31	A	1521	G
31	A	1522	A
31	A	1524	G
31	A	1525	G
31	A	1528	U
31	A	1529	A
31	A	1531	A
31	A	1532	G
31	A	1544	A
31	A	1557	G
31	A	1558	U
31	A	1559	A

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Mol	Chain	Res	Type
31	A	1568	U
31	A	1569	A
31	A	1570	C
31	A	1571	G
31	A	1592	A
31	A	1593	U
31	A	1594	A
31	A	1600	A
31	A	1603	A
31	A	1612	A
31	A	1620	U
31	A	1621	C
31	A	1622	A
31	A	1628	A
31	A	1635	C
31	A	1643	G
31	A	1644	A
31	A	1662	A
31	A	1682	C
31	A	1683	G
31	A	1684	C
31	A	1708	C
31	A	1710	G
31	A	1711	C
31	A	1734	A
31	A	1750	C
31	A	1751	A
31	A	1752	C
31	A	1753	A
31	A	1755	A
31	A	1756	G
31	A	1762	C
31	A	1766	G
31	A	1774	G
31	A	1778	G
31	A	1783	A
31	A	1796	A
31	A	1801	A
31	A	1810	C
31	A	1812	A
31	A	1818	U
31	A	1819	A

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Mol	Chain	Res	Type
31	A	1821	G
31	A	1826	U
31	A	1829	A
31	A	1839	A
31	A	1882	U
31	A	1884	A
31	A	1885	C
31	A	1915	A
31	A	1920	G
31	A	1923	C
31	A	1926	A
31	A	1927	A
31	A	1928	C
31	A	1930	A
31	A	1931	U
31	A	1943	G
31	A	1944	G
31	A	1945	U
31	A	1950	A
31	A	1951	A
31	A	1957	U
31	A	1969	U
31	A	1974	A
31	A	1981	C
31	A	1984	A
31	A	1985	A
31	A	1986	G
31	A	1996	U
31	A	2005	U
31	A	2006	G
31	A	2007	U
31	A	2011	G
31	A	2034	C
31	A	2035	A
31	A	2037	G
31	A	2045	A
31	A	2046	G
31	A	2047	A
31	A	2048	U
31	A	2069	C
31	A	2070	A
31	A	2073	A

*Continued on next page...*

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Mol	Chain	Res	Type
31	A	2074	A
31	A	2075	G
31	A	2076	A
31	A	2077	C
31	A	2082	U
31	A	2083	G
31	A	2091	A
31	A	2094	G
31	A	2101	G
31	A	2103	G
31	A	2106	U
31	A	2107	G
31	A	2118	U
31	A	2122	C
31	A	2123	U
31	A	2124	G
31	A	2125	C
31	A	2126	G
31	A	2128	A
31	A	2129	G
31	A	2130	C
31	A	2132	U
31	A	2133	A
31	A	2134	G
31	A	2137	G
31	A	2139	A
31	A	2140	A
31	A	2142	G
31	A	2144	G
31	A	2145	A
31	A	2146	A
31	A	2147	G
31	A	2148	A
31	A	2151	G
31	A	2159	C
31	A	2160	C
31	A	2162	G
31	A	2163	G
31	A	2173	G
31	A	2174	C
31	A	2175	C
31	A	2176	A

*Continued on next page...*

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Mol	Chain	Res	Type
31	A	2178	C
31	A	2179	A
31	A	2181	U
31	A	2183	A
31	A	2184	G
31	A	2185	A
31	A	2186	U
31	A	2187	A
31	A	2189	C
31	A	2191	C
31	A	2192	U
31	A	2195	G
31	A	2198	A
31	A	2199	G
31	A	2201	G
31	A	2204	A
31	A	2209	U
31	A	2212	A
31	A	2220	G
31	A	2229	U
31	A	2230	A
31	A	2240	G
31	A	2242	A
31	A	2254	A
31	A	2255	G
31	A	2256	A
31	A	2266	U
31	A	2268	G
31	A	2269	G
31	A	2271	C
31	A	2272	G
31	A	2283	A
31	A	2286	A
31	A	2295	A
31	A	2297	G
31	A	2300	U
31	A	2304	A
31	A	2317	G
31	A	2322	A
31	A	2323	C
31	A	2325	G
31	A	2342	G

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Mol	Chain	Res	Type
31	A	2343	C
31	A	2344	A
31	A	2348	G
31	A	2352	A
31	A	2353	A
31	A	2361	U
31	A	2362	G
31	A	2364	C
31	A	2367	C
31	A	2374	C
31	A	2378	C
31	A	2394	A
31	A	2396	G
31	A	2400	G
31	A	2402	C
31	A	2405	A
31	A	2406	G
31	A	2408	G
31	A	2419	G
31	A	2423	A
31	A	2432	G
31	A	2436	U
31	A	2442	A
31	A	2443	A
31	A	2444	C
31	A	2445	G
31	A	2446	G
31	A	2452	A
31	A	2458	U
31	A	2464	G
31	A	2465	A
31	A	2466	U
31	A	2487	G
31	A	2493	A
31	A	2508	U
31	A	2509	U
31	A	2511	G
31	A	2515	C
31	A	2518	C
31	A	2519	G
31	A	2520	A
31	A	2521	U

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Mol	Chain	Res	Type
31	A	2522	G
31	A	2524	C
31	A	2535	C
31	A	2537	C
31	A	2549	G
31	A	2552	U
31	A	2579	U
31	A	2583	A
31	A	2584	G
31	A	2589	A
31	A	2590	C
31	A	2591	G
31	A	2593	G
31	A	2594	A
31	A	2597	U
31	A	2598	G
31	A	2599	G
31	A	2601	U
31	A	2602	U
31	A	2603	C
31	A	2619	A
31	A	2626	U
31	A	2627	C
31	A	2630	U
31	A	2632	U
31	A	2646	U
31	A	2647	A
31	A	2653	U
31	A	2671	A
31	A	2672	G
31	A	2674	A
31	A	2680	G
31	A	2690	G
31	A	2702	G
31	A	2706	U
31	A	2708	C
31	A	2719	G
31	A	2729	A
31	A	2731	C
31	A	2732	G
31	A	2736	G
31	A	2744	A

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Mol	Chain	Res	Type
31	A	2751	A
31	A	2753	C
31	A	2762	G
31	A	2764	U
31	A	2766	A
31	A	2768	A
31	A	2770	C
31	A	2771	A
31	A	2780	G
31	A	2783	A
31	A	2784	G
31	A	2796	A
52	a	5	A
52	a	6	U
52	a	7	G
52	a	10	G
52	a	31	U
52	a	32	G
52	a	33	A
52	a	40	G
52	a	45	A
52	a	48	C
52	a	49	U
52	a	50	U
52	a	52	A
52	a	55	C
52	a	62	G
52	a	72	A
52	a	75	U
52	a	82	U
52	a	83	C
52	a	85	A
52	a	90	C
52	a	92	G
52	a	100	A
52	a	104	A
52	a	105	C
52	a	106	G
52	a	114	A
52	a	115	C
52	a	121	C
52	a	127	A

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Mol	Chain	Res	Type
52	a	130	G
52	a	143	G
52	a	147	C
52	a	148	G
52	a	150	C
52	a	152	G
52	a	166	G
52	a	167	G
52	a	174	A
52	a	180	A
52	a	191	G
52	a	202	G
52	a	216	U
52	a	218	G
52	a	221	A
52	a	222	G
52	a	230	G
52	a	237	G
52	a	238	C
52	a	252	G
52	a	260	G
52	a	269	A
52	a	277	A
52	a	287	C
52	a	296	A
52	a	299	C
52	a	300	A
52	a	303	G
52	a	315	A
52	a	317	G
52	a	322	G
52	a	323	C
52	a	324	A
52	a	325	G
52	a	338	U
52	a	343	C
52	a	344	A
52	a	349	G
52	a	353	A
52	a	355	G
52	a	358	U
52	a	360	A

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Mol	Chain	Res	Type
52	a	369	U
52	a	377	G
52	a	382	C
52	a	383	A
52	a	384	G
52	a	392	A
52	a	393	C
52	a	395	G
52	a	399	G
52	a	400	U
52	a	410	U
52	a	411	U
52	a	416	G
52	a	423	A
52	a	424	G
52	a	426	A
52	a	429	G
52	a	432	G
52	a	433	G
52	a	434	U
52	a	443	A
52	a	444	A
52	a	447	A
52	a	453	G
52	a	456	U
52	a	459	C
52	a	466	C
52	a	469	G
52	a	472	G
52	a	475	G
52	a	478	G
52	a	479	U
52	a	481	A
52	a	495	A
52	a	507	A
52	a	510	G
52	a	511	A
52	a	512	U
52	a	514	G
52	a	520	A
52	a	521	A
52	a	524	C

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Mol	Chain	Res	Type
52	a	525	G
52	a	536	G
52	a	543	A
52	a	544	A
52	a	566	C
52	a	577	A
52	a	578	C
52	a	579	A
52	a	580	G
52	a	600	U
52	a	601	G
52	a	602	G
52	a	613	G
52	a	630	G
52	a	650	A
52	a	651	G
52	a	659	A
52	a	660	A
52	a	669	A
52	a	670	A
52	a	671	C
52	a	672	G
52	a	695	A
52	a	696	C
52	a	697	A
52	a	703	A
52	a	725	A
52	a	741	U
52	a	742	A
52	a	757	G
52	a	762	A
52	a	763	A
52	a	765	C
52	a	766	G
52	a	768	U
52	a	769	G
52	a	775	U
52	a	776	A
52	a	780	G
52	a	784	U
52	a	790	U
52	a	791	C

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Mol	Chain	Res	Type
52	a	794	C
52	a	795	C
52	a	796	C
52	a	797	G
52	a	798	U
52	a	799	G
52	a	821	A
52	a	822	A
52	a	825	A
52	a	834	G
52	a	838	A
52	a	849	A
52	a	851	G
52	a	863	A
52	a	875	G
52	a	876	G
52	a	883	C
52	a	884	A
52	a	909	U
52	a	915	G
52	a	918	A
52	a	920	G
52	a	924	A
52	a	925	G
52	a	926	A
52	a	938	G
52	a	941	U
52	a	942	G
52	a	945	A
52	a	946	U
52	a	948	C
52	a	953	A
52	a	954	A
52	a	958	U
52	a	961	U
52	a	963	A
52	a	964	A
52	a	969	A
52	a	973	G
52	a	974	U
52	a	975	G
52	a	978	U

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Mol	Chain	Res	Type
52	a	980	C
52	a	981	G
52	a	982	G
52	a	985	A
52	a	986	C
52	a	992	C
52	a	994	C
52	a	995	A
52	a	1003	C
52	a	1005	U
52	a	1014	U
52	a	1027	U
52	a	1034	U
52	a	1038	G
52	a	1041	A
52	a	1043	G
52	a	1044	U
52	a	1047	C
52	a	1050	A
52	a	1057	G
52	a	1066	G
52	a	1073	G
52	a	1074	U
52	a	1075	U
52	a	1079	A
52	a	1080	A
52	a	1082	G
52	a	1088	U
52	a	1089	U
52	a	1091	G
52	a	1095	C
52	a	1099	G
52	a	1100	A
52	a	1105	A
52	a	1107	U
52	a	1114	G
52	a	1115	A
52	a	1116	U
52	a	1119	G
52	a	1130	G
52	a	1131	U
52	a	1132	G

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Mol	Chain	Res	Type
52	a	1144	A
52	a	1149	A
52	a	1150	U
52	a	1160	U
52	a	1161	A
52	a	1162	U
52	a	1163	G
52	a	1174	C
52	a	1175	A
52	a	1184	A
52	a	1186	A
52	a	1187	A
52	a	1188	U
52	a	1189	G
52	a	1195	G
52	a	1198	A
52	a	1204	U
52	a	1205	C
52	a	1206	G
52	a	1208	G
52	a	1222	G
52	a	1223	A
52	a	1227	A
52	a	1229	C
52	a	1233	A
52	a	1234	A
52	a	1235	A
52	a	1243	C
52	a	1246	C
52	a	1247	A
52	a	1248	G
52	a	1250	U
52	a	1253	G
52	a	1265	C
52	a	1266	A
52	a	1267	A
52	a	1271	G
52	a	1280	A
52	a	1288	A
52	a	1294	A
52	a	1295	G
52	a	1311	C

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Mol	Chain	Res	Type
52	a	1312	A
52	a	1317	G
52	a	1319	G
52	a	1327	C
52	a	1328	G
52	a	1346	C
52	a	1347	A
52	a	1351	C
52	a	1368	G
52	a	1371	G
52	a	1390	A
52	a	1395	A
52	a	1397	C
52	a	1400	C
52	a	1401	A
52	a	1402	A
52	a	1403	G
52	a	1405	A
52	a	1418	A
52	a	1441	A
52	a	1443	G
52	a	1452	A
52	a	1454	G
52	a	1455	U
52	a	1466	G
52	a	1478	G
52	a	1479	G
52	a	1480	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	B	57	U
27	W	29	U
27	W	32	C
27	W	33	A
27	W	97	A
31	A	5	A
31	A	97	A
31	A	514	A
31	A	556	C

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

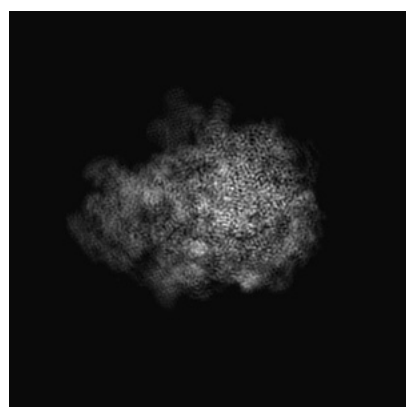
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6709. These allow visual inspection of the internal detail of the map and identification of artifacts.

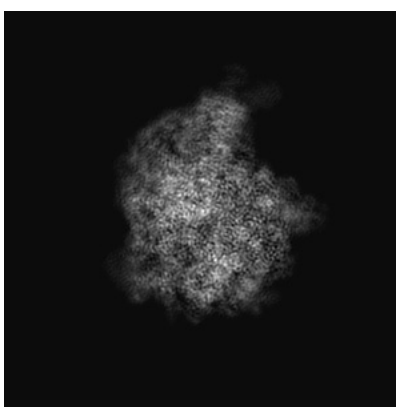
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

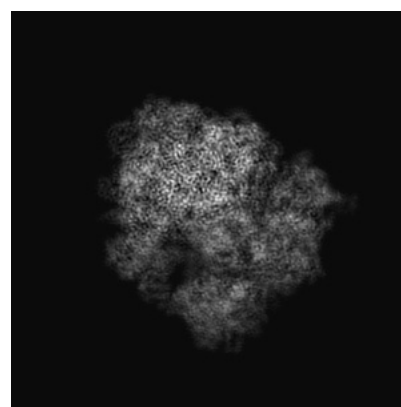
#### 6.1.1 Primary map



X



Y

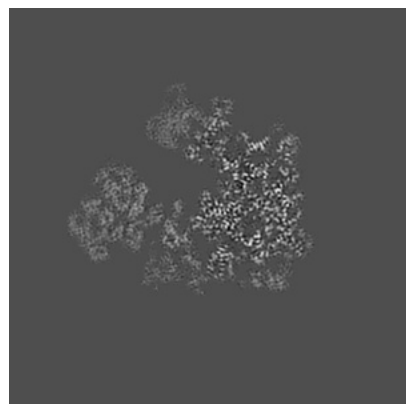


Z

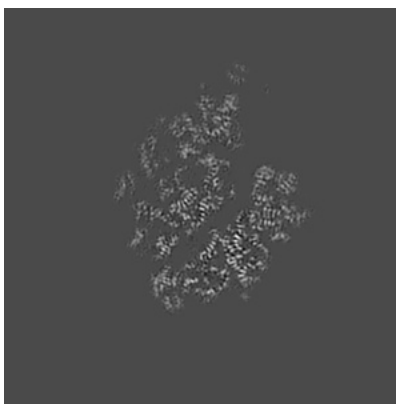
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

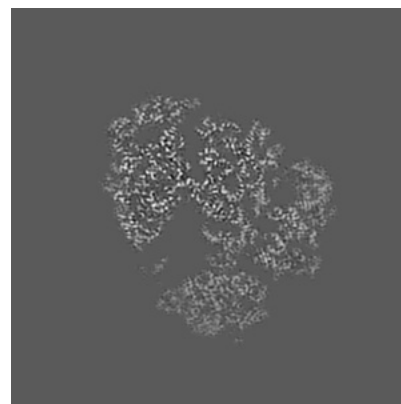
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

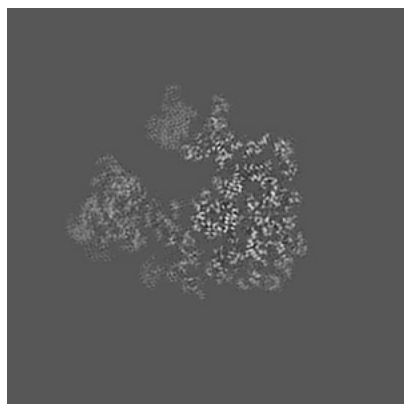


Z Index: 192

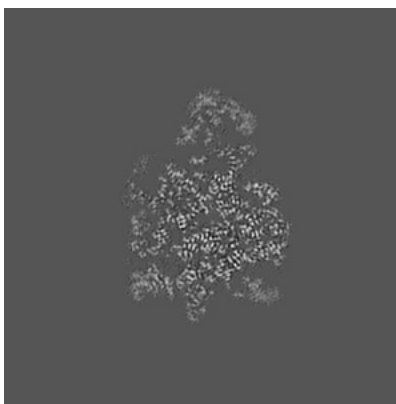
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

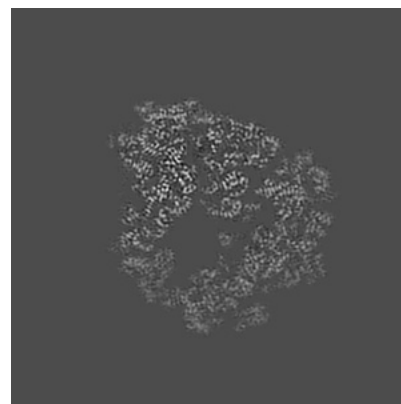
### 6.3.1 Primary map



X Index: 196



Y Index: 220



Z Index: 203

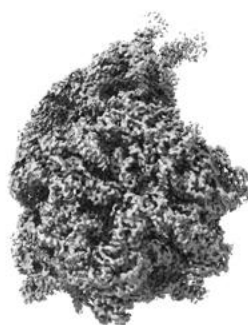
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

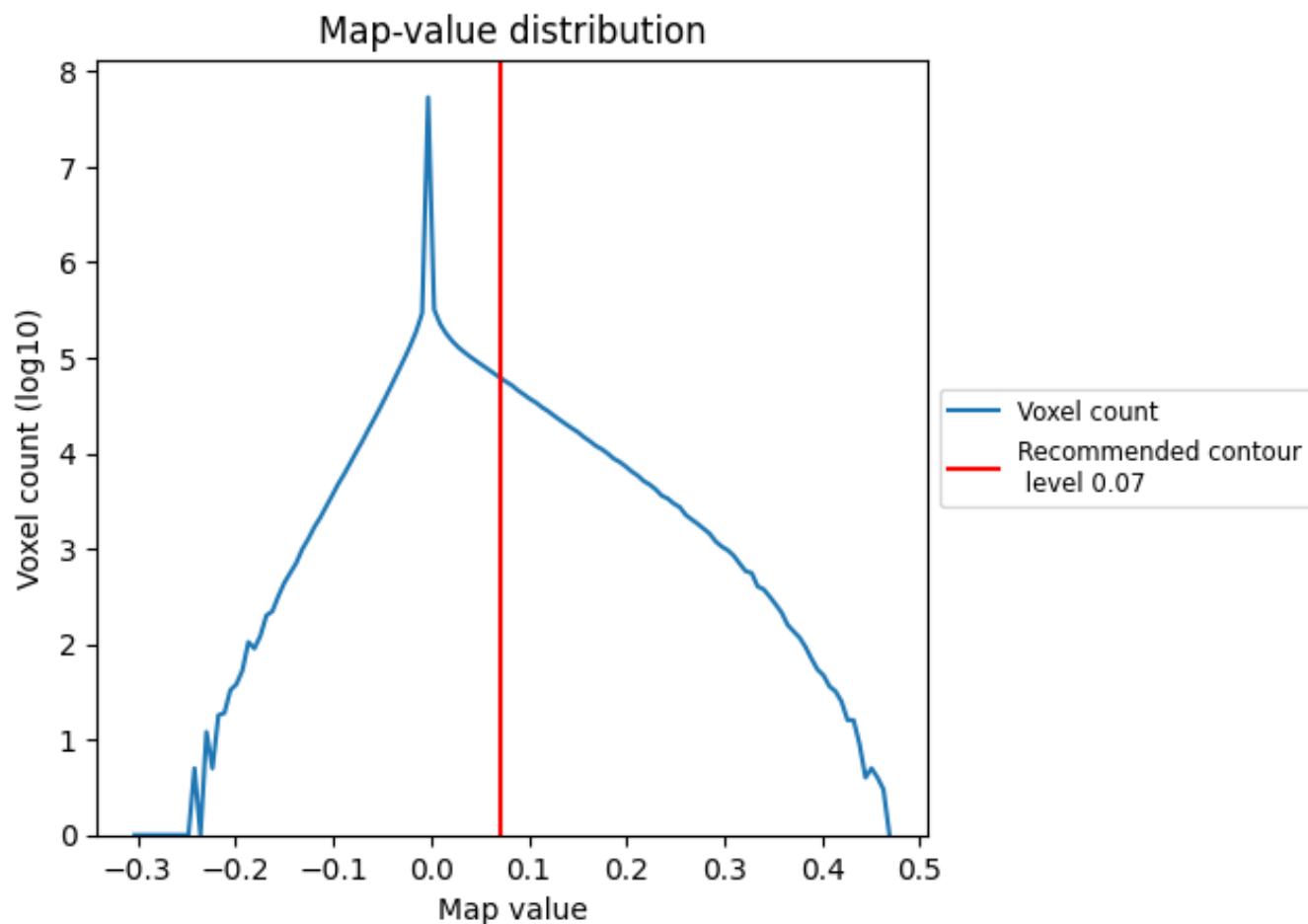
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

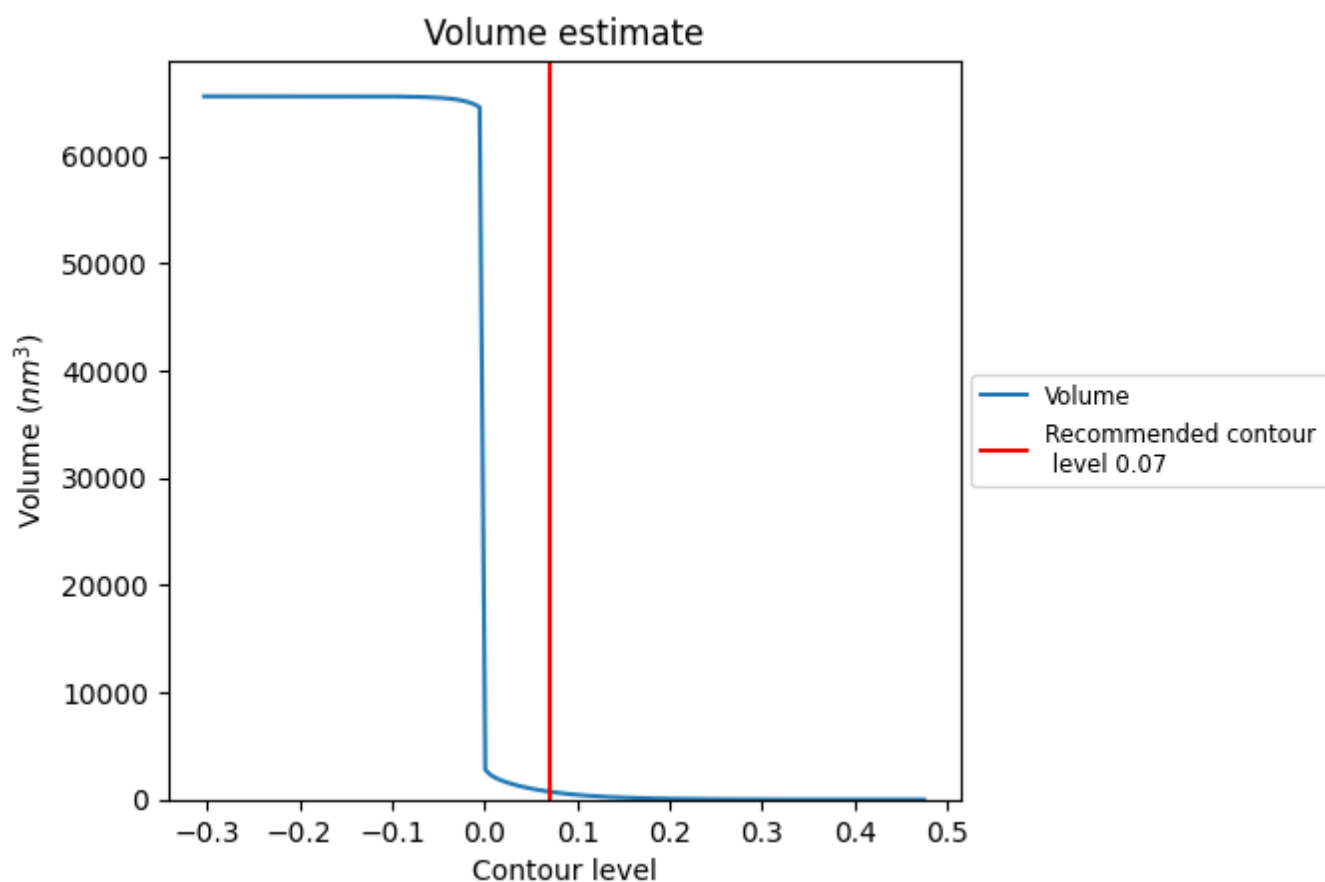
This section contains the results of statistical analysis of the map.

### 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.

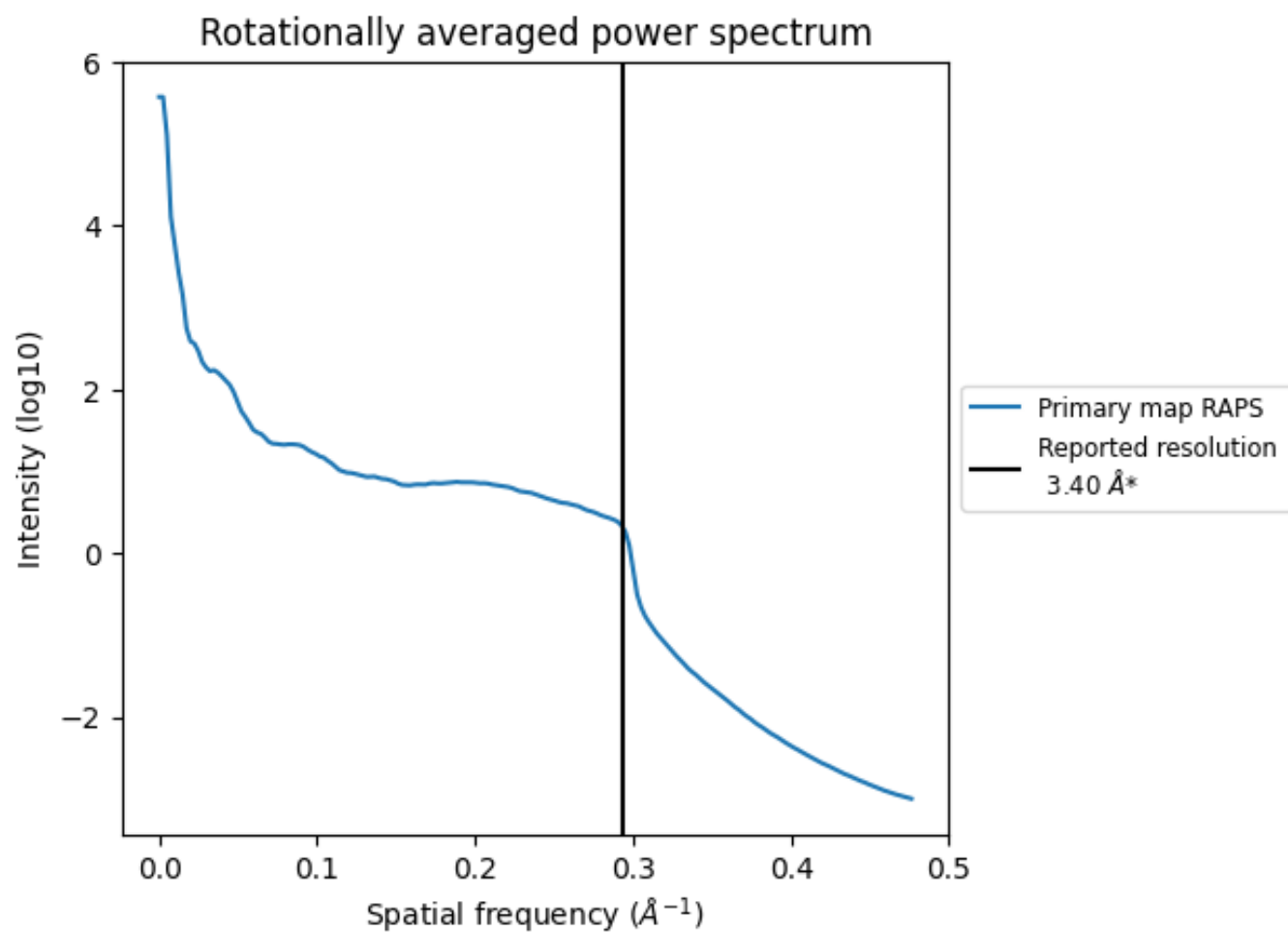
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 735 nm<sup>3</sup>; this corresponds to an approximate mass of 664 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 0.294 Å<sup>-1</sup>



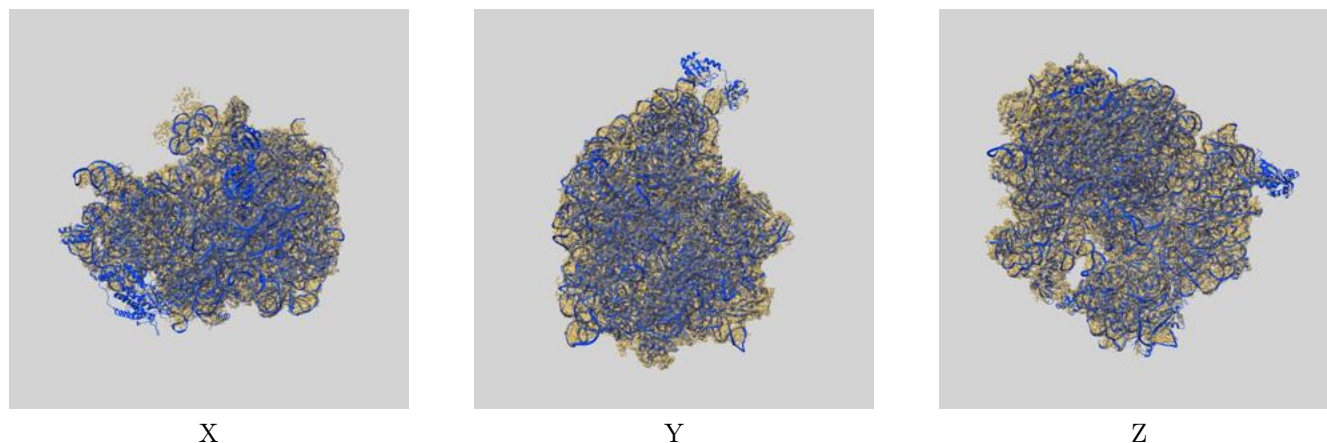
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

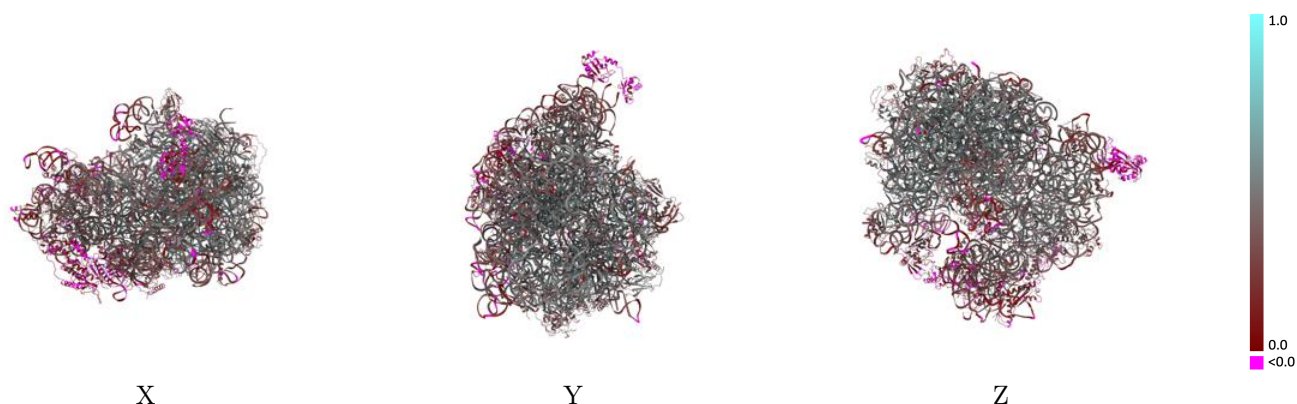
This section contains information regarding the fit between EMDB map EMD-6709 and PDB model 5X8P. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

### 9.1 Map-model overlay [i](#)



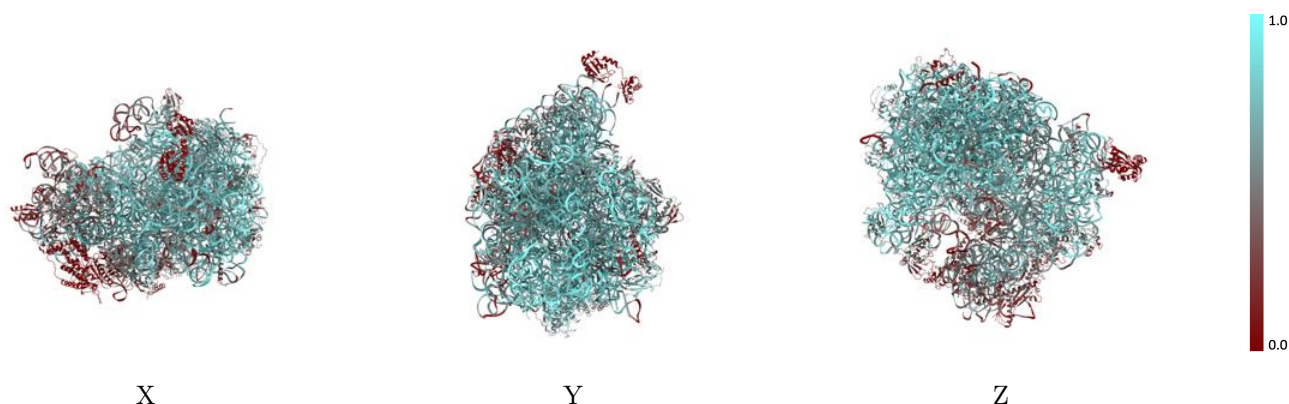
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



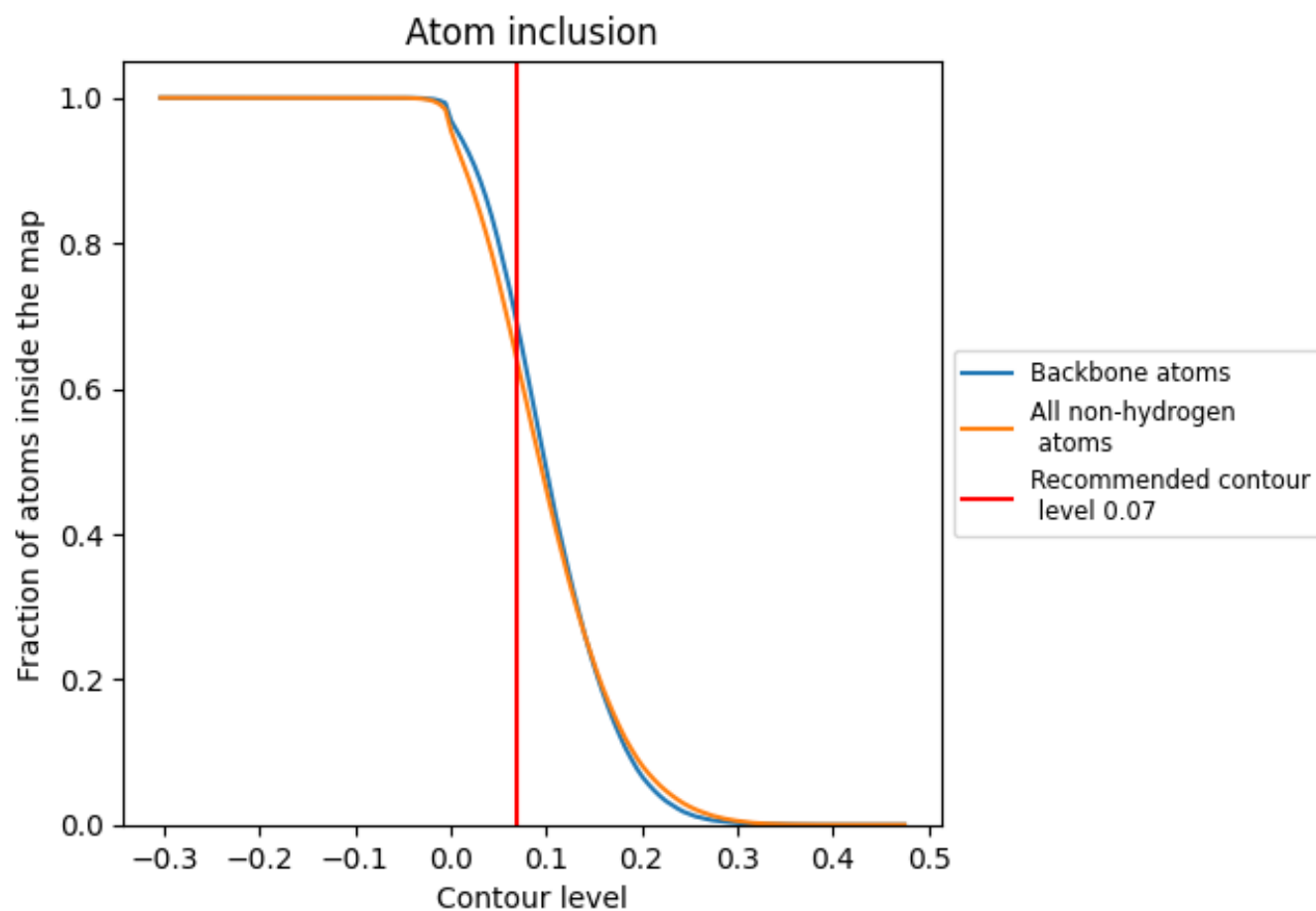
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 64% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6372	 0.3770
0	 0.1471	 0.1020
1	 0.6304	 0.4030
2	 0.5600	 0.3230
3	 0.6746	 0.4490
4	 0.6974	 0.4600
5	 0.6528	 0.3820
6	 0.4815	 0.3530
7	 0.6499	 0.4450
8	 0.0060	 0.0040
A	 0.7684	 0.4390
B	 0.7716	 0.3940
C	 0.5998	 0.4010
D	 0.6650	 0.4390
E	 0.6042	 0.3820
F	 0.3253	 0.2190
G	 0.4689	 0.3260
H	 0.2326	 0.2400
K	 0.5815	 0.4030
L	 0.5481	 0.3940
M	 0.6685	 0.4220
N	 0.6248	 0.3930
O	 0.6630	 0.4200
P	 0.5756	 0.3490
Q	 0.5941	 0.3900
R	 0.6494	 0.3930
S	 0.5480	 0.3760
T	 0.5484	 0.3770
U	 0.4931	 0.3680
V	 0.5189	 0.3490
W	 0.7952	 0.4450
X	 0.5954	 0.3980
Y	 0.6293	 0.4280
Z	 0.5090	 0.3550
a	 0.6890	 0.3720



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Chain	Atom inclusion	Q-score
b	 0.0586	 0.1410
c	 0.3419	 0.2870
d	 0.4053	 0.3200
e	 0.4774	 0.3310
f	 0.2462	 0.2140
g	 0.1644	 0.1820
h	 0.3788	 0.2850
i	 0.2495	 0.2130
j	 0.2455	 0.2480
k	 0.3143	 0.2520
l	 0.5381	 0.3930
m	 0.2451	 0.1450
n	 0.3367	 0.2590
o	 0.2598	 0.2480
p	 0.5016	 0.3410
q	 0.4417	 0.3440
r	 0.3373	 0.2620
s	 0.2293	 0.1610
t	 0.4346	 0.2550
u	 0.2043	 0.1680
v	 0.0188	 -0.0060
w	 0.0354	 0.0090
x	 0.3011	 0.2430
y	 0.3662	 0.3140