



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 01:58 PM JST

PDB ID : 8IE3 / pdb_00008ie3
EMDB ID : EMD-35375
Title : human nuclear pre-60S ribosomal particle - State E
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-02-15
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

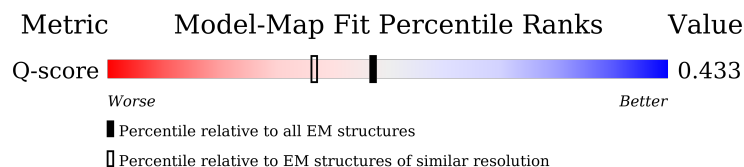
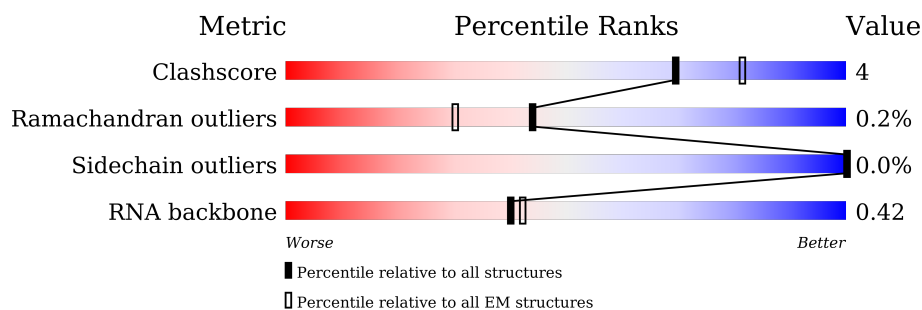
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



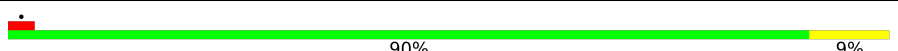
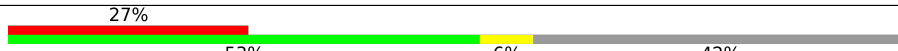
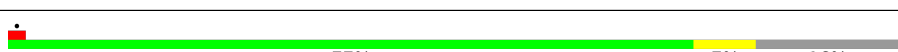
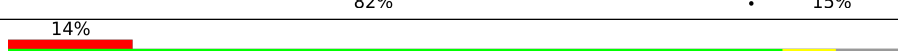
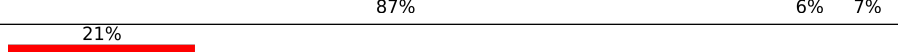
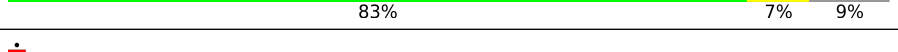
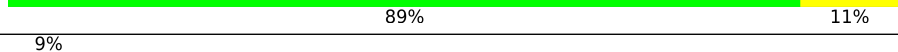
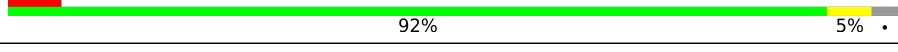
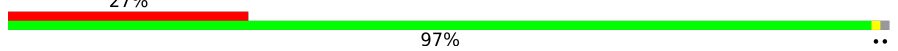
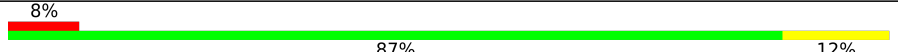
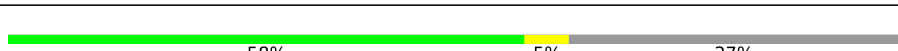
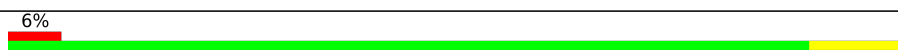
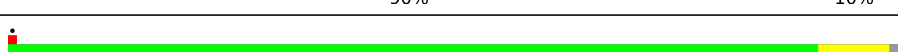
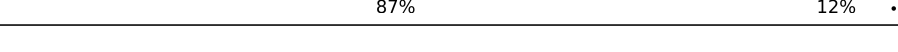
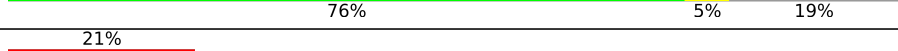
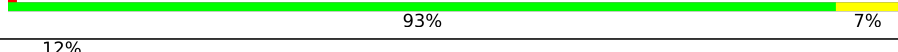
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	5	120	
2	6	245	
3	7	163	

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Mol	Chain	Length	Quality of chain
4	8	156	
5	9	134	
6	B	403	
7	C	159	
8	D	427	
9	E	115	
10	F	117	
11	G	266	
12	H	123	
13	I	192	
14	K	105	
15	L	148	
16	M	97	
17	O	70	
18	P	51	
19	Q	211	
20	S	215	
21	U	204	
22	V	203	
23	X	92	
24	Z	188	
25	a	196	
26	b	176	
27	c	160	
28	e	140	

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Mol	Chain	Length	Quality of chain
29	g	156	
30	h	145	
31	i	136	
32	l	137	
33	m	257	
34	n	110	
35	o	288	
36	p	248	
37	z	129	
38	A	731	
39	4	634	
40	R	260	
41	2	5054	
42	r	297	
43	d	128	
44	j	125	
45	k	135	
46	Y	184	
47	J	239	
48	T	178	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 145205 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 3 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	135	Total	C	N	O	S	0	0
			1159	737	225	187	10		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 5 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	9	97	Total	C	N	O	S	0	0
			787	481	168	134	4		

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	402	Total	C	N	O	S	1	0
			3244	2065	609	556	14		

- Molecule 7 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	93	Total	C	N	O	S	0	0
			764	476	167	117	4		

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 9 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 10 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 12 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 14 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 15 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	131	Total	C	N	O	S	0	0
			1043	666	205	169	3		

- Molecule 16 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 17 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 18 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 19 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 20 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 21 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 22 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 23 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 24 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	152	Total	C	N	O	S	0	0
			1227	770	248	204	5		

- Molecule 25 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	148	Total	C	N	O	S	0	0
			1239	772	266	192	9		

- Molecule 26 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 27 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	155	Total	C	N	O	S	0	0
			1264	801	248	210	5		

- Molecule 28 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 30 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 31 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 32 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 33 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	n	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 35 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	o	235	Total	C	N	O	S	0	0
			1897	1217	360	316	4		

- Molecule 36 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	p	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 37 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	z	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 38 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A	333	Total	C	N	O	S	0	0
			2672	1710	457	497	8		

- Molecule 39 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4	608	Total	C	N	O	S	0	0
			4992	3138	912	915	27		

- Molecule 40 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	225	Total	C	N	O	S	0	0
			1843	1178	350	307	8		

- Molecule 41 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	2	3519	Total	C	N	O	P	0	0
			75565	33698	13833	24516	3518		

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 43 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	d	104	Total	C	N	O	S	0	0
			850	542	149	157	2		

- Molecule 44 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	111	Total	C	N	O	S	0	0
			918	578	178	160	2		

- Molecule 45 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 46 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	167	Total	C	N	O	S	0	0
			1355	848	260	238	9		

- Molecule 47 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	J	203	Total	C	N	O	S	0	0
			1658	1058	289	300	11		

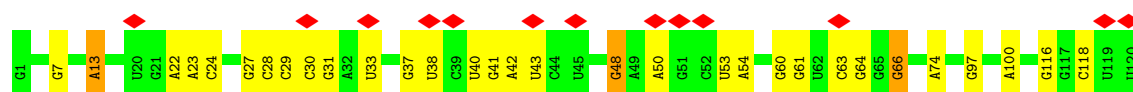
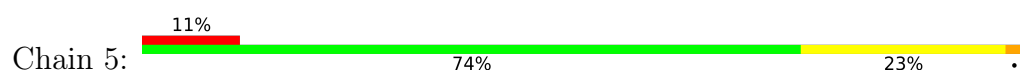
- Molecule 48 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	T	165	Total	C	N	O	S	0	0
			1319	836	245	233	5		

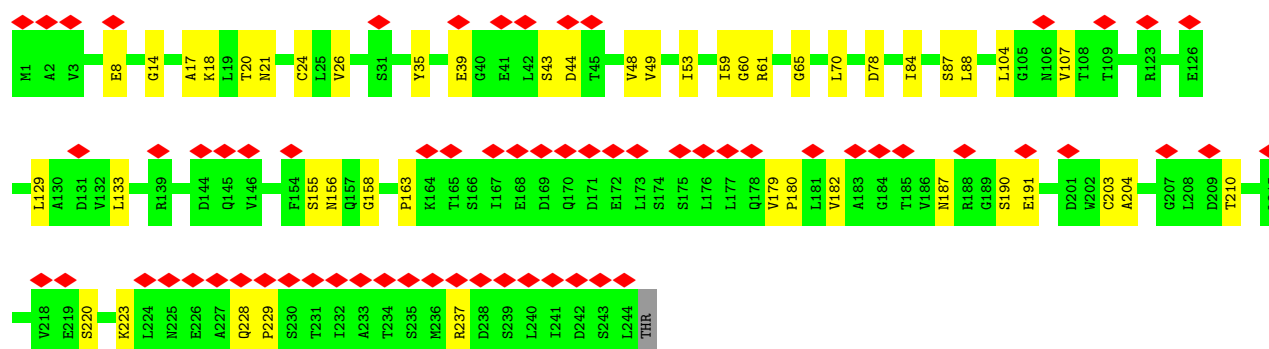
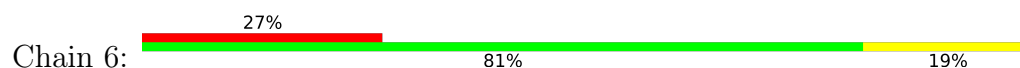
3 Residue-property plots [i](#)

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

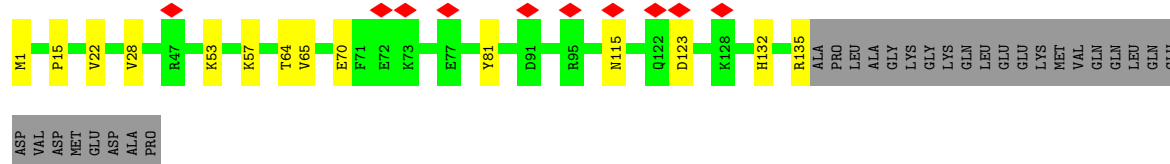
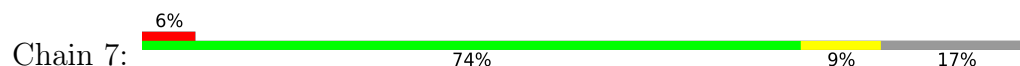
- Molecule 1: 5S rRNA



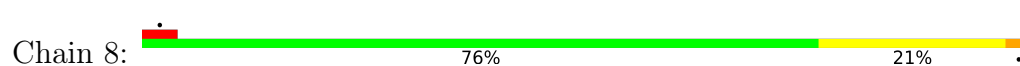
- Molecule 2: Eukaryotic translation initiation factor 6

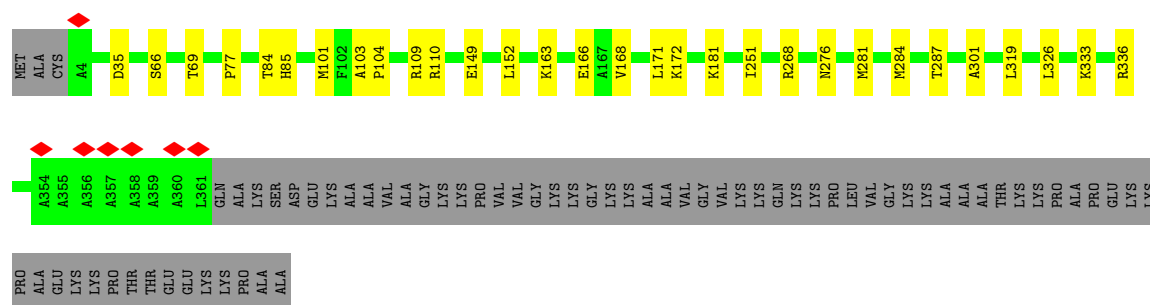


- Molecule 3: Probable ribosome biogenesis protein RLP24

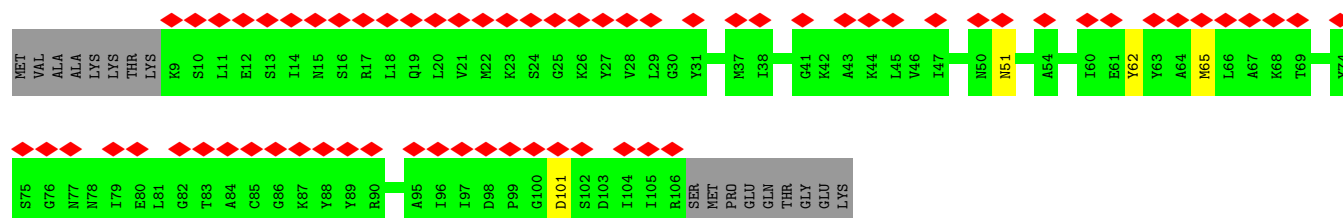
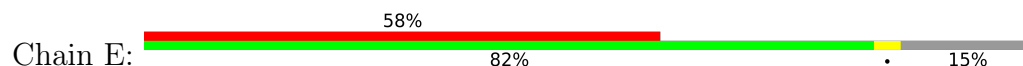


- Molecule 4: 5.8S rRNA

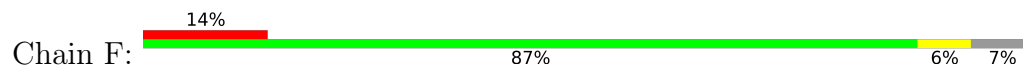




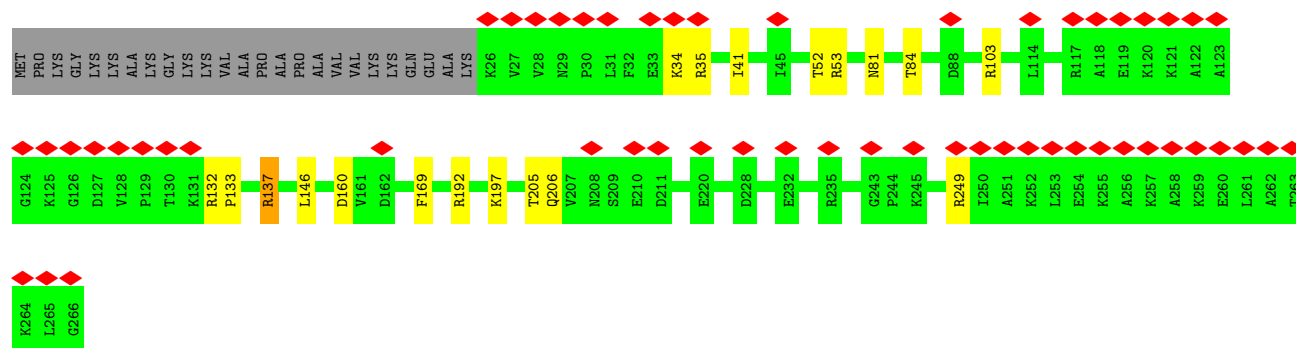
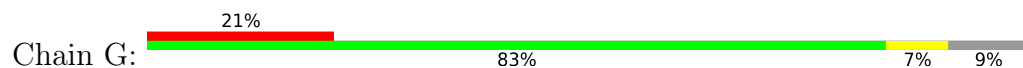
• Molecule 9: 60S ribosomal protein L30



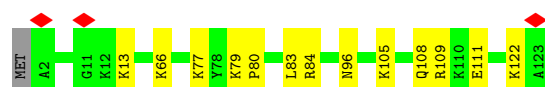
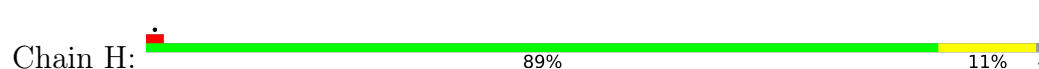
• Molecule 10: 60S ribosomal protein L34



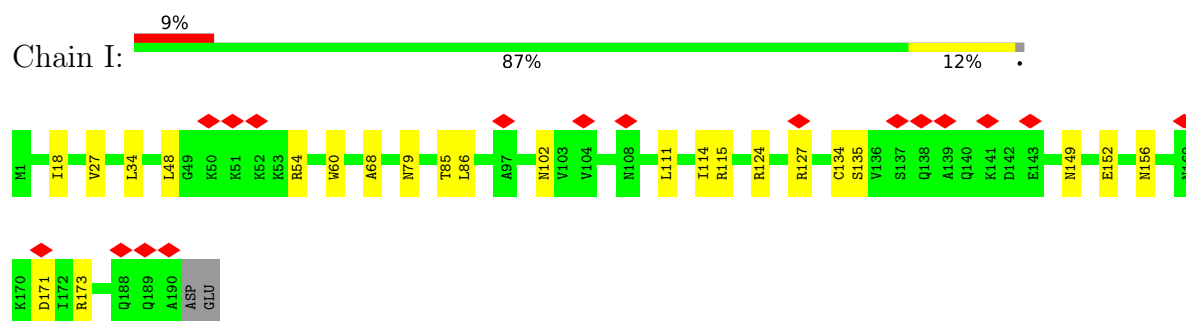
• Molecule 11: 60S ribosomal protein L7a



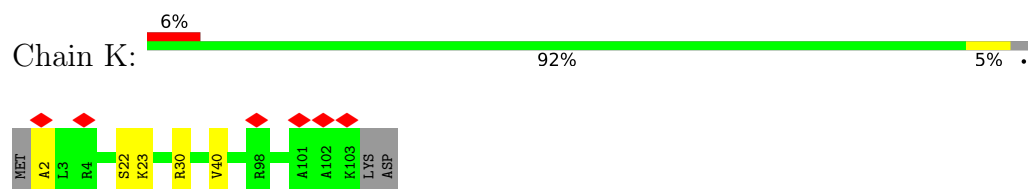
• Molecule 12: 60S ribosomal protein L35



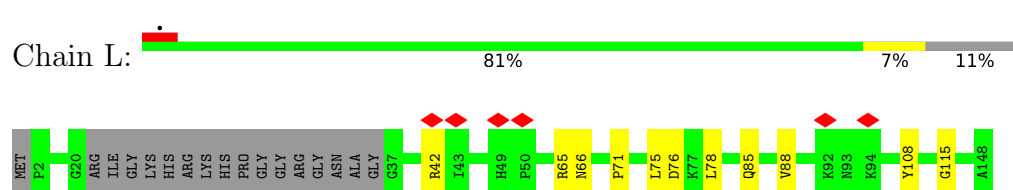
- Molecule 13: 60S ribosomal protein L9



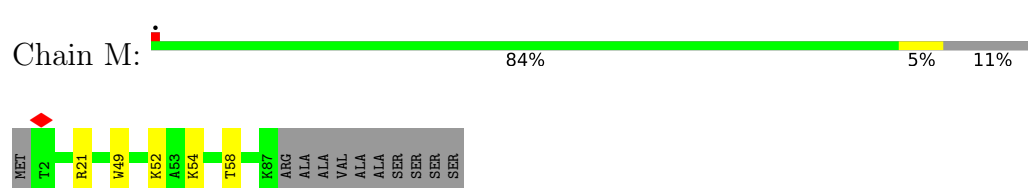
- Molecule 14: 60S ribosomal protein L36



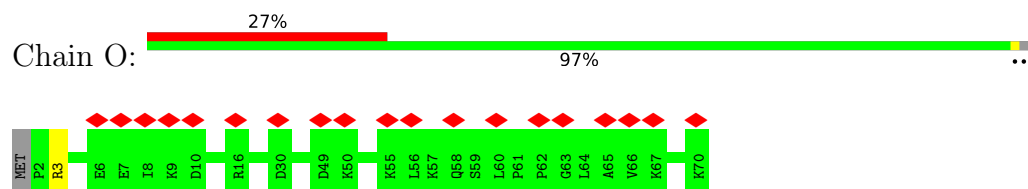
- Molecule 15: 60S ribosomal protein L27a



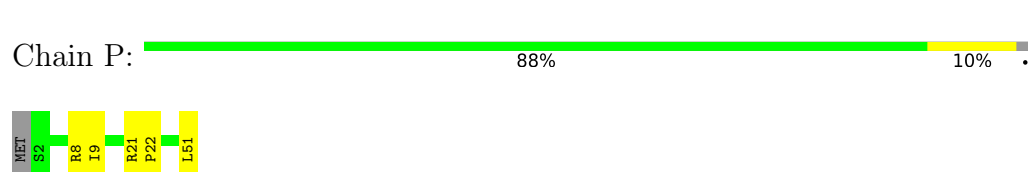
- Molecule 16: 60S ribosomal protein L37



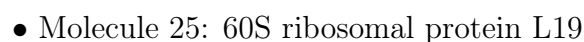
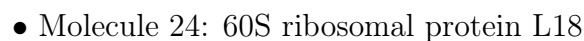
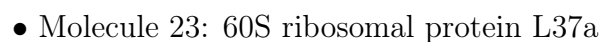
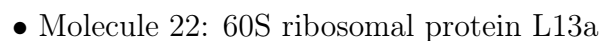
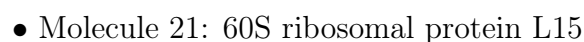
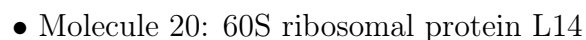
- Molecule 17: 60S ribosomal protein L38



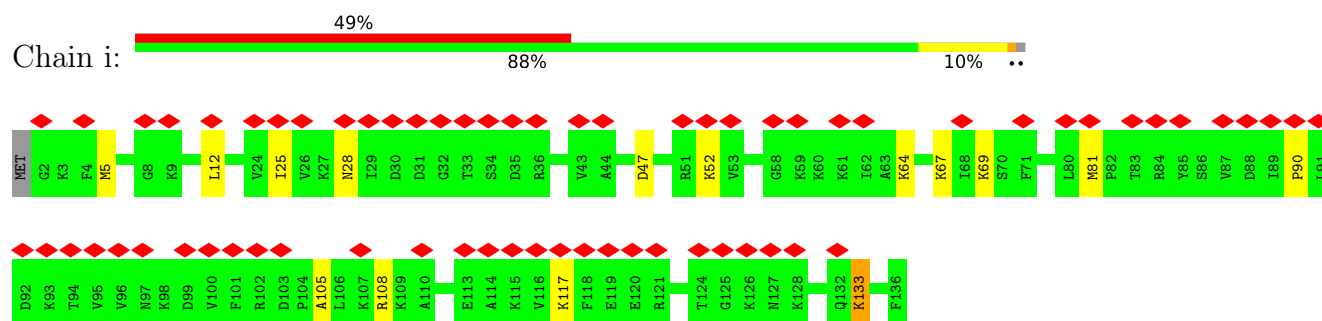
- Molecule 18: 60S ribosomal protein L39



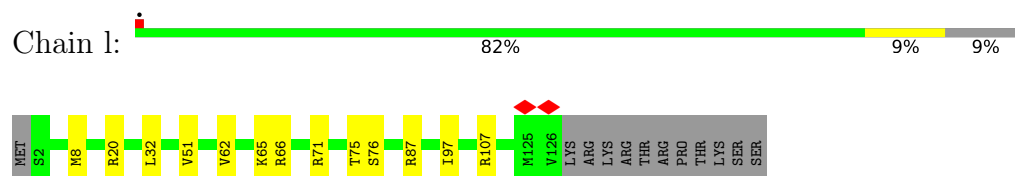
- Molecule 19: 60S ribosomal protein L13



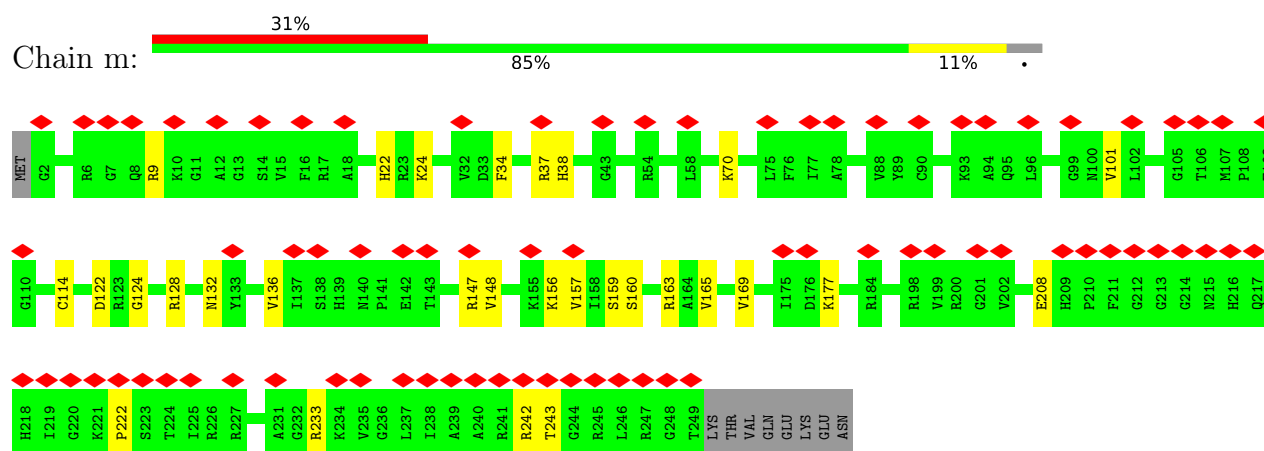
- Molecule 31: 60S ribosomal protein L27



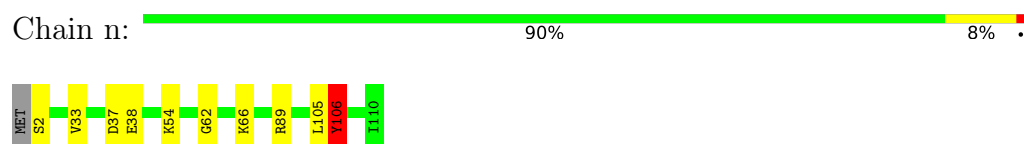
- Molecule 32: 60S ribosomal protein L28



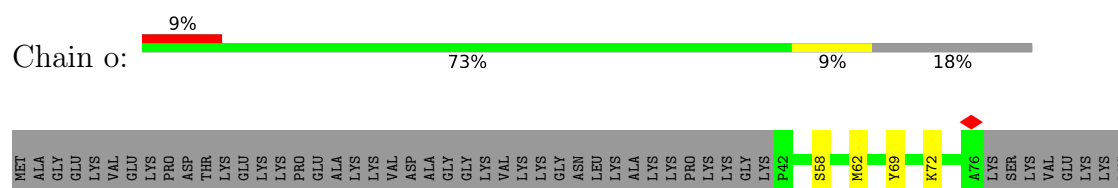
- Molecule 33: 60S ribosomal protein L8

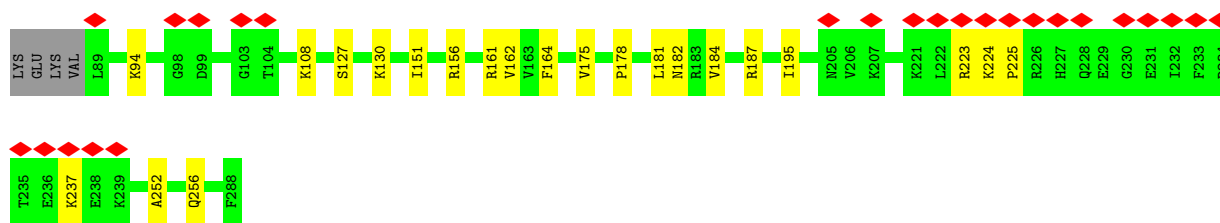


- Molecule 34: 60S ribosomal protein L35a



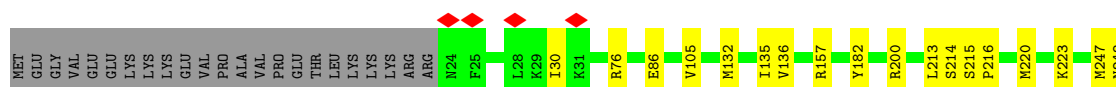
- Molecule 35: 60S ribosomal protein L6





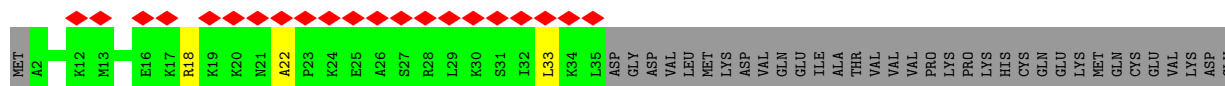
- Molecule 36: 60S ribosomal protein L7

Chain p: 83% 7% 9%



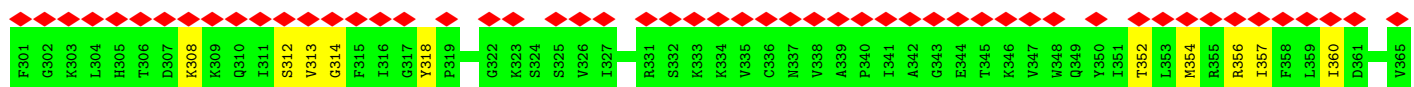
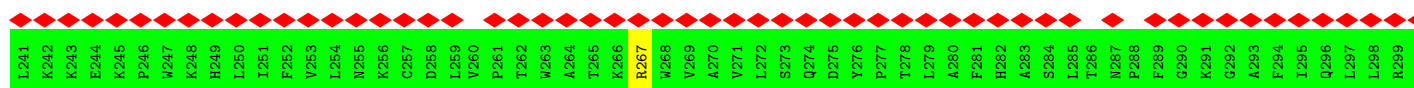
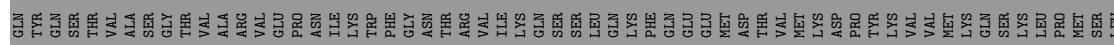
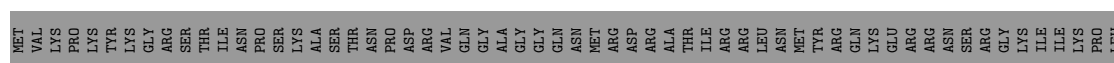
- Molecule 37: Protein LLP homolog

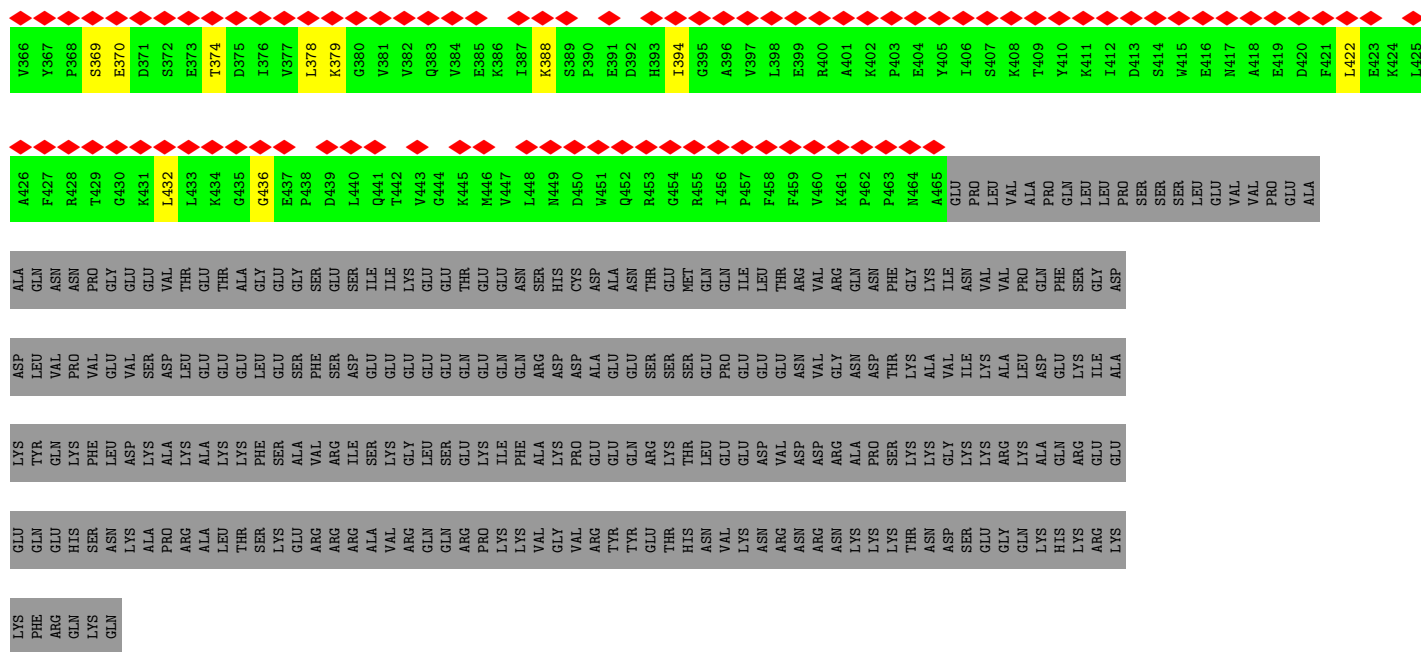
Chain z: 36% 45% 7% 48%



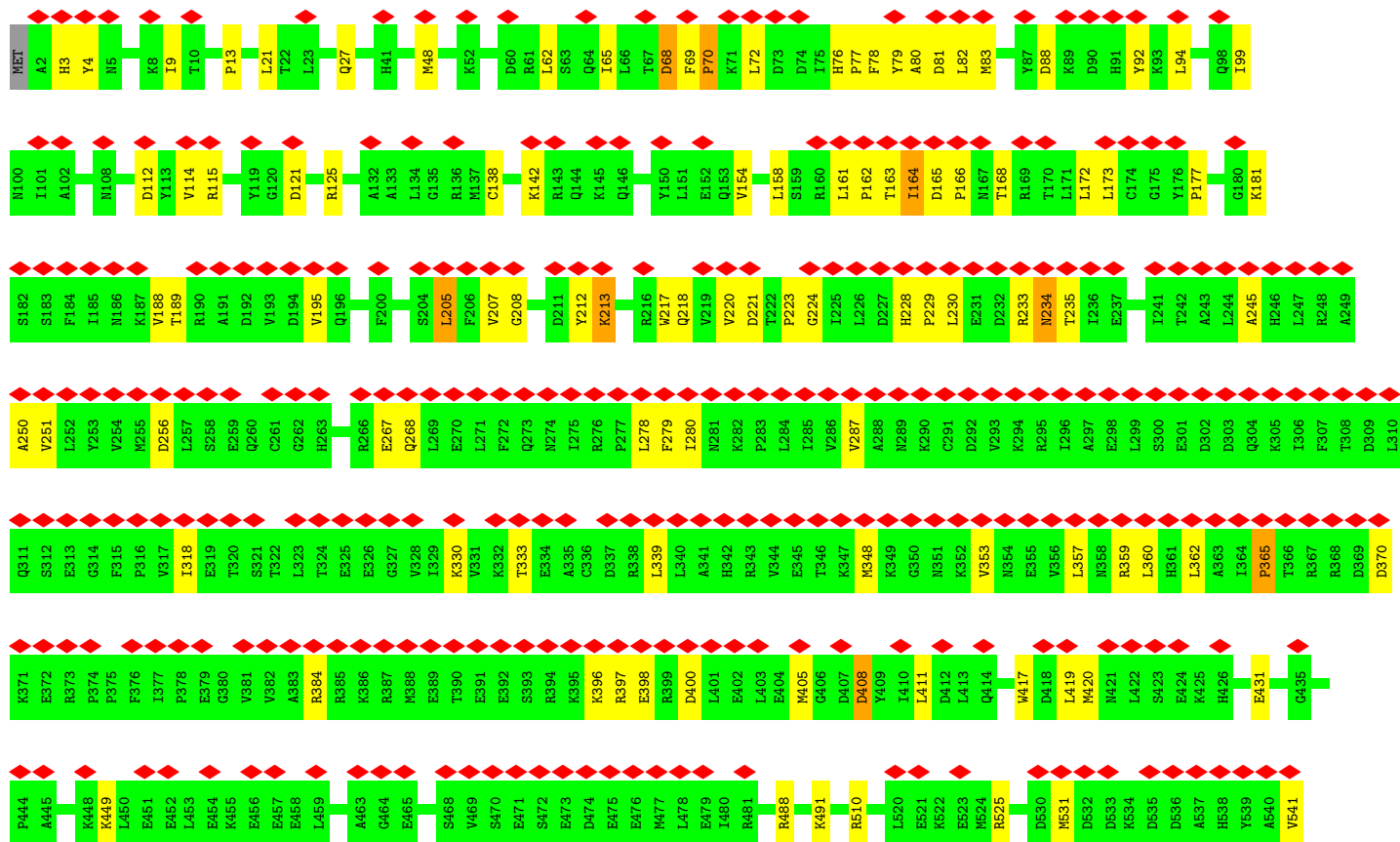
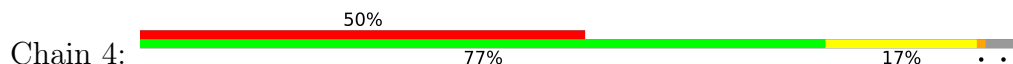
- Molecule 38: G Protein Nucleolar 2

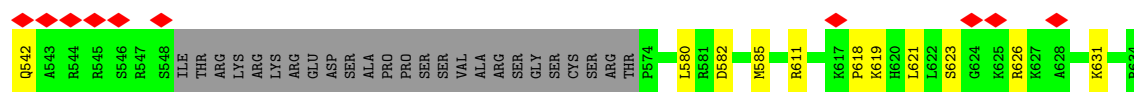
Chain A: 42% 40% 5% 54%



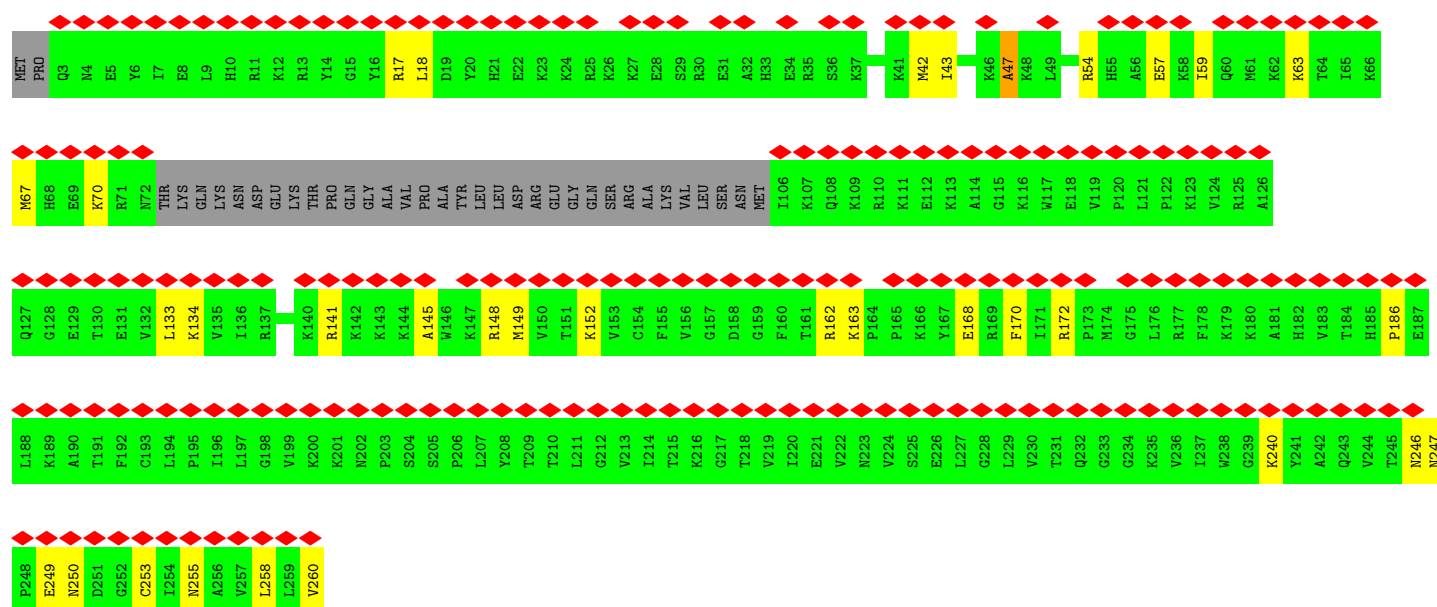
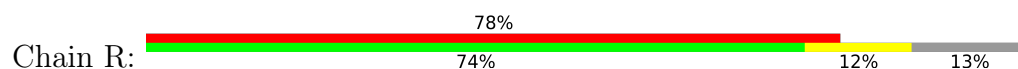


• Molecule 39: GTP-binding protein 4

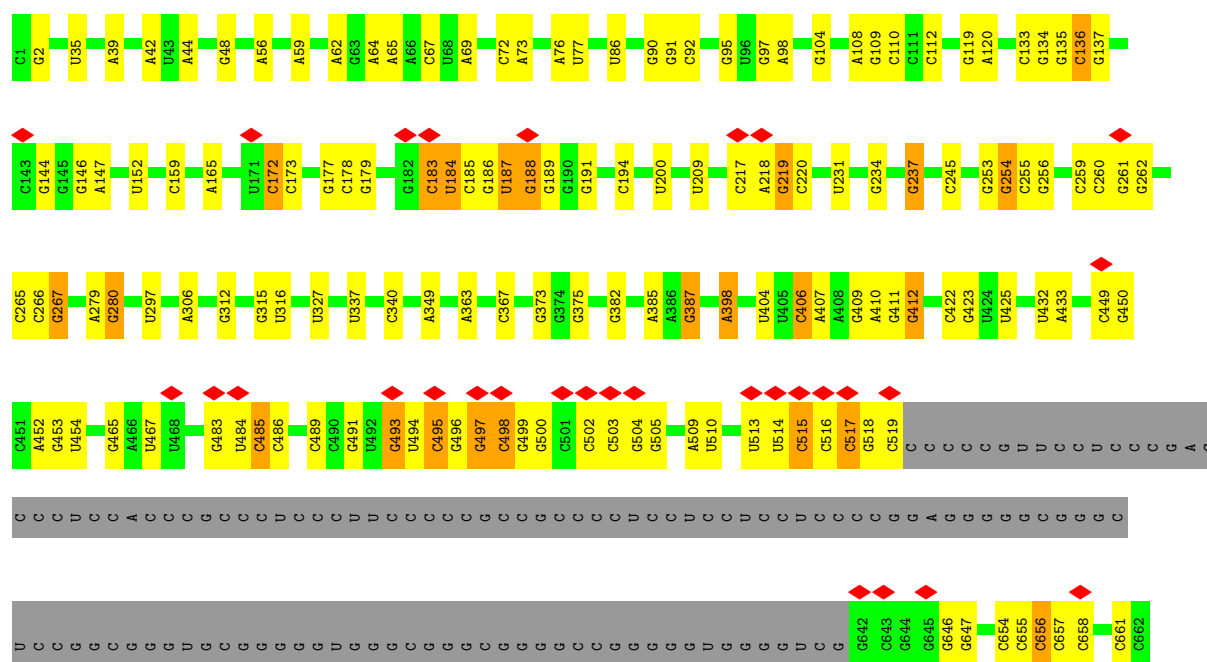




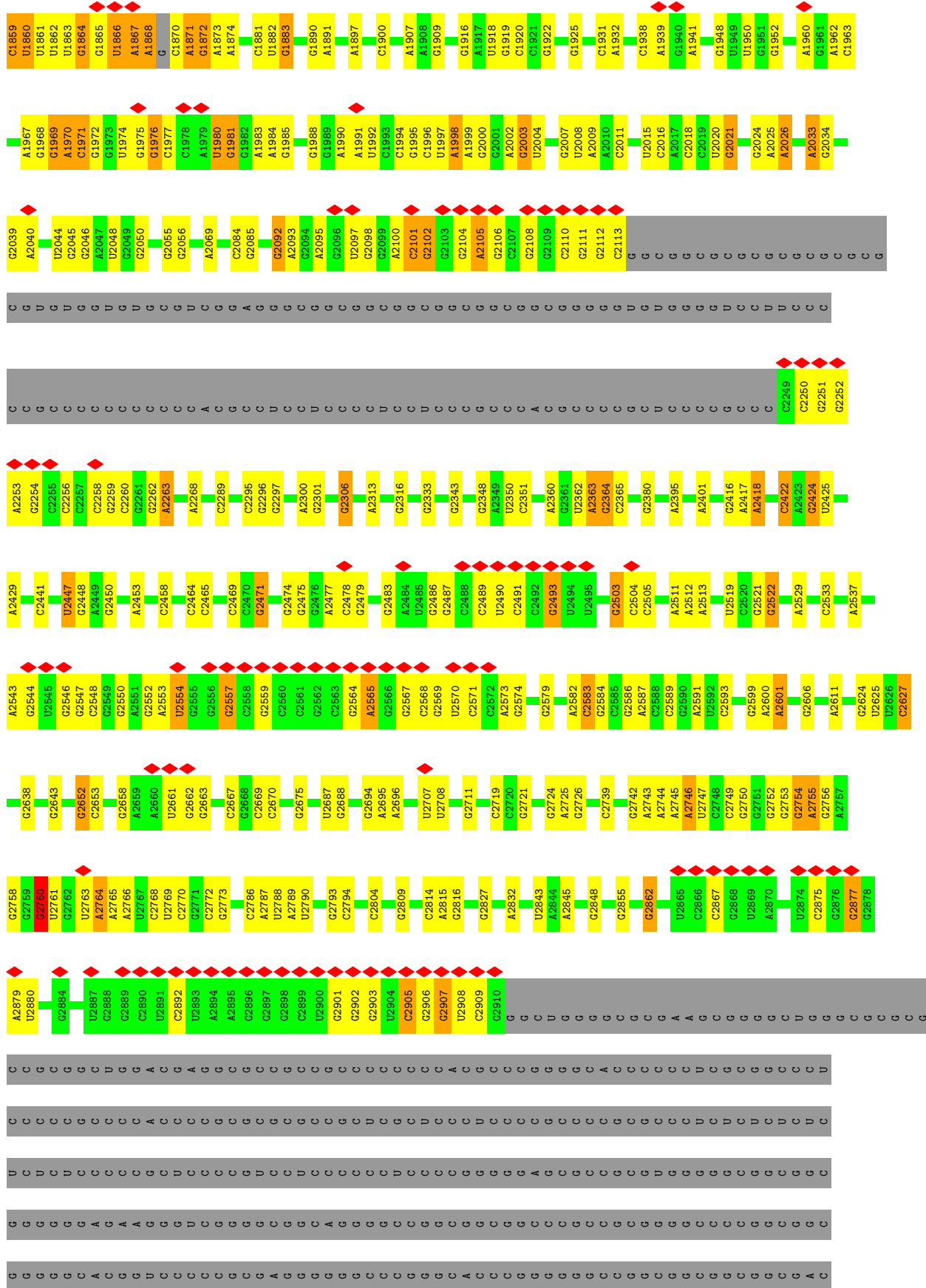
- Molecule 40: Ribosome biogenesis protein NSA2 homolog

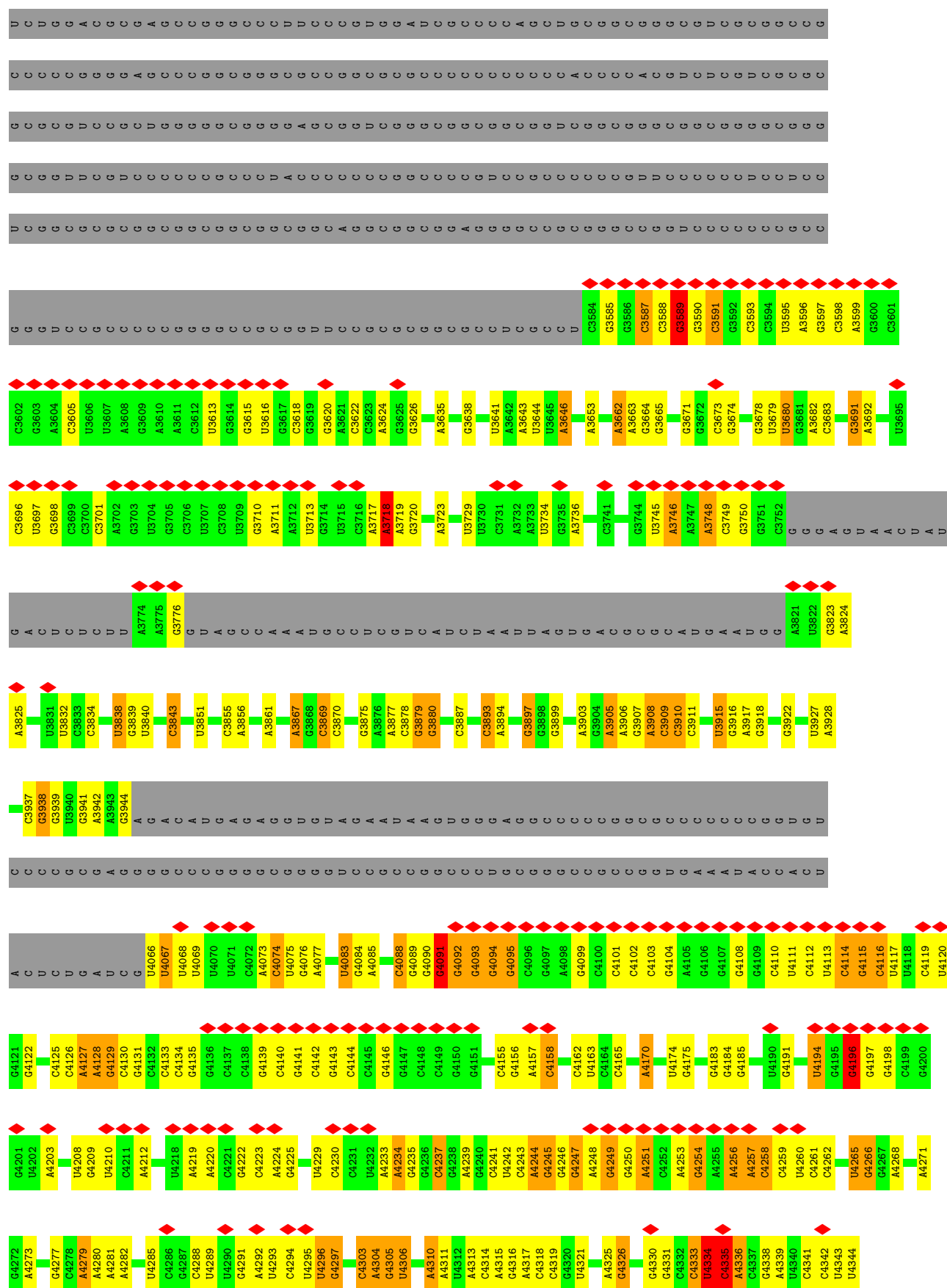


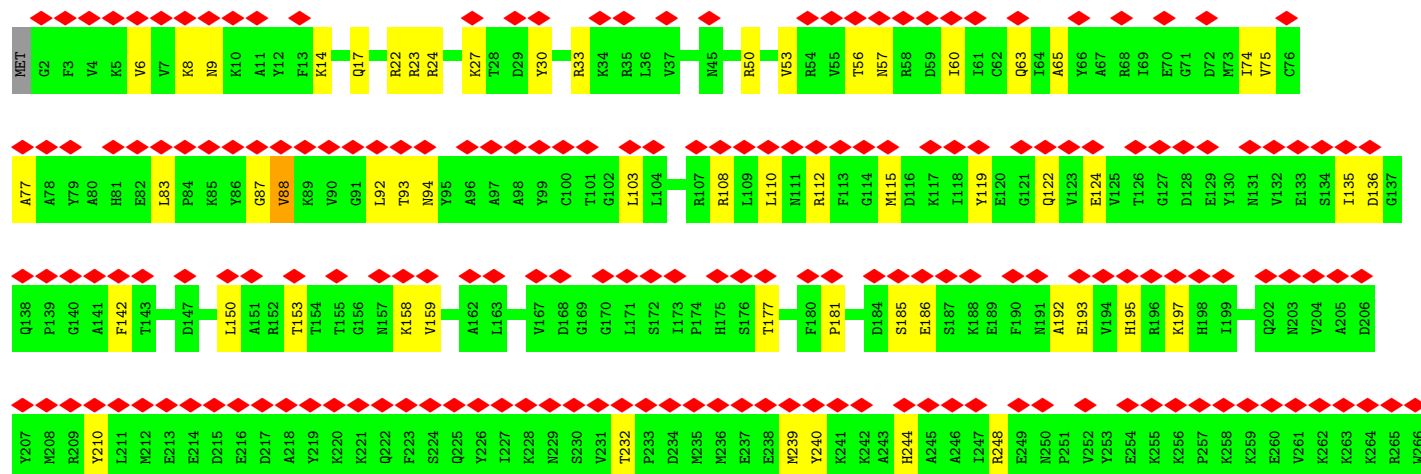
- Molecule 41: 28S rRNA





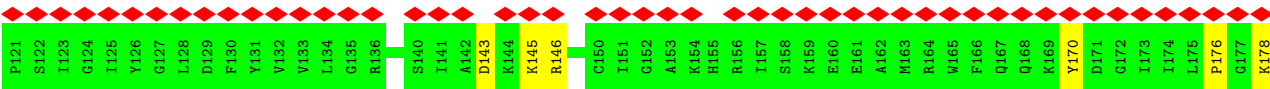
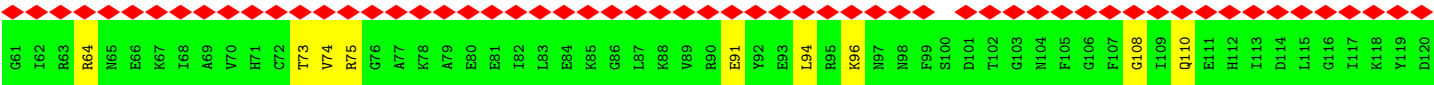
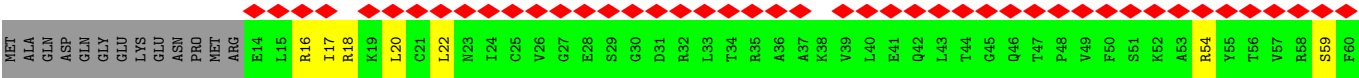
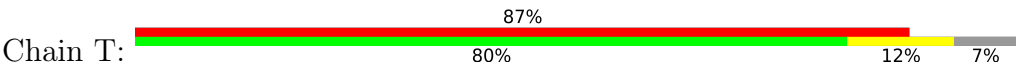








• Molecule 48: 60S ribosomal protein L11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34292	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	548.0, 548.0, 548.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: E7G, P7G, 6MZ, 7MG, 5MU, B8T, 1MA, E6G, 2MG, BGH, MHG, A2M, B8W, OMG, OMU, B8Q, B8K, B9H, B9B, I4U, P4U, UR3, OMC, M7A

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	5	0.24	0/2858	0.44	0/4455
2	6	0.35	0/1877	0.86	4/2554 (0.2%)
3	7	0.36	0/1181	0.74	0/1563
4	8	0.27	0/3679	0.46	0/5732
5	9	0.31	0/802	0.80	4/1069 (0.4%)
6	B	0.29	0/3315	0.70	3/4435 (0.1%)
7	C	0.31	0/777	0.74	1/1026 (0.1%)
8	D	0.31	0/2907	0.71	2/3905 (0.1%)
9	E	0.31	0/774	0.73	0/1038
10	F	0.31	0/878	0.70	0/1170
11	G	0.34	0/1971	0.71	2/2651 (0.1%)
12	H	0.31	0/1023	0.63	0/1351
13	I	0.31	0/1537	0.75	2/2066 (0.1%)
14	K	0.30	0/843	0.68	0/1115
15	L	0.26	0/1068	0.58	0/1428
16	M	0.30	0/720	0.72	0/952
17	O	0.31	0/575	0.72	0/761
18	P	0.27	0/454	0.55	0/599
19	Q	0.32	0/1732	0.69	0/2315
20	S	0.30	0/1133	0.65	0/1516
21	U	0.28	0/1746	0.60	0/2338
22	V	0.29	0/1682	0.62	1/2250 (0.0%)
23	X	0.29	0/718	0.70	0/953
24	Z	0.26	0/1243	0.55	0/1663
25	a	0.33	0/1255	0.78	4/1662 (0.2%)
26	b	0.25	0/1501	0.56	0/2013
27	c	0.28	0/1291	0.72	2/1725 (0.1%)
28	e	0.26	0/993	0.69	2/1332 (0.2%)
29	g	0.28	0/984	0.59	0/1323
30	h	0.28	0/1132	0.68	0/1504
31	i	0.37	0/1130	0.81	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	l	0.27	0/1017	0.62	2/1364 (0.1%)
33	m	0.29	0/1936	0.73	1/2596 (0.0%)
34	n	0.26	0/895	0.79	5/1198 (0.4%)
35	o	0.28	0/1935	0.70	2/2596 (0.1%)
36	p	0.33	0/1916	0.68	2/2553 (0.1%)
37	z	0.38	1/587 (0.2%)	0.67	0/767
38	A	0.31	0/2733	0.67	1/3697 (0.0%)
39	4	0.39	1/5075 (0.0%)	0.94	18/6807 (0.3%)
40	R	0.33	0/1878	0.78	1/2503 (0.0%)
41	2	0.66	8/82657 (0.0%)	0.48	23/128870 (0.0%)
42	r	0.41	1/2428 (0.0%)	1.06	13/3252 (0.4%)
43	d	0.35	0/864	0.90	5/1160 (0.4%)
44	j	0.28	0/933	0.65	0/1256
45	k	0.30	0/1082	0.69	1/1443 (0.1%)
46	Y	0.28	0/1383	0.61	0/1856
47	J	0.30	0/1692	0.68	1/2270 (0.0%)
48	T	0.33	0/1341	0.84	7/1793 (0.4%)
All	All	0.53	11/154131 (0.0%)	0.59	109/225952 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	6	0	1
6	B	0	1
19	Q	0	1
31	i	0	1
34	n	0	1
35	o	0	1
38	A	0	2
39	4	0	2
40	R	0	2
41	2	0	1
42	r	0	3
48	T	0	1
All	All	0	17

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	4605	A	C6-N1	76.65	2.88	1.35
41	2	4605	A	N3-C4	75.29	2.85	1.34
41	2	4605	A	C2-N3	72.32	2.78	1.33
41	2	4605	A	N1-C2	71.70	2.77	1.34
41	2	4605	A	C5-C6	70.99	2.83	1.41
41	2	4605	A	C5-C4	63.49	2.65	1.38
39	4	228	HIS	C-N	7.95	1.41	1.33
37	z	22	ALA	C-N	6.73	1.40	1.33
41	2	3718	A2M	O3'-P	5.11	1.61	1.56
42	r	232	THR	C-N	5.04	1.40	1.33
41	2	2401	A2M	O3'-P	5.00	1.61	1.56

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	4335	C	O5'-P-OP1	-23.68	36.96	108.00
41	2	4335	C	O5'-P-OP2	9.77	137.30	108.00
39	4	69	PHE	CA-C-N	-9.45	108.03	119.84
39	4	69	PHE	C-N-CA	-9.45	108.03	119.84
2	6	229	PRO	CA-N-CD	-8.85	99.62	112.00
41	2	4605	A	C4-C5-N7	-7.97	86.80	110.70
34	n	62	GLY	CA-C-N	7.77	132.48	120.68
34	n	62	GLY	C-N-CA	7.77	132.48	120.68
41	2	4605	A	N7-C8-N9	7.72	136.97	113.80
34	n	105	LEU	CA-C-N	7.67	140.52	121.80
34	n	105	LEU	C-N-CA	7.67	140.52	121.80
42	r	177	THR	N-CA-C	-7.49	97.74	108.07
42	r	87	GLY	CA-C-N	7.47	135.41	121.97
42	r	87	GLY	C-N-CA	7.47	135.41	121.97
34	n	106	TYR	N-CA-C	7.33	126.00	109.81
42	r	119	TYR	CA-CB-CG	7.12	126.72	113.90
41	2	4334	U	O3'-P-O5'	-6.86	93.71	104.00
39	4	213	LYS	CA-CB-CG	6.81	127.73	114.10
41	2	4605	A	N3-C4-N9	6.55	147.06	127.40
42	r	9	ASN	CA-C-N	6.51	129.31	120.38
42	r	9	ASN	C-N-CA	6.51	129.31	120.38
41	2	3590	G	N9-C1'-C2'	6.49	121.73	112.00
28	e	90	ARG	CA-C-N	6.48	136.36	124.82
28	e	90	ARG	C-N-CA	6.48	136.36	124.82
25	a	38	ARG	CA-C-N	6.46	133.87	121.54
25	a	38	ARG	C-N-CA	6.46	133.87	121.54
39	4	3	HIS	CA-C-N	6.44	133.84	121.54
39	4	3	HIS	C-N-CA	6.44	133.84	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	99	MET	CA-CB-CG	-6.28	101.55	114.10
48	T	170	TYR	CA-C-N	6.27	131.72	122.82
48	T	170	TYR	C-N-CA	6.27	131.72	122.82
48	T	18	ARG	CA-C-N	6.20	129.94	120.82
48	T	18	ARG	C-N-CA	6.20	129.94	120.82
25	a	78	ILE	N-CA-C	-6.16	106.94	112.12
8	D	171	LEU	CA-CB-CG	6.16	137.84	116.30
41	2	4335	C	OP1-P-OP2	-6.12	101.23	119.60
38	A	155	LEU	CA-CB-CG	6.11	137.68	116.30
41	2	4605	A	C6-C5-N7	5.99	150.27	132.30
41	2	914	U	P-O3'-C3'	5.95	129.12	120.20
39	4	88	ASP	CA-C-N	5.94	129.73	120.82
39	4	88	ASP	C-N-CA	5.94	129.73	120.82
27	c	80	VAL	N-CA-C	-5.88	101.28	109.45
40	R	149	MET	CB-CG-SD	5.88	130.34	112.70
41	2	2760	G	P-O3'-C3'	5.75	128.83	120.20
39	4	398	GLU	N-CA-C	-5.75	106.10	113.23
48	T	91	GLU	CA-CB-CG	5.73	125.57	114.10
2	6	237	ARG	CA-C-N	5.70	128.19	120.38
2	6	237	ARG	C-N-CA	5.70	128.19	120.38
42	r	210	TYR	N-CA-C	-5.68	105.62	113.18
36	p	220	MET	CA-C-N	5.67	132.37	121.54
36	p	220	MET	C-N-CA	5.67	132.37	121.54
41	2	2033	A	P-O3'-C3'	5.65	128.68	120.20
8	D	319	LEU	CA-CB-CG	5.65	136.07	116.30
47	J	114	GLU	N-CA-CB	5.64	118.98	110.30
6	B	360	LEU	CA-CB-CG	5.57	135.79	116.30
27	c	68	THR	OG1-CB-CG2	-5.54	98.22	109.30
41	2	3590	G	O4'-C1'-N9	5.53	116.80	108.50
41	2	1980	U	P-O3'-C3'	5.53	128.50	120.20
43	d	54	GLY	CA-C-N	5.53	132.09	121.54
43	d	54	GLY	C-N-CA	5.53	132.09	121.54
39	4	195	VAL	CA-C-N	5.46	129.76	121.03
39	4	195	VAL	C-N-CA	5.46	129.76	121.03
39	4	213	LYS	CB-CA-C	5.45	119.47	111.73
22	V	110	PRO	N-CA-C	5.44	117.34	110.70
39	4	279	PHE	CA-C-N	5.44	131.76	121.97
39	4	279	PHE	C-N-CA	5.44	131.76	121.97
41	2	406	C	C2'-C3'-O3'	5.37	121.76	113.70
13	I	60	TRP	CA-C-N	5.35	130.17	122.35
13	I	60	TRP	C-N-CA	5.35	130.17	122.35
41	2	406	C	P-O3'-C3'	5.33	128.20	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	T	64	ARG	CA-C-N	5.29	131.65	121.54
48	T	64	ARG	C-N-CA	5.29	131.65	121.54
41	2	3905	A	P-O3'-C3'	5.29	128.14	120.20
42	r	153	THR	CA-C-N	5.28	131.63	121.54
42	r	153	THR	C-N-CA	5.28	131.63	121.54
39	4	365	PRO	CA-C-N	5.27	131.61	121.54
39	4	365	PRO	C-N-CA	5.27	131.61	121.54
43	d	43	LEU	CA-CB-CG	5.26	134.72	116.30
32	l	32	LEU	CA-C-N	5.26	131.58	121.54
32	l	32	LEU	C-N-CA	5.26	131.58	121.54
39	4	408	ASP	N-CA-C	-5.26	106.65	114.64
41	2	485	C	C2-N1-C1'	5.24	134.52	118.80
5	9	98	SER	CA-C-N	5.22	131.52	121.54
5	9	98	SER	C-N-CA	5.22	131.52	121.54
41	2	914	U	C2'-C3'-O3'	5.22	117.33	109.50
6	B	29	VAL	CA-C-N	5.20	131.47	121.54
6	B	29	VAL	C-N-CA	5.20	131.47	121.54
39	4	205	LEU	CA-CB-CG	5.16	134.37	116.30
41	2	3587	C	C2-N1-C1'	5.16	134.28	118.80
39	4	164	ILE	N-CA-C	-5.14	100.88	108.23
42	r	57	ASN	N-CA-C	5.12	117.26	111.11
42	r	56	THR	CA-C-N	5.12	127.45	120.54
42	r	56	THR	C-N-CA	5.12	127.45	120.54
41	2	4091	G	C4-N9-C1'	5.11	141.84	126.50
42	r	119	TYR	CB-CA-C	5.10	119.56	112.11
35	o	127	SER	CA-C-N	5.10	131.05	123.05
35	o	127	SER	C-N-CA	5.10	131.05	123.05
7	C	9	THR	OG1-CB-CG2	-5.08	99.14	109.30
41	2	4913	G	P-O3'-C3'	5.07	127.81	120.20
41	2	3589	G	N9-C1'-C2'	5.07	119.61	112.00
45	k	66	THR	OG1-CB-CG2	-5.06	99.18	109.30
33	m	124	GLY	N-CA-C	5.05	117.73	111.93
11	G	169	PHE	CA-C-N	5.04	126.40	120.09
11	G	169	PHE	C-N-CA	5.04	126.40	120.09
43	d	66	SER	CA-C-N	5.04	131.16	121.54
43	d	66	SER	C-N-CA	5.04	131.16	121.54
5	9	4	SER	CA-C-N	5.03	133.14	121.87
5	9	4	SER	C-N-CA	5.03	133.14	121.87
2	6	223	LYS	CA-CB-CG	5.02	124.13	114.10

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	2	3589	G	Sidechain
39	4	163	THR	Peptide
39	4	234	ASN	Peptide
2	6	8	GLU	Peptide
38	A	150	ARG	Peptide
38	A	154	ASN	Peptide
6	B	241	PRO	Peptide
19	Q	154	VAL	Peptide
40	R	42	MET	Peptide
40	R	47	ALA	Peptide
48	T	94	LEU	Peptide
31	i	133	LYS	Peptide
34	n	106	TYR	Peptide
35	o	225	PRO	Peptide
42	r	142	PHE	Peptide
42	r	181	PRO	Peptide
42	r	60	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	2558	0	1296	19	0
2	6	1852	0	1828	25	0
3	7	1159	0	1224	10	0
4	8	3315	0	1685	10	0
5	9	787	0	796	9	0
6	B	3244	0	3389	27	0
7	C	764	0	822	6	0
8	D	2853	0	3028	20	0
9	E	764	0	804	3	0
10	F	868	0	963	4	0
11	G	1935	0	2087	16	0
12	H	1015	0	1148	11	0
13	I	1518	0	1601	12	0
14	K	832	0	917	4	0
15	L	1043	0	1089	7	0
16	M	705	0	741	4	0
17	O	569	0	637	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	P	444	0	483	3	0
19	Q	1701	0	1818	19	0
20	S	1111	0	1174	9	0
21	U	1701	0	1749	13	0
22	V	1650	0	1794	10	0
23	X	708	0	760	8	0
24	Z	1227	0	1333	7	0
25	a	1239	0	1363	8	0
26	b	1461	0	1502	9	0
27	c	1264	0	1337	7	0
28	e	979	0	1039	6	0
29	g	967	0	1040	2	0
30	h	1115	0	1205	11	0
31	i	1107	0	1182	10	0
32	l	1002	0	1068	9	0
33	m	1898	0	1993	23	0
34	n	876	0	912	5	0
35	o	1897	0	2046	15	0
36	p	1878	0	2009	11	0
37	z	581	0	656	9	0
38	A	2672	0	2696	30	0
39	4	4992	0	5129	84	0
40	R	1843	0	1979	19	0
41	2	75565	0	38004	409	0
42	r	2382	0	2410	52	0
43	d	850	0	868	4	0
44	j	918	0	964	6	0
45	k	1064	0	1160	6	0
46	Y	1355	0	1389	7	0
47	J	1658	0	1674	32	0
48	T	1319	0	1358	75	0
All	All	145205	0	108149	849	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (849) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2:4083:5MU:C5	41:2:4083:5MU:C4	1.79	1.66
41:2:4251:A:P	48:T:108:GLY:HA3	1.35	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:27:LYS:HZ3	48:T:146:ARG:CZ	0.92	1.55
41:2:4256:A:N1	48:T:59:SER:CB	1.70	1.49
42:r:27:LYS:NZ	48:T:146:ARG:CZ	1.81	1.44
41:2:4251:A:P	48:T:108:GLY:CA	2.12	1.35
42:r:27:LYS:CE	48:T:146:ARG:HH21	1.38	1.35
42:r:27:LYS:NZ	48:T:146:ARG:NH2	1.77	1.29
41:2:4256:A:C2	48:T:59:SER:OG	1.72	1.29
41:2:4296:U:O2	41:2:4315:A:C2	1.87	1.27
41:2:4296:U:O2	41:2:4315:A:N1	1.67	1.26
42:r:27:LYS:HZ3	48:T:146:ARG:NE	1.33	1.25
41:2:4256:A:N1	48:T:59:SER:HB3	1.32	1.25
42:r:27:LYS:NZ	48:T:146:ARG:NE	1.85	1.24
42:r:27:LYS:HZ3	48:T:146:ARG:NH2	1.33	1.24
41:2:4251:A:O4'	48:T:110:GLN:HG3	1.34	1.23
41:2:4251:A:OP1	48:T:108:GLY:HA3	1.11	1.22
42:r:27:LYS:HE2	48:T:146:ARG:HH21	1.04	1.20
41:2:4251:A:OP1	48:T:108:GLY:CA	1.91	1.19
42:r:27:LYS:CE	48:T:146:ARG:NH2	2.11	1.13
41:2:4251:A:C4'	48:T:110:GLN:HE21	1.66	1.08
41:2:4251:A:H4'	48:T:110:GLN:HE21	0.92	1.08
1:5:42:A:H1'	48:T:75:ARG:HH21	0.97	1.07
41:2:4128:A:H3'	41:2:4129:G:H8	1.20	1.06
1:5:42:A:H1'	48:T:75:ARG:NH2	1.72	1.04
41:2:4251:A:H4'	48:T:110:GLN:NE2	1.71	1.04
41:2:4256:A:N1	48:T:59:SER:OG	1.77	1.03
41:2:4251:A:OP2	48:T:108:GLY:O	1.75	1.03
39:4:72:LEU:HD21	39:4:83:MET:HG2	1.40	1.01
41:2:4094:G:H3'	41:2:4095:G:H4'	1.41	1.01
41:2:4251:A:C4'	48:T:110:GLN:NE2	2.24	1.00
38:A:174:TYR:CE1	39:4:76:HIS:HD2	1.80	0.99
41:2:4256:A:H2	48:T:59:SER:HG	1.11	0.98
41:2:4256:A:C6	48:T:59:SER:CB	2.47	0.97
41:2:4256:A:C6	48:T:59:SER:HB3	1.98	0.97
39:4:72:LEU:HD21	39:4:83:MET:CG	1.95	0.97
41:2:2554:U:H3	41:2:2764:A:H62	1.09	0.97
41:2:4128:A:H3'	41:2:4129:G:C8	2.00	0.95
41:2:4251:A:OP2	48:T:108:GLY:C	2.10	0.94
41:2:4251:A:OP2	48:T:108:GLY:CA	2.13	0.94
41:2:4251:A:O4'	48:T:110:GLN:CG	2.16	0.93
41:2:4251:A:C1'	48:T:110:GLN:HG3	1.97	0.92
1:5:42:A:C1'	48:T:75:ARG:HH21	1.83	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2:1998:A:H62	47:J:50:ASN:ND2	1.66	0.91
41:2:1550:G:H1	41:2:1578:U:H3	1.11	0.91
42:r:289:ARG:O	42:r:293:ARG:HB2	1.72	0.89
39:4:72:LEU:CD2	39:4:83:MET:HG2	2.01	0.89
41:2:1998:A:H62	47:J:50:ASN:HD21	0.92	0.88
41:2:4344:U:H3	41:2:4368:G:H1	1.18	0.87
42:r:27:LYS:HE2	48:T:146:ARG:NH2	1.80	0.87
42:r:27:LYS:CE	48:T:146:ARG:HE	1.88	0.86
41:2:1976:G:N1	41:2:1991:A:C8	2.43	0.86
38:A:174:TYR:CD1	39:4:76:HIS:CD2	2.63	0.86
41:2:4091:G:N2	41:2:4093:G:OP1	2.09	0.85
41:2:4605:A:C5	41:2:4605:A:C4	2.65	0.84
34:n:2:SER:N	41:2:4946:U:HO2'	1.76	0.84
42:r:27:LYS:NZ	48:T:146:ARG:HE	1.74	0.84
41:2:4256:A:H2	48:T:59:SER:OG	1.55	0.83
41:2:1865:G:H2'	41:2:1866:U:H1'	1.61	0.82
41:2:4251:A:C5'	48:T:110:GLN:NE2	2.42	0.82
38:A:174:TYR:CE1	39:4:76:HIS:CD2	2.67	0.81
41:2:1998:A:N6	47:J:50:ASN:HD21	1.76	0.81
41:2:4113:U:H3'	41:2:4114:C:O2	1.79	0.81
21:U:165:THR:O	21:U:169:ARG:HB2	1.82	0.80
41:2:4251:A:P	48:T:108:GLY:C	2.64	0.80
41:2:2845:A:H61	41:2:3843:C:H42	1.29	0.79
41:2:4094:G:OP2	41:2:4095:G:O2'	2.00	0.79
41:2:1970:A:H4'	41:2:1971:C:OP2	1.84	0.78
41:2:4296:U:C2	41:2:4315:A:N1	2.53	0.75
38:A:174:TYR:CD1	39:4:76:HIS:HD2	2.03	0.75
42:r:27:LYS:CE	48:T:146:ARG:NE	2.48	0.74
39:4:138:CYS:O	39:4:142:LYS:HB2	1.86	0.74
38:A:174:TYR:HB2	39:4:77:PRO:HD3	1.69	0.73
1:5:42:A:C1'	48:T:75:ARG:NH2	2.46	0.73
41:2:1998:A:C8	47:J:67:PHE:HE2	2.07	0.72
41:2:1863:U:H3	41:2:1871:A:H61	1.35	0.71
41:2:4246:G:H2'	41:2:4247:G:C8	2.26	0.71
41:2:4258:C:OP2	48:T:54:ARG:HD3	1.89	0.71
11:G:34:LYS:HA	41:2:4128:A:H2	1.55	0.70
42:r:27:LYS:HZ1	48:T:146:ARG:NE	1.88	0.70
1:5:42:A:O4'	48:T:75:ARG:NE	2.24	0.69
39:4:154:VAL:O	39:4:158:LEU:HB2	1.92	0.69
41:2:1969:G:H2'	41:2:1970:A:C1'	2.22	0.69
41:2:1865:G:H2'	41:2:1866:U:C1'	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:230:GLY:O	6:B:234:ARG:HB2	1.95	0.66
41:2:4251:A:H5'	48:T:110:GLN:NE2	2.10	0.66
41:2:4310:A:H4'	41:2:4335:C:C5'	2.26	0.66
41:2:4605:A:C5	41:2:4605:A:C6	2.83	0.66
41:2:1998:A:N7	47:J:67:PHE:HE2	1.94	0.66
41:2:4321:U:H3	41:2:4326:G:H1	1.42	0.66
41:2:1969:G:H2'	41:2:1970:A:H1'	1.78	0.65
41:2:1976:G:C6	41:2:1991:A:N7	2.64	0.65
41:2:4115:G:H4'	41:2:4116:C:OP2	1.96	0.65
41:2:4251:A:OP2	48:T:108:GLY:N	2.29	0.65
41:2:4310:A:H4'	41:2:4335:C:O5'	1.95	0.65
11:G:34:LYS:HA	41:2:4128:A:C2	2.31	0.65
41:2:4256:A:C6	48:T:59:SER:HB2	2.30	0.65
41:2:961:G:N2	41:2:964:A:N6	2.45	0.64
38:A:174:TYR:CZ	39:4:76:HIS:HD2	2.14	0.64
41:2:1864:G:H3'	41:2:1865:G:C8	2.32	0.64
41:2:1866:U:H2'	41:2:1867:A:C5	2.32	0.64
41:2:4303:C:H2'	41:2:4305:G:N3	2.12	0.64
42:r:150:LEU:CD1	48:T:145:LYS:HG3	2.27	0.64
41:2:2554:U:H3	41:2:2764:A:N6	1.91	0.63
41:2:2752:G:H2'	41:2:2753:G:C8	2.33	0.63
41:2:3944:G:H22	41:2:4069:U:H3	1.46	0.62
41:2:4256:A:N1	48:T:59:SER:HB2	2.02	0.62
31:i:12:LEU:HB2	31:i:81:MET:HB3	1.80	0.62
41:2:1860:U:H2'	41:2:1861:U:C6	2.35	0.62
41:2:1998:A:N6	47:J:50:ASN:ND2	2.42	0.62
42:r:27:LYS:HZ2	48:T:146:ARG:NH2	1.94	0.62
41:2:4296:U:O2	41:2:4315:A:H2	1.70	0.62
41:2:4258:C:OP2	48:T:54:ARG:NH1	2.31	0.61
27:c:9:ARG:HD2	41:2:4208:U:H5''	1.82	0.61
39:4:72:LEU:HD21	39:4:83:MET:CB	2.29	0.61
41:2:4251:A:P	48:T:108:GLY:N	2.73	0.60
41:2:1864:G:C6	41:2:1865:G:C2	2.88	0.60
41:2:4256:A:N6	48:T:59:SER:HB3	2.15	0.60
41:2:4310:A:H4'	41:2:4335:C:H5''	1.83	0.60
41:2:1998:A:C8	47:J:67:PHE:CE2	2.89	0.60
41:2:497:G:H21	41:2:498:C:H41	1.50	0.59
41:2:1866:U:H2'	41:2:1867:A:C4	2.38	0.59
41:2:1866:U:H2'	41:2:1867:A:C8	2.38	0.59
41:2:4570:G:H2'	41:2:4571:A2M:H8	1.85	0.59
38:A:183:VAL:HG21	39:4:4:TYR:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2:3697:U:H5''	41:2:3698:G:H5'	1.85	0.59
39:4:77:PRO:O	39:4:78:PHE:C	2.45	0.58
41:2:961:G:N2	41:2:964:A:C6	2.71	0.58
41:2:2845:A:N6	41:2:3843:C:H42	1.99	0.58
4:8:90:C:HO2'	30:h:24:HIS:HD1	1.51	0.58
41:2:4926:C:H5''	41:2:4927:G:H21	1.69	0.58
41:2:1860:U:O2'	41:2:1861:U:H5'	2.04	0.57
41:2:1865:G:N2	41:2:1870:C:N3	2.52	0.57
39:4:76:HIS:HB3	39:4:79:TYR:HD2	1.69	0.57
38:A:352:THR:HG23	41:2:4539:U:H5''	1.85	0.57
39:4:72:LEU:HD21	39:4:83:MET:HB3	1.87	0.57
41:2:2845:A:H61	41:2:3843:C:N4	1.98	0.57
31:i:133:LYS:NZ	41:2:2754:G:OP2	2.28	0.57
41:2:515:C:H42	41:2:647:G:H1	1.51	0.57
41:2:3717:A:H2'	41:2:3718:A2M:H8	1.87	0.57
41:2:1976:G:O6	41:2:1991:A:N7	2.38	0.56
27:c:44:GLY:H	27:c:95:HIS:HB3	1.71	0.56
41:2:1098:G:H1	41:2:1197:C:H42	1.54	0.56
39:4:188:VAL:HG23	39:4:189:THR:HG23	1.88	0.56
41:2:1860:U:H2'	41:2:1861:U:H6	1.71	0.56
41:2:4113:U:O5'	41:2:4114:C:O2	2.24	0.56
39:4:165:ASP:HB3	39:4:168:THR:HG22	1.88	0.55
41:2:4113:U:OP1	41:2:4114:C:H3'	2.06	0.55
41:2:4295:U:H2'	41:2:4296:U:H5'	1.88	0.55
41:2:4333:C:H2'	41:2:4334:U:C4	2.42	0.55
41:2:4254:G:C6	41:2:4257:A:N6	2.75	0.55
41:2:4492:U:H5''	41:2:4493:U:H5'	1.88	0.55
20:S:62:LEU:HD21	20:S:82:ILE:HD11	1.89	0.55
41:2:3911:C:H5''	41:2:4197:G:H1'	1.88	0.55
42:r:185:SER:OG	42:r:186:GLU:N	2.39	0.55
8:D:168:VAL:O	8:D:172:LYS:HB2	2.07	0.55
39:4:234:ASN:ND2	41:2:1981:G:OP2	2.40	0.55
40:R:162:ARG:NH2	40:R:172:ARG:O	2.40	0.55
41:2:1972:G:OP1	47:J:51:SER:HB3	2.06	0.55
3:7:81:TYR:HB3	39:4:419:LEU:HD21	1.89	0.54
3:7:1:MET:N	39:4:431:GLU:OE2	2.40	0.54
41:2:4310:A:O2'	41:2:4334:U:O3'	2.24	0.54
42:r:30:TYR:HA	42:r:33:ARG:HB3	1.89	0.54
41:2:188:G:N2	41:2:191:G:O6	2.41	0.54
23:X:29:ILE:HG21	33:m:177:LYS:HB2	1.89	0.54
33:m:34:PHE:O	33:m:38:HIS:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:40:U:O2	48:T:73:THR:OG1	2.21	0.54
39:4:205:LEU:HD23	39:4:223:PRO:HD3	1.88	0.54
41:2:4113:U:P	41:2:4114:C:H3'	2.47	0.54
39:4:348:MET:HA	39:4:353:VAL:HG11	1.90	0.54
47:J:214:ARG:NH2	47:J:216:GLN:OE1	2.41	0.54
24:Z:64:SER:HG	41:2:1501:C:HO2'	1.55	0.54
40:R:163:LYS:HD2	40:R:168:GLU:HG3	1.89	0.53
41:2:4114:C:H5''	41:2:4115:G:OP2	2.08	0.53
41:2:4246:G:H2'	41:2:4247:G:H8	1.70	0.53
6:B:353:VAL:O	37:z:18:ARG:NH1	2.41	0.53
8:D:109:ARG:NH2	41:2:2343:G:OP2	2.41	0.53
41:2:2469:C:H5	41:2:2471:G:H1	1.56	0.53
8:D:149:GLU:OE2	32:l:71:ARG:NH1	2.42	0.53
41:2:1256:G:OP2	41:2:1257:A:N6	2.42	0.53
10:F:41:ALA:O	10:F:52:ARG:NH1	2.42	0.53
22:V:7:LEU:HB2	22:V:31:ARG:HH21	1.74	0.53
41:2:35:U:O2'	41:2:1651:G:N3	2.41	0.53
41:2:1562:G:N2	41:2:1565:A:OP2	2.42	0.53
41:2:2554:U:O4	41:2:2764:A:N7	2.42	0.53
41:2:3907:G:C2	41:2:3908:A:H1'	2.44	0.53
8:D:326:LEU:HD21	8:D:333:LYS:HB2	1.91	0.53
41:2:1872:G:O2'	41:2:4219:A:N1	2.42	0.53
39:4:510:ARG:NH2	41:2:2625:U:OP2	2.42	0.53
28:e:69:LYS:O	28:e:73:ARG:HB2	2.08	0.53
19:Q:197:LYS:HD2	41:2:4358:U:H4'	1.90	0.53
41:2:2557:G:H22	41:2:2570:U:H3	1.57	0.53
41:2:4605:A:C2	41:2:4605:A:N1	2.77	0.53
42:r:63:GLN:HE22	42:r:65:ALA:HB2	1.74	0.53
11:G:41:ILE:HD11	41:2:4115:G:N3	2.24	0.52
41:2:1675:C:N4	41:2:1677:U:H1'	2.24	0.52
7:C:95:ARG:NH1	41:2:1265:G:OP1	2.42	0.52
41:2:493:G:N1	41:2:661:C:O2	2.42	0.52
41:2:4605:A:C2	41:2:4605:A:N3	2.78	0.52
41:2:186:G:N3	41:2:1366:G:N2	2.57	0.52
41:2:4251:A:H1'	48:T:110:GLN:HG3	1.86	0.52
12:H:122:LYS:HE2	19:Q:146:LEU:HD23	1.90	0.52
33:m:122:ASP:O	33:m:163:ARG:NH2	2.43	0.52
41:2:4448:G:N1	41:2:4502:C:OP1	2.42	0.52
1:5:66:G:OP1	42:r:14:LYS:NZ	2.42	0.52
2:6:203:CYS:SG	2:6:204:ALA:N	2.82	0.52
26:b:71:SER:O	26:b:76:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:z:98:ASN:ND2	41:2:4726:G:OP2	2.43	0.52
4:8:110:U:OP2	18:P:8:ARG:NH2	2.43	0.52
8:D:152:LEU:HD23	8:D:251:ILE:HG12	1.90	0.52
36:p:105:VAL:HG13	36:p:136:VAL:HG12	1.91	0.52
37:z:100:ARG:NH2	41:2:4726:G:N7	2.56	0.52
42:r:83:LEU:HD23	42:r:92:LEU:HG	1.91	0.52
39:4:9:ILE:HG23	39:4:68:ASP:OD2	2.09	0.51
40:R:133:LEU:HD22	40:R:148:ARG:HB3	1.92	0.51
42:r:150:LEU:CD1	48:T:145:LYS:CG	2.88	0.51
47:J:54:LYS:HG3	47:J:57:ARG:HH11	1.76	0.51
11:G:53:ARG:NH2	41:2:4165:C:OP1	2.42	0.51
33:m:101:VAL:HG22	33:m:165:VAL:HG22	1.90	0.51
41:2:4114:C:H5	41:2:4158:C:C4	2.28	0.51
6:B:57:VAL:HG23	6:B:366:LYS:HB3	1.92	0.51
20:S:59:ASP:OD1	20:S:59:ASP:N	2.44	0.51
39:4:164:ILE:HG23	39:4:166:PRO:HD3	1.91	0.51
41:2:2905:C:N4	41:2:3589:G:H1	2.07	0.51
41:2:1994:C:H2'	41:2:1995:G:H8	1.75	0.51
21:U:116:LEU:HD22	21:U:135:ILE:HD11	1.92	0.51
39:4:173:LEU:HD13	39:4:181:LYS:HB2	1.92	0.51
6:B:2:SER:N	41:2:4516:G:OP2	2.44	0.51
41:2:2599:G:N2	41:2:2747:U:O4	2.43	0.51
41:2:4294:C:C4	41:2:4295:U:C4	2.99	0.51
41:2:1871:A:H3'	41:2:1872:G:C4'	2.41	0.51
41:2:2753:G:H5''	41:2:2754:G:OP2	2.10	0.51
42:r:77:ALA:O	42:r:108:ARG:NH1	2.43	0.51
8:D:301:ALA:HB1	24:Z:132:LYS:HD3	1.91	0.51
16:M:52:LYS:NZ	41:2:375:G:OP2	2.43	0.51
39:4:256:ASP:OD1	39:4:256:ASP:N	2.44	0.51
5:9:33:ARG:NH1	5:9:94:VAL:O	2.43	0.51
11:G:41:ILE:HD11	41:2:4115:G:H1'	1.92	0.51
33:m:37:ARG:NH2	41:2:4088:C:OP1	2.43	0.51
41:2:1552:G:O2'	41:2:1574:B9B:N2	2.44	0.51
41:2:5025:C:O2'	41:2:5028:G:N3	2.43	0.51
6:B:69:LYS:NZ	39:4:411:LEU:O	2.42	0.51
39:4:48:MET:HE2	39:4:114:VAL:HG13	1.93	0.51
39:4:79:TYR:C	39:4:81:ASP:N	2.68	0.51
39:4:79:TYR:O	39:4:82:LEU:N	2.44	0.51
39:4:510:ARG:NH1	43:d:98:ASP:OD1	2.44	0.51
41:2:1676:C:H4'	41:2:1677:U:OP2	2.10	0.51
8:D:84:THR:OG1	8:D:85:HIS:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:o:164:PHE:HA	35:o:175:VAL:HG12	1.94	0.50
39:4:287:VAL:HG23	39:4:318:ILE:HB	1.93	0.50
8:D:336:ARG:NH1	41:2:947:C:OP1	2.44	0.50
14:K:30:ARG:NH1	41:2:327:U:O2'	2.45	0.50
40:R:246:ASN:ND2	40:R:253:CYS:SG	2.84	0.50
41:2:90:G:OP2	41:2:92:C:N4	2.44	0.50
35:o:161:ARG:O	35:o:182:ASN:ND2	2.45	0.50
39:4:79:TYR:O	39:4:81:ASP:N	2.43	0.50
41:2:253:G:N2	41:2:254:G:O6	2.44	0.50
41:2:2021:G:O3'	47:J:98:GLY:HA2	2.11	0.50
41:2:4303:C:H4'	41:2:4306:U:H5	1.75	0.50
28:e:76:VAL:HB	38:A:190:ARG:HB2	1.93	0.50
30:h:121:ARG:NH1	41:2:194:C:O2	2.44	0.50
40:R:152:LYS:HG3	40:R:249:GLU:HB2	1.91	0.50
41:2:2418:A:N1	41:2:2429:A:O2'	2.44	0.50
47:J:151:PRO:HG3	47:J:154:ARG:HH21	1.76	0.50
6:B:237:THR:HG21	6:B:251:VAL:HG22	1.93	0.50
32:l:87:ARG:NH1	41:2:690:C:OP1	2.45	0.50
47:J:20:LEU:HA	47:J:23:LYS:HD2	1.94	0.50
3:7:65:VAL:HG22	5:9:110:SER:HB2	1.94	0.50
9:E:101:ASP:N	9:E:101:ASP:OD1	2.45	0.50
10:F:76:ARG:NH1	41:2:2583:C:OP2	2.45	0.50
38:A:174:TYR:CG	39:4:76:HIS:CD2	2.99	0.50
40:R:54:ARG:NH1	40:R:57:GLU:OE1	2.45	0.50
41:2:1595:G:O2'	41:2:1597:G:N2	2.44	0.50
41:2:3641:U:OP2	41:2:3646:A:N6	2.44	0.50
36:p:182:TYR:HB3	36:p:200:ARG:HG3	1.94	0.50
41:2:1675:C:C4	41:2:1677:U:H1'	2.47	0.50
41:2:4251:A:OP1	48:T:108:GLY:C	2.51	0.50
9:E:51:ASN:ND2	23:X:40:SER:O	2.44	0.50
31:i:90:PRO:O	31:i:117:LYS:NZ	2.43	0.50
38:A:388:LYS:NZ	41:2:3834:C:OP1	2.45	0.50
39:4:357:LEU:HD23	39:4:360:LEU:HD12	1.94	0.50
39:4:405:MET:HB3	39:4:408:ASP:HB3	1.93	0.50
41:2:4237:C:O2'	41:2:4326:G:N2	2.45	0.50
42:r:88:VAL:HG22	42:r:239:MET:HE2	1.94	0.50
33:m:243:THR:HG23	41:2:3746:A:H5'	1.93	0.50
6:B:234:ARG:NH1	6:B:268:ARG:O	2.45	0.49
38:A:203:SER:OG	38:A:204:LYS:N	2.41	0.49
41:2:4335:C:H4'	41:2:4336:A:OP1	2.09	0.49
18:P:21:ARG:NH1	18:P:22:PRO:O	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:T:96:LYS:HB3	48:T:176:PRO:HG3	1.93	0.49
6:B:218:ASP:OD2	6:B:348:ARG:NH1	2.45	0.49
34:n:89:ARG:NH2	41:2:709:C:OP1	2.45	0.49
35:o:156:ARG:NH1	41:2:4940:C:OP1	2.44	0.49
41:2:1524:A2M:N6	41:2:3915:U:O2'	2.45	0.49
42:r:193:GLU:O	42:r:197:LYS:HB2	2.13	0.49
11:G:197:LYS:NZ	41:2:147:A:OP1	2.45	0.49
20:S:98:ARG:NH1	41:2:4872:2MG:O6	2.46	0.49
15:L:42:ARG:NH1	41:2:4376:A:O2'	2.45	0.49
40:R:145:ALA:O	41:2:4198:G:N2	2.45	0.49
46:Y:8:PRO:HD3	46:Y:149:ILE:HD13	1.93	0.49
47:J:42:ILE:HD12	47:J:206:TYR:HB2	1.94	0.49
6:B:222:VAL:O	6:B:343:ARG:NH1	2.46	0.49
34:n:33:VAL:HG23	34:n:38:GLU:HB2	1.95	0.49
38:A:308:LYS:O	38:A:356:ARG:NH2	2.46	0.49
41:2:4127:A:H1'	41:2:4128:A:C8	2.47	0.49
47:J:56:ILE:HG22	47:J:65:MET:HE1	1.93	0.49
2:6:65:GLY:HA3	2:6:70:LEU:HD23	1.95	0.49
20:S:81:ASP:OD1	20:S:81:ASP:N	2.45	0.49
30:h:8:THR:HG21	30:h:13:LYS:HD2	1.94	0.49
6:B:174:ARG:NH1	41:2:4985:U:O2	2.45	0.49
6:B:198:ARG:HA	6:B:201:LEU:HD13	1.94	0.49
21:U:17:ASP:OD1	21:U:20:ARG:NH2	2.44	0.49
42:r:63:GLN:HE21	42:r:74:ILE:HG12	1.77	0.49
41:2:992:C:N4	41:2:995:C:O2'	2.46	0.49
47:J:132:ALA:H	47:J:197:MET:HE1	1.77	0.49
19:Q:16:LYS:NZ	41:2:97:G:OP1	2.45	0.49
1:5:48:G:OP1	42:r:94:ASN:ND2	2.46	0.48
2:6:44:ASP:OD2	39:4:384:ARG:NH2	2.46	0.48
19:Q:35:ARG:NH2	41:2:337:U:OP1	2.44	0.48
41:2:1859:C:H1'	41:2:1860:U:C5	2.48	0.48
41:2:4296:U:H2'	41:2:4297:G:C8	2.48	0.48
8:D:181:LYS:NZ	41:2:219:G:O6	2.45	0.48
41:2:664:G:N2	41:2:666:G:O6	2.46	0.48
41:2:1316:OMG:OP1	45:k:43:ASN:ND2	2.46	0.48
41:2:2624:G:OP2	43:d:97:ARG:NH2	2.46	0.48
3:7:22:VAL:HG22	3:7:28:VAL:HG12	1.96	0.48
15:L:71:PRO:HG2	15:L:108:TYR:HA	1.96	0.48
39:4:62:LEU:HD23	39:4:65:ILE:HD12	1.96	0.48
40:R:240:LYS:HE2	40:R:260:VAL:HA	1.96	0.48
5:9:90:LYS:NZ	41:2:3613:U:OP2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:65:ARG:NH2	41:2:86:U:O2'	2.45	0.48
25:a:92:LYS:NZ	41:2:1574:B9B:OP2	2.44	0.48
35:o:94:LYS:NZ	41:2:688:U:OP1	2.46	0.48
38:A:318:TYR:HE2	38:A:379:LYS:HD3	1.78	0.48
40:R:186:PRO:HD3	40:R:258:LEU:HB3	1.95	0.48
2:6:220:SER:HA	2:6:228:GLN:HB3	1.96	0.48
23:X:26:VAL:HG23	33:m:177:LYS:HG3	1.96	0.48
27:c:130:ARG:NH1	41:2:1837:A:OP2	2.46	0.48
1:5:60:G:H2'	1:5:61:G:H8	1.78	0.48
16:M:54:LYS:O	16:M:58:THR:HB	2.13	0.48
32:l:66:ARG:NH1	32:l:75:THR:O	2.47	0.48
33:m:132:ASN:ND2	41:2:3683:C:OP1	2.42	0.48
41:2:4265:U:H4'	41:2:4266:G:C8	2.49	0.48
42:r:103:LEU:HD22	42:r:248:ARG:HH21	1.79	0.48
47:J:33:CYS:O	47:J:37:TYR:HB2	2.13	0.48
4:8:141:C:OP1	21:U:38:ARG:NH1	2.45	0.48
7:C:92:LYS:HG2	7:C:95:ARG:HH21	1.78	0.48
14:K:22:SER:OG	14:K:23:LYS:N	2.47	0.48
32:l:51:VAL:HG22	32:l:62:VAL:HG12	1.95	0.48
40:R:67:MET:HA	40:R:70:LYS:HB2	1.96	0.48
2:6:129:LEU:O	2:6:133:LEU:HB2	2.13	0.48
3:7:70:GLU:OE2	39:4:449:LYS:NZ	2.47	0.48
13:I:18:ILE:HG22	13:I:27:VAL:HG13	1.95	0.48
41:2:3589:G:N3	41:2:3591:C:N4	2.61	0.48
44:j:64:ILE:HG23	44:j:68:LEU:HD23	1.95	0.48
15:L:75:LEU:HD12	15:L:78:LEU:HD13	1.96	0.48
17:O:3:ARG:NH1	41:2:2643:G:O2'	2.44	0.48
32:l:65:LYS:NZ	32:l:76:SER:OG	2.47	0.48
41:2:1871:A:H3'	41:2:1872:G:O4'	2.14	0.48
38:A:354:MET:HB2	38:A:357:ILE:H	1.79	0.47
39:4:626:ARG:HB2	39:4:631:LYS:HE3	1.96	0.47
41:2:1177:U:H3'	41:2:1180:C:H41	1.79	0.47
41:2:2601:A:N6	41:2:2744:A:OP2	2.46	0.47
41:2:4310:A:O2'	41:2:4335:C:P	2.72	0.47
45:k:22:ARG:HB3	45:k:25:SER:HB3	1.96	0.47
29:g:139:ARG:NH1	41:2:2533:C:OP1	2.47	0.47
41:2:4304:A:H5'	41:2:4304:A:H8	1.79	0.47
2:6:158:GLY:HA2	2:6:179:VAL:HB	1.97	0.47
48:T:96:LYS:HE2	48:T:178:LYS:HD3	1.96	0.47
41:2:1669:A:N3	41:2:1852:U:O2'	2.46	0.47
41:2:2752:G:H2'	41:2:2753:G:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2:3620:G:OP1	41:2:3622:C:N4	2.48	0.47
20:S:117:LYS:NZ	41:2:4882:U:OP1	2.48	0.47
26:b:149:LYS:NZ	41:2:908:G:OP2	2.46	0.47
27:c:100:LYS:HB2	41:2:1730:U:H4'	1.95	0.47
42:r:240:TYR:O	42:r:244:HIS:ND1	2.47	0.47
47:J:54:LYS:O	47:J:57:ARG:HG3	2.13	0.47
33:m:70:LYS:NZ	41:2:2503:G:O6	2.47	0.47
36:p:214:SER:OG	36:p:215:SER:N	2.48	0.47
39:4:121:ASP:OD1	40:R:134:LYS:NZ	2.45	0.47
41:2:2101:C:H2'	41:2:2102:G:H2'	1.96	0.47
41:2:2905:C:H2'	41:2:2905:C:O2	2.13	0.47
2:6:104:LEU:HA	2:6:107:VAL:HG12	1.97	0.47
7:C:103:LYS:NZ	41:2:1707:C:O2'	2.43	0.47
8:D:101:MET:HE3	8:D:104:PRO:HA	1.97	0.47
8:D:103:ALA:HA	41:2:1517:2MG:HN2	1.79	0.47
35:o:69:TYR:O	35:o:72:LYS:NZ	2.47	0.47
37:z:82:ASN:ND2	41:2:4903:G:OP2	2.47	0.47
39:4:212:TYR:O	39:4:217:TRP:NE1	2.44	0.47
41:2:1962:A:N6	41:2:2026:A:O2'	2.47	0.47
41:2:1976:G:N1	41:2:1991:A:H8	2.08	0.47
41:2:3855:C:H2'	41:2:3856:A:H8	1.80	0.47
47:J:42:ILE:HD11	47:J:92:VAL:HG13	1.96	0.47
5:9:89:LEU:HA	5:9:92:LEU:HD12	1.95	0.47
12:H:79:LYS:O	12:H:84:ARG:NH2	2.47	0.47
25:a:13:SER:OG	25:a:38:ARG:NH2	2.48	0.47
33:m:114:CYS:HB2	33:m:169:VAL:HG13	1.97	0.47
33:m:128:ARG:NH2	41:2:3680:U:OP2	2.48	0.47
41:2:2579:G:N2	41:2:2582:A:OP2	2.45	0.47
41:2:3938:G:N2	41:2:4170:A:O3'	2.48	0.47
2:6:14:GLY:O	2:6:61:ARG:NH1	2.47	0.47
13:I:102:ASN:HB3	13:I:115:ARG:HB2	1.97	0.47
38:A:374:THR:O	38:A:378:LEU:HB2	2.13	0.47
42:r:136:ASP:OD1	42:r:136:ASP:N	2.45	0.47
23:X:59:SER:O	41:2:2652:G:N2	2.40	0.47
38:A:158:SER:OG	38:A:159:ASP:N	2.40	0.47
39:4:491:LYS:NZ	41:2:2627:C:O2'	2.43	0.47
42:r:192:ALA:HA	42:r:195:HIS:HB3	1.96	0.47
25:a:43:LYS:NZ	25:a:47:ASP:OD2	2.48	0.46
38:A:174:TYR:HB2	39:4:77:PRO:CD	2.42	0.46
39:4:62:LEU:HD22	39:4:99:ILE:HG23	1.97	0.46
42:r:292:GLU:OE2	42:r:293:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:i:67:LYS:NZ	41:2:2574:G:OP2	2.46	0.46
41:2:3917:A:H2'	41:2:3918:G:H8	1.80	0.46
44:j:95:ASP:OD1	44:j:95:ASP:N	2.46	0.46
6:B:8:ALA:HB2	28:e:49:LEU:HD22	1.98	0.46
28:e:60:MET:HE1	28:e:108:ASN:HA	1.97	0.46
41:2:3718:A2M:HM'2	41:2:3719:A:H5'	1.97	0.46
41:2:4245:G:C2	41:2:4246:G:C5	3.03	0.46
5:9:28:LEU:HB3	5:9:31:ILE:HG13	1.98	0.46
19:Q:83:VAL:HG12	19:Q:114:VAL:HG21	1.98	0.46
33:m:233:ARG:O	33:m:233:ARG:NH1	2.47	0.46
41:2:4304:A:H5'	41:2:4304:A:C8	2.51	0.46
3:7:57:LYS:HG2	3:7:64:THR:HG22	1.97	0.46
41:2:495:C:N3	41:2:656:C:N4	2.64	0.46
41:2:4453:C:OP1	41:2:4519:C:N4	2.47	0.46
42:r:53:VAL:HB	42:r:159:VAL:HG12	1.97	0.46
15:L:85:GLN:HA	15:L:88:VAL:HG12	1.98	0.46
19:Q:80:GLU:OE2	19:Q:102:ARG:NH2	2.48	0.46
24:Z:70:MET:HE3	24:Z:70:MET:HB3	1.84	0.46
31:i:25:ILE:HD11	31:i:28:ASN:HB3	1.98	0.46
41:2:1985:G:N2	41:2:2003:G:O2'	2.49	0.46
4:8:126:C:H5''	41:2:2493:G:H21	1.81	0.46
26:b:139:ARG:O	26:b:143:LYS:HB2	2.16	0.46
44:j:19:GLU:OE1	44:j:92:ARG:NH1	2.49	0.46
21:U:47:LYS:NZ	41:2:280:G:OP1	2.45	0.46
41:2:183:C:H1'	41:2:184:U:H5	1.81	0.46
41:2:1245:C:H2'	41:2:1246:G:H8	1.81	0.46
41:2:2816:G:N3	41:2:3622:C:O2'	2.49	0.46
2:6:155:SER:OG	2:6:156:ASN:N	2.49	0.46
13:I:171:ASP:OD1	13:I:173:ARG:NH1	2.48	0.46
39:4:618:PRO:HG2	39:4:621:LEU:HD12	1.98	0.46
41:2:1865:G:N2	41:2:1868:A:H61	2.14	0.46
8:D:35:ASP:OD1	8:D:35:ASP:N	2.48	0.45
41:2:3875:G:H22	41:2:3879:G:H5'	1.81	0.45
11:G:103:ARG:NH2	11:G:192:ARG:O	2.50	0.45
3:7:53:LYS:HG2	5:9:106:ALA:HB2	1.97	0.45
4:8:103:A:OP1	16:M:21:ARG:NH2	2.44	0.45
6:B:95:THR:HG22	41:2:4910:G:H4'	1.98	0.45
7:C:112:ILE:O	7:C:116:LEU:HB2	2.15	0.45
30:h:4:ASN:HB3	30:h:7:VAL:HG22	1.98	0.45
6:B:66:LYS:NZ	28:e:12:ALA:O	2.48	0.45
12:H:80:PRO:HD2	12:H:83:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:68:ALA:O	41:2:4691:A:O2'	2.34	0.45
14:K:2:ALA:N	19:Q:172:GLU:OE1	2.49	0.45
26:b:93:MET:HG2	41:2:1952:G:H4'	1.99	0.45
39:4:207:VAL:HG22	39:4:220:VAL:HG13	1.99	0.45
39:4:619:LYS:O	39:4:623:SER:HB2	2.17	0.45
47:J:50:ASN:HA	47:J:53:LEU:HG	1.99	0.45
1:5:74:A:N3	26:b:53:LYS:NZ	2.58	0.45
19:Q:11:LYS:NZ	41:2:95:G:OP2	2.49	0.45
33:m:22:HIS:O	33:m:24:LYS:NZ	2.50	0.45
39:4:582:ASP:N	39:4:582:ASP:OD1	2.49	0.45
41:2:2606:G:O2'	41:2:2667:C:N3	2.49	0.45
47:J:87:ASP:OD1	47:J:87:ASP:N	2.45	0.45
21:U:44:ARG:NH1	21:U:120:TRP:O	2.47	0.45
24:Z:81:VAL:HG12	24:Z:101:CYS:HB3	1.98	0.45
29:g:152:LYS:HE2	29:g:152:LYS:HB3	1.83	0.45
41:2:187:U:O2'	41:2:189:G:OP2	2.34	0.45
41:2:2092:G:O2'	41:2:2262:G:N2	2.49	0.45
42:r:27:LYS:HE3	48:T:146:ARG:HE	1.78	0.45
6:B:301:ASN:OD1	6:B:301:ASN:N	2.48	0.45
22:V:168:TYR:OH	41:2:4768:G:OP1	2.35	0.45
35:o:187:ARG:NH1	41:2:4939:C:OP1	2.50	0.45
39:4:229:PRO:HB2	39:4:233:ARG:HG2	1.98	0.45
40:R:43:ILE:HA	40:R:47:ALA:HB3	1.99	0.45
41:2:2362:U:H2'	41:2:2363:A2M:H8	1.99	0.45
11:G:160:ASP:OD1	11:G:160:ASP:N	2.50	0.45
22:V:47:PHE:HZ	22:V:144:GLU:HG3	1.81	0.45
23:X:10:ILE:HG23	23:X:11:VAL:HG13	1.99	0.45
25:a:114:LYS:O	25:a:146:LYS:NZ	2.47	0.45
36:p:76:ARG:NE	41:2:730:G:OP2	2.48	0.45
42:r:27:LYS:CE	48:T:146:ARG:CZ	2.64	0.45
5:9:14:SER:HB2	41:2:2843:U:H5''	1.98	0.45
23:X:86:LEU:HA	23:X:89:LEU:HG	1.98	0.45
31:i:47:ASP:HB3	31:i:69:LYS:HB3	1.98	0.45
39:4:541:VAL:HG12	39:4:542:GLN:HG3	1.99	0.45
41:2:4066:U:O2	41:2:4067:U:N3	2.49	0.45
42:r:6:VAL:HG22	42:r:8:LYS:H	1.82	0.45
1:5:23:A:N3	1:5:118:C:O2'	2.47	0.45
3:7:132:HIS:HA	3:7:135:ARG:HB2	1.99	0.45
4:8:150:C:N4	11:G:52:THR:O	2.48	0.45
6:B:206:PRO:HG2	6:B:209:GLN:HG3	1.98	0.45
20:S:114:LYS:NZ	41:2:4929:C:OP1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:140:LYS:HA	21:U:143:ARG:HB3	1.98	0.45
39:4:83:MET:HE2	39:4:83:MET:HB2	1.89	0.45
41:2:2574:G:N7	41:2:2760:G:N2	2.64	0.45
41:2:4605:A:C4	41:2:4605:A:N3	2.85	0.45
1:5:7:G:OP2	42:r:22:ARG:NH2	2.47	0.44
26:b:116:ARG:NH1	41:2:1950:U:O2'	2.50	0.44
30:h:8:THR:HB	30:h:10:ASP:H	1.81	0.44
41:2:4093:G:N3	41:2:4093:G:H2'	2.31	0.44
6:B:28:LYS:NZ	41:2:4582:C:OP2	2.46	0.44
13:I:114:ILE:HB	13:I:124:ARG:HB2	1.98	0.44
21:U:125:SER:HB3	41:2:3937:C:H1'	2.00	0.44
32:l:107:ARG:NH2	41:2:2263:A:OP1	2.50	0.44
36:p:223:LYS:HE3	41:2:1907:A:H4'	1.99	0.44
41:2:1100:U:O2	41:2:1195:G:O6	2.35	0.44
42:r:150:LEU:HD12	48:T:145:LYS:HG3	1.97	0.44
6:B:396:ARG:NH2	41:2:5040:U:OP2	2.46	0.44
8:D:66:SER:O	8:D:66:SER:OG	2.35	0.44
25:a:145:LEU:O	25:a:149:LYS:HB2	2.17	0.44
30:h:87:ARG:NH2	41:2:404:U:O3'	2.51	0.44
30:h:43:ASN:ND2	30:h:127:GLN:OE1	2.50	0.44
36:p:157:ARG:HE	36:p:248:ASN:HB2	1.83	0.44
41:2:62:A:N3	41:2:77:U:O2'	2.44	0.44
41:2:4256:A:H61	48:T:59:SER:HB3	1.83	0.44
41:2:4451:G:H21	41:2:4452:U:H3	1.64	0.44
41:2:4452:U:O2'	41:2:4522:G:O6	2.35	0.44
42:r:93:THR:O	42:r:158:LYS:NZ	2.44	0.44
42:r:110:LEU:HD22	42:r:115:MET:HG2	1.99	0.44
8:D:281:MET:HE3	8:D:281:MET:HB3	1.84	0.44
39:4:77:PRO:C	39:4:79:TYR:N	2.74	0.44
39:4:112:ASP:OD1	39:4:115:ARG:NH1	2.50	0.44
45:k:4:LEU:HB2	45:k:121:ARG:HG3	1.99	0.44
8:D:66:SER:HA	8:D:77:PRO:HA	2.00	0.44
10:F:45:ALA:HB3	10:F:82:MET:HG2	1.99	0.44
31:i:5:MET:SD	31:i:5:MET:N	2.90	0.44
35:o:252:ALA:O	35:o:256:GLN:NE2	2.43	0.44
41:2:4251:A:C1'	48:T:110:GLN:CG	2.81	0.44
42:r:23:ARG:HD2	42:r:23:ARG:HA	1.82	0.44
8:D:110:ARG:NH2	41:2:1508:A:OP1	2.44	0.44
21:U:155:VAL:O	21:U:162:ARG:NH2	2.50	0.44
3:7:1:MET:HE3	3:7:15:PRO:HG2	1.99	0.44
4:8:96:C:H5''	12:H:66:LYS:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:o:178:PRO:HB2	35:o:181:LEU:HD23	2.00	0.44
41:2:1788:A:O2'	41:2:4209:G:O2'	2.35	0.44
41:2:1969:G:C2	41:2:1970:A:C4	3.05	0.44
41:2:1971:C:O2'	41:2:1972:G:H8	2.01	0.44
41:2:4223:C:H2'	41:2:4224:A:H8	1.82	0.44
47:J:74:MET:HG3	47:J:93:SER:HB3	2.00	0.44
2:6:17:ALA:O	2:6:18:LYS:NZ	2.40	0.44
4:8:13:G:O2'	46:Y:121:LYS:O	2.35	0.44
8:D:163:LYS:HB2	8:D:166:GLU:HG3	2.00	0.44
24:Z:50:ARG:HA	24:Z:53:MET:HG3	1.99	0.44
30:h:10:ASP:HB3	30:h:13:LYS:HB2	1.99	0.44
41:2:1366:G:O2'	41:2:1367:C:O2	2.34	0.44
41:2:2458:C:O2'	41:2:3671:G:N3	2.49	0.44
41:2:3653:A:N6	41:2:3691:G:O2'	2.45	0.44
41:2:4250:G:O3'	48:T:108:GLY:HA3	2.07	0.44
2:6:84:ILE:HG23	2:6:88:LEU:HD13	1.98	0.43
12:H:122:LYS:HE3	19:Q:125:ILE:HD11	1.99	0.43
13:I:79:ASN:ND2	41:2:4690:B8K:OP1	2.46	0.43
24:Z:30:LYS:HE3	32:l:8:MET:HE3	2.00	0.43
37:z:83:LYS:NZ	41:2:4905:C:OP2	2.41	0.43
38:A:312:SER:HB3	38:A:360:ILE:HD11	2.00	0.43
38:A:432:LEU:HD12	38:A:436:GLY:HA2	2.00	0.43
39:4:177:PRO:HD3	39:4:224:GLY:HA3	2.00	0.43
41:2:961:G:N2	41:2:964:A:H61	2.16	0.43
41:2:3664:G:H2'	41:2:3665:G:H8	1.82	0.43
2:6:187:ASN:OD1	2:6:210:THR:OG1	2.36	0.43
22:V:187:LYS:HA	22:V:187:LYS:HD2	1.89	0.43
33:m:159:SER:OG	33:m:160:SER:N	2.51	0.43
38:A:369:SER:OG	38:A:370:GLU:N	2.49	0.43
38:A:394:ILE:HG13	38:A:422:LEU:HD11	2.00	0.43
41:2:187:U:O4	41:2:245:C:N4	2.52	0.43
10:F:15:THR:O	10:F:19:LYS:NZ	2.51	0.43
11:G:41:ILE:HD11	41:2:4115:G:C1'	2.48	0.43
22:V:34:VAL:HG12	22:V:103:LYS:HB2	2.00	0.43
35:o:130:LYS:HG3	41:2:1284:G:H21	1.83	0.43
41:2:1969:G:H2'	41:2:1970:A:O4'	2.17	0.43
41:2:2045:G:O6	41:2:3870:C:O2'	2.36	0.43
41:2:4113:U:O5'	41:2:4114:C:H3'	2.18	0.43
41:2:4321:U:O2	41:2:4326:G:N2	2.41	0.43
41:2:4495:G:H2'	41:2:4496:A:H8	1.83	0.43
47:J:54:LYS:HA	47:J:57:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:235:PRO:HA	38:A:238:GLU:HB2	1.99	0.43
39:4:161:LEU:HD12	39:4:162:PRO:HD2	2.01	0.43
39:4:330:LYS:HA	39:4:333:THR:HG22	2.01	0.43
41:2:2745:A:H2'	41:2:2746:A:H8	1.82	0.43
41:2:2862:G:N3	41:2:3624:A:H2'	2.34	0.43
47:J:27:ILE:HG12	47:J:76:ALA:HB2	1.99	0.43
48:T:20:LEU:HD13	48:T:22:LEU:HD21	2.00	0.43
2:6:163:PRO:HG3	39:4:359:ARG:HE	1.84	0.43
6:B:113:GLU:HA	6:B:116:ARG:HD2	2.01	0.43
14:K:40:VAL:HG11	21:U:5:LYS:HG2	2.00	0.43
39:4:125:ARG:NH1	40:R:250:ASN:OD1	2.51	0.43
39:4:370:ASP:OD1	39:4:370:ASP:N	2.51	0.43
41:2:172:C:H4'	41:2:173:C:H5'	2.01	0.43
42:r:27:LYS:CD	48:T:146:ARG:HH21	2.20	0.43
48:T:16:ARG:NH1	48:T:17:ILE:O	2.50	0.43
36:p:132:MET:HA	36:p:135:ILE:HD12	2.01	0.43
40:R:17:ARG:HH11	40:R:18:LEU:H	1.66	0.43
41:2:1972:G:H1	41:2:1994:C:H5	1.67	0.43
19:Q:140:SER:HA	19:Q:143:GLU:HG2	2.00	0.43
33:m:147:ARG:HG2	33:m:157:VAL:HG22	2.00	0.43
33:m:242:ARG:HG3	41:2:3745:U:H4'	2.01	0.43
41:2:4127:A:O2'	41:2:4156:G:N2	2.47	0.43
43:d:52:LYS:HE2	43:d:52:LYS:HB2	1.89	0.43
46:Y:127:ARG:HB2	46:Y:139:TYR:HB3	2.01	0.43
21:U:98:LEU:HA	21:U:101:VAL:HG12	2.00	0.43
22:V:121:PRO:HA	22:V:124:LEU:HD12	2.00	0.43
30:h:34:LEU:HD23	30:h:38:LEU:HB3	2.00	0.43
35:o:151:ILE:HB	35:o:195:ILE:HG23	2.01	0.43
41:2:1050:C:H3'	41:2:1051:G:H3'	1.99	0.43
41:2:1255:A:OP1	41:2:1257:A:N6	2.50	0.43
2:6:18:LYS:HG2	2:6:60:GLY:HA2	1.99	0.43
2:6:49:VAL:HG21	2:6:87:SER:HB2	2.00	0.43
11:G:81:ASN:O	11:G:84:THR:OG1	2.36	0.43
39:4:397:ARG:HB3	39:4:400:ASP:H	1.83	0.43
41:2:517:C:N4	41:2:646:G:O5'	2.48	0.43
41:2:4090:G:H2'	41:2:4091:G:H8	1.82	0.43
41:2:4092:G:O2'	41:2:4093:G:OP1	2.35	0.43
19:Q:139:SER:HB3	19:Q:142:GLU:HG2	2.01	0.43
23:X:30:GLU:HA	23:X:33:GLN:HG2	1.99	0.43
39:4:173:LEU:HD12	39:4:221:ASP:HA	2.01	0.43
41:2:1870:C:C4	41:2:1871:A:N7	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:150:LEU:HD11	48:T:145:LYS:CG	2.49	0.43
4:8:126:C:H4'	41:2:2493:G:H1'	2.00	0.42
8:D:69:THR:OG1	41:2:4390:A:OP1	2.36	0.42
21:U:77:LYS:HA	21:U:77:LYS:HD2	1.77	0.42
21:U:165:THR:HG23	21:U:168:GLY:H	1.84	0.42
28:e:16:ILE:HD11	28:e:57:VAL:H	1.84	0.42
33:m:38:HIS:CG	41:2:4115:G:C2	3.06	0.42
38:A:267:ARG:HD2	38:A:267:ARG:HA	1.83	0.42
41:2:1684:A:H4'	41:2:4305:G:OP2	2.19	0.42
41:2:1998:A:N6	47:J:50:ASN:OD1	2.52	0.42
41:2:2591:A:C4	41:2:2755:A:C2	3.07	0.42
41:2:3907:G:C4	41:2:3908:A:C8	3.08	0.42
41:2:4089:G:H2'	41:2:4090:G:H8	1.84	0.42
2:6:26:VAL:HG21	2:6:35:TYR:HD1	1.83	0.42
13:I:134:CYS:SG	13:I:135:SER:N	2.92	0.42
32:l:20:ARG:NH1	45:k:84:GLU:OE1	2.49	0.42
38:A:174:TYR:CG	38:A:174:TYR:O	2.70	0.42
39:4:13:PRO:HG3	39:4:21:LEU:HD21	2.00	0.42
40:R:247:ASN:OD1	40:R:250:ASN:ND2	2.52	0.42
41:2:1676:C:H41	41:2:4378:A:H5''	1.84	0.42
41:2:1976:G:C6	41:2:1990:A:N1	2.87	0.42
12:H:77:LYS:O	41:2:136:C:N4	2.52	0.42
26:b:77:ASN:HB3	26:b:98:ARG:HG2	2.00	0.42
35:o:223:ARG:HA	35:o:224:LYS:HA	1.83	0.42
39:4:267:GLU:OE2	39:4:268:GLN:NE2	2.51	0.42
41:2:67:C:OP2	41:2:312:G:N2	2.45	0.42
41:2:92:C:OP2	41:2:4341:C:O2'	2.36	0.42
41:2:1969:G:C6	41:2:1970:A:C5	3.07	0.42
41:2:2521:G:H2'	41:2:2522:7MG:H82	2.02	0.42
41:2:2583:C:H2'	41:2:2584:G:H8	1.83	0.42
41:2:4509:U:O2'	41:2:4511:A:N7	2.47	0.42
41:2:5015:G:H21	41:2:5034:A:H62	1.66	0.42
1:5:7:G:OP1	42:r:33:ARG:NH2	2.53	0.42
6:B:229:LYS:HA	6:B:229:LYS:HD2	1.95	0.42
16:M:49:TRP:O	41:2:1646:A:O2'	2.34	0.42
22:V:107:GLY:HA3	41:2:4910:G:H22	1.84	0.42
22:V:202:LEU:H	41:2:4872:2MG:HM21	1.84	0.42
25:a:60:ARG:NH2	41:2:2809:G:OP1	2.52	0.42
33:m:243:THR:OG1	41:2:3748:A:OP1	2.37	0.42
41:2:382:G:N1	41:2:385:A:OP2	2.50	0.42
41:2:2295:C:H2'	41:2:2296:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2:3910:C:H2'	41:2:3911:C:H6	1.85	0.42
44:j:101:LYS:HA	44:j:101:LYS:HD2	1.89	0.42
2:6:18:LYS:HA	2:6:18:LYS:HD3	1.89	0.42
4:8:14:OMU:HM22	4:8:14:OMU:H1'	1.71	0.42
35:o:58:SER:O	35:o:62:MET:HB2	2.20	0.42
39:4:70:PRO:HD2	39:4:92:TYR:OH	2.19	0.42
41:2:4266:G:N2	41:2:4279:A:C8	2.88	0.42
6:B:136:LYS:HB3	37:z:96:TRP:HB2	2.02	0.42
20:S:94:LYS:NZ	41:2:4872:2MG:OP2	2.48	0.42
23:X:23:ARG:HA	23:X:26:VAL:HG12	2.01	0.42
41:2:2848:G:O2'	41:2:3838:U:O4	2.38	0.42
41:2:3908:A:C5	41:2:3909:C:C4	3.08	0.42
41:2:3927:U:H2'	41:2:3928:A:H8	1.84	0.42
41:2:4249:G:H2'	41:2:4250:G:C8	2.54	0.42
1:5:42:A:C1'	48:T:75:ARG:HE	2.31	0.42
12:H:96:ASN:HD22	41:2:136:C:H5''	1.83	0.42
12:H:108:GLN:HA	12:H:111:GLU:HG2	2.00	0.42
41:2:1996:C:O3'	47:J:57:ARG:CZ	2.68	0.42
41:2:4244:A:H2'	41:2:4245:G:O4'	2.20	0.42
41:2:4306:U:H3	41:2:4376:A:H61	1.67	0.42
5:9:28:LEU:H	5:9:31:ILE:HD12	1.84	0.42
11:G:205:THR:OG1	11:G:206:GLN:N	2.52	0.42
13:I:34:LEU:HD11	13:I:149:ASN:HB3	2.00	0.42
39:4:525:ARG:NH2	39:4:531:MET:O	2.53	0.42
41:2:2877:G:N2	41:2:3824:A:O2'	2.44	0.42
42:r:50:ARG:HG3	42:r:65:ALA:HB3	2.01	0.42
1:5:13:A:N3	42:r:24:ARG:NH2	2.67	0.42
36:p:216:PRO:HD3	36:p:247:MET:HE2	2.02	0.42
38:A:219:VAL:HB	38:A:313:VAL:HG22	2.01	0.42
41:2:753:C:H41	41:2:910:G:H1	1.68	0.42
41:2:4127:A:H1'	41:2:4128:A:H8	1.84	0.42
41:2:4196:OMG:HM22	41:2:4196:OMG:H1'	1.75	0.42
41:2:4344:U:O4	41:2:4368:G:O6	2.38	0.42
46:Y:94:MET:HE2	46:Y:148:MET:HE2	2.02	0.42
47:J:147:HIS:HA	47:J:167:VAL:HG23	2.02	0.42
48:T:20:LEU:HD12	48:T:74:VAL:HB	2.02	0.42
39:4:168:THR:HG23	39:4:218:GLN:HE22	1.85	0.42
41:2:1861:U:H2'	41:2:1862:U:O4'	2.20	0.42
41:2:1969:G:N3	41:2:1970:A:H1'	2.35	0.42
42:r:108:ARG:O	42:r:112:ARG:HB2	2.20	0.42
47:J:53:LEU:O	47:J:57:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:182:VAL:HG22	39:4:362:LEU:HA	2.01	0.41
5:9:4:SER:HB2	41:2:1604:G:H1'	2.01	0.41
6:B:19:ARG:NH2	41:2:4623:OMG:OP1	2.53	0.41
11:G:137[A]:ARG:HD2	11:G:146:LEU:HD11	2.01	0.41
18:P:9:ILE:HG23	18:P:51:LEU:HD21	2.01	0.41
36:p:157:ARG:HD2	36:p:213:LEU:HD23	2.02	0.41
38:A:135:LEU:HA	39:4:94:LEU:HD21	2.01	0.41
39:4:189:THR:HG21	39:4:208:GLY:HA3	2.00	0.41
41:2:1865:G:C2	41:2:1866:U:C2	3.08	0.41
41:2:4256:A:N6	48:T:59:SER:CB	2.79	0.41
46:Y:140:MET:HE3	46:Y:140:MET:HB3	1.87	0.41
1:5:13:A:O3'	42:r:24:ARG:NH1	2.53	0.41
3:7:123:ASP:OD2	39:4:488:ARG:NH2	2.53	0.41
13:I:111:LEU:HD13	13:I:127:ARG:HE	1.85	0.41
19:Q:159:ASN:H	41:2:1378:C:H42	1.67	0.41
31:i:105:ALA:HA	31:i:108:ARG:HE	1.85	0.41
36:p:30:ILE:HD12	36:p:30:ILE:HA	1.97	0.41
39:4:417:TRP:CD1	39:4:419:LEU:HD13	2.54	0.41
41:2:753:C:H5	41:2:910:G:H22	1.68	0.41
41:2:1735:U:H2'	41:2:1736:A:H8	1.85	0.41
41:2:1967:A:H2'	41:2:1968:G:H8	1.83	0.41
6:B:224:LYS:HG2	6:B:340:THR:HB	2.02	0.41
19:Q:66:TYR:OH	41:2:1382:G:OP1	2.33	0.41
27:c:135:PRO:HB3	36:p:86:GLU:HG3	2.02	0.41
31:i:64:LYS:NZ	41:2:2760:G:O6	2.53	0.41
40:R:59:ILE:O	40:R:63:LYS:N	2.47	0.41
41:2:1550:G:O6	41:2:1578:U:O4	2.38	0.41
41:2:1971:C:N4	41:2:2000:G:N3	2.67	0.41
2:6:20:THR:OG1	2:6:21:ASN:N	2.53	0.41
6:B:29:VAL:HA	6:B:220:ILE:HD13	2.02	0.41
12:H:109:ARG:NH2	41:2:267:G:OP1	2.52	0.41
19:Q:70:VAL:H	19:Q:159:ASN:HD21	1.68	0.41
30:h:103:LYS:NZ	41:2:231:U:O2	2.45	0.41
39:4:72:LEU:CG	39:4:83:MET:HG2	2.47	0.41
39:4:250:ALA:HB2	39:4:339:LEU:HD12	2.03	0.41
41:2:679:C:H2'	41:2:680:G:H8	1.85	0.41
41:2:1440:U:H3	41:2:2105:A:H2	1.67	0.41
41:2:1584:G:H1	41:2:1609:U:H3	1.66	0.41
41:2:4251:A:O4'	48:T:110:GLN:CD	2.63	0.41
41:2:4620:OMU:HM23	41:2:4620:OMU:H1'	1.76	0.41
47:J:49:ARG:NH1	47:J:51:SER:OG	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:180:PRO:HD3	39:4:365:PRO:HG3	2.02	0.41
6:B:220:ILE:HB	6:B:346:THR:HB	2.02	0.41
7:C:38:LYS:HD2	41:2:4315:A:H4'	2.02	0.41
34:n:54:LYS:O	34:n:66:LYS:NZ	2.52	0.41
39:4:611:ARG:NH2	41:2:367:C:OP1	2.53	0.41
41:2:1890:G:OP2	41:2:1890:G:N2	2.44	0.41
44:j:111:VAL:HG21	44:j:117:LEU:HD11	2.02	0.41
6:B:352:LEU:HB2	37:z:18:ARG:HH12	1.84	0.41
8:D:284:MET:HE2	8:D:287:THR:HA	2.02	0.41
12:H:13:LYS:HA	12:H:13:LYS:HD3	1.88	0.41
33:m:208:GLU:HG2	41:2:1629:G:H1	1.85	0.41
41:2:1676:C:H41	41:2:4378:A:C5'	2.34	0.41
41:2:4605:A:C6	41:2:4605:A:N1	2.88	0.41
1:5:42:A:C1'	48:T:75:ARG:CZ	2.98	0.41
11:G:132:ARG:HA	11:G:133:PRO:HD3	1.83	0.41
11:G:249:ARG:HH12	41:2:4074:C:H4'	1.86	0.41
25:a:44:LEU:HD22	25:a:49:LEU:HD22	2.02	0.41
26:b:94:TYR:O	26:b:139:ARG:NH2	2.47	0.41
27:c:80:VAL:HG21	27:c:85:LEU:HD12	2.03	0.41
34:n:37:ASP:N	34:n:37:ASP:OD1	2.49	0.41
38:A:314:GLY:HA2	38:A:360:ILE:HB	2.03	0.41
41:2:1332:C:H2'	41:2:1333:A:H8	1.86	0.41
41:2:1676:C:O5'	41:2:1677:U:H5	2.04	0.41
41:2:1859:C:H1'	41:2:1860:U:C6	2.56	0.41
41:2:2447:U:H2'	41:2:2448:G:H8	1.86	0.41
41:2:2574:G:C5	41:2:2760:G:N2	2.88	0.41
41:2:4075:U:H3	41:2:4170:A:H62	1.69	0.41
47:J:69:LYS:HE2	47:J:69:LYS:HB2	1.90	0.41
1:5:30:C:N4	1:5:31:G:O6	2.54	0.41
7:C:36:ASP:HB3	7:C:39:PHE:HB2	2.02	0.41
11:G:35:ARG:HH12	31:i:52:LYS:HE3	1.85	0.41
33:m:136:VAL:HA	33:m:148:VAL:HG12	2.03	0.41
35:o:108:LYS:HB3	35:o:108:LYS:HE2	1.92	0.41
38:A:137:THR:OG1	38:A:138:GLU:N	2.53	0.41
39:4:213:LYS:HE2	39:4:213:LYS:HB3	1.89	0.41
41:2:5022:U:O2'	41:2:5025:C:N4	2.51	0.41
47:J:147:HIS:HB3	47:J:166:VAL:HA	2.02	0.41
2:6:39:GLU:O	2:6:43:SER:HB3	2.20	0.41
2:6:190:SER:OG	2:6:191:GLU:N	2.52	0.41
19:Q:79:GLU:HG2	19:Q:110:LEU:HD11	2.02	0.41
32:l:97:ILE:HG21	32:l:107:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:m:9:ARG:NH1	41:2:1628:C:OP2	2.48	0.41
33:m:222:PRO:HG3	41:2:3749:C:H1'	2.03	0.41
39:4:27:GLN:HG3	41:2:4405:G:H8	1.86	0.41
41:2:3893:C:H2'	41:2:3894:A:H8	1.86	0.41
41:2:4174:U:H2'	41:2:4175:G:H8	1.85	0.41
41:2:4230:C:O2'	41:2:4234:A:N6	2.53	0.41
41:2:4244:A:C8	41:2:4245:G:C8	3.09	0.41
41:2:4599:A:H61	41:2:4610:A:H5''	1.86	0.41
42:r:122:GLN:HE21	42:r:124:GLU:HB2	1.84	0.41
46:Y:64:ASN:HB2	46:Y:80:GLN:NE2	2.35	0.41
2:6:53:ILE:HG12	2:6:59:ILE:HG22	2.03	0.41
9:E:62:TYR:HA	9:E:65:MET:HG3	2.02	0.41
12:H:105:LYS:HA	12:H:108:GLN:HG2	2.03	0.41
19:Q:74:ARG:NH2	41:2:76:A:N7	2.68	0.41
22:V:106:ASP:O	41:2:4910:G:N2	2.54	0.41
24:Z:72:LEU:HB2	24:Z:75:ARG:HD2	2.03	0.41
25:a:15:LEU:HD13	25:a:52:ARG:HB2	2.03	0.41
30:h:47:MET:HE3	30:h:47:MET:HB3	1.82	0.41
35:o:162:VAL:HG12	35:o:184:VAL:HG21	2.02	0.41
39:4:580:LEU:HB3	39:4:585:MET:HG3	2.03	0.41
40:R:141:ARG:NH2	41:2:4531:U:OP2	2.43	0.41
41:2:422:C:H2'	41:2:423:G:H8	1.86	0.41
41:2:1675:C:H3'	41:2:1677:U:C5	2.56	0.41
41:2:2564:G:O2'	41:2:2565:A:O4'	2.38	0.41
43:d:56:LEU:HD22	43:d:61:VAL:HB	2.03	0.41
8:D:268:ARG:NH1	41:2:655:C:OP2	2.54	0.40
13:I:48:LEU:HD23	13:I:54:ARG:HE	1.87	0.40
37:z:33:LEU:HA	37:z:33:LEU:HD23	1.89	0.40
37:z:86:LEU:HD12	37:z:86:LEU:HA	1.98	0.40
38:A:151:LYS:HG2	39:4:235:THR:H	1.85	0.40
41:2:387:G:O2'	41:2:412:G:N1	2.44	0.40
41:2:1270:A:O2'	41:2:1439:C:O2	2.37	0.40
41:2:4265:U:N3	42:r:17:GLN:O	2.44	0.40
2:6:24:CYS:HB3	2:6:48:VAL:HG22	2.02	0.40
13:I:152:GLU:O	13:I:156:ASN:HB2	2.21	0.40
33:m:156:LYS:NZ	41:2:3662:A:OP2	2.53	0.40
35:o:237:LYS:HB2	35:o:237:LYS:HE2	1.97	0.40
41:2:387:G:HO2'	41:2:412:G:H1	1.67	0.40
41:2:425:U:OP1	46:Y:37:LYS:NZ	2.54	0.40
41:2:1596:U:O2	41:2:3861:A:O2'	2.32	0.40
42:r:197:LYS:HB2	42:r:197:LYS:HE3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:111:GLN:HA	19:Q:114:VAL:HG12	2.02	0.40
19:Q:155:MET:HA	19:Q:156:PRO:HD3	1.76	0.40
20:S:86:TRP:O	20:S:89:THR:OG1	2.38	0.40
22:V:43:ILE:HD11	22:V:138:LEU:HD13	2.03	0.40
39:4:172:LEU:HD12	39:4:251:VAL:HG12	2.03	0.40
39:4:245:ALA:HA	39:4:278:LEU:HD13	2.03	0.40
40:R:170:PHE:O	40:R:172:ARG:NH1	2.54	0.40
41:2:2611:A:H5'	41:2:2688:G:H4'	2.03	0.40
41:2:2832:A:OP1	44:j:47:LYS:NZ	2.45	0.40
41:2:4638:U:OP1	41:2:5044:A:O2'	2.38	0.40
45:k:67:LYS:O	45:k:75:ARG:NH2	2.54	0.40
1:5:43:U:H4'	48:T:143:ASP:O	2.22	0.40
2:6:78:ASP:OD1	2:6:78:ASP:N	2.53	0.40
15:L:66:ASN:OD1	19:Q:65:ARG:NH1	2.51	0.40
15:L:76:ASP:HB3	15:L:115:GLY:HA3	2.02	0.40
20:S:3:PHE:H	26:b:175:PHE:HZ	1.69	0.40
40:R:246:ASN:ND2	40:R:255:ASN:OD1	2.54	0.40
41:2:2306:G:OP1	45:k:128:ARG:NH1	2.54	0.40
41:2:2749:C:H2'	41:2:2750:G:H8	1.86	0.40
41:2:4736:C:H2'	41:2:4737:G:H8	1.86	0.40
47:J:137:LEU:HD12	47:J:173:TYR:HB3	2.04	0.40
13:I:85:THR:HG23	13:I:86:LEU:HD12	2.03	0.40
27:c:116:LYS:HB3	27:c:116:LYS:HE2	1.98	0.40
41:2:1556:C:O2'	41:2:2669:C:OP1	2.33	0.40
41:2:1865:G:H21	41:2:1868:A:N6	2.20	0.40
41:2:2905:C:C2	41:2:2907:G:C6	3.09	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	6	242/245 (99%)	221 (91%)	21 (9%)	0	100	100
3	7	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
5	9	93/134 (69%)	80 (86%)	12 (13%)	1 (1%)	11	39
6	B	401/403 (100%)	381 (95%)	20 (5%)	0	100	100
7	C	89/159 (56%)	85 (96%)	4 (4%)	0	100	100
8	D	356/427 (83%)	334 (94%)	22 (6%)	0	100	100
9	E	96/115 (84%)	92 (96%)	4 (4%)	0	100	100
10	F	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
11	G	240/266 (90%)	229 (95%)	11 (5%)	0	100	100
12	H	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
13	I	188/192 (98%)	174 (93%)	14 (7%)	0	100	100
14	K	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
15	L	127/148 (86%)	120 (94%)	7 (6%)	0	100	100
16	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
17	O	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
18	P	48/51 (94%)	48 (100%)	0	0	100	100
19	Q	208/211 (99%)	192 (92%)	16 (8%)	0	100	100
20	S	133/215 (62%)	125 (94%)	8 (6%)	0	100	100
21	U	201/204 (98%)	189 (94%)	12 (6%)	0	100	100
22	V	199/203 (98%)	195 (98%)	4 (2%)	0	100	100
23	X	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
24	Z	150/188 (80%)	148 (99%)	2 (1%)	0	100	100
25	a	146/196 (74%)	141 (97%)	5 (3%)	0	100	100
26	b	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
27	c	153/160 (96%)	143 (94%)	10 (6%)	0	100	100
28	e	129/140 (92%)	118 (92%)	11 (8%)	0	100	100
29	g	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
30	h	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
31	i	133/136 (98%)	122 (92%)	11 (8%)	0	100	100
32	l	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
33	m	246/257 (96%)	219 (89%)	27 (11%)	0	100	100
34	n	107/110 (97%)	100 (94%)	6 (6%)	1 (1%)	14	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	o	231/288 (80%)	215 (93%)	16 (7%)	0	100	100
36	p	224/248 (90%)	214 (96%)	10 (4%)	0	100	100
37	z	63/129 (49%)	60 (95%)	3 (5%)	0	100	100
38	A	331/731 (45%)	311 (94%)	18 (5%)	2 (1%)	21	52
39	4	604/634 (95%)	540 (89%)	57 (9%)	7 (1%)	10	37
40	R	221/260 (85%)	212 (96%)	9 (4%)	0	100	100
42	r	291/297 (98%)	251 (86%)	37 (13%)	3 (1%)	12	40
43	d	102/128 (80%)	98 (96%)	4 (4%)	0	100	100
44	j	109/125 (87%)	105 (96%)	4 (4%)	0	100	100
45	k	127/135 (94%)	120 (94%)	7 (6%)	0	100	100
46	Y	165/184 (90%)	154 (93%)	11 (7%)	0	100	100
47	J	201/239 (84%)	189 (94%)	12 (6%)	0	100	100
48	T	163/178 (92%)	147 (90%)	16 (10%)	0	100	100
All	All	7762/9117 (85%)	7267 (94%)	481 (6%)	14 (0%)	44	71

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	n	106	TYR
39	4	280	ILE
42	r	75	VAL
42	r	88	VAL
5	9	99	GLN
38	A	153	PRO
39	4	68	ASP
39	4	80	ALA
39	4	396	LYS
38	A	156	PHE
39	4	230	LEU
39	4	420	MET
42	r	135	ILE
39	4	70	PRO

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	6	212/213 (100%)	212 (100%)	0	100	100
3	7	126/149 (85%)	125 (99%)	1 (1%)	73	79
5	9	81/114 (71%)	81 (100%)	0	100	100
6	B	349/349 (100%)	349 (100%)	0	100	100
7	C	78/126 (62%)	78 (100%)	0	100	100
8	D	298/348 (86%)	297 (100%)	1 (0%)	86	86
9	E	83/97 (86%)	83 (100%)	0	100	100
10	F	94/100 (94%)	94 (100%)	0	100	100
11	G	204/223 (92%)	202 (99%)	2 (1%)	68	76
12	H	109/110 (99%)	109 (100%)	0	100	100
13	I	169/171 (99%)	169 (100%)	0	100	100
14	K	86/89 (97%)	86 (100%)	0	100	100
15	L	110/121 (91%)	110 (100%)	0	100	100
16	M	73/80 (91%)	73 (100%)	0	100	100
17	O	64/65 (98%)	64 (100%)	0	100	100
18	P	47/48 (98%)	47 (100%)	0	100	100
19	Q	176/177 (99%)	176 (100%)	0	100	100
20	S	115/161 (71%)	115 (100%)	0	100	100
21	U	171/172 (99%)	171 (100%)	0	100	100
22	V	173/174 (99%)	173 (100%)	0	100	100
23	X	74/75 (99%)	74 (100%)	0	100	100
24	Z	136/165 (82%)	136 (100%)	0	100	100
25	a	133/175 (76%)	133 (100%)	0	100	100
26	b	157/157 (100%)	157 (100%)	0	100	100
27	c	136/140 (97%)	136 (100%)	0	100	100
28	e	101/107 (94%)	101 (100%)	0	100	100
29	g	106/133 (80%)	106 (100%)	0	100	100
30	h	124/135 (92%)	124 (100%)	0	100	100
31	i	117/118 (99%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	l	109/121 (90%)	109 (100%)	0	100	100
33	m	190/199 (96%)	190 (100%)	0	100	100
34	n	88/89 (99%)	88 (100%)	0	100	100
35	o	208/252 (82%)	208 (100%)	0	100	100
36	p	195/215 (91%)	195 (100%)	0	100	100
37	z	61/115 (53%)	61 (100%)	0	100	100
38	A	296/654 (45%)	296 (100%)	0	100	100
39	4	551/574 (96%)	551 (100%)	0	100	100
40	R	198/228 (87%)	198 (100%)	0	100	100
42	r	246/250 (98%)	246 (100%)	0	100	100
43	d	94/115 (82%)	94 (100%)	0	100	100
44	j	101/110 (92%)	101 (100%)	0	100	100
45	k	115/121 (95%)	115 (100%)	0	100	100
46	Y	147/163 (90%)	147 (100%)	0	100	100
47	J	180/214 (84%)	180 (100%)	0	100	100
48	T	138/149 (93%)	138 (100%)	0	100	100
All	All	6819/7861 (87%)	6815 (100%)	4 (0%)	100	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	7	115	ASN
8	D	276	ASN
11	G	137[A]	ARG
11	G	137[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
2	6	50	HIS
2	6	140	GLN
2	6	145	GLN
2	6	156	ASN
3	7	17	HIS
3	7	110	ASN

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Mol	Chain	Res	Type
3	7	122	GLN
3	7	132	HIS
5	9	61	HIS
6	B	68	ASN
6	B	109	HIS
7	C	58	GLN
7	C	61	ASN
8	D	38	ASN
8	D	41	HIS
8	D	43	ASN
8	D	142	HIS
8	D	187	GLN
8	D	203	GLN
8	D	317	ASN
8	D	338	ASN
8	D	347	HIS
9	E	51	ASN
11	G	64	GLN
11	G	100	HIS
11	G	108	GLN
12	H	20	GLN
12	H	96	ASN
12	H	107	GLN
13	I	189	GLN
15	L	14	HIS
15	L	67	GLN
18	P	19	GLN
18	P	33	ASN
19	Q	40	GLN
19	Q	149	GLN
19	Q	175	ASN
20	S	125	ASN
21	U	32	GLN
21	U	37	HIS
21	U	109	HIS
21	U	156	HIS
21	U	158	HIS
22	V	5	GLN
22	V	50	ASN
22	V	180	GLN
23	X	34	HIS
24	Z	44	ASN

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Mol	Chain	Res	Type
26	b	23	HIS
28	e	50	ASN
30	h	14	ASN
30	h	20	ASN
32	l	100	ASN
33	m	22	HIS
33	m	187	HIS
33	m	215	ASN
34	n	21	GLN
34	n	56	ASN
36	p	24	ASN
36	p	58	HIS
36	p	80	ASN
36	p	110	GLN
36	p	126	ASN
36	p	248	ASN
37	z	92	GLN
37	z	99	GLN
37	z	101	GLN
38	A	274	GLN
38	A	287	ASN
38	A	305	HIS
39	4	76	HIS
39	4	144	GLN
39	4	218	GLN
39	4	268	GLN
39	4	516	GLN
39	4	612	HIS
40	R	3	GLN
40	R	60	GLN
40	R	127	GLN
42	r	63	GLN
42	r	138	GLN
43	d	17	GLN
43	d	55	ASN
44	j	34	HIS
44	j	121	ASN
45	k	23	HIS
45	k	24	GLN
45	k	63	ASN
45	k	80	HIS
45	k	92	ASN

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Mol	Chain	Res	Type
47	J	50	ASN
47	J	70	ASN
47	J	90	HIS
48	T	23	ASN
48	T	65	ASN
48	T	71	HIS
48	T	110	GLN
48	T	155	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	119/120 (99%)	20 (16%)	0
4	8	155/156 (99%)	32 (20%)	0
41	2	3501/5054 (69%)	960 (27%)	21 (0%)
All	All	3775/5330 (70%)	1012 (26%)	21 (0%)

All (1012) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	13	A
1	5	22	A
1	5	24	C
1	5	27	G
1	5	28	C
1	5	29	C
1	5	33	U
1	5	37	G
1	5	38	U
1	5	41	G
1	5	48	G
1	5	50	A
1	5	53	U
1	5	54	A
1	5	63	C
1	5	64	G
1	5	66	G
1	5	97	G
1	5	100	A
1	5	116	G
4	8	24	G

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Mol	Chain	Res	Type
4	8	25	G
4	8	34	U
4	8	35	C
4	8	39	G
4	8	48	A
4	8	49	G
4	8	52	A
4	8	59	A
4	8	60	G
4	8	62	A
4	8	63	U
4	8	80	A
4	8	82	A
4	8	84	A
4	8	85	U
4	8	87	G
4	8	93	C
4	8	103	A
4	8	104	A
4	8	105	C
4	8	110	U
4	8	111	U
4	8	112	G
4	8	114	G
4	8	123	U
4	8	124	U
4	8	125	C
4	8	126	C
4	8	127	U
4	8	150	C
4	8	151	G
41	2	2	G
41	2	39	A
41	2	42	A
41	2	44	A
41	2	48	G
41	2	56	A
41	2	59	A
41	2	64	A
41	2	65	A
41	2	69	A
41	2	72	C

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Mol	Chain	Res	Type
41	2	73	A
41	2	91	G
41	2	98	A
41	2	104	G
41	2	108	A
41	2	109	G
41	2	110	C
41	2	112	C
41	2	119	G
41	2	120	A
41	2	133	C
41	2	134	G
41	2	135	G
41	2	136	C
41	2	137	G
41	2	144	G
41	2	146	G
41	2	152	U
41	2	159	C
41	2	165	A
41	2	172	C
41	2	177	G
41	2	178	C
41	2	179	G
41	2	183	C
41	2	184	U
41	2	185	C
41	2	187	U
41	2	188	G
41	2	200	U
41	2	209	U
41	2	217	C
41	2	218	A
41	2	219	G
41	2	220	C
41	2	234	G
41	2	237	B9B
41	2	254	G
41	2	255	C
41	2	256	G
41	2	259	C
41	2	260	C

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Mol	Chain	Res	Type
41	2	261	G
41	2	262	G
41	2	265	C
41	2	266	C
41	2	267	G
41	2	279	A
41	2	280	G
41	2	297	U
41	2	306	A
41	2	315	G
41	2	316	U
41	2	340	C
41	2	349	A
41	2	363	A
41	2	387	G
41	2	398	A2M
41	2	406	C
41	2	407	A
41	2	409	G
41	2	410	A
41	2	411	G
41	2	412	G
41	2	432	U
41	2	433	A
41	2	449	C
41	2	450	G
41	2	452	A
41	2	453	G
41	2	454	U
41	2	465	G
41	2	467	U
41	2	483	G
41	2	484	U
41	2	485	C
41	2	486	C
41	2	489	C
41	2	491	G
41	2	493	G
41	2	494	U
41	2	495	C
41	2	496	G
41	2	497	G

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Mol	Chain	Res	Type
41	2	498	C
41	2	499	G
41	2	500	G
41	2	502	C
41	2	503	C
41	2	504	G
41	2	505	G
41	2	509	A
41	2	510	U
41	2	513	U
41	2	514	U
41	2	515	C
41	2	516	C
41	2	517	C
41	2	518	G
41	2	519	C
41	2	654	C
41	2	656	C
41	2	657	C
41	2	658	C
41	2	663	G
41	2	667	A
41	2	668	C
41	2	670	G
41	2	673	C
41	2	686	A
41	2	688	U
41	2	690	C
41	2	692	A
41	2	696	C
41	2	697	G
41	2	704	C
41	2	708	G
41	2	731	G
41	2	738	C
41	2	739	G
41	2	740	G
41	2	743	G
41	2	746	A
41	2	747	A
41	2	759	G
41	2	904	C

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Mol	Chain	Res	Type
41	2	905	C
41	2	910	G
41	2	913	U
41	2	914	U
41	2	915	A
41	2	916	C
41	2	917	A
41	2	918	G
41	2	924	C
41	2	925	C
41	2	926	G
41	2	929	A
41	2	932	A
41	2	933	G
41	2	934	C
41	2	936	C
41	2	941	C
41	2	943	A
41	2	944	A
41	2	945	U
41	2	946	C
41	2	956	A
41	2	959	G
41	2	960	A
41	2	962	C
41	2	964	A
41	2	965	G
41	2	966	A
41	2	967	C
41	2	969	C
41	2	970	G
41	2	971	U
41	2	972	C
41	2	982	U
41	2	984	C
41	2	985	C
41	2	986	C
41	2	989	U
41	2	990	C
41	2	991	C
41	2	992	C
41	2	993	G

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Mol	Chain	Res	Type
41	2	994	G
41	2	995	C
41	2	996	G
41	2	1048	G
41	2	1049	C
41	2	1050	C
41	2	1051	G
41	2	1067	G
41	2	1070	G
41	2	1072	C
41	2	1081	C
41	2	1092	G
41	2	1100	U
41	2	1168	G
41	2	1172	C
41	2	1173	G
41	2	1178	G
41	2	1179	U
41	2	1180	C
41	2	1181	C
41	2	1182	C
41	2	1183	C
41	2	1184	A
41	2	1187	G
41	2	1189	G
41	2	1194	G
41	2	1198	G
41	2	1199	G
41	2	1200	G
41	2	1201	U
41	2	1202	C
41	2	1203	G
41	2	1210	C
41	2	1211	G
41	2	1215	C
41	2	1222	A
41	2	1241	C
41	2	1242	G
41	2	1245	C
41	2	1252	C
41	2	1253	G
41	2	1254	A

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Mol	Chain	Res	Type
41	2	1255	A
41	2	1260	G
41	2	1266	G
41	2	1269	G
41	2	1270	A
41	2	1271	G
41	2	1272	C
41	2	1273	G
41	2	1275	G
41	2	1279	A
41	2	1280	C
41	2	1283	G
41	2	1284	G
41	2	1285	U
41	2	1287	G
41	2	1293	G
41	2	1294	A
41	2	1295	C
41	2	1296	G
41	2	1301	C
41	2	1302	U
41	2	1303	A
41	2	1314	C
41	2	1319	U
41	2	1324	A
41	2	1326	A2M
41	2	1327	C
41	2	1337	A
41	2	1353	G
41	2	1354	A
41	2	1358	G
41	2	1359	G
41	2	1365	C
41	2	1366	G
41	2	1370	G
41	2	1371	A
41	2	1377	G
41	2	1378	C
41	2	1379	C
41	2	1387	A
41	2	1394	G
41	2	1397	A

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Mol	Chain	Res	Type
41	2	1398	A
41	2	1402	C
41	2	1404	G
41	2	1405	C
41	2	1406	G
41	2	1407	C
41	2	1409	C
41	2	1410	U
41	2	1411	C
41	2	1414	C
41	2	1420	A
41	2	1438	U
41	2	1439	C
41	2	1441	C
41	2	1442	C
41	2	1444	G
41	2	1447	C
41	2	1458	C
41	2	1482	G
41	2	1483	C
41	2	1494	U
41	2	1497	A
41	2	1498	G
41	2	1503	A
41	2	1512	G
41	2	1523	A
41	2	1534	A2M
41	2	1543	G
41	2	1547	A
41	2	1557	C
41	2	1564	A
41	2	1565	A
41	2	1566	C
41	2	1571	G
41	2	1574	B9B
41	2	1578	U
41	2	1592	G
41	2	1595	G
41	2	1596	U
41	2	1611	C
41	2	1612	G
41	2	1613	A

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Mol	Chain	Res	Type
41	2	1624	G
41	2	1625	OMG
41	2	1626	G
41	2	1631	A
41	2	1633	G
41	2	1634	A
41	2	1637	A
41	2	1638	A
41	2	1641	G
41	2	1650	A
41	2	1654	G
41	2	1661	C
41	2	1671	U
41	2	1676	C
41	2	1677	U
41	2	1678	C
41	2	1685	G
41	2	1691	G
41	2	1694	C
41	2	1697	G
41	2	1699	A
41	2	1700	G
41	2	1701	A
41	2	1702	C
41	2	1703	C
41	2	1704	C
41	2	1705	G
41	2	1707	C
41	2	1708	G
41	2	1715	C
41	2	1716	G
41	2	1718	C
41	2	1719	A
41	2	1721	G
41	2	1724	G
41	2	1734	G
41	2	1789	C
41	2	1791	U
41	2	1796	U
41	2	1803	G
41	2	1804	A
41	2	1806	G

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Mol	Chain	Res	Type
41	2	1808	C
41	2	1810	G
41	2	1811	G
41	2	1813	U
41	2	1814	C
41	2	1817	U
41	2	1819	G
41	2	1821	G
41	2	1822	U
41	2	1832	C
41	2	1833	G
41	2	1836	G
41	2	1837	A
41	2	1842	G
41	2	1854	G
41	2	1855	G
41	2	1856	C
41	2	1857	C
41	2	1859	C
41	2	1860	U
41	2	1864	G
41	2	1866	U
41	2	1867	A
41	2	1868	A
41	2	1871	A
41	2	1872	G
41	2	1873	A
41	2	1874	A
41	2	1881	C
41	2	1882	U
41	2	1883	OMG
41	2	1891	A
41	2	1897	A
41	2	1900	C
41	2	1916	G
41	2	1918	U
41	2	1919	G
41	2	1920	C
41	2	1922	G
41	2	1925	G
41	2	1931	C
41	2	1932	A

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Mol	Chain	Res	Type
41	2	1938	C
41	2	1939	A
41	2	1941	A
41	2	1948	G
41	2	1960	A
41	2	1963	C
41	2	1969	G
41	2	1970	A
41	2	1971	C
41	2	1974	U
41	2	1975	G
41	2	1976	G
41	2	1977	C
41	2	1980	U
41	2	1981	G
41	2	1983	A
41	2	1984	A
41	2	1988	G
41	2	1992	U
41	2	1997	U
41	2	1998	A
41	2	1999	A
41	2	2002	A
41	2	2003	G
41	2	2004	U
41	2	2007	G
41	2	2008	U
41	2	2009	A
41	2	2011	C
41	2	2016	C
41	2	2018	C
41	2	2020	U
41	2	2021	G
41	2	2024	G
41	2	2025	A
41	2	2026	A
41	2	2033	A
41	2	2034	G
41	2	2039	G
41	2	2040	A
41	2	2044	U
41	2	2046	G

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Mol	Chain	Res	Type
41	2	2048	U
41	2	2055	G
41	2	2056	G
41	2	2069	A
41	2	2084	C
41	2	2085	G
41	2	2092	G
41	2	2093	A
41	2	2095	A
41	2	2097	U
41	2	2098	G
41	2	2100	A
41	2	2101	C
41	2	2102	G
41	2	2104	G
41	2	2105	A
41	2	2106	G
41	2	2108	G
41	2	2110	C
41	2	2111	G
41	2	2112	G
41	2	2113	C
41	2	2250	C
41	2	2251	G
41	2	2252	G
41	2	2253	A
41	2	2254	G
41	2	2256	C
41	2	2258	C
41	2	2259	G
41	2	2260	C
41	2	2263	A
41	2	2268	A
41	2	2289	C
41	2	2300	A
41	2	2301	G
41	2	2306	G
41	2	2313	A
41	2	2316	G
41	2	2333	G
41	2	2348	G
41	2	2350	U

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Mol	Chain	Res	Type
41	2	2351	C
41	2	2360	A
41	2	2364	OMG
41	2	2395	A
41	2	2416	G
41	2	2417	A
41	2	2418	A
41	2	2422	OMC
41	2	2424	OMG
41	2	2425	U
41	2	2441	C
41	2	2447	U
41	2	2450	G
41	2	2453	A
41	2	2464	C
41	2	2465	C
41	2	2471	G
41	2	2474	G
41	2	2475	G
41	2	2477	A
41	2	2478	C
41	2	2479	G
41	2	2483	G
41	2	2486	G
41	2	2487	G
41	2	2489	C
41	2	2490	U
41	2	2491	C
41	2	2493	G
41	2	2503	G
41	2	2504	C
41	2	2505	C
41	2	2511	A
41	2	2512	A
41	2	2513	A
41	2	2519	U
41	2	2529	A
41	2	2537	A
41	2	2543	A
41	2	2544	G
41	2	2546	G
41	2	2547	G

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Mol	Chain	Res	Type
41	2	2548	C
41	2	2550	G
41	2	2552	G
41	2	2553	A
41	2	2554	U
41	2	2557	G
41	2	2559	G
41	2	2565	A
41	2	2567	G
41	2	2568	C
41	2	2569	G
41	2	2571	C
41	2	2573	A
41	2	2583	C
41	2	2586	G
41	2	2587	A
41	2	2589	C
41	2	2593	C
41	2	2600	A
41	2	2601	A
41	2	2627	C
41	2	2638	G
41	2	2652	G
41	2	2653	C
41	2	2658	G
41	2	2661	U
41	2	2662	G
41	2	2663	G
41	2	2670	C
41	2	2675	G
41	2	2687	U
41	2	2694	G
41	2	2695	A
41	2	2696	A
41	2	2707	U
41	2	2708	U
41	2	2711	G
41	2	2719	C
41	2	2721	G
41	2	2724	G
41	2	2725	A
41	2	2726	G

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Mol	Chain	Res	Type
41	2	2739	C
41	2	2742	G
41	2	2743	A
41	2	2746	A
41	2	2754	G
41	2	2755	A
41	2	2756	G
41	2	2758	G
41	2	2760	G
41	2	2761	U
41	2	2763	U
41	2	2764	A
41	2	2765	A
41	2	2766	A
41	2	2768	C
41	2	2769	U
41	2	2770	C
41	2	2772	C
41	2	2787	A
41	2	2788	U
41	2	2789	A
41	2	2790	U
41	2	2793	G
41	2	2794	C
41	2	2814	C
41	2	2815	A
41	2	2827	G
41	2	2855	G
41	2	2862	G
41	2	2867	C
41	2	2875	C
41	2	2877	G
41	2	2879	A
41	2	2880	U
41	2	2892	C
41	2	2901	G
41	2	2902	G
41	2	2903	G
41	2	2905	C
41	2	2906	G
41	2	2907	G
41	2	2908	U

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Mol	Chain	Res	Type
41	2	2909	C
41	2	3585	G
41	2	3587	C
41	2	3588	C
41	2	3591	C
41	2	3593	C
41	2	3595	U
41	2	3596	A
41	2	3597	G
41	2	3598	C
41	2	3599	A
41	2	3605	C
41	2	3615	G
41	2	3616	U
41	2	3618	C
41	2	3626	G
41	2	3635	A
41	2	3638	G
41	2	3643	A
41	2	3644	U
41	2	3646	A
41	2	3662	A
41	2	3663	A
41	2	3673	C
41	2	3674	G
41	2	3678	G
41	2	3679	U
41	2	3680	U
41	2	3682	A
41	2	3691	G
41	2	3692	A
41	2	3696	C
41	2	3710	G
41	2	3711	A
41	2	3713	U
41	2	3718	A2M
41	2	3720	G
41	2	3729	U
41	2	3734	U
41	2	3736	A
41	2	3746	A
41	2	3748	A

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Mol	Chain	Res	Type
41	2	3750	G
41	2	3776	G
41	2	3823	G
41	2	3832	U
41	2	3838	U
41	2	3839	G
41	2	3840	U
41	2	3843	C
41	2	3851	U
41	2	3867	A2M
41	2	3869	OMC
41	2	3877	A
41	2	3878	C
41	2	3879	G
41	2	3880	P7G
41	2	3893	C
41	2	3897	B8K
41	2	3903	A
41	2	3905	A
41	2	3906	A
41	2	3908	A
41	2	3909	C
41	2	3910	C
41	2	3915	U
41	2	3916	G
41	2	3922	G
41	2	3938	G
41	2	3939	G
41	2	3941	G
41	2	3942	A
41	2	4067	U
41	2	4068	U
41	2	4073	A
41	2	4074	C
41	2	4076	G
41	2	4077	A
41	2	4084	G
41	2	4085	A
41	2	4088	C
41	2	4091	G
41	2	4092	G
41	2	4093	G

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Mol	Chain	Res	Type
41	2	4094	G
41	2	4095	G
41	2	4099	G
41	2	4101	C
41	2	4102	C
41	2	4103	C
41	2	4104	G
41	2	4108	G
41	2	4110	C
41	2	4111	U
41	2	4112	C
41	2	4114	C
41	2	4115	G
41	2	4116	C
41	2	4117	U
41	2	4119	C
41	2	4120	U
41	2	4122	G
41	2	4125	C
41	2	4126	C
41	2	4127	A
41	2	4128	A
41	2	4129	G
41	2	4130	C
41	2	4131	G
41	2	4133	C
41	2	4134	C
41	2	4135	G
41	2	4139	G
41	2	4140	C
41	2	4141	G
41	2	4142	C
41	2	4143	G
41	2	4144	C
41	2	4146	G
41	2	4155	C
41	2	4157	A
41	2	4158	C
41	2	4162	C
41	2	4163	U
41	2	4170	A
41	2	4183	G

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Mol	Chain	Res	Type
41	2	4184	G
41	2	4191	G
41	2	4194	I4U
41	2	4196	OMG
41	2	4203	A
41	2	4210	U
41	2	4212	A
41	2	4222	G
41	2	4225	G
41	2	4229	U
41	2	4233	A
41	2	4234	A
41	2	4235	G
41	2	4237	C
41	2	4239	A
41	2	4241	C
41	2	4242	U
41	2	4243	C
41	2	4244	A
41	2	4245	G
41	2	4247	G
41	2	4248	A
41	2	4249	G
41	2	4251	A
41	2	4253	A
41	2	4254	G
41	2	4256	A
41	2	4257	A
41	2	4258	C
41	2	4259	C
41	2	4260	U
41	2	4261	C
41	2	4262	C
41	2	4265	U
41	2	4266	G
41	2	4268	A
41	2	4271	A
41	2	4273	A
41	2	4277	G
41	2	4279	A
41	2	4280	A
41	2	4281	A

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Mol	Chain	Res	Type
41	2	4282	A
41	2	4285	U
41	2	4288	C
41	2	4289	U
41	2	4291	G
41	2	4292	A
41	2	4293	U
41	2	4296	U
41	2	4297	G
41	2	4303	C
41	2	4304	A
41	2	4305	G
41	2	4306	U
41	2	4310	A
41	2	4311	A
41	2	4313	A
41	2	4314	C
41	2	4316	G
41	2	4317	A
41	2	4318	C
41	2	4319	C
41	2	4325	A
41	2	4326	G
41	2	4330	G
41	2	4331	G
41	2	4334	U
41	2	4335	C
41	2	4336	A
41	2	4338	G
41	2	4339	A
41	2	4342	C
41	2	4343	U
41	2	4348	A
41	2	4349	C
41	2	4350	C
41	2	4354	U
41	2	4360	U
41	2	4365	C
41	2	4367	G
41	2	4371	MHG
41	2	4373	G
41	2	4376	A

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Mol	Chain	Res	Type
41	2	4377	G
41	2	4378	A
41	2	4380	A
41	2	4381	A
41	2	4386	C
41	2	4387	C
41	2	4395	U
41	2	4396	A
41	2	4407	G
41	2	4415	1MA
41	2	4418	G
41	2	4421	C
41	2	4422	A
41	2	4428	A
41	2	4451	G
41	2	4452	U
41	2	4453	C
41	2	4465	U
41	2	4466	C
41	2	4475	G
41	2	4476	C
41	2	4484	A
41	2	4488	A
41	2	4498	U
41	2	4499	G
41	2	4500	U
41	2	4502	C
41	2	4503	A
41	2	4508	C
41	2	4510	A
41	2	4512	U
41	2	4513	A
41	2	4518	A
41	2	4519	C
41	2	4520	G
41	2	4523	A2M
41	2	4524	G
41	2	4529	B8W
41	2	4538	G
41	2	4545	G
41	2	4549	G
41	2	4550	7MG

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Mol	Chain	Res	Type
41	2	4555	U
41	2	4556	U
41	2	4557	U
41	2	4558	U
41	2	4560	C
41	2	4567	G
41	2	4570	G
41	2	4575	G
41	2	4584	A
41	2	4589	A
41	2	4590	A
41	2	4597	UR3
41	2	4599	A
41	2	4600	G
41	2	4601	U
41	2	4606	G
41	2	4607	A
41	2	4608	G
41	2	4618	G
41	2	4634	U
41	2	4635	A
41	2	4636	U
41	2	4637	OMG
41	2	4656	A
41	2	4670	C
41	2	4672	A
41	2	4677	U
41	2	4678	G
41	2	4684	A
41	2	4687	A
41	2	4694	G
41	2	4695	C
41	2	4708	A
41	2	4709	U
41	2	4719	G
41	2	4720	C
41	2	4730	C
41	2	4731	G
41	2	4732	G
41	2	4733	C
41	2	4734	A
41	2	4735	G

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Mol	Chain	Res	Type
41	2	4740	G
41	2	4741	C
41	2	4742	G
41	2	4745	G
41	2	4754	G
41	2	4757	C
41	2	4759	C
41	2	4761	G
41	2	4764	A
41	2	4765	G
41	2	4771	C
41	2	4775	C
41	2	4776	G
41	2	4860	G
41	2	4870	OMG
41	2	4871	C
41	2	4872	2MG
41	2	4873	G
41	2	4877	G
41	2	4882	U
41	2	4883	C
41	2	4887	C
41	2	4889	G
41	2	4895	C
41	2	4900	C
41	2	4901	G
41	2	4903	G
41	2	4910	G
41	2	4912	G
41	2	4914	C
41	2	4915	G
41	2	4923	C
41	2	4927	G
41	2	4928	C
41	2	4934	A
41	2	4937	C
41	2	4938	A
41	2	4940	C
41	2	4941	G
41	2	4943	A
41	2	4951	G
41	2	4955	A

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Mol	Chain	Res	Type
41	2	4960	G
41	2	4961	G
41	2	4976	U
41	2	4979	A
41	2	4989	U
41	2	4990	C
41	2	4991	U
41	2	5014	A
41	2	5017	G
41	2	5020	G
41	2	5022	U
41	2	5026	U
41	2	5027	C
41	2	5028	G
41	2	5030	U
41	2	5031	G
41	2	5034	A
41	2	5041	G
41	2	5047	C
41	2	5050	C
41	2	5054	C
41	2	5055	G
41	2	5058	A
41	2	5061	A
41	2	5069	U

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
41	2	406	C
41	2	914	U
41	2	1322	1MA
41	2	1625	OMG
41	2	1676	C
41	2	1859	C
41	2	1970	A
41	2	1976	G
41	2	1980	U
41	2	2015	U
41	2	2033	A
41	2	2760	G
41	2	3905	A

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Mol	Chain	Res	Type
41	2	4092	G
41	2	4130	C
41	2	4266	G
41	2	4333	C
41	2	4334	U
41	2	4335	C
41	2	4555	U
41	2	4913	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
41	OMG	2	4623	41	23,26,27	2.63	8 (34%)	33,38,41	2.72	12 (36%)
41	OMG	2	4637	41	23,26,27	2.68	8 (34%)	33,38,41	2.79	10 (30%)
41	OMG	2	4370	41	23,26,27	2.72	8 (34%)	33,38,41	2.87	12 (36%)
41	OMG	2	1625	41	23,26,27	2.73	8 (34%)	33,38,41	2.80	10 (30%)
41	P7G	2	1909	41	24,28,29	4.01	11 (45%)	27,41,44	1.51	3 (11%)
41	B8K	2	3897	41	24,28,29	3.41	11 (45%)	30,42,45	2.50	11 (36%)
41	A2M	2	3718	41	22,25,26	3.17	9 (40%)	31,36,39	2.90	11 (35%)
41	I4U	2	4194	41	21,24,25	3.61	9 (42%)	27,34,37	0.96	1 (3%)
41	OMC	2	4536	41	19,22,23	3.04	8 (42%)	26,31,34	1.19	3 (11%)
41	OMG	2	4196	41	23,26,27	2.74	8 (34%)	33,38,41	3.13	9 (27%)
41	OMC	2	2365	41	19,22,23	2.90	8 (42%)	26,31,34	0.81	0
41	B8T	2	4671	41	19,22,23	3.58	8 (42%)	26,31,34	0.95	1 (3%)
41	B8W	2	2380	41	23,26,27	2.72	5 (21%)	33,38,41	2.55	14 (42%)
41	OMG	2	1883	41	23,26,27	2.70	8 (34%)	33,38,41	2.71	11 (33%)
41	OMG	2	2050	41	23,26,27	2.65	8 (34%)	33,38,41	2.71	10 (30%)
41	B8T	2	4483	41	19,22,23	3.67	8 (42%)	26,31,34	1.23	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A2M	2	3723	41	22,25,26	3.18	9 (40%)	31,36,39	3.01	11 (35%)
41	1MA	2	1322	41	21,25,26	3.04	5 (23%)	31,37,40	1.79	6 (19%)
41	OMG	2	1316	41	23,26,27	2.66	8 (34%)	33,38,41	2.74	11 (33%)
41	2MG	2	4872	41	23,26,27	2.84	9 (39%)	32,38,41	2.31	9 (28%)
41	B9H	2	2786	41	20,25,26	3.36	4 (20%)	22,35,38	2.67	7 (31%)
41	OMG	2	373	41	23,26,27	2.65	9 (39%)	33,38,41	2.68	13 (39%)
41	A2M	2	4571	41	22,25,26	3.17	9 (40%)	31,36,39	2.93	10 (32%)
41	B8K	2	4690	41	24,28,29	3.36	11 (45%)	30,42,45	2.64	12 (40%)
41	A2M	2	2401	41	22,25,26	3.24	10 (45%)	31,36,39	3.00	11 (35%)
41	E6G	2	4355	41	24,27,28	2.02	4 (16%)	34,39,42	2.69	15 (44%)
41	A2M	2	1534	41	22,25,26	3.21	9 (40%)	31,36,39	3.06	12 (38%)
41	OMC	2	2422	41	19,22,23	3.00	8 (42%)	26,31,34	1.16	3 (11%)
41	OMC	2	2804	41	19,22,23	2.91	8 (42%)	26,31,34	1.31	3 (11%)
41	MHG	2	4371	41	29,32,33	4.00	12 (41%)	34,46,49	2.30	12 (35%)
41	E7G	2	2297	41	24,27,28	4.01	11 (45%)	30,40,43	2.19	11 (36%)
41	A2M	2	2363	41	22,25,26	3.21	9 (40%)	31,36,39	2.98	11 (35%)
41	OMG	2	2773	41	23,26,27	2.70	8 (34%)	33,38,41	2.77	9 (27%)
41	1MA	2	4415	41	21,25,26	3.01	5 (23%)	31,37,40	1.88	7 (22%)
41	UR3	2	4530	41	19,22,23	2.93	6 (31%)	26,32,35	1.32	2 (7%)
41	A2M	2	398	41	22,25,26	3.19	9 (40%)	31,36,39	2.98	10 (32%)
41	B8W	2	4529	41	23,26,27	2.81	6 (26%)	33,38,41	2.68	15 (45%)
41	A2M	2	1326	41	22,25,26	3.14	9 (40%)	31,36,39	2.99	10 (32%)
41	OMG	2	1522	41	23,26,27	2.64	8 (34%)	33,38,41	2.75	9 (27%)
41	2MG	2	978	41	23,26,27	2.99	7 (30%)	32,38,41	2.21	9 (28%)
41	B8W	2	4185	41	23,26,27	2.76	6 (26%)	33,38,41	2.61	14 (42%)
41	UR3	2	4597	41	19,22,23	2.82	7 (36%)	26,32,35	1.91	3 (11%)
41	OMC	2	3887	41	19,22,23	3.04	8 (42%)	26,31,34	0.84	1 (3%)
41	7MG	2	4550	41	22,26,27	3.83	10 (45%)	29,39,42	1.92	8 (27%)
41	BGH	2	3899	41	25,29,30	4.64	17 (68%)	31,43,46	2.60	11 (35%)
41	P4U	2	1348	41	21,24,25	3.50	8 (38%)	27,33,36	1.07	2 (7%)
41	B8W	2	4472	41	23,26,27	2.76	6 (26%)	33,38,41	2.65	15 (45%)
41	2MG	2	729	41	23,26,27	2.96	8 (34%)	32,38,41	2.21	8 (25%)
41	B8Q	2	1456	41	17,22,23	2.95	5 (29%)	22,32,35	2.36	6 (27%)
41	7MG	2	2522	41	22,26,27	3.72	10 (45%)	29,39,42	1.95	8 (27%)
41	P7G	2	3880	41	24,28,29	4.18	11 (45%)	27,41,44	1.40	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A2M	2	3825	41	22,25,26	3.18	9 (40%)	31,36,39	2.91	10 (32%)
41	OMG	2	4494	41	23,26,27	2.71	8 (34%)	33,38,41	2.80	9 (27%)
41	OMG	2	2424	41	23,26,27	2.70	8 (34%)	33,38,41	2.85	10 (30%)
41	2MG	2	1517	41	23,26,27	2.98	8 (34%)	32,38,41	2.34	8 (25%)
41	OMG	2	2364	41	23,26,27	2.63	8 (34%)	33,38,41	2.71	11 (33%)
41	A2M	2	3867	41	22,25,26	3.16	9 (40%)	31,36,39	3.07	12 (38%)
41	5MU	2	4083	41	19,22,23	7.18	8 (42%)	28,32,35	3.45	10 (35%)
41	OMG	2	4870	41	23,26,27	2.69	8 (34%)	33,38,41	3.03	9 (27%)
41	A2M	2	4523	41	22,25,26	3.15	9 (40%)	31,36,39	3.08	12 (38%)
41	OMC	2	3701	41	19,22,23	3.03	8 (42%)	26,31,34	0.78	0
41	OMC	2	3869	41	19,22,23	3.07	8 (42%)	26,31,34	1.41	4 (15%)
41	A2M	2	1524	41	22,25,26	3.17	9 (40%)	31,36,39	3.04	12 (38%)
41	M7A	2	4564	41	20,25,26	2.02	3 (15%)	28,37,40	3.92	8 (28%)
41	B9B	2	237	41	25,28,29	1.78	6 (24%)	35,40,43	5.24	11 (31%)
41	6MZ	2	4220	41	22,25,26	2.59	3 (13%)	30,36,39	3.36	10 (33%)
41	7MG	2	1605	41	22,26,27	3.82	10 (45%)	29,39,42	1.96	9 (31%)
4	OMU	8	14	4,41	19,22,23	2.97	8 (42%)	26,31,34	1.87	6 (23%)
41	B9B	2	1574	41	25,28,29	1.73	6 (24%)	35,40,43	5.29	11 (31%)
41	I4U	2	1659	41	21,24,25	3.53	9 (42%)	27,34,37	1.19	2 (7%)
41	OMU	2	4620	41	19,22,23	2.96	8 (42%)	26,31,34	1.68	5 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	OMG	2	4623	41	-	0/9/27/28	0/3/3/3
41	OMG	2	4637	41	-	3/9/27/28	0/3/3/3
41	OMG	2	4370	41	-	0/9/27/28	0/3/3/3
41	OMG	2	1625	41	-	3/9/27/28	0/3/3/3
41	P7G	2	1909	41	-	2/10/40/41	0/3/3/3
41	B8K	2	3897	41	-	3/11/41/42	0/3/3/3
41	A2M	2	3718	41	-	3/9/27/28	0/3/3/3
41	I4U	2	4194	41	-	8/9/29/30	0/2/2/2
41	OMC	2	4536	41	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	OMG	2	4196	41	-	4/9/27/28	0/3/3/3
41	OMC	2	2365	41	-	0/9/27/28	0/2/2/2
41	B8T	2	4671	41	-	0/7/27/28	0/2/2/2
41	B8W	2	2380	41	-	2/9/27/28	0/3/3/3
41	OMG	2	1883	41	-	2/9/27/28	0/3/3/3
41	OMG	2	2050	41	-	0/9/27/28	0/3/3/3
41	B8T	2	4483	41	-	0/7/27/28	0/2/2/2
41	A2M	2	3723	41	-	1/9/27/28	0/3/3/3
41	1MA	2	1322	41	-	1/7/25/26	0/3/3/3
41	OMG	2	1316	41	-	0/9/27/28	0/3/3/3
41	2MG	2	4872	41	-	2/9/27/28	0/3/3/3
41	B9H	2	2786	41	-	1/12/47/48	0/2/2/2
41	OMG	2	373	41	-	1/9/27/28	0/3/3/3
41	A2M	2	4571	41	-	1/9/27/28	0/3/3/3
41	B8K	2	4690	41	-	0/11/41/42	0/3/3/3
41	A2M	2	2401	41	-	3/9/27/28	0/3/3/3
41	E6G	2	4355	41	-	2/10/28/29	0/3/3/3
41	A2M	2	1534	41	-	3/9/27/28	0/3/3/3
41	OMC	2	2422	41	-	1/9/27/28	0/2/2/2
41	OMC	2	2804	41	-	0/9/27/28	0/2/2/2
41	MHG	2	4371	41	-	8/16/46/47	0/3/3/3
41	E7G	2	2297	41	-	1/9/39/40	0/3/3/3
41	A2M	2	2363	41	-	0/9/27/28	0/3/3/3
41	OMG	2	2773	41	-	0/9/27/28	0/3/3/3
41	1MA	2	4415	41	-	2/7/25/26	0/3/3/3
41	UR3	2	4530	41	-	0/7/25/26	0/2/2/2
41	A2M	2	398	41	-	2/9/27/28	0/3/3/3
41	B8W	2	4529	41	-	0/9/27/28	0/3/3/3
41	A2M	2	1326	41	-	1/9/27/28	0/3/3/3
41	OMG	2	1522	41	-	0/9/27/28	0/3/3/3
41	2MG	2	978	41	-	0/9/27/28	0/3/3/3
41	B8W	2	4185	41	-	2/9/27/28	0/3/3/3
41	UR3	2	4597	41	-	2/7/25/26	0/2/2/2
41	OMC	2	3887	41	-	1/9/27/28	0/2/2/2
41	7MG	2	4550	41	-	2/7/37/38	0/3/3/3
41	BGH	2	3899	41	-	0/13/43/44	0/3/3/3
41	P4U	2	1348	41	-	1/10/29/30	0/2/2/2
41	B8W	2	4472	41	-	2/9/27/28	0/3/3/3
41	2MG	2	729	41	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	B8Q	2	1456	41	-	0/7/42/43	0/2/2/2
41	7MG	2	2522	41	-	0/7/37/38	0/3/3/3
41	P7G	2	3880	41	-	4/10/40/41	0/3/3/3
41	A2M	2	3825	41	-	0/9/27/28	0/3/3/3
41	OMG	2	4494	41	-	0/9/27/28	0/3/3/3
41	OMG	2	2424	41	-	2/9/27/28	0/3/3/3
41	2MG	2	1517	41	-	1/9/27/28	0/3/3/3
41	OMG	2	2364	41	-	2/9/27/28	0/3/3/3
41	A2M	2	3867	41	-	3/9/27/28	0/3/3/3
41	5MU	2	4083	41	-	0/7/25/26	0/2/2/2
41	OMG	2	4870	41	-	3/9/27/28	0/3/3/3
41	A2M	2	4523	41	-	4/9/27/28	0/3/3/3
41	OMC	2	3701	41	-	4/9/27/28	0/2/2/2
41	OMC	2	3869	41	-	5/9/27/28	0/2/2/2
41	A2M	2	1524	41	-	1/9/27/28	0/3/3/3
41	M7A	2	4564	41	-	0/7/37/38	0/3/3/3
41	B9B	2	237	41	-	4/11/29/30	0/3/3/3
41	6MZ	2	4220	41	-	1/9/27/28	0/3/3/3
41	7MG	2	1605	41	-	0/7/37/38	0/3/3/3
4	OMU	8	14	4,41	-	1/9/27/28	0/2/2/2
41	B9B	2	1574	41	-	5/11/29/30	0/3/3/3
41	I4U	2	1659	41	-	1/9/29/30	0/2/2/2
41	OMU	2	4620	41	-	1/9/27/28	0/2/2/2

All (575) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	4083	5MU	C4-C5	20.75	1.79	1.44
41	2	4083	5MU	C6-N1	15.72	1.64	1.38
41	2	4083	5MU	C6-C5	-11.53	1.15	1.34
41	2	4220	6MZ	C6-N6	11.04	1.46	1.34
41	2	4083	5MU	C4-N3	-10.94	1.18	1.38
41	2	4194	I4U	C4-N3	10.85	1.45	1.31
41	2	2786	B9H	C2-N3	10.70	1.50	1.37
41	2	1659	I4U	C4-N3	10.55	1.45	1.31
41	2	1348	P4U	C4-N3	10.38	1.44	1.31
41	2	1322	1MA	C2-N3	9.79	1.48	1.30
41	2	4415	1MA	C2-N3	9.66	1.48	1.30
41	2	4371	MHG	C8-N9	9.60	1.51	1.46
41	2	2297	E7G	C5-N7	9.50	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	3880	P7G	C5-N7	9.48	1.46	1.35
41	2	4550	7MG	C8-N9	9.35	1.51	1.46
41	2	3880	P7G	C8-N9	9.33	1.51	1.46
41	2	1909	P7G	C8-N9	9.27	1.51	1.46
41	2	1909	P7G	C5-N7	9.15	1.45	1.35
41	2	1605	7MG	C8-N9	9.09	1.51	1.46
41	2	3897	B8K	C8-N9	9.09	1.51	1.46
41	2	4371	MHG	C5-N7	9.07	1.45	1.35
41	2	4529	B8W	O6-C6	8.93	1.49	1.35
41	2	3899	BGH	O4'-C1'	8.91	1.63	1.42
41	2	4690	B8K	C8-N9	8.90	1.50	1.46
41	2	3899	BGH	C8-N9	8.89	1.50	1.46
41	2	398	A2M	C3'-C4'	-8.86	1.30	1.53
41	2	1524	A2M	C3'-C4'	-8.86	1.30	1.53
41	2	2297	E7G	C8-N9	8.85	1.50	1.46
41	2	2401	A2M	C3'-C4'	-8.84	1.30	1.53
41	2	3867	A2M	C3'-C4'	-8.83	1.30	1.53
41	2	4550	7MG	C5-N7	8.82	1.45	1.35
41	2	1534	A2M	C3'-C4'	-8.78	1.30	1.53
41	2	2363	A2M	C3'-C4'	-8.78	1.30	1.53
41	2	4185	B8W	O6-C6	8.76	1.49	1.35
41	2	1605	7MG	C5-N7	8.74	1.45	1.35
41	2	3723	A2M	C3'-C4'	-8.74	1.30	1.53
41	2	4571	A2M	C3'-C4'	-8.74	1.30	1.53
41	2	3899	BGH	C2'-C1'	-8.73	1.30	1.53
41	2	1326	A2M	C3'-C4'	-8.71	1.30	1.53
41	2	3825	A2M	C3'-C4'	-8.71	1.30	1.53
41	2	2522	7MG	C8-N9	8.67	1.50	1.46
41	2	4472	B8W	O6-C6	8.62	1.48	1.35
41	2	3718	A2M	C3'-C4'	-8.59	1.31	1.53
41	2	2522	7MG	C5-N7	8.58	1.45	1.35
41	2	4523	A2M	C3'-C4'	-8.48	1.31	1.53
41	2	2380	B8W	O6-C6	8.46	1.48	1.35
41	2	4371	MHG	C2-N3	8.25	1.47	1.31
41	2	1456	B8Q	C6-C5	8.17	1.51	1.33
41	2	978	2MG	C2-N3	8.03	1.47	1.31
41	2	4529	B8W	C2-N2	8.01	1.49	1.33
41	2	4472	B8W	C2-N2	8.01	1.49	1.33
41	2	1517	2MG	C2-N3	7.98	1.47	1.31
41	2	4185	B8W	C2-N2	7.95	1.49	1.33
41	2	729	2MG	C2-N3	7.92	1.47	1.31
41	2	3718	A2M	O4'-C4'	7.87	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	2380	B8W	C2-N2	7.81	1.49	1.33
41	2	4872	2MG	C2-N3	7.75	1.46	1.31
41	2	3825	A2M	O4'-C4'	7.71	1.62	1.45
41	2	1534	A2M	O4'-C4'	7.69	1.62	1.45
41	2	2401	A2M	O4'-C4'	7.63	1.62	1.45
41	2	3899	BGH	O4'-C4'	-7.61	1.28	1.45
41	2	4523	A2M	O4'-C4'	7.60	1.62	1.45
41	2	398	A2M	O4'-C4'	7.60	1.62	1.45
41	2	2363	A2M	O4'-C4'	7.59	1.62	1.45
41	2	3723	A2M	O4'-C4'	7.58	1.61	1.45
41	2	4483	B8T	C2-N3	7.47	1.51	1.36
41	2	1524	A2M	O4'-C4'	7.41	1.61	1.45
41	2	4571	A2M	O4'-C4'	7.38	1.61	1.45
41	2	3867	A2M	O4'-C4'	7.36	1.61	1.45
41	2	1326	A2M	O4'-C4'	7.36	1.61	1.45
41	2	4483	B8T	C4-N3	7.32	1.45	1.32
41	2	4671	B8T	C2-N3	7.21	1.51	1.36
41	2	2786	B9H	C2-N1	7.18	1.48	1.38
41	2	4530	UR3	C2-N1	7.14	1.48	1.38
41	2	4671	B8T	C4-N3	7.11	1.45	1.32
41	2	4415	1MA	C4-N3	7.11	1.50	1.35
41	2	1322	1MA	C4-N3	7.04	1.50	1.35
41	2	4671	B8T	C6-C5	6.84	1.51	1.35
41	2	4620	OMU	C2-N1	6.83	1.49	1.38
41	2	4530	UR3	C6-C5	6.82	1.50	1.35
41	2	978	2MG	C2-N2	6.77	1.48	1.33
41	2	3880	P7G	C8-N7	6.77	1.52	1.45
41	2	1517	2MG	C2-N2	6.74	1.48	1.33
41	2	4597	UR3	C6-C5	6.73	1.50	1.35
41	2	729	2MG	C4-N3	6.71	1.50	1.34
41	2	2786	B9H	C6-C5	6.69	1.48	1.33
41	2	1517	2MG	C4-N3	6.69	1.50	1.34
4	8	14	OMU	C2-N3	6.69	1.49	1.38
41	2	4483	B8T	C6-C5	6.69	1.50	1.35
41	2	4620	OMU	C2-N3	6.68	1.49	1.38
4	8	14	OMU	C2-N1	6.68	1.49	1.38
41	2	1456	B8Q	C2-N3	6.67	1.46	1.35
41	2	978	2MG	C4-N3	6.62	1.50	1.34
41	2	729	2MG	C2-N2	6.61	1.48	1.33
41	2	4690	B8K	C2-N3	6.61	1.49	1.33
41	2	3897	B8K	C2-N3	6.58	1.49	1.33
41	2	4371	MHG	C8-N7	6.58	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	2297	E7G	C8-N7	6.53	1.52	1.45
41	2	3880	P7G	C4-N9	6.49	1.44	1.35
41	2	1625	OMG	C2-N3	6.45	1.48	1.33
41	2	4483	B8T	C4-N4	6.42	1.49	1.35
41	2	4196	OMG	C2-N3	6.41	1.48	1.33
41	2	4536	OMC	C2-N3	6.40	1.49	1.36
41	2	3701	OMC	C2-N3	6.39	1.49	1.36
41	2	3869	OMC	C2-N3	6.38	1.49	1.36
41	2	3887	OMC	C2-N3	6.37	1.49	1.36
41	2	4370	OMG	C2-N3	6.34	1.48	1.33
41	2	4196	OMG	C4-N3	6.33	1.49	1.34
41	2	2773	OMG	C2-N3	6.32	1.48	1.33
41	2	4371	MHG	C2-N1	6.31	1.46	1.36
41	2	1625	OMG	C4-N3	6.30	1.49	1.34
41	2	2422	OMC	C2-N3	6.29	1.49	1.36
41	2	4194	I4U	C6-C5	6.28	1.49	1.35
41	2	4494	OMG	C2-N3	6.27	1.48	1.33
41	2	4370	OMG	C4-N3	6.24	1.49	1.34
41	2	3880	P7G	C4-N3	6.24	1.48	1.37
41	2	2424	OMG	C2-N3	6.24	1.48	1.33
41	2	4194	I4U	C2-N3	6.23	1.49	1.36
41	2	4870	OMG	C2-N3	6.23	1.48	1.33
41	2	4597	UR3	C2-N3	6.23	1.51	1.39
41	2	4671	B8T	C4-N4	6.23	1.48	1.35
41	2	1909	P7G	C4-N3	6.21	1.48	1.37
41	2	4597	UR3	C2-N1	6.21	1.47	1.38
41	2	4870	OMG	C4-N3	6.21	1.49	1.34
41	2	4872	2MG	C2-N2	6.18	1.47	1.33
41	2	2424	OMG	C4-N3	6.17	1.48	1.34
41	2	4637	OMG	C4-N3	6.17	1.48	1.34
41	2	4494	OMG	C4-N3	6.17	1.48	1.34
41	2	1659	I4U	C2-N3	6.16	1.48	1.36
41	2	1348	P4U	C2-N3	6.14	1.48	1.36
41	2	3899	BGH	C4-N9	6.13	1.44	1.37
41	2	3701	OMC	C6-C5	6.13	1.49	1.35
41	2	2773	OMG	C4-N3	6.10	1.48	1.34
41	2	4637	OMG	C2-N3	6.10	1.47	1.33
41	2	1883	OMG	C2-N3	6.09	1.47	1.33
41	2	2773	OMG	C2-N2	6.09	1.48	1.34
41	2	4370	OMG	C2-N2	6.08	1.48	1.34
41	2	2804	OMC	C2-N3	6.06	1.48	1.36
41	2	4196	OMG	C2-N2	6.06	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	1659	I4U	C6-C5	6.06	1.49	1.35
41	2	1883	OMG	C4-N3	6.06	1.48	1.34
41	2	1883	OMG	C2-N2	6.05	1.48	1.34
41	2	2365	OMC	C2-N3	6.05	1.48	1.36
41	2	3887	OMC	C6-C5	6.04	1.49	1.35
41	2	4870	OMG	C2-N2	6.03	1.48	1.34
41	2	1316	OMG	C4-N3	6.02	1.48	1.34
41	2	4355	E6G	C2-N2	6.02	1.45	1.33
41	2	4494	OMG	C2-N2	6.02	1.48	1.34
41	2	1625	OMG	C2-N2	6.01	1.48	1.34
41	2	2424	OMG	C2-N2	5.99	1.48	1.34
41	2	1348	P4U	C6-C5	5.99	1.49	1.35
41	2	1909	P7G	C4-N9	5.99	1.44	1.35
41	2	4536	OMC	C6-C5	5.99	1.49	1.35
41	2	373	OMG	C4-N3	5.97	1.48	1.34
41	2	1316	OMG	C2-N3	5.97	1.47	1.33
41	2	4872	2MG	C4-N3	5.94	1.48	1.34
41	2	1522	OMG	C2-N3	5.94	1.47	1.33
41	2	1522	OMG	C4-N3	5.94	1.48	1.34
41	2	2050	OMG	C2-N3	5.93	1.47	1.33
41	2	1909	P7G	C2-N2	5.93	1.48	1.34
41	2	373	OMG	C2-N2	5.92	1.48	1.34
41	2	2050	OMG	C4-N3	5.91	1.48	1.34
41	2	2422	OMC	C6-C5	5.89	1.48	1.35
41	2	1316	OMG	C2-N2	5.89	1.48	1.34
41	2	3880	P7G	C2-N2	5.88	1.48	1.34
41	2	2364	OMG	C2-N3	5.88	1.47	1.33
41	2	4623	OMG	C2-N2	5.88	1.48	1.34
41	2	2804	OMC	C6-C5	5.86	1.48	1.35
41	2	2365	OMC	C6-C5	5.86	1.48	1.35
41	2	4623	OMG	C2-N3	5.86	1.47	1.33
41	2	1522	OMG	C2-N2	5.86	1.48	1.34
41	2	2364	OMG	C4-N3	5.85	1.48	1.34
41	2	4623	OMG	C4-N3	5.85	1.48	1.34
41	2	4530	UR3	C2-N3	5.85	1.50	1.39
41	2	2050	OMG	C2-N2	5.85	1.48	1.34
41	2	3869	OMC	C6-C5	5.84	1.48	1.35
41	2	4564	M7A	C4-N9	5.84	1.49	1.38
41	2	4355	E6G	O6-C6	5.83	1.44	1.35
41	2	4637	OMG	C2-N2	5.82	1.48	1.34
41	2	2364	OMG	C2-N2	5.82	1.48	1.34
41	2	2297	E7G	C4-N3	5.80	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	373	OMG	C2-N3	5.79	1.47	1.33
41	2	3899	BGH	C2-N3	5.79	1.47	1.33
41	2	4371	MHG	C4-N9	5.78	1.44	1.37
41	2	2297	E7G	C4-N9	5.76	1.44	1.37
41	2	4371	MHG	C2-N2	5.75	1.46	1.33
41	2	3897	B8K	C4-N9	5.74	1.44	1.37
41	2	3899	BGH	C4-N3	5.72	1.47	1.34
41	2	1574	B9B	C2-N2	5.71	1.45	1.33
41	2	237	B9B	C2-N2	5.69	1.45	1.33
41	2	2297	E7G	C2-N3	5.67	1.46	1.33
41	2	4371	MHG	C4-N3	5.66	1.47	1.34
41	2	4550	7MG	C2-N3	5.64	1.46	1.33
41	2	2522	7MG	C2-N3	5.61	1.46	1.33
41	2	1605	7MG	C2-N3	5.58	1.46	1.33
41	2	3869	OMC	C2-N1	5.57	1.52	1.40
41	2	1909	P7G	C8-N7	5.55	1.51	1.45
41	2	4620	OMU	C6-C5	5.55	1.48	1.35
41	2	4690	B8K	C4-N9	5.51	1.44	1.37
4	8	14	OMU	C6-C5	5.46	1.47	1.35
41	2	1605	7MG	C4-N3	5.44	1.47	1.34
41	2	4550	7MG	C4-N3	5.43	1.47	1.34
41	2	2522	7MG	C4-N3	5.40	1.47	1.34
41	2	1605	7MG	C4-N9	5.32	1.43	1.37
41	2	3880	P7G	C2-N1	5.22	1.45	1.33
41	2	3701	OMC	C4-N3	5.16	1.44	1.34
41	2	3887	OMC	C4-N3	5.16	1.44	1.34
41	2	4483	B8T	C2-N1	5.16	1.51	1.40
41	2	1909	P7G	C2-N1	5.12	1.45	1.33
41	2	4536	OMC	C2-N1	5.08	1.51	1.40
41	2	2297	E7G	C2-N2	5.06	1.46	1.34
41	2	2422	OMC	C2-N1	5.06	1.51	1.40
41	2	4536	OMC	C4-N3	4.98	1.44	1.34
41	2	3701	OMC	C4-N4	4.95	1.45	1.33
41	2	2522	7MG	C4-N9	4.95	1.43	1.37
41	2	1456	B8Q	C2-N1	4.92	1.45	1.38
41	2	3869	OMC	C4-N4	4.89	1.45	1.33
41	2	3869	OMC	C4-N3	4.89	1.44	1.34
41	2	2422	OMC	C4-N3	4.87	1.44	1.34
41	2	3899	BGH	C2-N2	4.86	1.45	1.34
41	2	3887	OMC	C4-N4	4.86	1.45	1.33
41	2	4536	OMC	C4-N4	4.83	1.45	1.33
41	2	2422	OMC	C4-N4	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	4194	I4U	C5-C4	4.83	1.49	1.43
41	2	2365	OMC	C4-N3	4.80	1.44	1.34
41	2	2365	OMC	C4-N4	4.80	1.45	1.33
41	2	2804	OMC	C2-N1	4.80	1.50	1.40
41	2	2401	A2M	O4'-C1'	-4.74	1.30	1.42
41	2	1605	7MG	C2-N2	4.74	1.45	1.34
41	2	4550	7MG	C2-N2	4.74	1.45	1.34
41	2	4550	7MG	C4-N9	4.73	1.43	1.37
41	2	3887	OMC	C2-N1	4.69	1.50	1.40
41	2	2804	OMC	C4-N4	4.69	1.45	1.33
41	2	2522	7MG	C2-N2	4.69	1.45	1.34
41	2	1659	I4U	C5-C4	4.67	1.49	1.43
41	2	4571	A2M	O4'-C1'	-4.67	1.30	1.42
41	2	2363	A2M	O4'-C1'	-4.64	1.31	1.42
41	2	4523	A2M	O4'-C1'	-4.64	1.31	1.42
41	2	1524	A2M	O4'-C1'	-4.62	1.31	1.42
41	2	3723	A2M	O4'-C1'	-4.61	1.31	1.42
41	2	1534	A2M	O4'-C1'	-4.61	1.31	1.42
41	2	2804	OMC	C4-N3	4.60	1.43	1.34
41	2	3899	BGH	C5-N7	4.60	1.47	1.39
41	2	3825	A2M	C6-N6	4.59	1.45	1.34
41	2	3718	A2M	C6-N6	4.58	1.45	1.34
41	2	1326	A2M	O4'-C1'	-4.57	1.31	1.42
41	2	4671	B8T	C2-N1	4.56	1.49	1.40
41	2	4083	5MU	C2-N3	4.56	1.46	1.38
41	2	4523	A2M	C6-N6	4.55	1.45	1.34
41	2	3867	A2M	C6-N6	4.53	1.45	1.34
41	2	398	A2M	O4'-C1'	-4.52	1.31	1.42
41	2	398	A2M	C6-N6	4.52	1.45	1.34
41	2	2401	A2M	C6-N6	4.52	1.45	1.34
41	2	3867	A2M	O4'-C1'	-4.51	1.31	1.42
41	2	1524	A2M	C6-N6	4.50	1.45	1.34
41	2	1534	A2M	C6-N6	4.49	1.45	1.34
41	2	1348	P4U	O4-C4	4.48	1.40	1.35
41	2	3825	A2M	O4'-C1'	-4.47	1.31	1.42
41	2	1326	A2M	C6-N6	4.46	1.45	1.34
41	2	3897	B8K	C4-N3	4.46	1.44	1.34
41	2	4571	A2M	C6-N6	4.45	1.45	1.34
41	2	3723	A2M	C6-N6	4.44	1.45	1.34
41	2	3718	A2M	O4'-C1'	-4.42	1.31	1.42
41	2	1322	1MA	C5-C6	4.42	1.55	1.43
41	2	4690	B8K	C4-N3	4.41	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	4415	1MA	C5-C6	4.40	1.55	1.43
41	2	2363	A2M	C6-N6	4.39	1.45	1.34
41	2	2365	OMC	C2-N1	4.36	1.49	1.40
41	2	3701	OMC	C2-N1	4.35	1.49	1.40
41	2	3897	B8K	C5-C6	4.32	1.54	1.43
41	2	4564	M7A	C6-N6	4.32	1.45	1.34
41	2	4194	I4U	C2-N1	4.30	1.49	1.40
41	2	3899	BGH	C5-C6	4.29	1.54	1.43
41	2	1322	1MA	C2-N1	4.25	1.43	1.35
41	2	3897	B8K	C5-N7	4.22	1.46	1.39
41	2	1348	P4U	C2-N1	4.19	1.49	1.40
41	2	729	2MG	C2-N1	4.18	1.43	1.36
41	2	1659	I4U	C2-N1	4.16	1.49	1.40
41	2	4690	B8K	C5-N7	4.16	1.46	1.39
4	8	14	OMU	C4-N3	4.15	1.46	1.38
41	2	978	2MG	C2-N1	4.13	1.43	1.36
41	2	4415	1MA	C2-N1	4.07	1.43	1.35
41	2	4690	B8K	C5-C6	4.05	1.54	1.43
41	2	4564	M7A	C5-N7	4.03	1.49	1.39
41	2	4637	OMG	C5-N7	-4.02	1.31	1.39
41	2	4620	OMU	C4-N3	4.01	1.45	1.38
41	2	1517	2MG	C2-N1	3.98	1.43	1.36
41	2	4872	2MG	C2-N1	3.97	1.43	1.36
41	2	1348	P4U	C5-C4	3.95	1.48	1.43
41	2	2050	OMG	C5-N7	-3.94	1.31	1.39
41	2	1316	OMG	C5-N7	-3.91	1.31	1.39
41	2	1522	OMG	C5-N7	-3.89	1.31	1.39
41	2	2773	OMG	C5-N7	-3.89	1.31	1.39
41	2	4371	MHG	C5-C6	3.87	1.53	1.43
41	2	2424	OMG	C5-N7	-3.86	1.31	1.39
41	2	4671	B8T	C5-C4	3.84	1.49	1.40
41	2	2364	OMG	C5-N7	-3.83	1.31	1.39
41	2	1883	OMG	C5-N7	-3.82	1.31	1.39
41	2	4550	7MG	C5-C6	3.81	1.53	1.43
41	2	1625	OMG	C5-N7	-3.80	1.31	1.39
41	2	4494	OMG	C5-N7	-3.77	1.31	1.39
41	2	1605	7MG	C5-C6	3.76	1.53	1.43
41	2	2297	E7G	C5-C6	3.76	1.53	1.43
41	2	373	OMG	C5-N7	-3.71	1.31	1.39
41	2	3899	BGH	O2'-C2'	3.71	1.52	1.42
41	2	2522	7MG	C5-C6	3.71	1.53	1.43
41	2	3880	P7G	C6-N1	3.71	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	3899	BGH	C71-N7	3.70	1.47	1.39
41	2	4196	OMG	C5-N7	-3.69	1.31	1.39
41	2	4623	OMG	C5-N7	-3.66	1.32	1.39
41	2	3880	P7G	C2-N3	3.64	1.46	1.37
41	2	1909	P7G	C2-N3	3.63	1.46	1.37
41	2	1605	7MG	C2-N1	3.63	1.46	1.37
41	2	4483	B8T	C5-C4	3.63	1.48	1.40
41	2	4870	OMG	C5-N7	-3.63	1.32	1.39
41	2	4550	7MG	C2-N1	3.62	1.46	1.37
41	2	3897	B8K	C6-N1	3.60	1.45	1.38
41	2	4370	OMG	C5-N7	-3.59	1.32	1.39
41	2	4690	B8K	C71-N7	3.57	1.47	1.39
41	2	3897	B8K	C2-N2	3.56	1.42	1.34
41	2	2522	7MG	C2-N1	3.53	1.46	1.37
41	2	4690	B8K	C6-N1	3.51	1.45	1.38
41	2	1883	OMG	O6-C6	-3.51	1.16	1.23
41	2	4690	B8K	C2-N2	3.49	1.42	1.34
41	2	2297	E7G	C2-N1	3.48	1.46	1.37
41	2	3897	B8K	C71-N7	3.47	1.47	1.39
41	2	1909	P7G	C6-N1	3.47	1.44	1.38
41	2	237	B9B	O6-C6	3.46	1.40	1.35
41	2	4371	MHG	C6-N1	3.45	1.45	1.38
41	2	4550	7MG	C6-N1	3.43	1.45	1.38
41	2	4483	B8T	C6-N1	3.42	1.46	1.38
41	2	1574	B9B	O6-C6	3.41	1.40	1.35
41	2	4530	UR3	C6-N1	3.41	1.46	1.38
41	2	3899	BGH	C6-N1	3.40	1.45	1.38
41	2	3899	BGH	C2-N1	3.40	1.46	1.37
41	2	4194	I4U	C6-N1	3.39	1.46	1.38
41	2	3887	OMC	C6-N1	3.39	1.46	1.38
41	2	3869	OMC	C6-N1	3.37	1.46	1.38
41	2	1605	7MG	C6-N1	3.37	1.45	1.38
41	2	3897	B8K	C2-N1	3.34	1.45	1.37
41	2	3880	P7G	C5-C4	3.30	1.43	1.37
41	2	4536	OMC	C6-N1	3.29	1.45	1.38
41	2	373	OMG	C6-N1	3.28	1.44	1.38
41	2	4690	B8K	C2-N1	3.27	1.45	1.37
41	2	4494	OMG	C6-N1	3.25	1.44	1.38
41	2	2297	E7G	C6-N1	3.25	1.44	1.38
41	2	2522	7MG	C6-N1	3.23	1.44	1.38
41	2	4083	5MU	C2-N1	3.22	1.43	1.38
41	2	4355	E6G	C5-C4	-3.22	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	2422	OMC	C6-N1	3.21	1.45	1.38
41	2	4623	OMG	C6-N1	3.20	1.44	1.38
41	2	4196	OMG	C6-N1	3.19	1.44	1.38
41	2	1522	OMG	O6-C6	-3.19	1.17	1.23
41	2	1659	I4U	C6-N1	3.19	1.45	1.38
41	2	4370	OMG	O6-C6	-3.19	1.17	1.23
41	2	2380	B8W	C5-N7	-3.18	1.33	1.39
41	2	1316	OMG	O6-C6	-3.18	1.17	1.23
41	2	3701	OMC	C6-N1	3.17	1.45	1.38
41	2	1348	P4U	C6-N1	3.17	1.45	1.38
41	2	2424	OMG	O6-C6	-3.15	1.17	1.23
41	2	4623	OMG	O6-C6	-3.15	1.17	1.23
41	2	2050	OMG	O6-C6	-3.15	1.17	1.23
41	2	2364	OMG	O6-C6	-3.15	1.17	1.23
41	2	2364	OMG	C6-N1	3.15	1.44	1.38
41	2	373	OMG	O6-C6	-3.15	1.17	1.23
41	2	1909	P7G	C5-C4	3.15	1.43	1.37
41	2	1909	P7G	O6-C6	-3.14	1.18	1.23
41	2	2804	OMC	C6-N1	3.14	1.45	1.38
41	2	1316	OMG	C6-N1	3.13	1.44	1.38
41	2	4597	UR3	C6-N1	3.13	1.45	1.38
41	2	4870	OMG	O6-C6	-3.12	1.17	1.23
41	2	4637	OMG	O6-C6	-3.12	1.17	1.23
41	2	4671	B8T	C6-N1	3.12	1.45	1.38
41	2	1517	2MG	C5-N7	-3.12	1.33	1.39
41	2	1625	OMG	C6-N1	3.11	1.44	1.38
41	2	2365	OMC	C6-N1	3.10	1.45	1.38
41	2	3880	P7G	O6-C6	-3.09	1.18	1.23
41	2	4870	OMG	C6-N1	3.09	1.44	1.38
41	2	4370	OMG	C6-N1	3.08	1.44	1.38
41	2	2050	OMG	C6-N1	3.07	1.44	1.38
41	2	4637	OMG	C6-N1	3.07	1.44	1.38
41	2	4194	I4U	O4-C41	-3.06	1.40	1.47
41	2	3718	A2M	O3'-C3'	3.05	1.50	1.43
41	2	4083	5MU	O4-C4	-3.05	1.17	1.23
41	2	1625	OMG	O6-C6	-3.04	1.17	1.23
4	8	14	OMU	O4-C4	-3.04	1.18	1.24
41	2	1883	OMG	C6-N1	3.04	1.44	1.38
41	2	2773	OMG	C6-N1	3.03	1.44	1.38
41	2	2380	B8W	C5-C4	-3.02	1.33	1.39
41	2	729	2MG	C5-N7	-3.01	1.33	1.39
41	2	237	B9B	C5-C4	-3.01	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	2424	OMG	C6-N1	3.01	1.44	1.38
41	2	4872	2MG	C5-N7	-3.00	1.33	1.39
41	2	4671	B8T	O2-C2	-2.98	1.18	1.23
41	2	4529	B8W	C5-N7	-2.96	1.33	1.39
41	2	4494	OMG	O6-C6	-2.95	1.18	1.23
41	2	3825	A2M	O3'-C3'	2.95	1.49	1.43
41	2	3899	BGH	O3'-C3'	-2.94	1.36	1.43
41	2	2773	OMG	O6-C6	-2.93	1.18	1.23
41	2	3897	B8K	C5-C4	2.93	1.47	1.38
41	2	2401	A2M	O3'-C3'	2.93	1.49	1.43
41	2	4620	OMU	O4-C4	-2.92	1.18	1.24
41	2	1534	A2M	O3'-C3'	2.92	1.49	1.43
41	2	2401	A2M	C5-C4	-2.91	1.33	1.39
41	2	3723	A2M	O3'-C3'	2.91	1.49	1.43
41	2	4472	B8W	C5-C4	-2.91	1.33	1.39
41	2	4196	OMG	O6-C6	-2.91	1.18	1.23
41	2	2363	A2M	O3'-C3'	2.90	1.49	1.43
41	2	4690	B8K	C5-C4	2.89	1.47	1.38
41	2	1524	A2M	O3'-C3'	2.89	1.49	1.43
41	2	4523	A2M	O3'-C3'	2.87	1.49	1.43
41	2	1522	OMG	C6-N1	2.87	1.44	1.38
41	2	237	B9B	C5-N7	-2.87	1.33	1.39
41	2	4185	B8W	C5-N7	-2.86	1.33	1.39
41	2	398	A2M	O3'-C3'	2.85	1.49	1.43
41	2	978	2MG	C5-N7	-2.85	1.33	1.39
41	2	1659	I4U	O4-C4	2.84	1.41	1.35
41	2	1348	P4U	O2-C2	-2.84	1.18	1.23
41	2	1574	B9B	C5-C4	-2.84	1.33	1.39
41	2	3867	A2M	O3'-C3'	2.84	1.49	1.43
41	2	4529	B8W	C5-C4	-2.83	1.33	1.39
41	2	2804	OMC	O2-C2	-2.80	1.18	1.23
41	2	3723	A2M	C5-C4	-2.80	1.33	1.39
41	2	4571	A2M	O3'-C3'	2.79	1.49	1.43
41	2	4472	B8W	C5-N7	-2.79	1.33	1.39
41	2	1534	A2M	O2'-C2'	-2.79	1.35	1.42
41	2	4185	B8W	C5-C4	-2.78	1.33	1.39
41	2	1326	A2M	O3'-C3'	2.78	1.49	1.43
41	2	2401	A2M	O2'-C2'	-2.78	1.35	1.42
41	2	2363	A2M	C5-C4	-2.77	1.33	1.39
41	2	2363	A2M	O2'-C2'	-2.77	1.35	1.42
41	2	2365	OMC	O2-C2	-2.77	1.18	1.23
41	2	1659	I4U	O2-C2	-2.76	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	978	2MG	C5-C6	2.75	1.54	1.44
41	2	3899	BGH	O6-C6	-2.73	1.18	1.23
4	8	14	OMU	C6-N1	2.73	1.44	1.38
41	2	1659	I4U	O4-C41	-2.71	1.40	1.47
41	2	398	A2M	C5-C4	-2.70	1.34	1.39
41	2	3701	OMC	O2-C2	-2.69	1.18	1.23
41	2	1534	A2M	C8-N9	-2.68	1.32	1.37
41	2	4220	6MZ	C5-N7	-2.67	1.34	1.39
41	2	4872	2MG	C5-C6	2.67	1.54	1.44
41	2	4483	B8T	O2-C2	-2.66	1.18	1.23
41	2	3701	OMC	C5-C4	2.66	1.49	1.42
41	2	4083	5MU	O2-C2	-2.66	1.18	1.23
41	2	2422	OMC	O2-C2	-2.64	1.18	1.23
41	2	4620	OMU	C6-N1	2.64	1.44	1.38
41	2	4571	A2M	C5-C4	-2.63	1.34	1.39
41	2	4571	A2M	C8-N9	-2.63	1.32	1.37
41	2	4536	OMC	O2-C2	-2.63	1.18	1.23
41	2	4370	OMG	C5-C6	2.63	1.54	1.44
41	2	1326	A2M	C5-C4	-2.62	1.34	1.39
41	2	729	2MG	C5-C6	2.62	1.54	1.44
41	2	4196	OMG	C5-C6	2.62	1.54	1.44
41	2	1625	OMG	C5-C6	2.62	1.54	1.44
41	2	4494	OMG	C5-C6	2.61	1.54	1.44
41	2	3867	A2M	O2'-C2'	-2.61	1.35	1.42
41	2	2773	OMG	C5-C6	2.61	1.54	1.44
41	2	398	A2M	O2'-C2'	-2.61	1.35	1.42
41	2	1574	B9B	C5-N7	-2.61	1.34	1.39
41	2	3869	OMC	O2-C2	-2.60	1.18	1.23
41	2	1517	2MG	C5-C6	2.60	1.54	1.44
41	2	4523	A2M	C5-C4	-2.59	1.34	1.39
41	2	1524	A2M	O2'-C2'	-2.59	1.36	1.42
41	2	3867	A2M	C5-C4	-2.59	1.34	1.39
41	2	4194	I4U	O2-C2	-2.58	1.18	1.23
41	2	2363	A2M	C8-N9	-2.57	1.32	1.37
41	2	3718	A2M	O2'-C2'	-2.57	1.36	1.42
41	2	3887	OMC	O2-C2	-2.56	1.19	1.23
41	2	1625	OMG	C2-N1	2.56	1.44	1.37
41	2	2773	OMG	C2-N1	2.56	1.44	1.37
41	2	2401	A2M	C8-N9	-2.56	1.32	1.37
41	2	1534	A2M	C5-C4	-2.55	1.34	1.39
41	2	1326	A2M	O2'-C2'	-2.55	1.36	1.42
41	2	4571	A2M	O2'-C2'	-2.54	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	1605	7MG	O6-C6	-2.54	1.18	1.23
41	2	4194	I4U	O4-C4	2.54	1.40	1.35
41	2	4637	OMG	C5-C6	2.53	1.53	1.44
41	2	4620	OMU	O2-C2	-2.53	1.18	1.23
41	2	4523	A2M	O2'-C2'	-2.53	1.36	1.42
41	2	4623	OMG	C5-C6	2.53	1.53	1.44
41	2	4870	OMG	C5-C6	2.52	1.53	1.44
41	2	4494	OMG	C2-N1	2.52	1.43	1.37
41	2	4196	OMG	C2-N1	2.52	1.43	1.37
41	2	4872	2MG	C4-N9	-2.52	1.31	1.38
41	2	3825	A2M	O2'-C2'	-2.51	1.36	1.42
41	2	2522	7MG	O6-C6	-2.51	1.18	1.23
41	2	3825	A2M	C5-C4	-2.51	1.34	1.39
41	2	3723	A2M	O2'-C2'	-2.50	1.36	1.42
41	2	1316	OMG	C5-C6	2.50	1.53	1.44
41	2	2364	OMG	C5-C6	2.50	1.53	1.44
41	2	2363	A2M	C5-N7	-2.50	1.34	1.39
41	2	4550	7MG	O6-C6	-2.49	1.18	1.23
41	2	2050	OMG	C5-C6	2.48	1.53	1.44
41	2	2297	E7G	O6-C6	-2.47	1.18	1.23
41	2	1524	A2M	C5-C4	-2.47	1.34	1.39
41	2	4571	A2M	C5-N7	-2.46	1.34	1.39
41	2	4220	6MZ	C5-C4	-2.46	1.34	1.39
41	2	398	A2M	C8-N9	-2.46	1.33	1.37
41	2	1522	OMG	C5-C6	2.46	1.53	1.44
41	2	4623	OMG	C2-N1	2.45	1.43	1.37
41	2	4370	OMG	C2-N1	2.45	1.43	1.37
41	2	2050	OMG	C2-N1	2.45	1.43	1.37
41	2	2424	OMG	C5-C6	2.45	1.53	1.44
41	2	373	OMG	C2-N1	2.44	1.43	1.37
41	2	4529	B8W	C8-N9	-2.44	1.33	1.37
41	2	1883	OMG	C2-N1	2.44	1.43	1.37
41	2	978	2MG	C6-N1	2.43	1.43	1.38
4	8	14	OMU	O2-C2	-2.43	1.18	1.23
41	2	2364	OMG	C2-N1	2.43	1.43	1.37
41	2	2424	OMG	C2-N1	2.42	1.43	1.37
41	2	373	OMG	C5-C6	2.42	1.53	1.44
41	2	4530	UR3	C4-N3	2.41	1.46	1.40
4	8	14	OMU	C5-C4	2.41	1.49	1.43
41	2	4870	OMG	C2-N1	2.40	1.43	1.37
41	2	1316	OMG	C2-N1	2.38	1.43	1.37
41	2	3887	OMC	C5-C4	2.38	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	1522	OMG	C2-N1	2.38	1.43	1.37
41	2	3718	A2M	C5-N7	-2.37	1.34	1.39
41	2	4637	OMG	C2-N1	2.36	1.43	1.37
41	2	4523	A2M	C8-N9	-2.36	1.33	1.37
41	2	4872	2MG	C6-N1	2.34	1.43	1.38
41	2	237	B9B	C8-N9	-2.34	1.33	1.37
41	2	3723	A2M	C8-N9	-2.33	1.33	1.37
41	2	3825	A2M	C8-N9	-2.33	1.33	1.37
41	2	3718	A2M	C5-C4	-2.33	1.34	1.39
41	2	729	2MG	C6-N1	2.33	1.43	1.38
41	2	2380	B8W	C8-N9	-2.33	1.33	1.37
41	2	1883	OMG	C5-C6	2.32	1.53	1.44
41	2	1524	A2M	C5-N7	-2.32	1.34	1.39
41	2	1326	A2M	C5-N7	-2.30	1.34	1.39
41	2	1524	A2M	C8-N9	-2.30	1.33	1.37
41	2	3867	A2M	C8-N9	-2.30	1.33	1.37
41	2	398	A2M	C5-N7	-2.29	1.34	1.39
41	2	2401	A2M	C5-N7	-2.28	1.34	1.39
41	2	1517	2MG	C6-N1	2.28	1.43	1.38
41	2	3825	A2M	C5-N7	-2.28	1.34	1.39
41	2	4530	UR3	C5-C4	2.27	1.49	1.43
41	2	3867	A2M	C5-N7	-2.27	1.34	1.39
41	2	1456	B8Q	C6-N1	2.27	1.43	1.38
41	2	4597	UR3	C4-N3	2.26	1.45	1.40
41	2	4536	OMC	C5-C4	2.25	1.48	1.42
41	2	4597	UR3	C5-C4	2.25	1.49	1.43
41	2	2422	OMC	C5-C4	2.25	1.48	1.42
41	2	3718	A2M	C8-N9	-2.25	1.33	1.37
41	2	2365	OMC	C5-C4	2.24	1.48	1.42
41	2	4371	MHG	O6-C6	-2.23	1.19	1.23
41	2	4472	B8W	C4-N3	2.22	1.37	1.34
41	2	1326	A2M	C8-N9	-2.21	1.33	1.37
41	2	4620	OMU	C5-C4	2.20	1.48	1.43
41	2	1534	A2M	C5-N7	-2.19	1.34	1.39
41	2	1517	2MG	O6-C6	-2.18	1.19	1.23
41	2	3723	A2M	C5-N7	-2.16	1.34	1.39
41	2	237	B9B	C5-C6	-2.15	1.37	1.41
41	2	2401	A2M	C4-N9	-2.15	1.32	1.37
41	2	3899	BGH	C5-C4	2.13	1.45	1.38
41	2	4523	A2M	C5-N7	-2.12	1.35	1.39
41	2	4872	2MG	O6-C6	-2.11	1.19	1.23
41	2	4355	E6G	C8-N9	-2.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	1456	B8Q	O2-C2	-2.10	1.18	1.22
41	2	4185	B8W	C4-N3	2.10	1.36	1.34
41	2	4597	UR3	O2-C2	-2.10	1.18	1.22
41	2	3869	OMC	C5-C4	2.09	1.47	1.42
41	2	4371	MHG	C5-C4	2.08	1.44	1.38
41	2	1574	B9B	C8-N9	-2.07	1.33	1.37
41	2	2786	B9H	C6-N1	2.06	1.43	1.38
41	2	4472	B8W	C8-N9	-2.06	1.33	1.37
41	2	1574	B9B	C5-C6	-2.06	1.37	1.41
41	2	4415	1MA	CM1-N1	2.06	1.50	1.46
41	2	2804	OMC	C5-C4	2.04	1.47	1.42
41	2	4185	B8W	C8-N9	-2.04	1.33	1.37
41	2	4529	B8W	C4-N3	2.03	1.36	1.34
41	2	729	2MG	O6-C6	-2.03	1.19	1.23
41	2	1322	1MA	CM1-N1	2.02	1.50	1.46
41	2	373	OMG	C4-N9	-2.01	1.32	1.38

All (597) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	1574	B9B	O6-C6-C5	21.73	144.09	116.57
41	2	237	B9B	O6-C6-C5	21.48	143.77	116.57
41	2	1574	B9B	O6-C6-N1	-18.66	94.01	120.00
41	2	237	B9B	O6-C6-N1	-18.47	94.27	120.00
41	2	4564	M7A	C5-C6-N6	13.81	147.33	123.74
41	2	4564	M7A	N6-C6-N1	-11.85	92.41	118.35
41	2	4083	5MU	C5-C4-N3	10.78	124.51	115.31
41	2	4196	OMG	C1'-N9-C8	-10.22	97.60	126.70
41	2	4196	OMG	C1'-N9-C4	10.21	156.84	126.50
41	2	4870	OMG	C1'-N9-C8	-10.09	97.97	126.70
41	2	4870	OMG	C1'-N9-C4	9.72	155.38	126.50
41	2	4220	6MZ	C1'-N9-C8	9.28	148.09	127.14
41	2	4220	6MZ	C4-N9-C1'	-9.25	104.56	126.59
41	2	2424	OMG	C1'-N9-C4	8.98	153.18	126.50
41	2	2773	OMG	C1'-N9-C4	8.97	153.16	126.50
41	2	4370	OMG	C1'-N9-C4	8.90	152.92	126.50
41	2	4370	OMG	C1'-N9-C8	-8.87	101.45	126.70
41	2	2424	OMG	C1'-N9-C8	-8.85	101.52	126.70
41	2	1625	OMG	C1'-N9-C4	8.76	152.52	126.50
41	2	4494	OMG	C1'-N9-C4	8.73	152.44	126.50
41	2	1522	OMG	C1'-N9-C4	8.59	152.03	126.50
41	2	4637	OMG	C1'-N9-C4	8.52	151.80	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	2773	OMG	C1'-N9-C8	-8.51	102.47	126.70
41	2	1522	OMG	C1'-N9-C8	-8.48	102.55	126.70
41	2	4494	OMG	C1'-N9-C8	-8.45	102.63	126.70
41	2	4623	OMG	C1'-N9-C4	8.36	151.35	126.50
41	2	4623	OMG	C1'-N9-C8	-8.36	102.91	126.70
41	2	2050	OMG	C1'-N9-C4	8.35	151.29	126.50
41	2	1625	OMG	C1'-N9-C8	-8.28	103.14	126.70
41	2	1316	OMG	C1'-N9-C4	8.26	151.05	126.50
41	2	2364	OMG	C1'-N9-C4	8.25	151.00	126.50
41	2	4637	OMG	C1'-N9-C8	-8.17	103.45	126.70
41	2	2050	OMG	C1'-N9-C8	-8.07	103.72	126.70
41	2	2786	B9H	C31-N3-C2	8.05	127.27	117.21
41	2	1316	OMG	C1'-N9-C8	-8.03	103.84	126.70
41	2	4083	5MU	C5-C6-N1	-8.02	115.09	123.34
41	2	1883	OMG	C1'-N9-C4	7.99	150.24	126.50
41	2	2364	OMG	C1'-N9-C8	-7.95	104.06	126.70
41	2	1883	OMG	C1'-N9-C8	-7.93	104.13	126.70
41	2	373	OMG	C1'-N9-C4	7.77	149.58	126.50
41	2	373	OMG	C1'-N9-C8	-7.75	104.63	126.70
41	2	4597	UR3	C4-N3-C2	-7.63	117.38	124.56
41	2	1534	A2M	N6-C6-N1	-7.24	102.49	118.35
41	2	1517	2MG	C2-N3-C4	7.23	121.00	112.04
41	2	4083	5MU	C4-N3-C2	-7.18	118.05	127.35
41	2	398	A2M	N6-C6-N1	-7.01	103.00	118.35
41	2	4185	B8W	C5-C4-N3	-7.00	119.32	127.19
41	2	4472	B8W	C5-C4-N3	-6.95	119.37	127.19
41	2	1326	A2M	N6-C6-N1	-6.92	103.19	118.35
41	2	3723	A2M	N6-C6-N1	-6.86	103.32	118.35
41	2	3867	A2M	N6-C6-N1	-6.84	103.36	118.35
41	2	4371	MHG	C2-N3-C4	6.82	120.49	112.04
41	2	1524	A2M	N6-C6-N1	-6.79	103.48	118.35
41	2	2363	A2M	N6-C6-N1	-6.78	103.49	118.35
41	2	3718	A2M	N6-C6-N1	-6.75	103.56	118.35
41	2	4355	E6G	N2-C2-N3	6.74	127.74	117.25
41	2	4529	B8W	C5-C4-N3	-6.73	119.62	127.19
41	2	3825	A2M	N6-C6-N1	-6.71	103.66	118.35
41	2	729	2MG	C2-N3-C4	6.70	120.35	112.04
41	2	237	B9B	C5-C4-N3	-6.70	119.66	127.19
41	2	4523	A2M	N6-C6-N1	-6.67	103.73	118.35
41	2	2380	B8W	C5-C4-N3	-6.67	119.68	127.19
41	2	978	2MG	C2-N3-C4	6.67	120.31	112.04
41	2	2401	A2M	N6-C6-N1	-6.66	103.76	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	4571	A2M	N6-C6-N1	-6.64	103.81	118.35
41	2	4690	B8K	C72-C71-N7	6.64	128.84	118.86
41	2	1574	B9B	C5-C4-N3	-6.56	119.81	127.19
41	2	4355	E6G	C5-C4-N3	-6.43	119.95	127.19
41	2	4472	B8W	N2-C2-N3	6.43	127.25	117.25
41	2	1326	A2M	N3-C2-N1	-6.43	118.55	128.60
41	2	2401	A2M	N3-C2-N1	-6.37	118.63	128.60
41	2	4529	B8W	N2-C2-N3	6.35	127.14	117.25
41	2	2786	B9H	C6-N1-C2	-6.35	116.10	121.79
41	2	4185	B8W	N2-C2-N3	6.34	127.12	117.25
41	2	4220	6MZ	N1-C2-N3	-6.34	118.68	128.60
41	2	1524	A2M	N3-C2-N1	-6.34	118.69	128.60
41	2	3899	BGH	C72-C71-N7	6.31	128.35	118.86
41	2	3723	A2M	N3-C2-N1	-6.29	118.77	128.60
41	2	2380	B8W	N2-C2-N3	6.28	127.02	117.25
41	2	398	A2M	N3-C2-N1	-6.26	118.81	128.60
41	2	2401	A2M	N9-C8-N7	-6.25	105.36	113.91
41	2	4523	A2M	N3-C2-N1	-6.24	118.84	128.60
41	2	2363	A2M	N3-C2-N1	-6.22	118.88	128.60
41	2	3867	A2M	N3-C2-N1	-6.22	118.88	128.60
41	2	3723	A2M	N9-C8-N7	-6.22	105.41	113.91
41	2	4571	A2M	N3-C2-N1	-6.21	118.89	128.60
41	2	1517	2MG	C5-C4-N3	-6.21	118.39	128.46
41	2	3825	A2M	N3-C2-N1	-6.19	118.91	128.60
41	2	4872	2MG	C2-N3-C4	6.17	119.68	112.04
41	2	4220	6MZ	C5-C4-N3	-6.16	118.71	126.75
41	2	1534	A2M	C5-C6-N6	6.14	136.79	123.43
41	2	3897	B8K	C72-C71-N7	6.12	128.06	118.86
41	2	4523	A2M	N9-C8-N7	-6.11	105.55	113.91
41	2	398	A2M	C5-C6-N6	6.05	136.59	123.43
41	2	4564	M7A	N3-C2-N1	-6.03	119.16	128.60
41	2	1326	A2M	C5-C6-N6	6.03	136.54	123.43
41	2	1534	A2M	N3-C2-N1	-5.99	119.23	128.60
41	2	4690	B8K	C5-C6-N1	5.92	121.42	110.99
41	2	398	A2M	N9-C8-N7	-5.92	105.82	113.91
41	2	4355	E6G	O6-C6-N1	5.89	128.20	120.00
41	2	3867	A2M	N9-C8-N7	-5.88	105.87	113.91
41	2	3723	A2M	C5-C6-N6	5.86	136.19	123.43
41	2	1524	A2M	C5-C6-N6	5.85	136.16	123.43
41	2	3867	A2M	C5-C6-N6	5.85	136.15	123.43
41	2	1326	A2M	N9-C8-N7	-5.84	105.92	113.91
41	2	3718	A2M	C5-C6-N6	5.84	136.15	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	729	2MG	C5-C4-N3	-5.84	118.99	128.46
41	2	3825	A2M	C5-C6-N6	5.80	136.05	123.43
41	2	3899	BGH	C5-C6-N1	5.80	121.20	110.99
41	2	3718	A2M	N3-C2-N1	-5.78	119.55	128.60
41	2	2363	A2M	N9-C8-N7	-5.73	106.07	113.91
41	2	4571	A2M	C5-C6-N6	5.73	135.91	123.43
41	2	4523	A2M	C5-C6-N6	5.73	135.89	123.43
41	2	2363	A2M	C5-C6-N6	5.73	135.89	123.43
41	2	2401	A2M	C5-C6-N6	5.71	135.86	123.43
41	2	2401	A2M	C4-N9-C8	5.71	111.91	105.73
41	2	3825	A2M	N9-C8-N7	-5.69	106.13	113.91
41	2	1534	A2M	N9-C8-N7	-5.69	106.13	113.91
41	2	4571	A2M	N9-C8-N7	-5.65	106.19	113.91
41	2	1524	A2M	N9-C8-N7	-5.64	106.20	113.91
41	2	1625	OMG	C5-C4-N3	-5.59	119.40	128.46
41	2	3897	B8K	C5-C6-N1	5.55	120.78	110.99
41	2	1456	B8Q	N3-C2-N1	5.55	123.66	117.13
41	2	978	2MG	C5-C4-N3	-5.53	119.49	128.46
41	2	3723	A2M	C4-N9-C8	5.53	111.72	105.73
41	2	4196	OMG	C5-C4-N3	-5.52	119.50	128.46
41	2	4523	A2M	C4-N9-C8	5.44	111.63	105.73
4	8	14	OMU	C4-N3-C2	-5.41	119.44	126.58
41	2	4637	OMG	C5-C4-N3	-5.37	119.76	128.46
41	2	4872	2MG	C5-C4-N3	-5.36	119.76	128.46
41	2	4872	2MG	C2-N1-C6	-5.36	118.31	124.48
41	2	3718	A2M	N9-C8-N7	-5.33	106.62	113.91
41	2	2773	OMG	C5-C4-N3	-5.33	119.82	128.46
41	2	1909	P7G	C4-C5-N7	5.31	109.47	106.67
41	2	4370	OMG	C5-C4-N3	-5.28	119.90	128.46
41	2	4494	OMG	C5-C4-N3	-5.27	119.92	128.46
41	2	4529	B8W	O6-C6-N1	5.26	126.27	119.01
41	2	2424	OMG	C5-C4-N3	-5.19	120.03	128.46
41	2	2297	E7G	C5-C6-N1	5.16	120.08	110.99
41	2	2297	E7G	C4-C5-N7	5.15	109.50	104.91
41	2	398	A2M	C4-N9-C8	5.13	111.29	105.73
41	2	1316	OMG	C5-C4-N3	-5.09	120.20	128.46
41	2	1534	A2M	C4-N9-C8	5.07	111.22	105.73
41	2	3867	A2M	C4-N9-C8	5.07	111.22	105.73
41	2	1326	A2M	C4-N9-C8	5.05	111.20	105.73
41	2	4415	1MA	C5-C4-N3	-5.04	119.75	127.26
41	2	4571	A2M	C4-N9-C8	5.03	111.18	105.73
41	2	4870	OMG	C5-C4-N3	-5.03	120.30	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	1574	B9B	N2-C2-N3	5.03	125.07	117.25
41	2	3899	BGH	C2-N3-C4	5.01	121.23	112.30
41	2	4371	MHG	C5-C6-N1	5.00	119.81	110.99
41	2	1456	B8Q	C31-N3-C4	5.00	121.79	114.25
41	2	2363	A2M	C4-N9-C8	5.00	111.14	105.73
41	2	4564	M7A	N3-C4-N9	4.99	133.18	126.87
41	2	4185	B8W	O6-C6-N1	4.99	125.90	119.01
41	2	4415	1MA	N1-C2-N3	-4.99	120.07	126.00
41	2	1456	B8Q	O2-C2-N3	-4.96	115.66	122.95
41	2	1883	OMG	C5-C4-N3	-4.96	120.42	128.46
41	2	1524	A2M	C4-N9-C8	4.94	111.08	105.73
41	2	4620	OMU	C4-N3-C2	-4.94	120.06	126.58
41	2	237	B9B	N2-C2-N3	4.92	124.91	117.25
41	2	1322	1MA	C5-C4-N3	-4.90	119.95	127.26
41	2	3825	A2M	C4-N9-C8	4.88	111.02	105.73
41	2	1605	7MG	C5-C6-N1	4.88	119.59	110.99
41	2	1517	2MG	C2-N1-C6	-4.88	118.87	124.48
41	2	2522	7MG	C5-C6-N1	4.87	119.58	110.99
41	2	2050	OMG	C5-C4-N3	-4.87	120.56	128.46
41	2	2364	OMG	C5-C4-N3	-4.87	120.56	128.46
41	2	4371	MHG	C4-C5-N7	4.85	109.23	104.91
41	2	1522	OMG	C5-C4-N3	-4.82	120.64	128.46
41	2	4550	7MG	C5-C6-N1	4.80	119.46	110.99
41	2	3867	A2M	C5-C4-N3	-4.79	120.50	126.75
41	2	4690	B8K	C2-N3-C4	4.78	120.81	112.30
41	2	3897	B8K	C2-N3-C4	4.77	120.80	112.30
41	2	1524	A2M	C5-C4-N3	-4.75	120.55	126.75
41	2	4083	5MU	O4-C4-C5	-4.75	119.40	124.90
41	2	2363	A2M	C5-C4-N3	-4.71	120.60	126.75
41	2	1322	1MA	N1-C2-N3	-4.71	120.40	126.00
41	2	4472	B8W	O6-C6-N1	4.71	125.51	119.01
41	2	1534	A2M	C5-C4-N3	-4.70	120.61	126.75
41	2	3718	A2M	C5-C4-N3	-4.70	120.62	126.75
41	2	2297	E7G	C2-N3-C4	4.69	120.66	112.30
41	2	4370	OMG	C2-N3-C4	4.63	120.54	112.30
41	2	4690	B8K	C4-C5-N7	4.63	109.03	104.91
41	2	4530	UR3	C4-N3-C2	-4.62	120.21	124.56
41	2	3880	P7G	C4-C5-N7	4.61	109.10	106.67
41	2	3718	A2M	C4-N9-C8	4.60	110.71	105.73
41	2	4637	OMG	C2-N3-C4	4.57	120.45	112.30
41	2	4185	B8W	N3-C4-N9	4.57	133.33	126.99
41	2	4523	A2M	C5-C4-N3	-4.57	120.79	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	1316	OMG	C2-N3-C4	4.57	120.44	112.30
41	2	4083	5MU	C5M-C5-C6	-4.57	116.75	122.85
41	2	4472	B8W	N3-C4-N9	4.56	133.32	126.99
41	2	4196	OMG	C2-N3-C4	4.56	120.42	112.30
41	2	373	OMG	C5-C4-N3	-4.55	121.08	128.46
41	2	729	2MG	C2-N1-C6	-4.55	119.25	124.48
41	2	4494	OMG	C2-N3-C4	4.54	120.38	112.30
41	2	978	2MG	C2-N1-C6	-4.53	119.26	124.48
41	2	1625	OMG	C2-N3-C4	4.52	120.35	112.30
41	2	2380	B8W	O6-C6-N1	4.52	125.24	119.01
41	2	4623	OMG	C5-C4-N3	-4.51	121.15	128.46
41	2	4872	2MG	CM2-N2-C2	-4.50	113.91	123.86
41	2	3825	A2M	C5-C4-N3	-4.49	120.89	126.75
41	2	3867	A2M	C1'-N9-C8	-4.49	117.00	127.14
41	2	1883	OMG	C2-N3-C4	4.47	120.26	112.30
41	2	1524	A2M	C1'-N9-C8	-4.47	117.05	127.14
41	2	2424	OMG	C2-N3-C4	4.44	120.21	112.30
41	2	4571	A2M	C5-C4-N3	-4.43	120.97	126.75
41	2	4870	OMG	C2-N3-C4	4.42	120.18	112.30
41	2	4083	5MU	N3-C2-N1	4.38	120.71	114.89
41	2	2364	OMG	C2-N3-C4	4.37	120.09	112.30
41	2	4220	6MZ	C2-N3-C4	4.37	122.07	111.75
41	2	2363	A2M	C1'-N9-C8	-4.37	117.27	127.14
41	2	398	A2M	C5-C4-N3	-4.36	121.06	126.75
41	2	4355	E6G	N9-C8-N7	-4.36	107.95	113.91
41	2	3869	OMC	O2-C2-N3	-4.36	115.24	122.33
41	2	1534	A2M	C1'-N9-C8	-4.36	117.30	127.14
41	2	1659	I4U	C5-C4-N3	-4.35	118.29	124.91
41	2	2050	OMG	C2-N3-C4	4.34	120.04	112.30
41	2	1574	B9B	N9-C8-N7	-4.34	107.97	113.91
41	2	373	OMG	C2-N3-C4	4.34	120.03	112.30
41	2	1456	B8Q	C6-N1-C2	-4.33	117.91	121.79
41	2	2773	OMG	C2-N3-C4	4.33	120.01	112.30
41	2	1517	2MG	N9-C4-N3	4.32	134.61	125.94
41	2	4472	B8W	N9-C8-N7	-4.30	108.03	113.91
41	2	1326	A2M	C5-C4-N3	-4.30	121.14	126.75
41	2	237	B9B	N3-C4-N9	4.29	132.94	126.99
41	2	2522	7MG	C2-N3-C4	4.29	119.94	112.30
41	2	3899	BGH	C4-C5-N7	4.28	108.72	104.91
41	2	1522	OMG	C2-N3-C4	4.26	119.88	112.30
41	2	4690	B8K	N9-C8-N7	4.24	109.03	103.33
41	2	1605	7MG	C2-N3-C4	4.24	119.85	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	4623	OMG	C2-N3-C4	4.23	119.84	112.30
41	2	4571	A2M	C1'-N9-C8	-4.23	117.58	127.14
41	2	4550	7MG	C2-N3-C4	4.23	119.83	112.30
41	2	1524	A2M	N3-C4-N9	4.20	134.00	127.08
41	2	2380	B8W	N3-C4-N9	4.18	132.79	126.99
41	2	3723	A2M	C5-C4-N3	-4.18	121.30	126.75
41	2	4415	1MA	C2-N3-C4	4.17	120.60	112.41
41	2	3899	BGH	C5-C4-N9	4.14	111.72	106.35
41	2	3899	BGH	N9-C8-N7	4.12	108.86	103.33
41	2	2401	A2M	C5-C4-N3	-4.12	121.38	126.75
41	2	3867	A2M	N3-C4-N9	4.11	133.85	127.08
41	2	4220	6MZ	N3-C4-N9	4.10	133.85	127.08
41	2	2363	A2M	N3-C4-N9	4.10	133.84	127.08
41	2	3897	B8K	C5-C4-N9	4.10	111.67	106.35
41	2	237	B9B	N9-C8-N7	-4.07	108.35	113.91
41	2	3718	A2M	N3-C4-N9	4.07	133.78	127.08
41	2	4523	A2M	C1'-N9-C8	-4.07	117.95	127.14
41	2	2380	B8W	N9-C8-N7	-4.05	108.38	113.91
41	2	4529	B8W	N3-C4-N9	4.04	132.59	126.99
41	2	1574	B9B	N3-C4-N9	4.02	132.57	126.99
41	2	4523	A2M	N3-C4-N9	4.01	133.70	127.08
41	2	1326	A2M	C1'-N9-C8	-4.01	118.08	127.14
41	2	1534	A2M	N3-C4-N9	4.01	133.69	127.08
41	2	3718	A2M	C1'-N9-C8	-3.98	118.16	127.14
41	2	4690	B8K	C5-C4-N9	3.98	111.51	106.35
41	2	4185	B8W	N9-C8-N7	-3.95	108.51	113.91
41	2	1322	1MA	C2-N3-C4	3.94	120.15	112.41
41	2	1605	7MG	C5-C4-N9	3.91	111.42	106.35
41	2	2297	E7G	C5-C4-N3	-3.90	120.71	128.13
41	2	2804	OMC	O2-C2-N3	-3.89	116.00	122.33
41	2	4620	OMU	N3-C2-N1	3.89	120.05	114.89
41	2	3897	B8K	C4-C5-N7	3.88	108.36	104.91
41	2	4083	5MU	C5M-C5-C4	3.88	123.04	118.77
41	2	4571	A2M	N3-C4-N9	3.87	133.46	127.08
41	2	729	2MG	N9-C4-N3	3.87	133.70	125.94
41	2	398	A2M	C1'-N9-C8	-3.85	118.44	127.14
41	2	2786	B9H	O3'-C3'-C2'	3.84	122.08	111.17
41	2	3825	A2M	N3-C4-N9	3.83	133.39	127.08
41	2	4371	MHG	C5-C4-N3	-3.80	120.88	128.13
41	2	3867	A2M	C2-N3-C4	3.78	120.68	111.75
41	2	3825	A2M	C1'-N9-C8	-3.76	118.65	127.14
41	2	4355	E6G	N3-C4-N9	3.72	132.15	126.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	398	A2M	N3-C4-N9	3.72	133.21	127.08
41	2	1326	A2M	N3-C4-N9	3.70	133.19	127.08
41	2	1524	A2M	C2-N3-C4	3.70	120.50	111.75
41	2	4355	E6G	O6-C6-C5	-3.70	111.88	116.57
41	2	3897	B8K	N9-C8-N7	3.70	108.30	103.33
41	2	2401	A2M	N3-C4-N9	3.70	133.17	127.08
41	2	3723	A2M	N3-C4-N9	3.69	133.16	127.08
41	2	4550	7MG	C5-C4-N9	3.68	111.12	106.35
41	2	2363	A2M	C2-N3-C4	3.67	120.41	111.75
41	2	2522	7MG	C5-C4-N9	3.66	111.10	106.35
41	2	4220	6MZ	N9-C8-N7	-3.66	108.91	113.91
41	2	4523	A2M	C2-N3-C4	3.65	120.38	111.75
4	8	14	OMU	C5-C4-N3	3.65	120.30	114.84
41	2	4523	A2M	C5-N7-C8	3.64	108.69	103.51
41	2	398	A2M	C2-N3-C4	3.63	120.32	111.75
41	2	1534	A2M	C2-N3-C4	3.62	120.31	111.75
41	2	3723	A2M	C1'-N9-C8	-3.61	118.98	127.14
41	2	2401	A2M	C1'-N9-C8	-3.61	118.98	127.14
41	2	1326	A2M	C2-N3-C4	3.61	120.28	111.75
41	2	237	B9B	N3-C2-N1	-3.60	119.77	125.42
41	2	3825	A2M	C2-N3-C4	3.59	120.23	111.75
41	2	3723	A2M	C5-N7-C8	3.58	108.59	103.51
41	2	3899	BGH	C5-C4-N3	-3.57	121.33	128.13
41	2	4571	A2M	C2-N3-C4	3.57	120.18	111.75
41	2	4564	M7A	C2-N3-C4	3.57	120.18	111.75
41	2	4355	E6G	N3-C2-N1	-3.56	119.84	125.42
4	8	14	OMU	N3-C2-N1	3.55	119.61	114.89
41	2	3723	A2M	C2-N3-C4	3.54	120.12	111.75
41	2	398	A2M	C5-N7-C8	3.54	108.53	103.51
41	2	1605	7MG	C5-C4-N3	-3.53	121.39	128.13
41	2	3867	A2M	C5-N7-C8	3.53	108.52	103.51
41	2	4472	B8W	N1-C2-N3	-3.51	119.91	125.42
41	2	978	2MG	N9-C4-N3	3.51	133.00	125.94
41	2	2401	A2M	C2-N3-C4	3.51	120.05	111.75
41	2	3718	A2M	C2-N3-C4	3.51	120.05	111.75
41	2	1574	B9B	N3-C2-N1	-3.51	119.92	125.42
41	2	1348	P4U	C5-C4-N3	-3.49	119.60	124.91
41	2	2401	A2M	C5-N7-C8	3.49	108.46	103.51
41	2	2522	7MG	C5-C4-N3	-3.47	121.51	128.13
41	2	1534	A2M	C5-N7-C8	3.45	108.42	103.51
41	2	3825	A2M	C5-N7-C8	3.44	108.39	103.51
41	2	2297	E7G	C5-C4-N9	3.44	110.81	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	1326	A2M	C5-N7-C8	3.42	108.36	103.51
41	2	4529	B8W	N1-C2-N3	-3.40	120.09	125.42
41	2	2363	A2M	C5-N7-C8	3.39	108.33	103.51
41	2	2422	OMC	O2-C2-N3	-3.37	116.85	122.33
41	2	4371	MHG	C5-C4-N9	3.35	110.70	106.35
41	2	1524	A2M	C5-N7-C8	3.35	108.27	103.51
41	2	4536	OMC	O2-C2-N3	-3.33	116.92	122.33
41	2	4194	I4U	C5-C4-N3	-3.33	119.85	124.91
41	2	4529	B8W	C4-N9-C1'	-3.33	118.67	126.59
41	2	1883	OMG	C2-N1-C6	-3.32	119.04	125.10
41	2	4185	B8W	N1-C2-N3	-3.32	120.21	125.42
41	2	4571	A2M	C5-N7-C8	3.31	108.21	103.51
41	2	4529	B8W	N9-C8-N7	-3.28	109.42	113.91
41	2	4550	7MG	C5-C4-N3	-3.28	121.88	128.13
41	2	1456	B8Q	C1'-N1-C2	3.27	122.51	116.99
41	2	4220	6MZ	C4-C5-C6	3.25	119.32	116.81
41	2	2364	OMG	C2-N1-C6	-3.24	119.20	125.10
41	2	1625	OMG	C2-N1-C6	-3.22	119.22	125.10
41	2	4637	OMG	C2-N1-C6	-3.22	119.23	125.10
41	2	3718	A2M	C5-N7-C8	3.22	108.08	103.51
41	2	2050	OMG	C2-N1-C6	-3.21	119.25	125.10
41	2	4690	B8K	C5-C4-N3	-3.21	122.02	128.13
41	2	4494	OMG	C2-N1-C6	-3.19	119.28	125.10
41	2	4690	B8K	C6-C5-C4	-3.19	116.05	122.62
41	2	2380	B8W	N1-C2-N3	-3.18	120.44	125.42
41	2	4529	B8W	C1'-N9-C8	3.17	134.30	127.14
41	2	4415	1MA	N9-C8-N7	-3.17	107.41	113.39
41	2	4370	OMG	C2-N1-C6	-3.16	119.33	125.10
41	2	3897	B8K	C6-C5-C4	-3.15	116.13	122.62
41	2	2424	OMG	C2-N1-C6	-3.15	119.36	125.10
41	2	4355	E6G	C5-N7-C8	3.15	107.98	103.51
41	2	1316	OMG	C2-N1-C6	-3.14	119.37	125.10
41	2	4371	MHG	C2-N1-C6	-3.13	120.88	124.48
41	2	3897	B8K	C5-C4-N3	-3.12	122.19	128.13
41	2	1322	1MA	N9-C8-N7	-3.12	107.52	113.39
41	2	4355	E6G	N2-C2-N1	-3.11	112.42	117.25
4	8	14	OMU	O4-C4-C5	-3.10	119.70	125.16
41	2	4196	OMG	C2-N1-C6	-3.09	119.46	125.10
41	2	4620	OMU	C5-C4-N3	3.08	119.45	114.84
41	2	1909	P7G	N9-C8-N7	3.08	107.78	103.38
41	2	2380	B8W	N2-C2-N1	-3.02	112.55	117.25
41	2	1574	B9B	C5-N7-C8	3.02	107.80	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	4472	B8W	C5-N7-C8	3.02	107.80	103.51
41	2	4870	OMG	C2-N1-C6	-3.02	119.60	125.10
4	8	14	OMU	CM2-O2'-C2'	3.02	122.44	114.52
41	2	1883	OMG	O6-C6-C5	-3.02	118.60	126.60
41	2	373	OMG	C2-N1-C6	-3.01	119.61	125.10
41	2	2786	B9H	O2-C2-N1	-3.00	115.71	122.72
41	2	4623	OMG	C2-N1-C6	-2.99	119.64	125.10
41	2	4597	UR3	C6-N1-C2	-2.97	119.13	121.79
41	2	4872	2MG	N9-C4-N3	2.97	131.90	125.94
41	2	1883	OMG	C5-C6-N1	2.97	120.72	113.19
41	2	4185	B8W	N2-C2-N1	-2.96	112.65	117.25
41	2	4220	6MZ	C5-N7-C8	2.95	107.70	103.51
41	2	2380	B8W	C5-N7-C8	2.94	107.68	103.51
41	2	2773	OMG	C2-N1-C6	-2.92	119.77	125.10
41	2	1517	2MG	C5-C6-N1	2.92	120.61	113.19
41	2	3899	BGH	C6-C5-C4	-2.92	116.60	122.62
41	2	4196	OMG	CM2-O2'-C2'	2.92	122.18	114.52
41	2	4355	E6G	C61-O6-C6	-2.92	114.75	117.59
41	2	1522	OMG	C2-N1-C6	-2.91	119.80	125.10
41	2	4371	MHG	N1-C2-N3	-2.91	119.46	123.95
41	2	4872	2MG	N9-C8-N7	-2.90	107.94	113.39
41	2	4529	B8W	N2-C2-N1	-2.88	112.77	117.25
41	2	4370	OMG	C5-C6-N1	2.88	120.50	113.19
41	2	978	2MG	N9-C8-N7	-2.86	108.00	113.39
41	2	4620	OMU	O4-C4-C5	-2.85	120.14	125.16
41	2	4083	5MU	O2-C2-N1	-2.84	119.00	122.79
41	2	4472	B8W	N2-C2-N1	-2.84	112.84	117.25
41	2	4185	B8W	C5-N7-C8	2.84	107.54	103.51
41	2	2364	OMG	C5-C4-N9	2.81	110.72	105.63
41	2	2786	B9H	C32-C31-N3	2.80	118.32	112.47
41	2	2297	E7G	N9-C8-N7	2.80	107.38	103.38
41	2	2804	OMC	C1'-N1-C2	2.79	124.64	118.42
41	2	2424	OMG	C5-C6-N1	2.78	120.26	113.19
41	2	1605	7MG	N9-C8-N7	2.78	107.36	103.38
41	2	1456	B8Q	C31-N3-C2	2.78	121.83	117.79
41	2	978	2MG	C5-C6-N1	2.77	120.23	113.19
41	2	237	B9B	C5-N7-C8	2.77	107.44	103.51
41	2	4597	UR3	C3U-N3-C2	2.77	122.16	117.31
41	2	4870	OMG	C5-C6-N1	2.76	120.20	113.19
41	2	4671	B8T	C6-C5-C4	2.76	120.34	116.96
41	2	4637	OMG	C5-C6-N1	2.76	120.20	113.19
41	2	3899	BGH	O6-C6-N1	-2.74	114.86	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	2522	7MG	N9-C8-N7	2.74	107.30	103.38
41	2	1316	OMG	C5-C6-N1	2.74	120.16	113.19
41	2	3869	OMC	C1'-N1-C2	2.74	124.53	118.42
41	2	4494	OMG	C5-C6-N1	2.73	120.11	113.19
41	2	1625	OMG	C5-C6-N1	2.72	120.10	113.19
41	2	2050	OMG	C5-C6-N1	2.72	120.10	113.19
41	2	729	2MG	C5-C6-N1	2.72	120.10	113.19
41	2	4872	2MG	C5-C6-N1	2.71	120.08	113.19
41	2	373	OMG	C5-C6-N1	2.71	120.07	113.19
41	2	2364	OMG	C5-C6-N1	2.71	120.07	113.19
41	2	2522	7MG	C4-C5-N7	2.69	109.26	105.53
41	2	1517	2MG	O6-C6-C5	-2.69	119.47	126.60
41	2	4415	1MA	N9-C4-N3	2.68	133.18	126.94
41	2	2050	OMG	C5-C4-N9	2.67	110.47	105.63
41	2	4196	OMG	C5-C6-N1	2.67	119.97	113.19
41	2	1316	OMG	C5-C4-N9	2.67	110.47	105.63
41	2	4550	7MG	C4-C5-N7	2.66	109.22	105.53
41	2	2401	A2M	C2'-C1'-N9	-2.65	109.06	113.53
41	2	4196	OMG	N9-C4-N3	2.65	131.27	125.94
41	2	4530	UR3	C6-N1-C2	-2.65	119.42	121.79
41	2	4185	B8W	O6-C6-C5	-2.64	113.65	116.97
41	2	4623	OMG	C5-C4-N9	2.64	110.43	105.63
41	2	3880	P7G	N9-C8-N7	2.64	107.15	103.38
41	2	4637	OMG	C5-C4-N9	2.64	110.42	105.63
41	2	4637	OMG	O4'-C1'-N9	2.63	114.36	108.36
41	2	4371	MHG	C71-C72-C73	-2.62	106.84	114.20
41	2	2786	B9H	O3'-C3'-C4'	2.62	118.63	111.05
41	2	4355	E6G	C2-N1-C6	2.62	120.09	115.93
41	2	2050	OMG	O6-C6-C5	-2.62	119.66	126.60
41	2	4623	OMG	C5-C6-N1	2.61	119.83	113.19
41	2	1322	1MA	N9-C4-N3	2.61	133.03	126.94
41	2	729	2MG	N9-C8-N7	-2.61	108.48	113.39
41	2	1522	OMG	C5-C6-N1	2.61	119.81	113.19
41	2	4083	5MU	C6-C5-C4	2.61	120.21	118.03
41	2	2424	OMG	O6-C6-C5	-2.60	119.69	126.60
41	2	4220	6MZ	C5-C6-N1	2.60	120.98	118.20
41	2	4690	B8K	C2-N1-C6	-2.60	120.35	125.10
41	2	373	OMG	C5-C4-N9	2.60	110.34	105.63
41	2	4529	B8W	O6-C6-C5	-2.59	113.72	116.97
41	2	2364	OMG	O6-C6-C5	-2.59	119.74	126.60
41	2	3869	OMC	O2-C2-N1	2.59	124.23	118.89
41	2	2804	OMC	O2-C2-N1	2.58	124.22	118.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	373	OMG	O6-C6-C5	-2.58	119.77	126.60
41	2	4483	B8T	O3'-C3'-C2'	2.57	120.14	111.82
41	2	4371	MHG	N9-C8-N7	2.56	107.03	103.38
41	2	1883	OMG	C2'-C1'-N9	-2.55	109.26	114.22
41	2	4196	OMG	O6-C6-C5	-2.55	119.83	126.60
41	2	2380	B8W	C61-O6-C6	-2.55	114.69	117.21
41	2	2773	OMG	C5-C4-N9	2.55	110.25	105.63
41	2	4355	E6G	C5-C6-N1	-2.55	119.92	123.46
41	2	1625	OMG	O6-C6-C5	-2.54	119.86	126.60
41	2	1625	OMG	C5-C4-N9	2.53	110.23	105.63
41	2	4472	B8W	C4-N9-C1'	-2.52	120.59	126.59
41	2	237	B9B	C2-N3-C4	2.52	120.85	113.89
41	2	1605	7MG	C2-N1-C6	-2.52	120.51	125.10
41	2	729	2MG	O6-C6-C5	-2.51	119.94	126.60
41	2	4494	OMG	O6-C6-C5	-2.51	119.94	126.60
41	2	3899	BGH	C2-N1-C6	-2.50	120.53	125.10
41	2	3897	B8K	O6-C6-N1	-2.50	115.32	120.12
41	2	1522	OMG	C5-C4-N9	2.49	110.15	105.63
41	2	4494	OMG	C5-C4-N9	2.49	110.15	105.63
41	2	1316	OMG	O6-C6-C5	-2.49	119.99	126.60
41	2	2422	OMC	C1'-N1-C2	2.49	123.98	118.42
41	2	4872	2MG	O6-C6-C5	-2.49	120.00	126.60
41	2	4529	B8W	C2-N1-C6	2.49	119.88	115.93
41	2	4415	1MA	C1'-N9-C4	-2.49	119.12	126.50
41	2	4529	B8W	C5-C6-N1	-2.48	120.01	123.46
41	2	4637	OMG	O6-C6-C5	-2.47	120.04	126.60
41	2	4870	OMG	O6-C6-C5	-2.47	120.04	126.60
41	2	4564	M7A	C5-C4-N3	-2.47	120.83	126.62
41	2	1605	7MG	C4-C5-N7	2.45	108.93	105.53
41	2	4529	B8W	C5-N7-C8	2.44	106.98	103.51
41	2	2773	OMG	C5-C6-N1	2.44	119.40	113.19
41	2	4870	OMG	N9-C8-N7	-2.44	108.80	113.39
41	2	978	2MG	O6-C6-C5	-2.43	120.14	126.60
41	2	4472	B8W	O6-C6-C5	-2.43	113.92	116.97
41	2	4523	A2M	C4'-O4'-C1'	-2.43	104.11	109.47
41	2	1316	OMG	O4'-C1'-N9	2.43	113.91	108.36
41	2	4564	M7A	C4-N9-C1'	-2.43	120.83	126.60
41	2	4483	B8T	O3'-C3'-C4'	2.43	118.07	111.05
41	2	373	OMG	O4'-C1'-N9	2.43	113.91	108.36
41	2	1522	OMG	O6-C6-C5	-2.42	120.17	126.60
41	2	1574	B9B	C2-N3-C4	2.42	120.58	113.89
41	2	4550	7MG	N9-C8-N7	2.41	106.83	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	2297	E7G	C2-N1-C6	-2.41	120.70	125.10
41	2	1909	P7G	C71-N7-C5	2.41	130.22	124.52
41	2	1517	2MG	N9-C8-N7	-2.40	108.87	113.39
41	2	4623	OMG	O6-C6-C5	-2.40	120.24	126.60
41	2	2364	OMG	O4'-C1'-N9	2.39	113.82	108.36
41	2	4370	OMG	O6-C6-C5	-2.39	120.27	126.60
41	2	2380	B8W	C4-N9-C1'	-2.38	120.91	126.59
41	2	1517	2MG	N1-C2-N3	-2.38	120.27	123.95
41	2	373	OMG	C2'-C1'-N9	-2.38	109.60	114.22
41	2	2050	OMG	O4'-C1'-N9	2.38	113.81	108.36
41	2	4483	B8T	O2-C2-N3	-2.37	118.47	122.33
41	2	3867	A2M	C4'-O4'-C1'	-2.37	104.24	109.47
41	2	2364	OMG	N2-C2-N1	2.37	121.75	116.71
41	2	4472	B8W	C2-N3-C4	2.36	120.42	113.89
41	2	4355	E6G	C2-N3-C4	2.36	120.40	113.89
41	2	4370	OMG	C5-C4-N9	2.34	109.88	105.63
41	2	4523	A2M	C2'-C1'-N9	-2.34	109.59	113.53
41	2	2522	7MG	C2-N1-C6	-2.33	120.85	125.10
41	2	4623	OMG	O4'-C1'-N9	2.32	113.68	108.36
41	2	1574	B9B	C4-N9-C8	2.32	108.25	105.73
41	2	3723	A2M	C2'-C1'-N9	-2.32	109.63	113.53
41	2	4494	OMG	O4'-C1'-N9	2.32	113.66	108.36
41	2	978	2MG	N1-C2-N3	-2.32	120.37	123.95
41	2	4620	OMU	O2-C2-N1	-2.31	119.71	122.79
41	2	3869	OMC	C6-N1-C2	-2.30	116.50	120.49
41	2	4472	B8W	C2-N1-C6	2.30	119.58	115.93
41	2	1883	OMG	C5-C4-N9	2.30	109.80	105.63
41	2	4185	B8W	C2-N3-C4	2.30	120.24	113.89
41	2	4370	OMG	O4'-C1'-N9	2.29	113.60	108.36
41	2	2424	OMG	O4'-C1'-N9	2.29	113.59	108.36
41	2	2773	OMG	O6-C6-C5	-2.28	120.54	126.60
41	2	2786	B9H	C1'-N1-C6	2.28	125.82	120.84
4	8	14	OMU	O2-C2-N1	-2.28	119.76	122.79
41	2	4870	OMG	N9-C4-N3	2.27	130.50	125.94
41	2	3897	B8K	C2-N1-C6	-2.27	120.96	125.10
41	2	373	OMG	N9-C8-N7	-2.27	109.12	113.39
41	2	4371	MHG	O6-C6-C5	-2.27	121.98	127.54
41	2	1625	OMG	O4'-C1'-N9	2.27	113.54	108.36
41	2	3899	BGH	N1-C2-N3	-2.26	119.10	123.32
41	2	4623	OMG	N2-C2-N1	2.25	121.51	116.71
41	2	1883	OMG	O4'-C1'-N9	2.25	113.51	108.36
41	2	4623	OMG	N9-C8-N7	-2.25	109.16	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	2424	OMG	C5-C4-N9	2.25	109.71	105.63
41	2	3897	B8K	N1-C2-N3	-2.24	119.15	123.32
41	2	729	2MG	N1-C2-N3	-2.24	120.49	123.95
41	2	4550	7MG	C2-N1-C6	-2.23	121.03	125.10
41	2	373	OMG	N2-C2-N1	2.23	121.46	116.71
41	2	1522	OMG	O4'-C1'-N9	2.23	113.46	108.36
41	2	4371	MHG	C71-N7-C5	2.22	129.78	124.52
41	2	4355	E6G	C4-N9-C8	2.22	108.14	105.73
41	2	1524	A2M	C4-N9-C1'	2.21	131.87	126.59
41	2	2380	B8W	C2-N1-C6	2.21	119.44	115.93
41	2	1625	OMG	N9-C4-N3	2.21	130.38	125.94
41	2	237	B9B	C4-N9-C8	2.21	108.12	105.73
41	2	1574	B9B	C61-O6-C6	-2.20	113.27	117.47
41	2	4529	B8W	C2-N3-C4	2.20	119.98	113.89
41	2	4550	7MG	C6-C5-C4	-2.20	118.09	122.62
41	2	4472	B8W	C4-N9-C8	2.20	108.11	105.73
41	2	4623	OMG	C4-C5-N7	-2.19	107.25	110.72
41	2	1524	A2M	C4'-O4'-C1'	-2.19	104.65	109.47
41	2	2380	B8W	C5-C6-N1	-2.18	120.42	123.46
41	2	4185	B8W	C6-C5-N7	-2.18	130.74	133.63
41	2	4185	B8W	C2-N1-C6	2.17	119.38	115.93
41	2	4185	B8W	C5-C6-N1	-2.17	120.45	123.46
41	2	2364	OMG	C4-C5-N7	-2.16	107.30	110.72
41	2	373	OMG	C4-C5-N7	-2.16	107.30	110.72
41	2	1316	OMG	C4-C5-N7	-2.16	107.30	110.72
41	2	2424	OMG	N9-C4-N3	2.15	130.26	125.94
41	2	3867	A2M	C4-N9-C1'	2.14	131.70	126.59
41	2	978	2MG	C8-N7-C5	2.14	108.11	104.24
41	2	4637	OMG	C4-C5-N7	-2.14	107.33	110.72
41	2	4472	B8W	C61-O6-C6	-2.14	115.09	117.21
41	2	1348	P4U	C41-O4-C4	-2.14	112.90	117.24
41	2	4690	B8K	N1-C2-N3	-2.13	119.34	123.32
41	2	4370	OMG	N9-C4-N3	2.13	130.22	125.94
41	2	2380	B8W	C2-N3-C4	2.13	119.78	113.89
41	2	4690	B8K	O6-C6-N1	-2.12	116.05	120.12
41	2	3880	P7G	N3-C2-N1	-2.12	119.36	123.32
41	2	4529	B8W	C6-C5-N7	-2.12	130.82	133.63
41	2	4536	OMC	C1'-N1-C2	2.12	123.15	118.42
41	2	4355	E6G	C4-C5-N7	-2.12	108.04	110.62
41	2	3718	A2M	C2'-C1'-N9	-2.11	109.97	113.53
41	2	4415	1MA	C8-N7-C5	2.11	108.06	104.24
41	2	2773	OMG	O4'-C1'-N9	2.11	113.18	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	2422	OMC	O2-C2-N1	2.10	123.23	118.89
41	2	2380	B8W	O6-C6-C5	-2.10	114.33	116.97
41	2	4083	5MU	O4-C4-N3	-2.10	116.09	120.12
41	2	3887	OMC	O2-C2-N3	-2.10	118.91	122.33
41	2	4564	M7A	C71-N7-C5	-2.10	115.95	124.01
41	2	2522	7MG	C6-C5-C4	-2.09	118.30	122.62
41	2	1605	7MG	O6-C6-C5	-2.09	122.41	127.54
41	2	1534	A2M	O4'-C1'-C2'	-2.09	102.90	106.57
41	2	2363	A2M	C4-N9-C1'	2.09	131.57	126.59
41	2	4472	B8W	C5-C6-N1	-2.08	120.57	123.46
41	2	1322	1MA	C8-N7-C5	2.08	108.00	104.24
41	2	4370	OMG	N9-C8-N7	-2.07	109.48	113.39
41	2	4536	OMC	O2-C2-N1	2.07	123.17	118.89
41	2	4872	2MG	C8-N7-C5	2.07	107.99	104.24
41	2	237	B9B	C61-O6-C6	-2.07	113.53	117.47
41	2	2297	E7G	N1-C2-N3	-2.07	119.47	123.32
41	2	4185	B8W	C4-N9-C1'	-2.06	121.69	126.59
41	2	2297	E7G	C6-C5-C4	-2.06	118.37	122.62
41	2	2050	OMG	N2-C2-N1	2.05	121.08	116.71
41	2	4690	B8K	O6-C6-C5	-2.04	122.53	127.54
41	2	1316	OMG	N2-C2-N1	2.04	121.06	116.71
41	2	1534	A2M	C4-N9-C1'	2.03	131.44	126.59
41	2	4370	OMG	C4-C5-N7	-2.03	107.50	110.72
41	2	2297	E7G	C8-N7-C71	2.02	125.30	120.50
41	2	1605	7MG	C6-C5-C4	-2.02	118.46	122.62
41	2	1659	I4U	O2-C2-N3	-2.01	119.06	122.33
41	2	2297	E7G	N9-C4-N3	2.01	128.48	125.47
41	2	1883	OMG	N9-C8-N7	-2.01	109.61	113.39
41	2	4371	MHG	C6-C5-C4	-2.01	118.48	122.62

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	8	14	OMU	C1'-C2'-O2'-CM2
41	2	237	B9B	C5-C6-O6-C61
41	2	237	B9B	N1-C6-O6-C61
41	2	237	B9B	C3'-C4'-C5'-O5'
41	2	237	B9B	O4'-C4'-C5'-O5'
41	2	398	A2M	O4'-C4'-C5'-O5'
41	2	1348	P4U	N3-C4-O4-C41
41	2	1574	B9B	C5-C6-O6-C61

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Mol	Chain	Res	Type	Atoms
41	2	1574	B9B	N1-C6-O6-C61
41	2	1625	OMG	C3'-C4'-C5'-O5'
41	2	1883	OMG	C3'-C4'-C5'-O5'
41	2	2364	OMG	O4'-C4'-C5'-O5'
41	2	2380	B8W	C5-C6-O6-C61
41	2	2380	B8W	N1-C6-O6-C61
41	2	2424	OMG	O4'-C4'-C5'-O5'
41	2	2424	OMG	C3'-C4'-C5'-O5'
41	2	3867	A2M	C3'-C4'-C5'-O5'
41	2	3869	OMC	O4'-C1'-N1-C2
41	2	3869	OMC	O4'-C1'-N1-C6
41	2	3880	P7G	C3'-C4'-C5'-O5'
41	2	3880	P7G	O4'-C4'-C5'-O5'
41	2	3897	B8K	O4'-C4'-C5'-O5'
41	2	4185	B8W	C5-C6-O6-C61
41	2	4185	B8W	N1-C6-O6-C61
41	2	4194	I4U	O4'-C4'-C5'-O5'
41	2	4196	OMG	C1'-C2'-O2'-CM2
41	2	4220	6MZ	N1-C6-N6-C9
41	2	4355	E6G	C5-C6-O6-C61
41	2	4355	E6G	N1-C6-O6-C61
41	2	4371	MHG	C71-C72-C73-C75
41	2	4415	1MA	O4'-C4'-C5'-O5'
41	2	4472	B8W	C5-C6-O6-C61
41	2	4620	OMU	C1'-C2'-O2'-CM2
41	2	4637	OMG	O4'-C4'-C5'-O5'
41	2	4637	OMG	C1'-C2'-O2'-CM2
41	2	4870	OMG	O4'-C4'-C5'-O5'
41	2	4870	OMG	C3'-C4'-C5'-O5'
41	2	729	2MG	O4'-C4'-C5'-O5'
41	2	1534	A2M	O4'-C4'-C5'-O5'
41	2	1883	OMG	O4'-C4'-C5'-O5'
41	2	2364	OMG	C3'-C4'-C5'-O5'
41	2	2401	A2M	C3'-C4'-C5'-O5'
41	2	3718	A2M	O4'-C4'-C5'-O5'
41	2	3897	B8K	C3'-C4'-C5'-O5'
41	2	4194	I4U	C3'-C4'-C5'-O5'
41	2	4371	MHG	O4'-C4'-C5'-O5'
41	2	4415	1MA	C3'-C4'-C5'-O5'
41	2	4550	7MG	C3'-C4'-C5'-O5'
41	2	4637	OMG	C3'-C4'-C5'-O5'
41	2	4872	2MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
41	2	3869	OMC	C2'-C1'-N1-C6
41	2	398	A2M	C3'-C4'-C5'-O5'
41	2	1625	OMG	O4'-C4'-C5'-O5'
41	2	3718	A2M	C3'-C4'-C5'-O5'
41	2	3867	A2M	O4'-C4'-C5'-O5'
41	2	4196	OMG	C3'-C4'-C5'-O5'
41	2	4523	A2M	O4'-C4'-C5'-O5'
41	2	4523	A2M	C3'-C4'-C5'-O5'
41	2	4550	7MG	O4'-C4'-C5'-O5'
41	2	4872	2MG	C3'-C4'-C5'-O5'
41	2	4472	B8W	N1-C6-O6-C61
41	2	4194	I4U	C2'-C1'-N1-C6
41	2	3869	OMC	C2'-C1'-N1-C2
41	2	4194	I4U	C2'-C1'-N1-C2
41	2	729	2MG	C3'-C4'-C5'-O5'
41	2	1534	A2M	C3'-C4'-C5'-O5'
41	2	4196	OMG	O4'-C4'-C5'-O5'
41	2	3701	OMC	C2'-C1'-N1-C6
41	2	4371	MHG	C72-C73-C74-C76
41	2	2401	A2M	O4'-C4'-C5'-O5'
41	2	3880	P7G	C72-C71-N7-C8
41	2	4371	MHG	C71-C72-C73-C74
41	2	1909	P7G	O4'-C4'-C5'-O5'
41	2	2786	B9H	C32-C31-N3-C2
41	2	4371	MHG	C3'-C4'-C5'-O5'
41	2	4371	MHG	C75-C73-C74-C76
41	2	4194	I4U	O4'-C1'-N1-C6
41	2	3718	A2M	C3'-C2'-O2'-CM'
41	2	4597	UR3	O4'-C4'-C5'-O5'
41	2	4371	MHG	C2'-C1'-N9-C8
41	2	1574	B9B	O4'-C4'-C5'-O5'
41	2	2297	E7G	C72-C71-N7-C8
41	2	1534	A2M	C4'-C5'-O5'-P
41	2	4523	A2M	C3'-C2'-O2'-CM'
41	2	4194	I4U	O4'-C1'-N1-C2
41	2	3701	OMC	O4'-C1'-N1-C6
41	2	1625	OMG	C4'-C5'-O5'-P
41	2	3723	A2M	O4'-C4'-C5'-O5'
41	2	4571	A2M	O4'-C4'-C5'-O5'
41	2	3701	OMC	C2'-C1'-N1-C2
41	2	4523	A2M	C4'-C5'-O5'-P
41	2	373	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
41	2	1517	2MG	C4'-C5'-O5'-P
41	2	3867	A2M	C4'-C5'-O5'-P
41	2	3887	OMC	C4'-C5'-O5'-P
41	2	3897	B8K	C4'-C5'-O5'-P
41	2	4196	OMG	C4'-C5'-O5'-P
41	2	4870	OMG	C4'-C5'-O5'-P
41	2	3869	OMC	C4'-C5'-O5'-P
41	2	1574	B9B	C3'-C4'-C5'-O5'
41	2	3701	OMC	O4'-C1'-N1-C2
41	2	4194	I4U	C43-C41-O4-C4
41	2	2401	A2M	C3'-C2'-O2'-CM'
41	2	1574	B9B	C4'-C5'-O5'-P
41	2	3880	P7G	C72-C71-N7-C5
41	2	1909	P7G	C3'-C4'-C5'-O5'
41	2	4371	MHG	O4'-C1'-N9-C8
41	2	2422	OMC	O4'-C4'-C5'-O5'
41	2	1322	1MA	C2'-C1'-N9-C8
41	2	1659	I4U	C43-C41-O4-C4
41	2	4194	I4U	C42-C41-O4-C4
41	2	4597	UR3	C3'-C4'-C5'-O5'
41	2	1326	A2M	C4'-C5'-O5'-P
41	2	1524	A2M	C4'-C5'-O5'-P

There are no ring outliers.

15 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	2	4623	OMG	1	0
41	2	3718	A2M	2	0
41	2	4196	OMG	1	0
41	2	1316	OMG	1	0
41	2	4872	2MG	3	0
41	2	4571	A2M	1	0
41	2	4690	B8K	1	0
41	2	2363	A2M	1	0
41	2	2522	7MG	1	0
41	2	1517	2MG	1	0
41	2	4083	5MU	1	0
41	2	1524	A2M	1	0
4	8	14	OMU	1	0
41	2	1574	B9B	2	0
41	2	4620	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

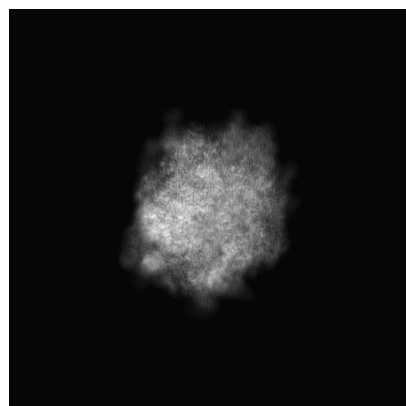
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35375. These allow visual inspection of the internal detail of the map and identification of artifacts.

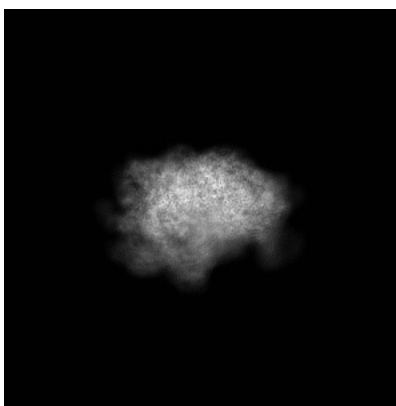
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

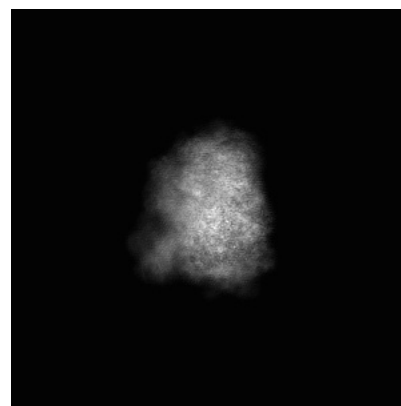
6.1.1 Primary map



X

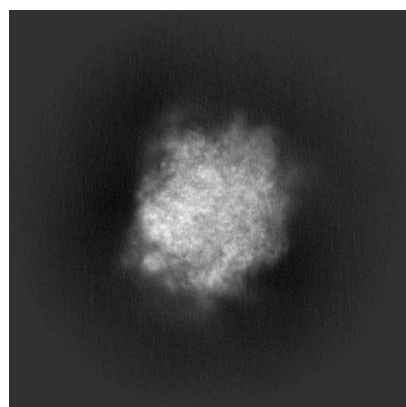


Y

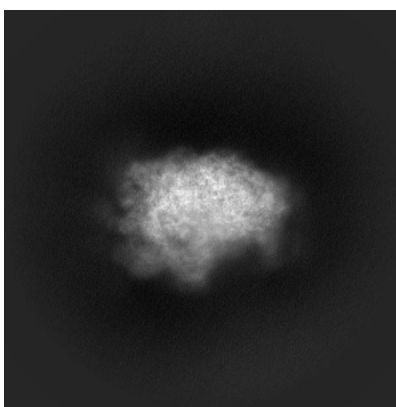


Z

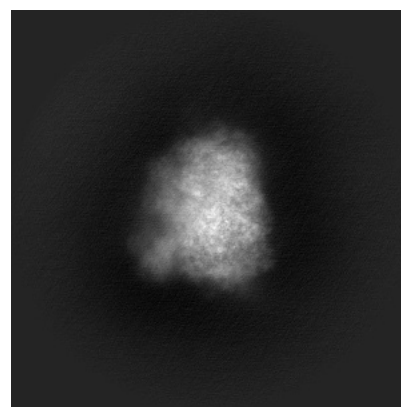
6.1.2 Raw map



X



Y

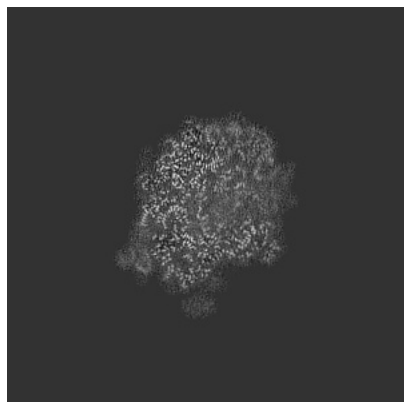


Z

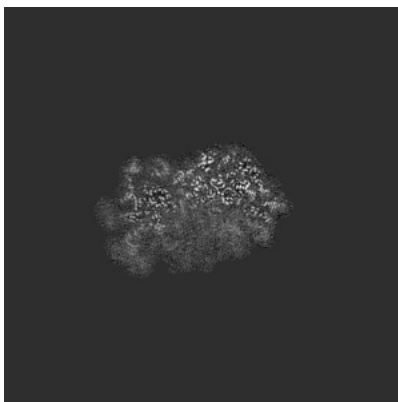
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200

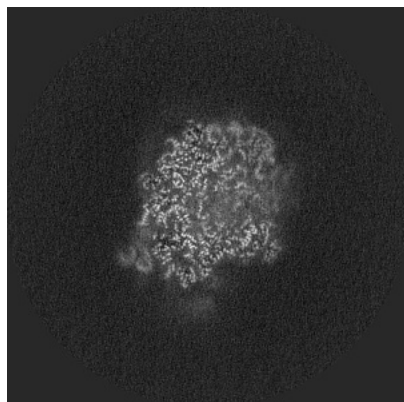


Y Index: 200

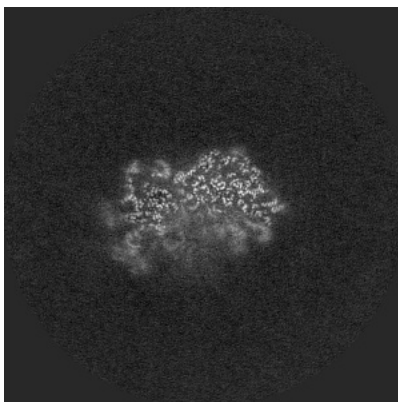


Z Index: 200

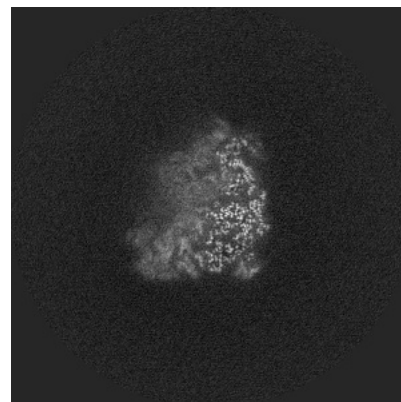
6.2.2 Raw map



X Index: 200



Y Index: 200

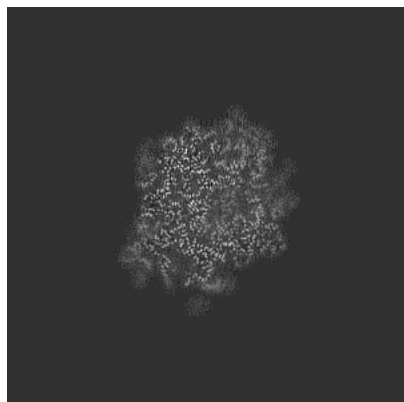


Z Index: 200

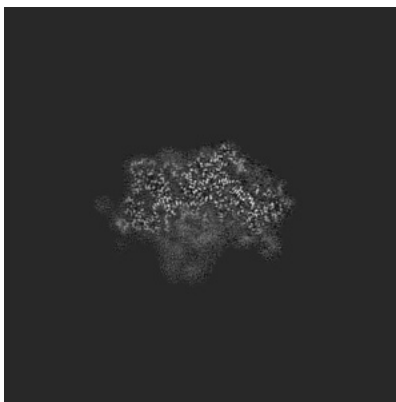
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

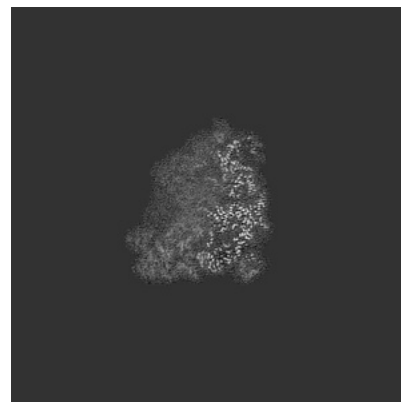
6.3.1 Primary map



X Index: 207

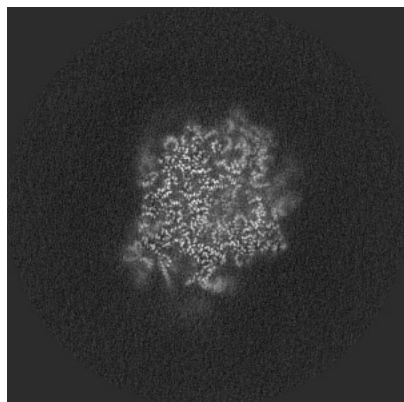


Y Index: 181

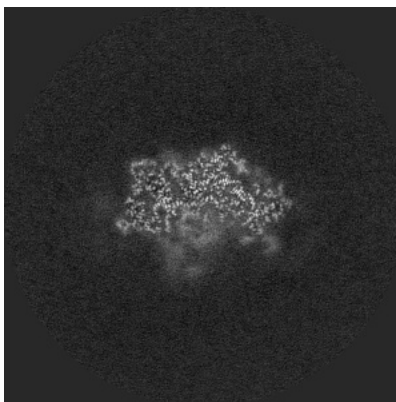


Z Index: 198

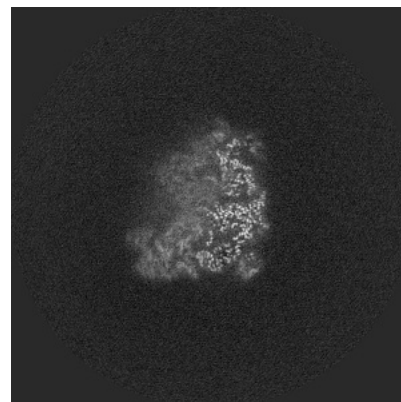
6.3.2 Raw map



X Index: 207



Y Index: 182

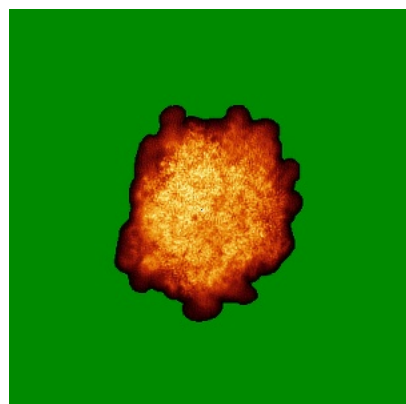


Z Index: 199

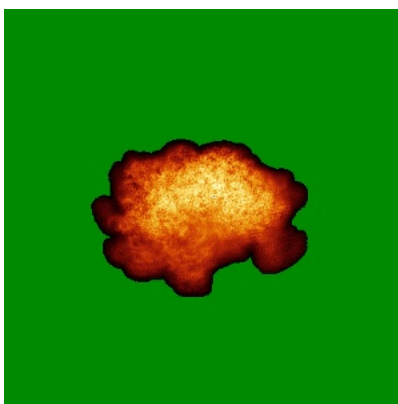
The images above show the largest variance slices of the map in three orthogonal directions.

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

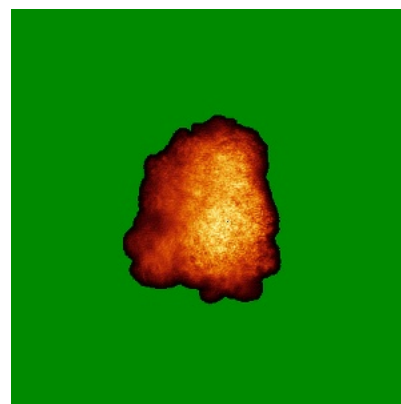
6.4.1 Primary map



X

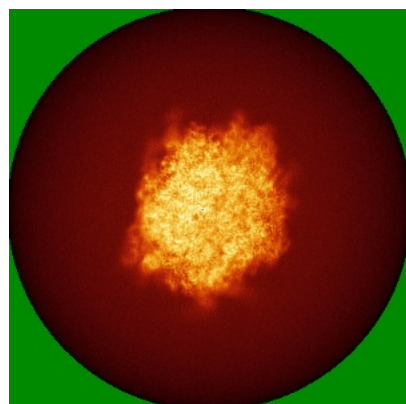


Y

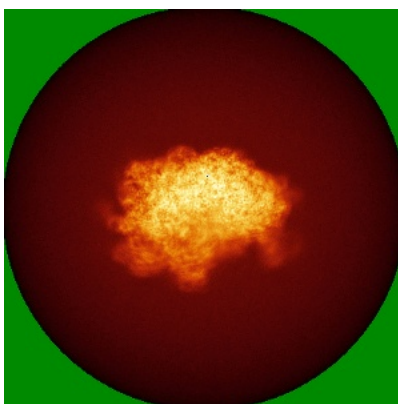


Z

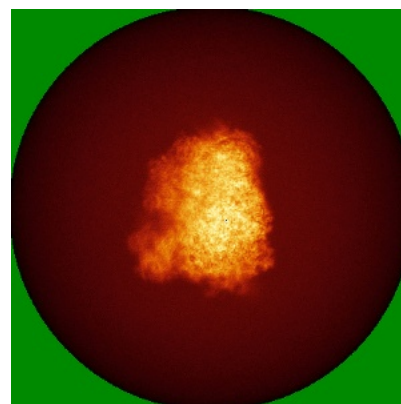
6.4.2 Raw map



X



Y

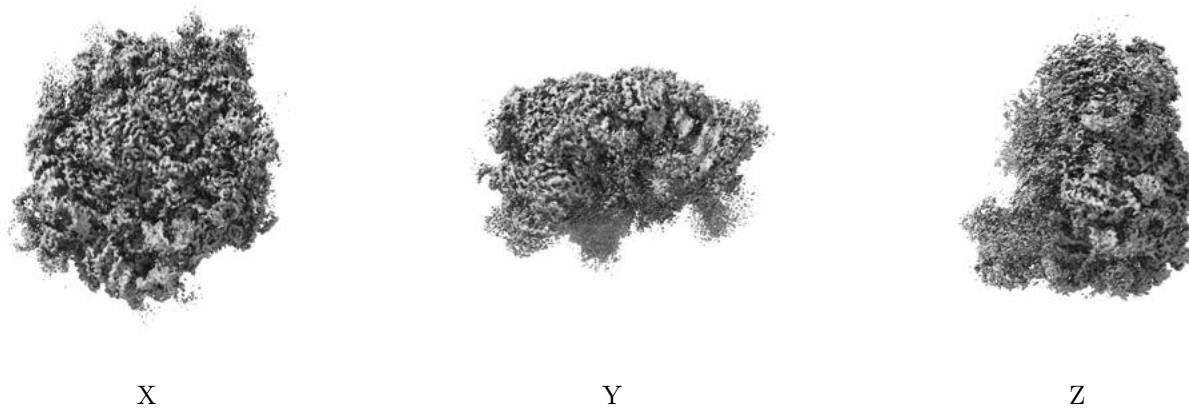


Z

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

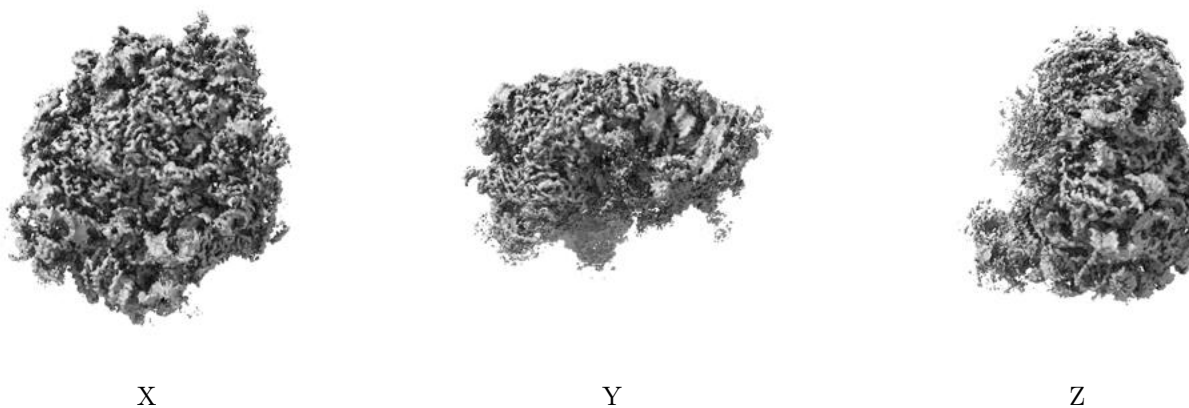
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

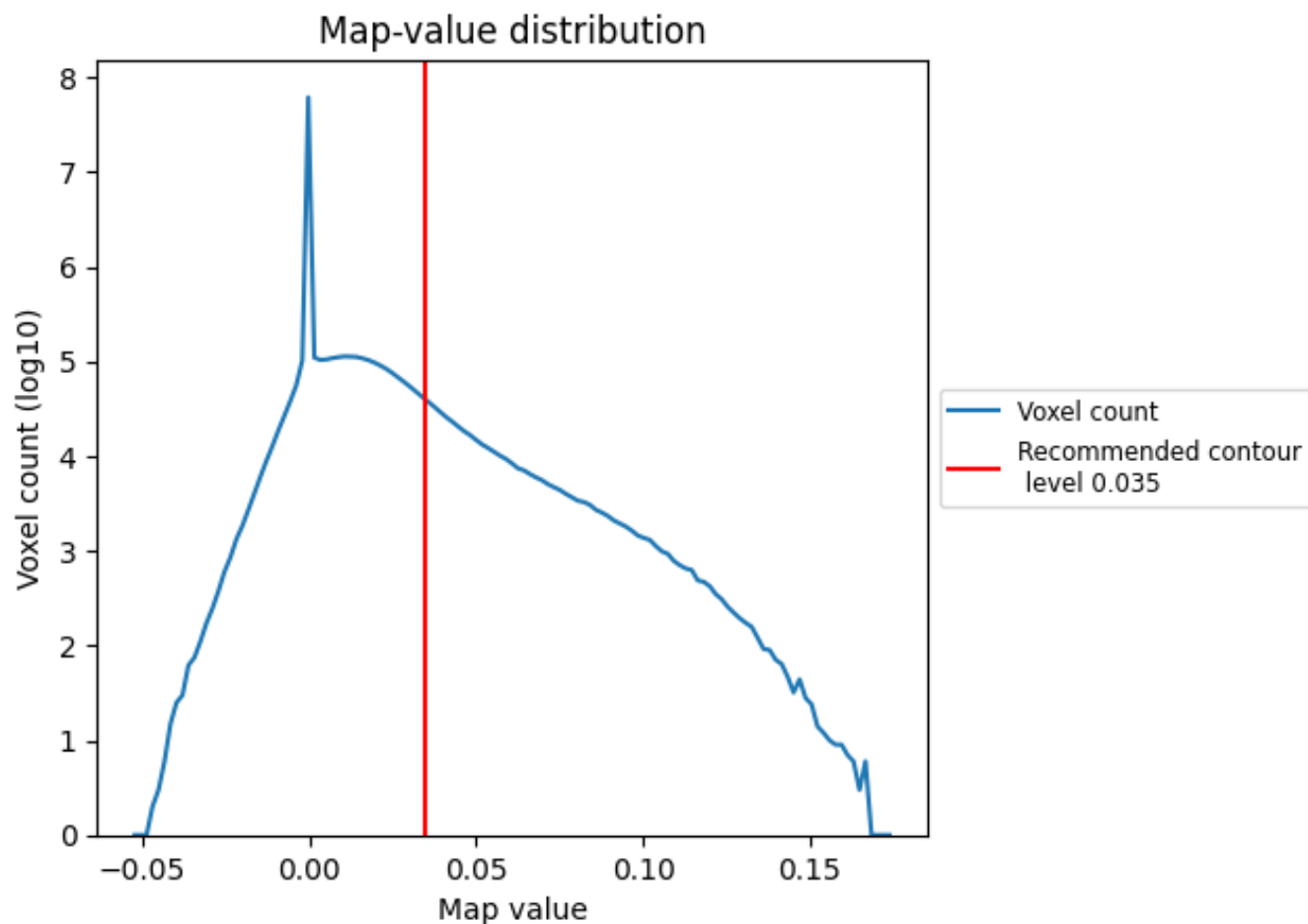
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

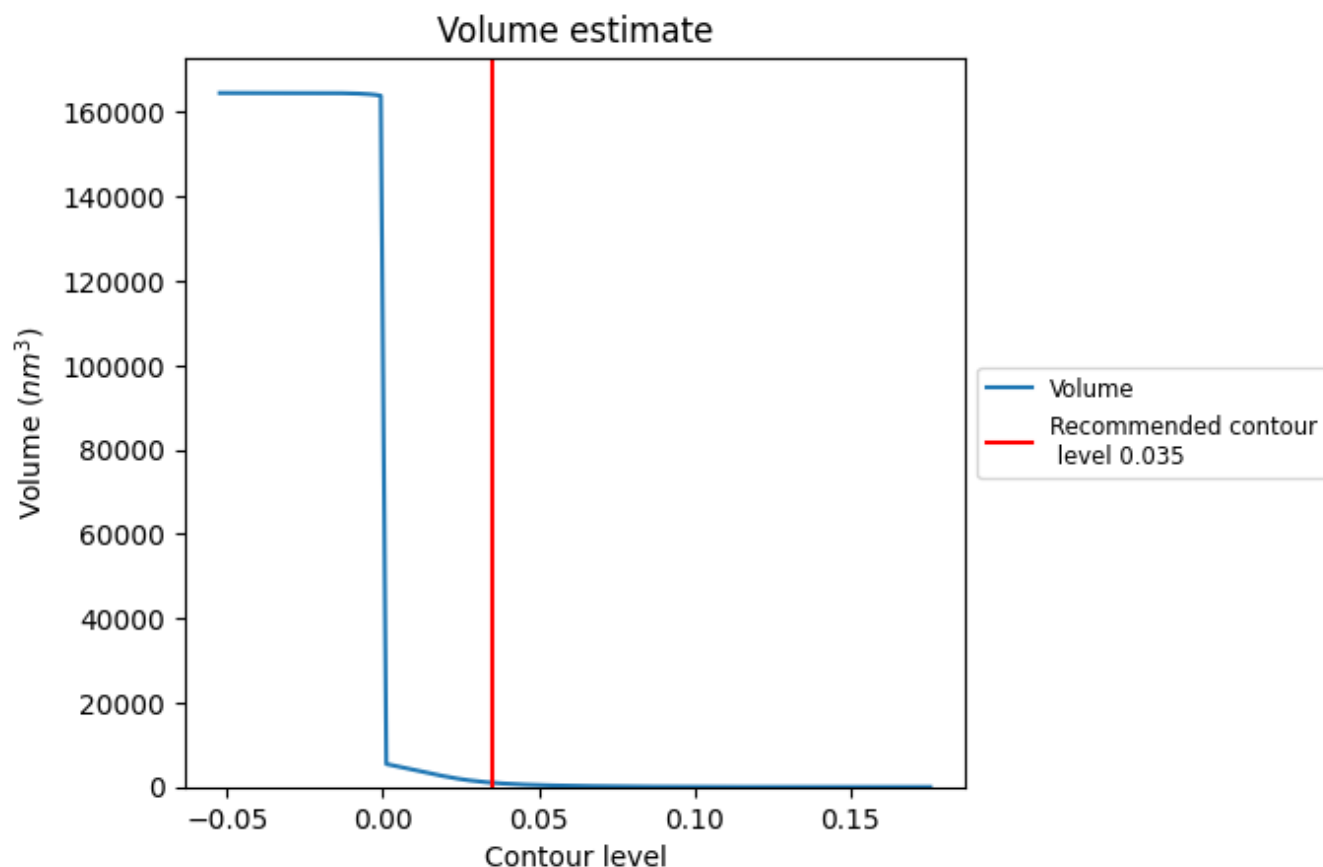
This section contains the results of statistical analysis of the map.

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.

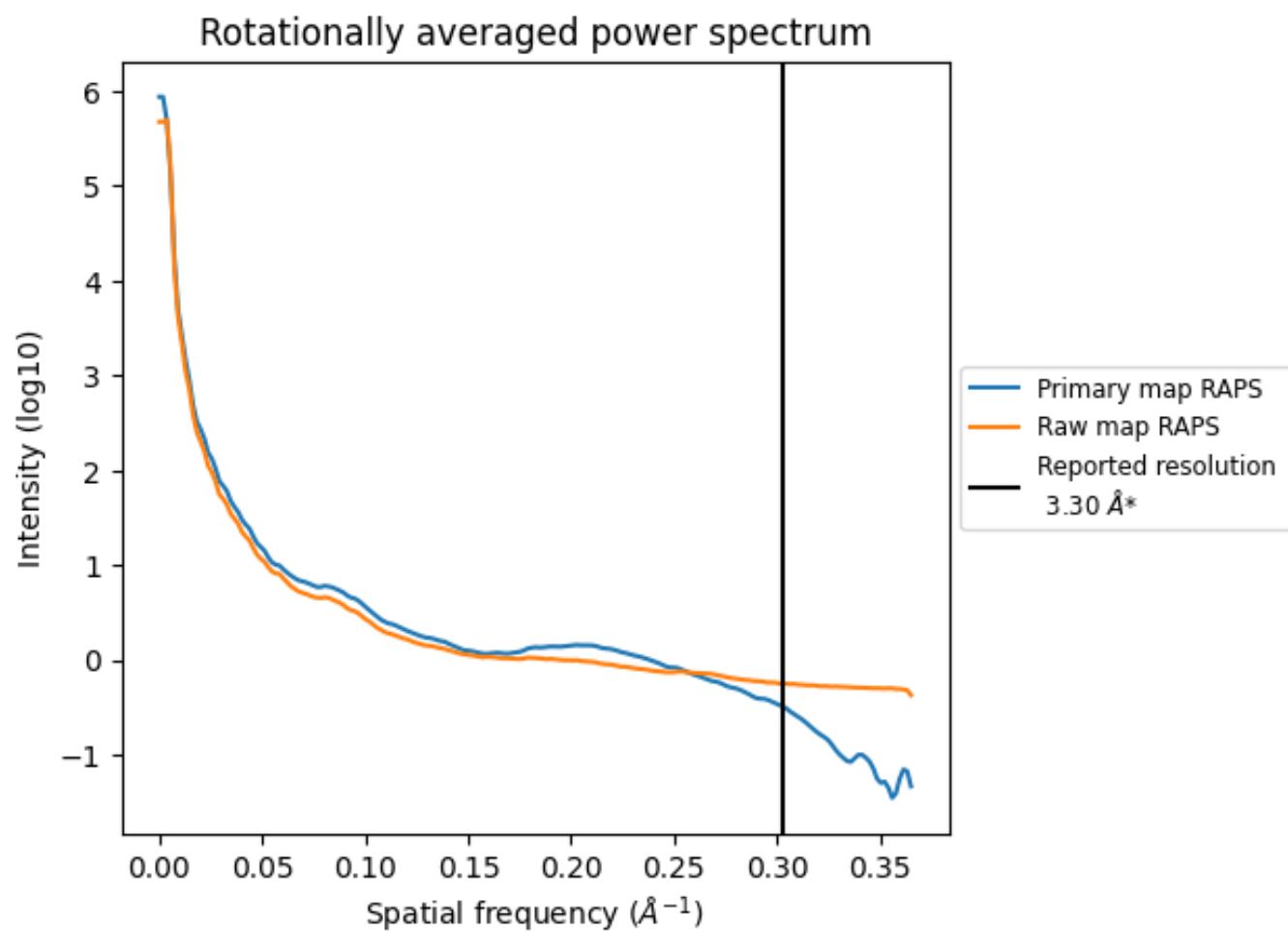
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1007 nm^3 ; this corresponds to an approximate mass of 910 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 ⓘ

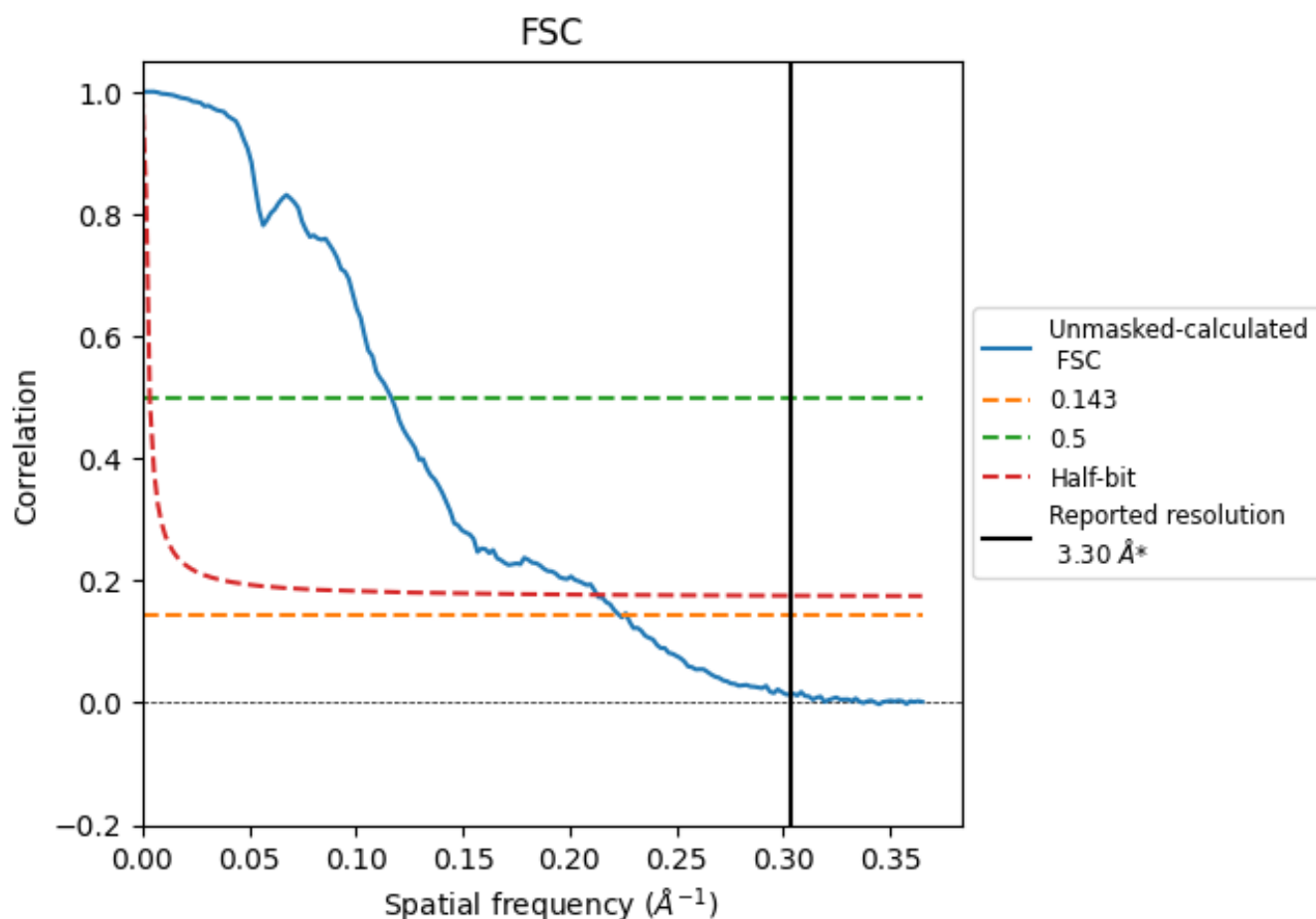


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

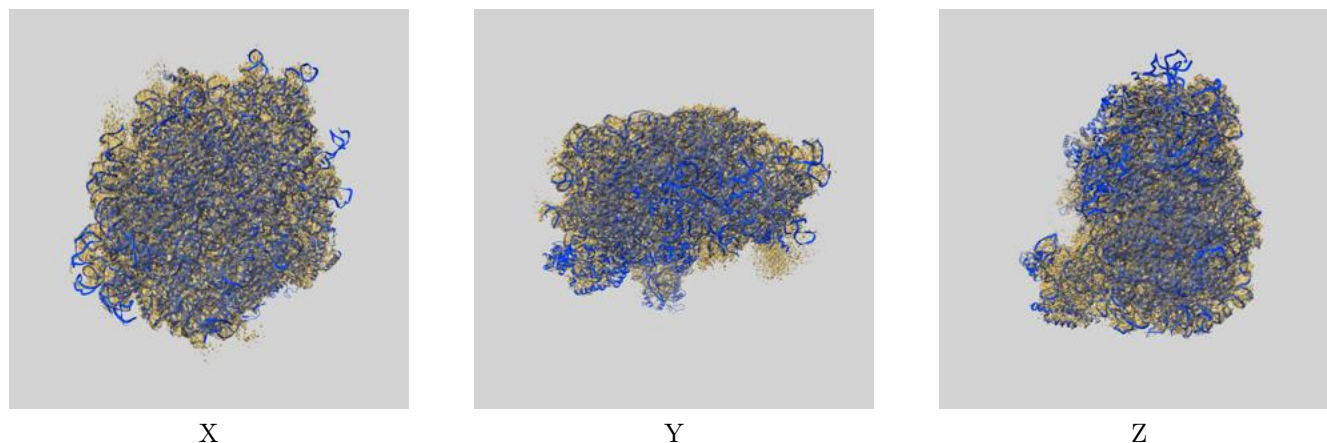
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.48	8.58	4.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.48 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

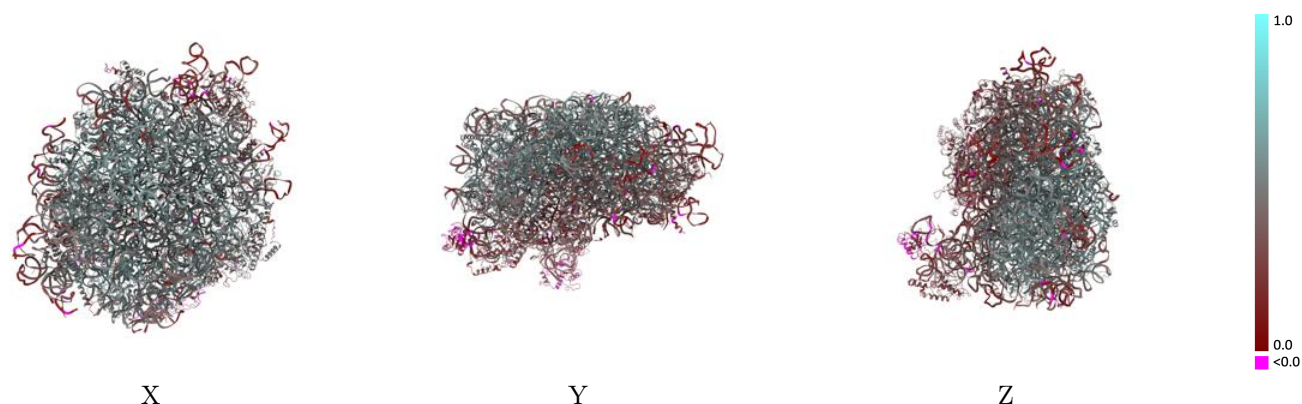
This section contains information regarding the fit between EMDB map EMD-35375 and PDB model 8IE3. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



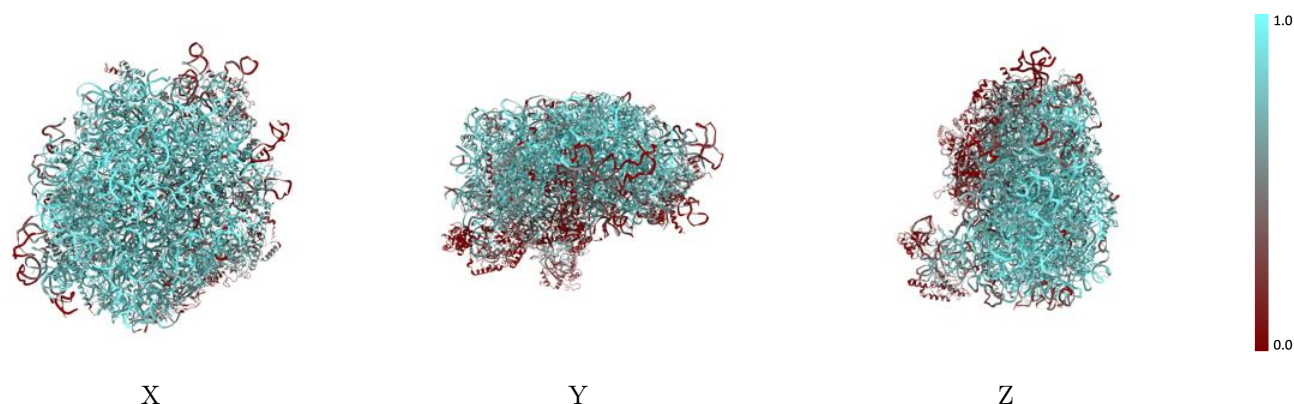
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



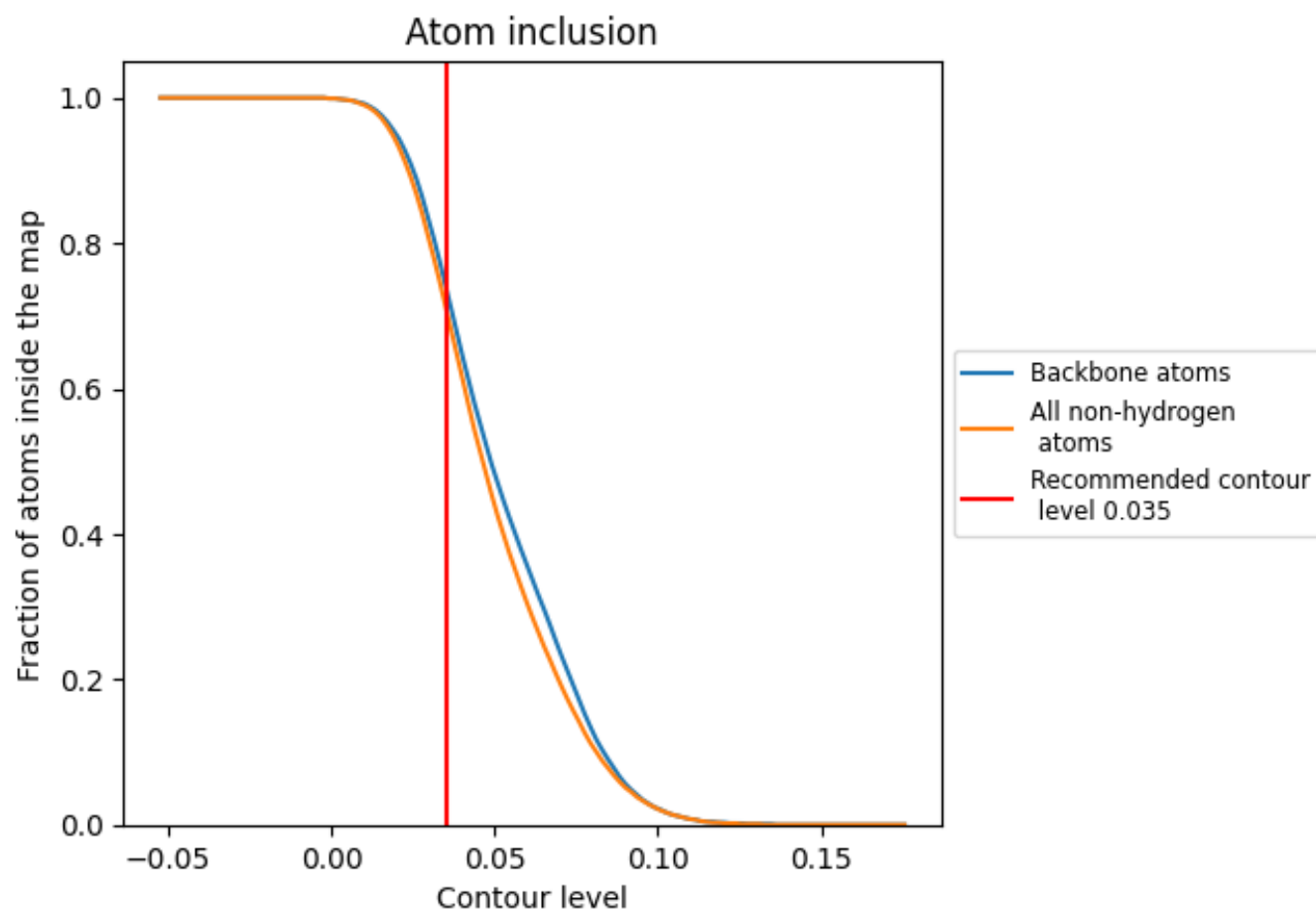
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 71% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7130	 0.4330
2	 0.7830	 0.4280
4	 0.3960	 0.3700
5	 0.7430	 0.3490
6	 0.5140	 0.4200
7	 0.7080	 0.4940
8	 0.9370	 0.5170
9	 0.0190	 0.2760
A	 0.1270	 0.3110
B	 0.8080	 0.5250
C	 0.4950	 0.3610
D	 0.8990	 0.5500
E	 0.2820	 0.3360
F	 0.7150	 0.4470
G	 0.6350	 0.4250
H	 0.8490	 0.5390
I	 0.6680	 0.4800
J	 0.0340	 0.0670
K	 0.7980	 0.4970
L	 0.8500	 0.5450
M	 0.9200	 0.5440
O	 0.5820	 0.4330
P	 0.9290	 0.5490
Q	 0.7920	 0.5080
R	 0.1550	 0.2590
S	 0.8340	 0.5220
T	 0.1020	 0.0780
U	 0.8880	 0.5480
V	 0.8570	 0.5340
X	 0.4810	 0.3740
Y	 0.8070	 0.5250
Z	 0.9000	 0.5710
a	 0.6220	 0.4370
b	 0.8690	 0.5470
c	 0.6460	 0.4150



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Chain	Atom inclusion	Q-score
d	 0.6810	 0.4720
e	 0.6840	 0.4720
g	 0.8460	 0.5310
h	 0.8610	 0.5440
i	 0.4390	 0.3340
j	 0.7830	 0.5170
k	 0.9110	 0.5640
l	 0.8740	 0.5510
m	 0.5320	 0.4030
n	 0.9250	 0.5660
o	 0.7080	 0.4820
p	 0.8440	 0.5390
r	 0.2790	 0.2800
z	 0.3000	 0.4130