



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:51 AM UTC

PDB ID : 8IR3 / pdb_00008ir3
EMDB ID : EMD-35673
Title : human nuclear pre-60S ribosomal particle - State B'
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-03-17
Resolution : 3.50 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:

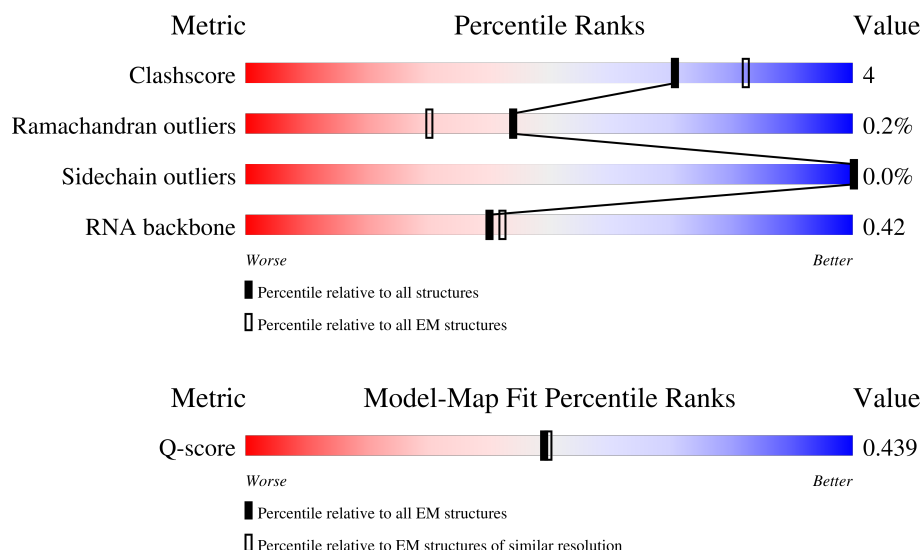
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 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	13950 (3.00 - 4.00)

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	y	165	
2	4	634	
3	6	245	

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Mol	Chain	Length	Quality of chain
4	7	163	
5	9	134	
6	B	403	
7	D	427	
8	E	115	
9	F	117	
10	G	266	
11	H	123	
12	I	192	
13	K	105	
14	L	148	
15	M	97	
16	P	51	
17	Q	211	
18	S	215	
19	U	204	
20	V	203	
21	X	92	
22	Z	188	
23	a	196	
24	b	176	
25	c	160	
26	e	140	
27	h	145	
28	l	137	

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Mol	Chain	Length	Quality of chain
29	m	257	
30	n	110	
31	o	288	
32	p	248	
33	z	129	
34	A	178	
35	C	297	
36	J	260	
37	N	485	
38	R	365	
39	u	549	
40	v	239	
41	w	731	
42	r	360	
43	8	156	
44	2	5054	
45	d	128	
46	j	125	
47	k	135	
48	Y	184	
49	t	293	
50	s	490	
51	i	136	
52	T	306	
53	5	120	

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Mol	Chain	Length	Quality of chain
54	q	588	
55	f	478	
56	O	70	
57	3	255	
58	g	156	
59	x	60	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 166429 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	y	165	Total	C	N	O	S	0	0
			1250	779	232	234	5		

- Molecule 2 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	620	Total	C	N	O	S	0	0
			5093	3198	935	933	27		

- Molecule 3 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 4 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	135	Total	C	N	O	S	0	0
			1159	737	225	187	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	9	86	Total	C	N	O	S	0	0
			711	433	154	121	3		

- 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 L4.

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

- Molecule 8 is a protein called 60S ribosomal protein L30.

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

- Molecule 9 is a protein called 60S ribosomal protein L34.

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

- Molecule 10 is a protein called 60S ribosomal protein L7a.

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

- Molecule 11 is a protein called 60S ribosomal protein L35.

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

- Molecule 12 is a protein called 60S ribosomal protein L9.

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

- Molecule 13 is a protein called 60S ribosomal protein L36.

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

- Molecule 14 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 15 is a protein called 60S ribosomal protein L37.

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

- Molecule 16 is a protein called 60S ribosomal protein L39.

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

- Molecule 17 is a protein called 60S ribosomal protein L13.

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

- Molecule 18 is a protein called 60S ribosomal protein L14.

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

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

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

- Molecule 21 is a protein called 60S ribosomal protein L37a.

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

- Molecule 22 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 23 is a protein called 60S ribosomal protein L19.

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

- Molecule 24 is a protein called 60S ribosomal protein L18a.

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

- Molecule 25 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	119	Total	C	N	O	S	0	0
			975	619	189	164	3		

- Molecule 26 is a protein called 60S ribosomal protein L23.

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

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L28.

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

- Molecule 29 is a protein called 60S ribosomal protein L8.

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

- Molecule 30 is a protein called 60S ribosomal protein L35a.

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

- Molecule 31 is a protein called 60S ribosomal protein L6.

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

- Molecule 32 is a protein called 60S ribosomal protein L7.

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

- Molecule 33 is a protein called Protein LLP homolog.

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

- Molecule 34 is a protein called 60S ribosomal protein L11.

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

- Molecule 35 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C	248	Total	C	N	O	S	0	0
			2027	1289	370	354	14		

- Molecule 36 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	J	259	Total	C	N	O	S	0	0
			2106	1339	399	359	9		

- Molecule 37 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	472	Total	C	N	O	S	0	0
			3669	2307	660	690	12		

- Molecule 38 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	R	199	Total	C	N	O	S	0	0
			1636	1022	315	296	3		

- Molecule 39 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	75	Total	C	N	O	S	0	0
			639	400	138	98	3		

- Molecule 40 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	206	Total	C	N	O	S	0	0
			1680	1072	293	304	11		

- Molecule 41 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	449	Total	C	N	O	S	0	0
			3623	2301	643	665	14		

- Molecule 42 is a protein called Coiled-coil domain-containing protein 86.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	24	Total	C	N	O	S	0	0
			217	134	45	37	1		

- Molecule 43 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	8	155	Total	C	N	O	P	0	0
			3295	1472	583	1086	154		

- Molecule 44 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	2	3541	Total	C	N	O	P	0	0
			75906	33833	13870	24663	3540		

- Molecule 45 is a protein called 60S ribosomal protein L22.

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

- Molecule 46 is a protein called 60S ribosomal protein L31.

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

- Molecule 47 is a protein called 60S ribosomal protein L32.

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

- Molecule 48 is a protein called 60S ribosomal protein L17.

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

- Molecule 49 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	111	Total	C	N	O	S	0	0
			928	601	157	167	3		

- Molecule 50 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	239	Total	C	N	O	S	0	0
			1924	1232	338	348	6		

- Molecule 51 is a protein called 60S ribosomal protein L27.

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

- Molecule 52 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	T	266	Total	C	N	O	S	0	0
			2166	1388	382	384	12		

- Molecule 53 is a RNA chain called 5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 54 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	q	404	Total	C	N	O	S	0	0
			3317	2140	582	582	13		

- Molecule 55 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	f	258	Total	C	N	O	S	0	0
			2137	1326	427	382	2		

- Molecule 56 is a protein called 60S ribosomal protein L38.

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

- Molecule 57 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	3	229	Total	C	N	O	S	0	0
			1892	1223	356	309	4		

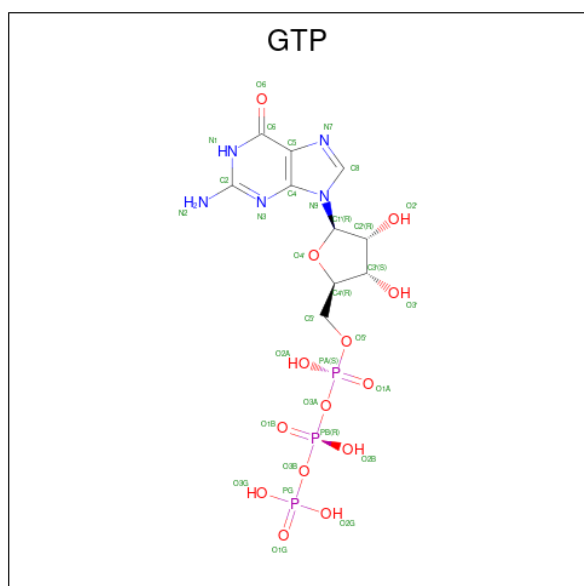
- Molecule 58 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	g	143	Total	C	N	O	S	0	0
			1156	740	220	195	1		

- Molecule 59 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	x	54	Total	C	N	O	P	0	0
			648	270	1	323	54		

- Molecule 60 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
60	w	1	Total	C	N	O	P	0
			32	10	5	14	3	

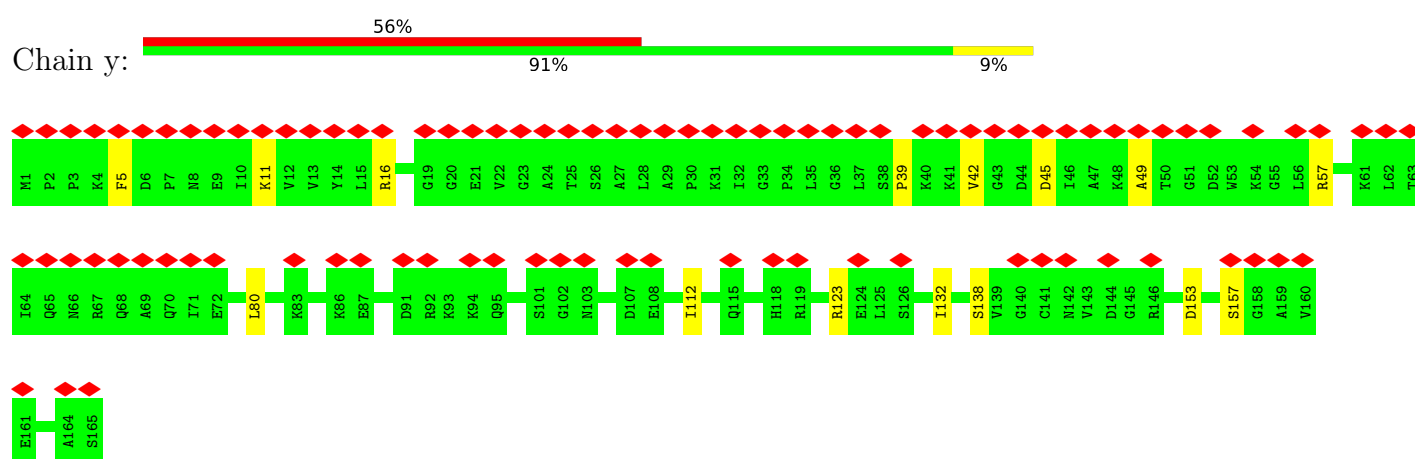
- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
61	w	1	Total	Mg	0
			1	1	

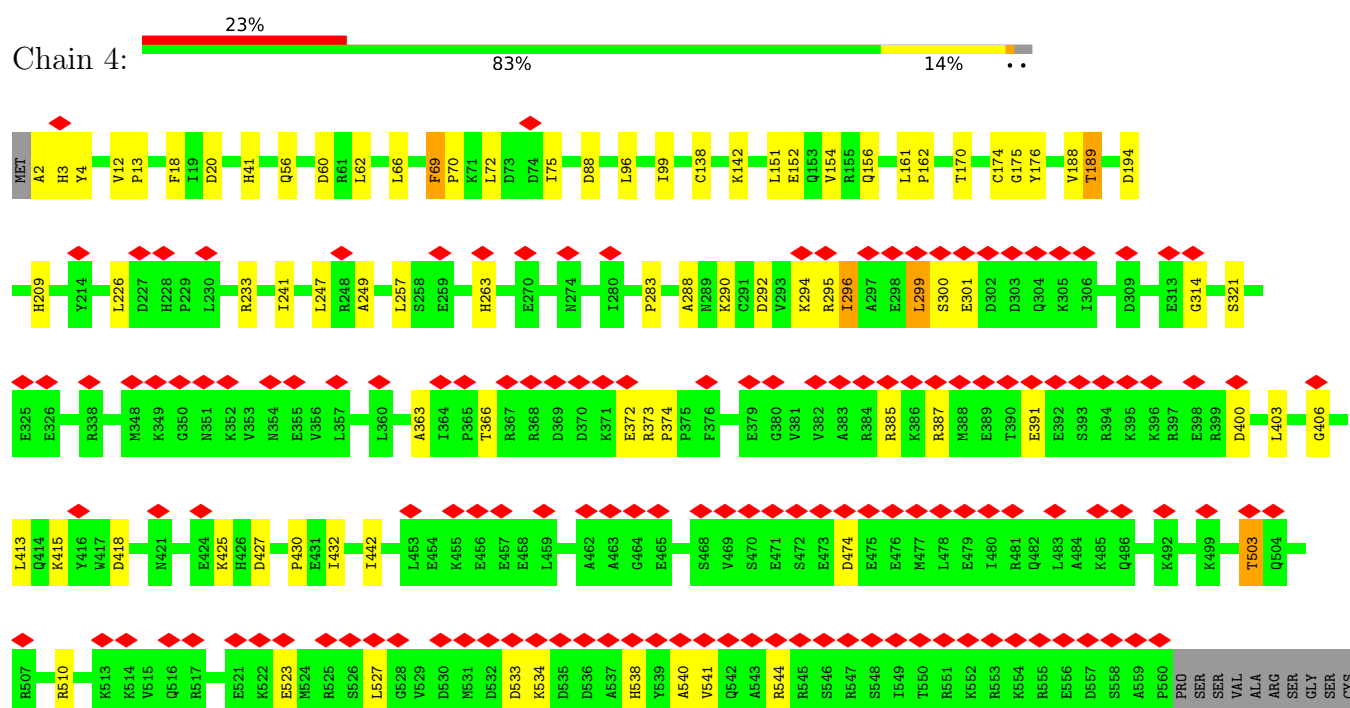
3 Residue-property plots [i](#)

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: 60S ribosomal protein L12

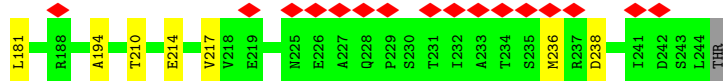
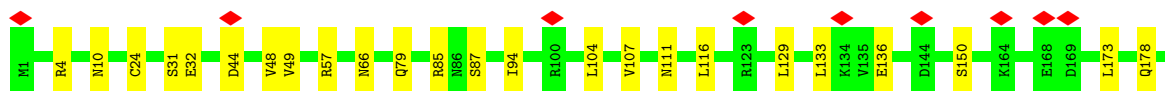
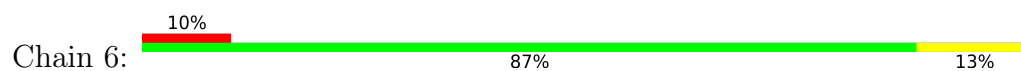


• Molecule 2: GTP-binding protein 4

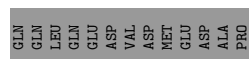
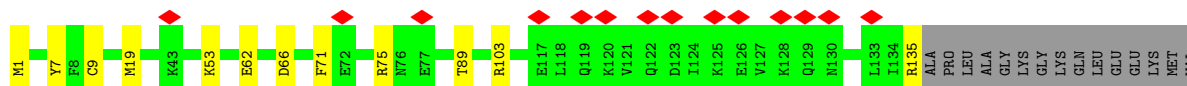
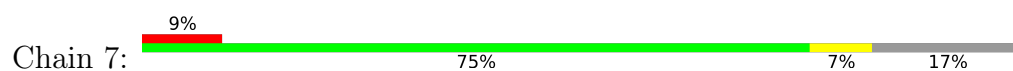




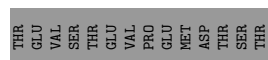
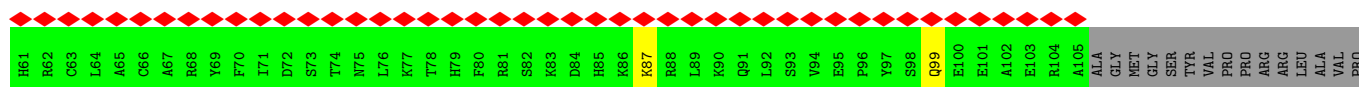
- Molecule 3: Eukaryotic translation initiation factor 6



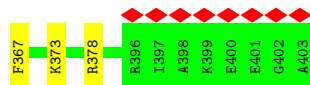
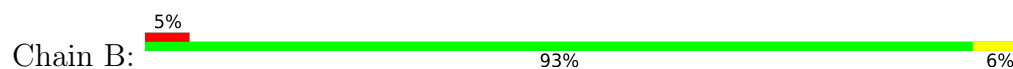
- Molecule 4: Probable ribosome biogenesis protein RLP24



- Molecule 5: Zinc finger protein 593

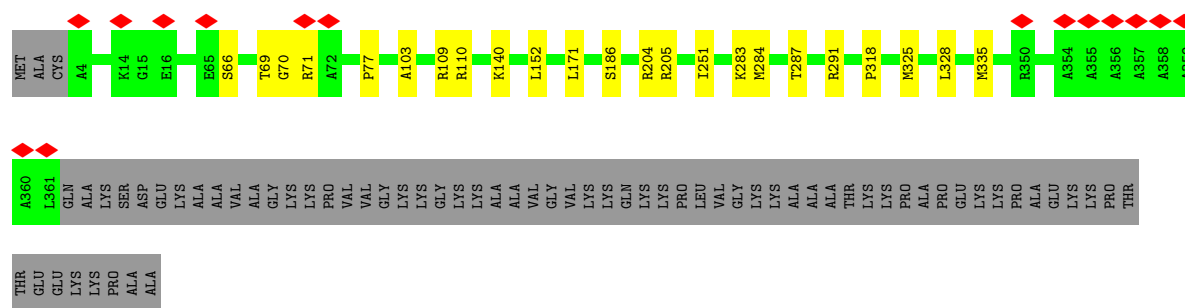


- Molecule 6: 60S ribosomal protein L3



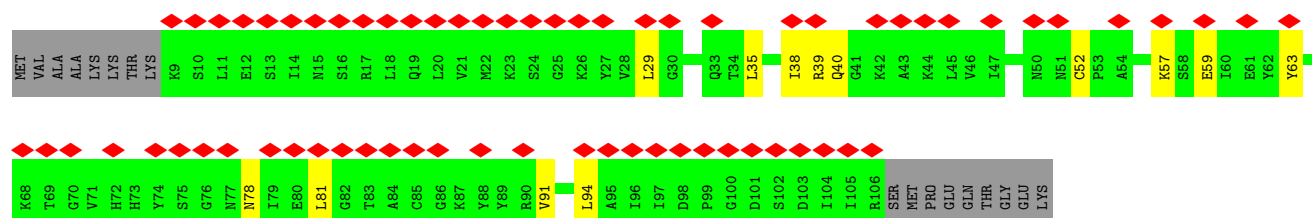
- Molecule 7: 60S ribosomal protein L4

Chain D: 



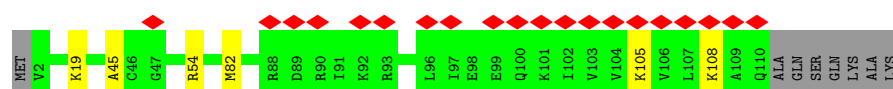
- Molecule 8: 60S ribosomal protein L30

Chain E: 



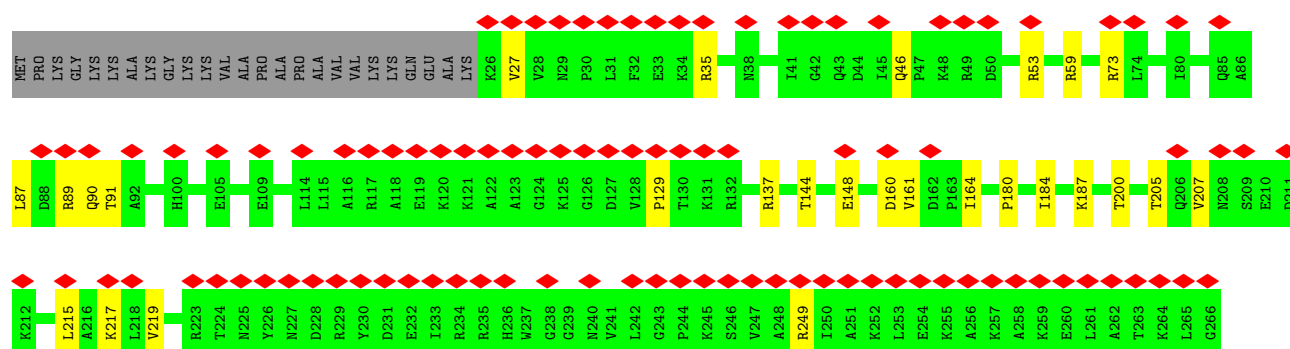
- Molecule 9: 60S ribosomal protein L34

Chain F: 



- Molecule 10: 60S ribosomal protein L7a

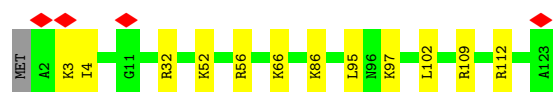
Chain G: 



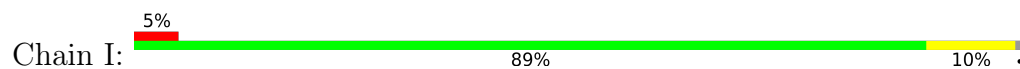
- Molecule 11: 60S ribosomal protein L35

Chain H: 

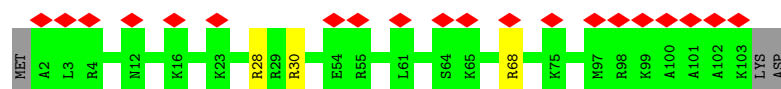




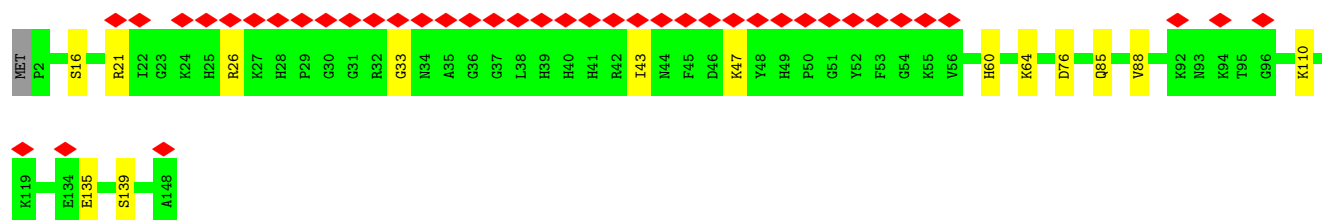
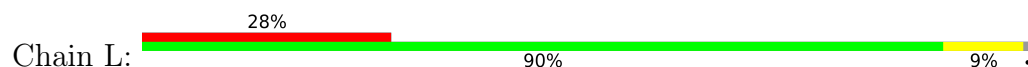
- Molecule 12: 60S ribosomal protein L9



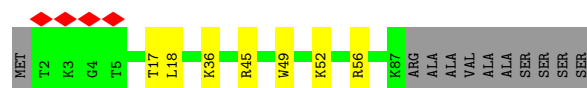
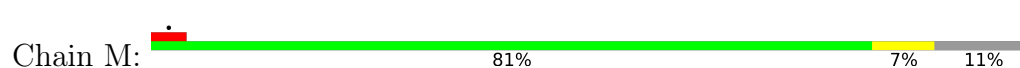
- Molecule 13: 60S ribosomal protein L36



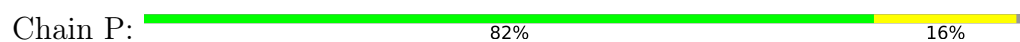
- Molecule 14: 60S ribosomal protein L27a



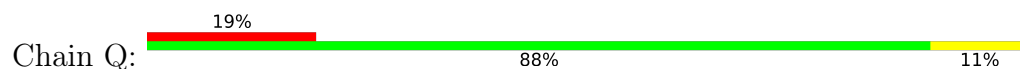
- Molecule 15: 60S ribosomal protein L37

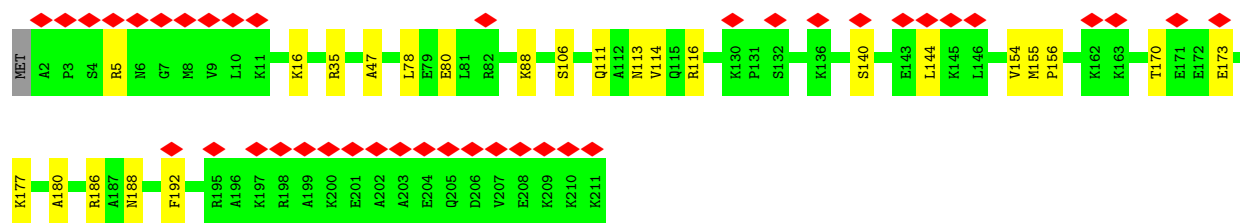


- Molecule 16: 60S ribosomal protein L39

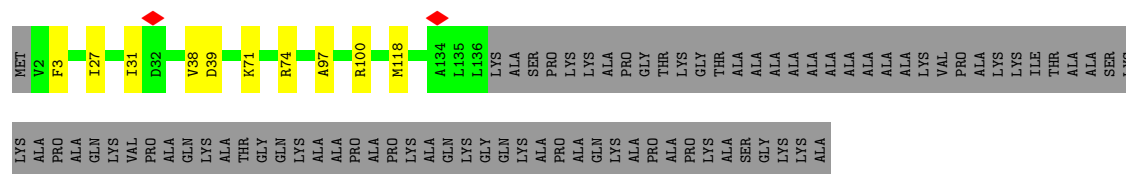


- Molecule 17: 60S ribosomal protein L13

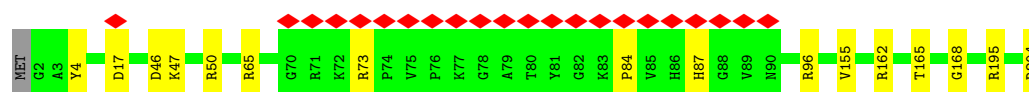
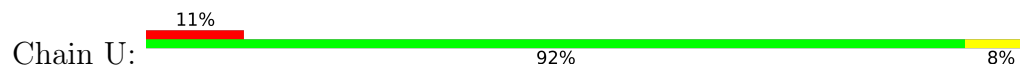




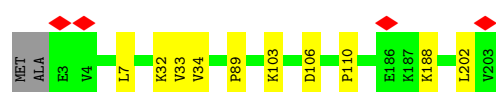
- Molecule 18: 60S ribosomal protein L14



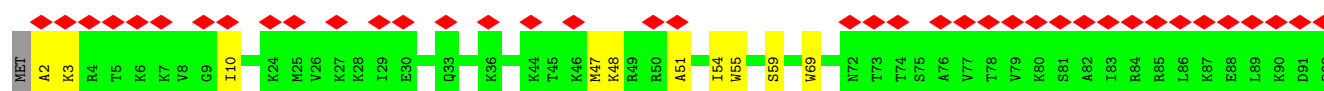
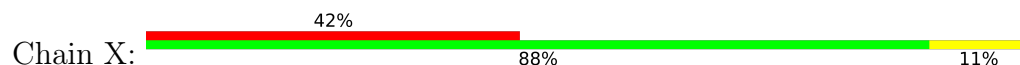
- Molecule 19: 60S ribosomal protein L15



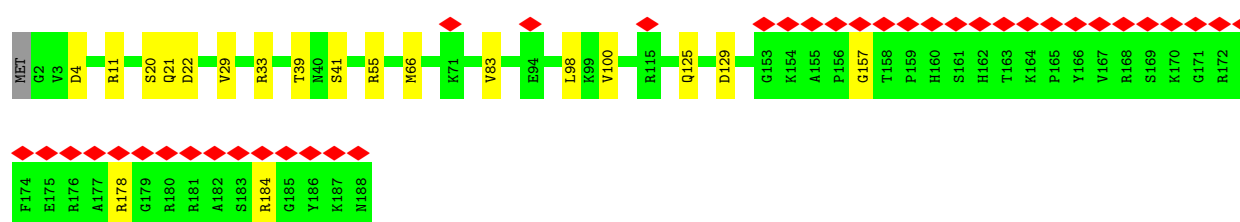
- Molecule 20: 60S ribosomal protein L13a



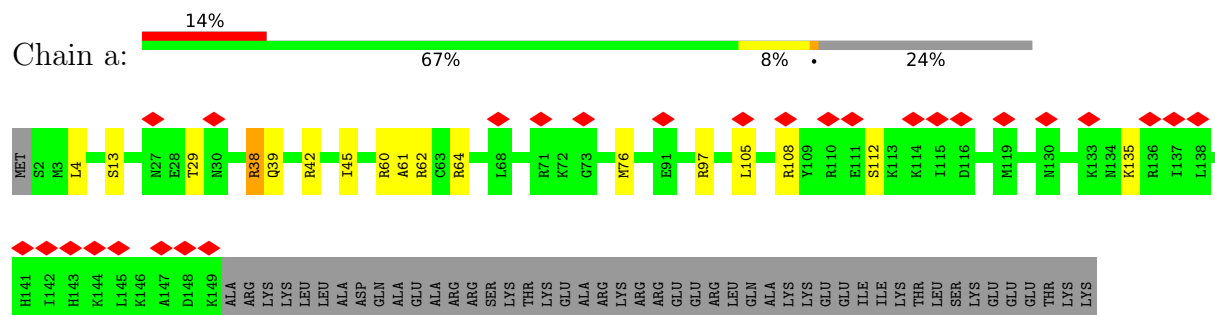
- Molecule 21: 60S ribosomal protein L37a



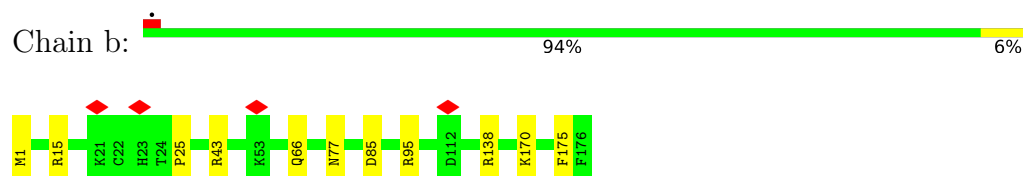
- Molecule 22: 60S ribosomal protein L18



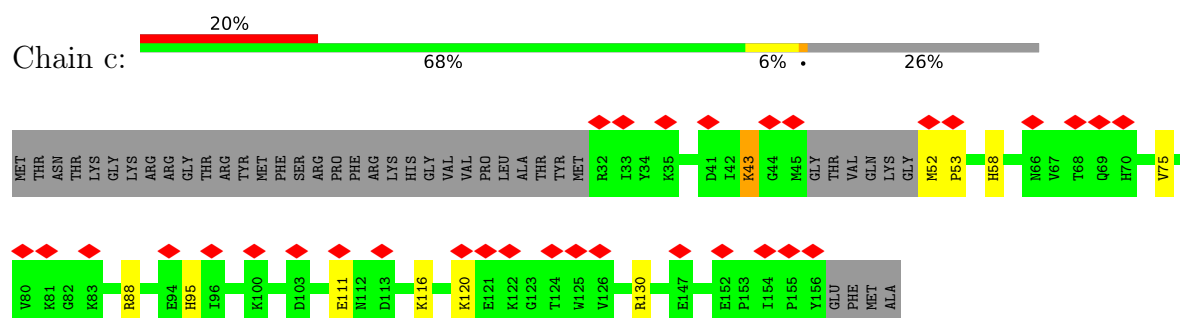
- Molecule 23: 60S ribosomal protein L19



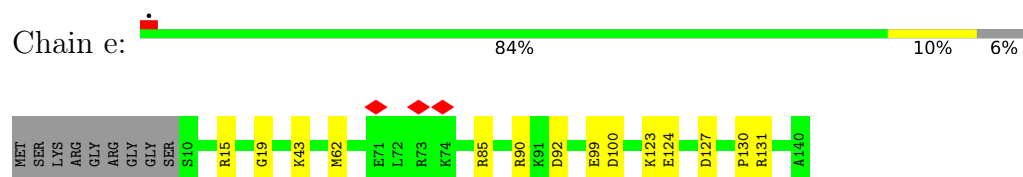
- Molecule 24: 60S ribosomal protein L18a



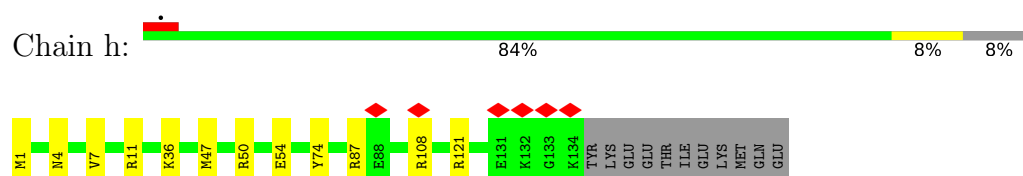
- Molecule 25: 60S ribosomal protein L21



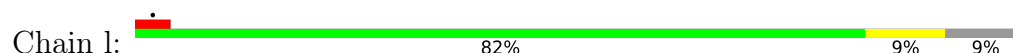
- Molecule 26: 60S ribosomal protein L23

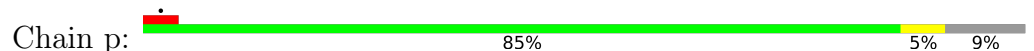


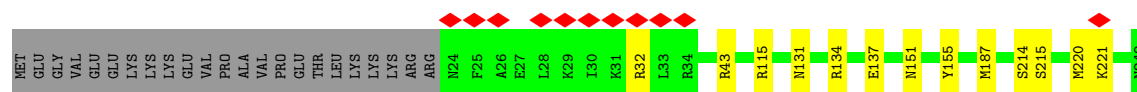
- Molecule 27: 60S ribosomal protein L26



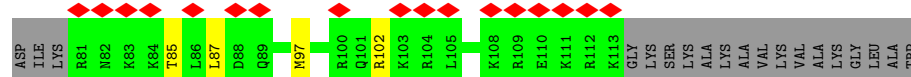
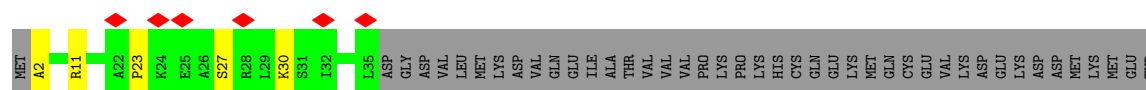
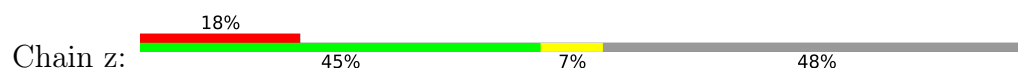
- Molecule 28: 60S ribosomal protein L28



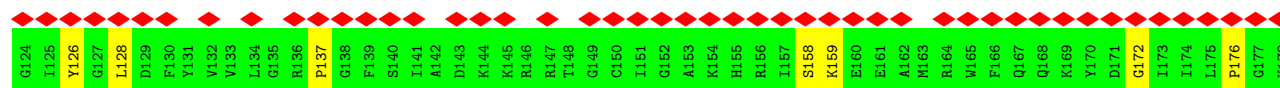
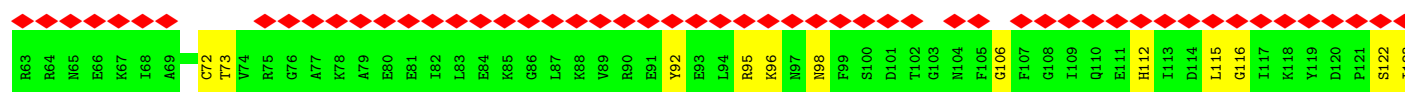
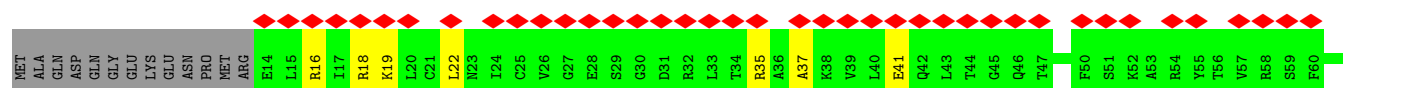
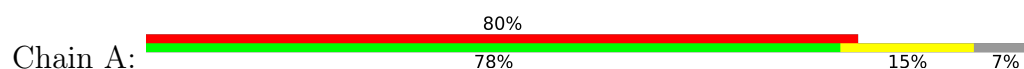




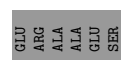
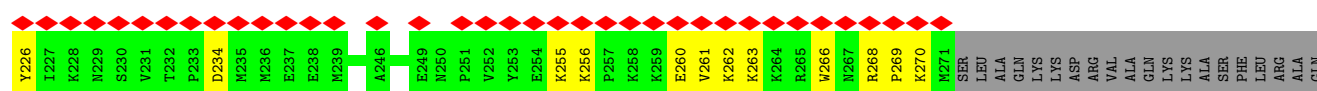
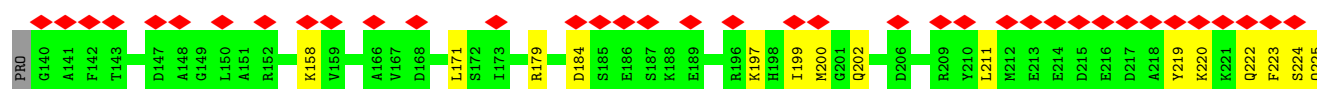
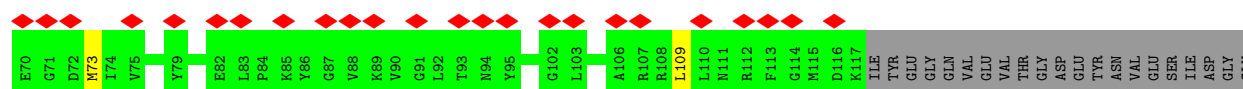
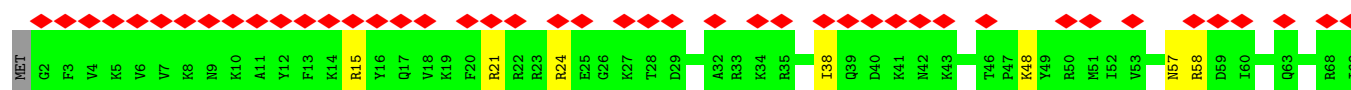
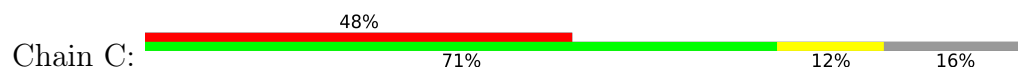
• Molecule 33: Protein LLP homolog

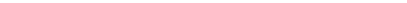


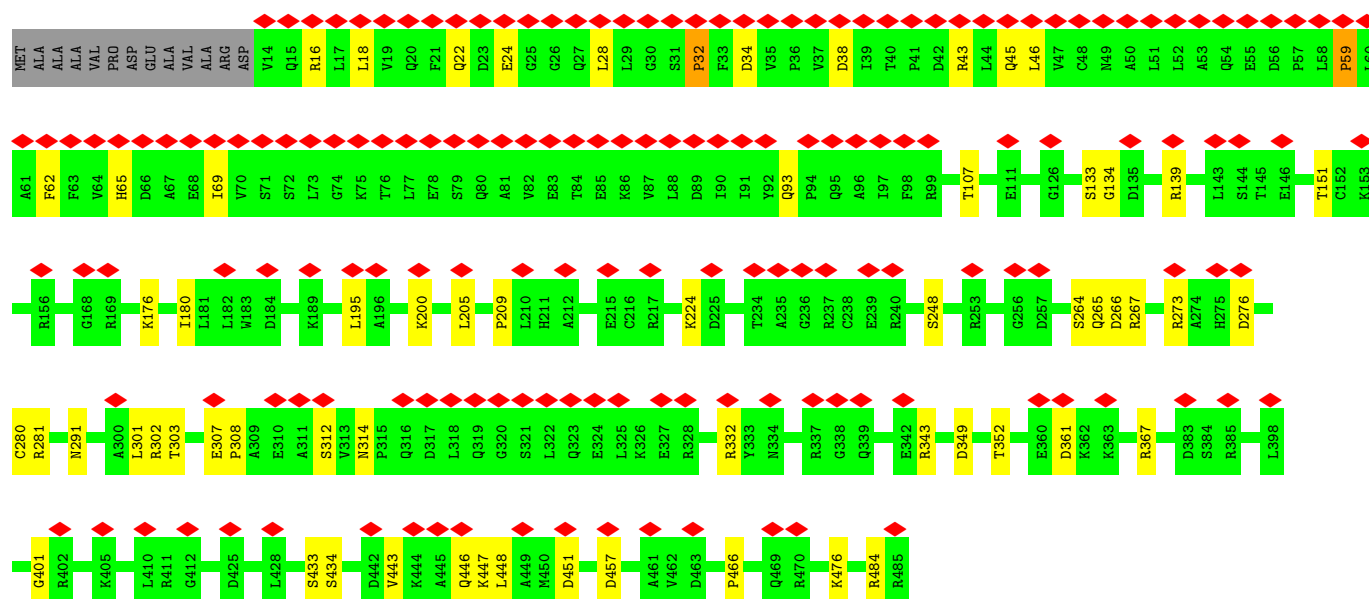
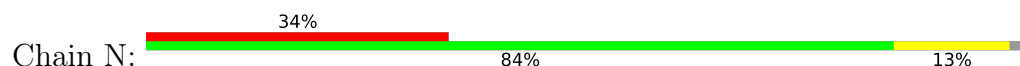
• Molecule 34: 60S ribosomal protein L11



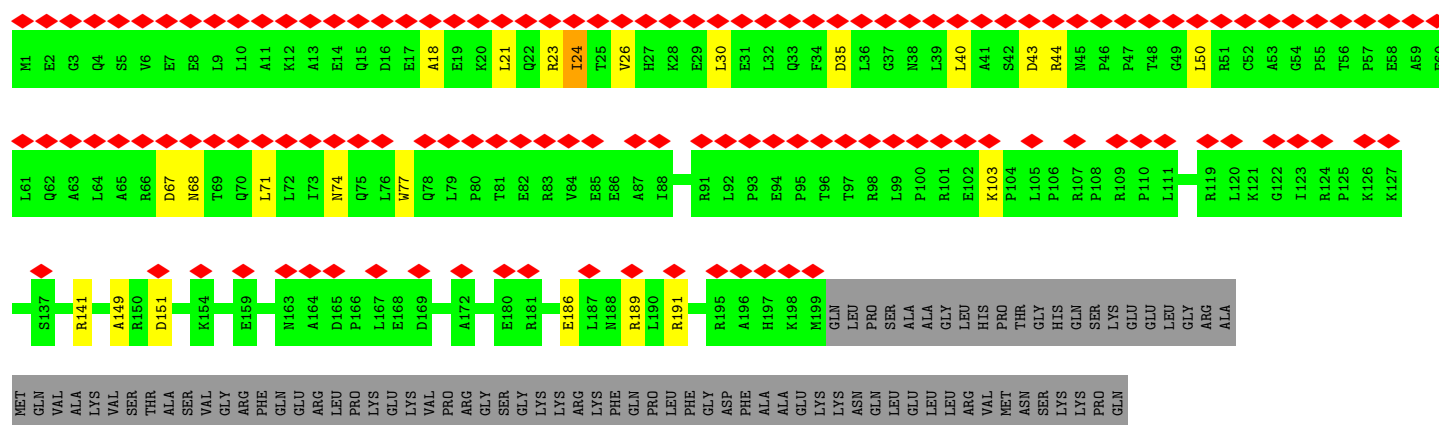
• Molecule 35: 60S ribosomal protein L5

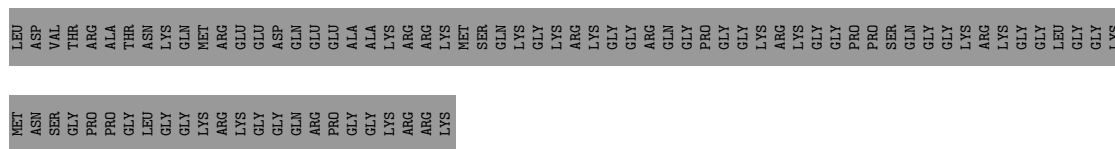


- Chain J:  8% 92% 8%

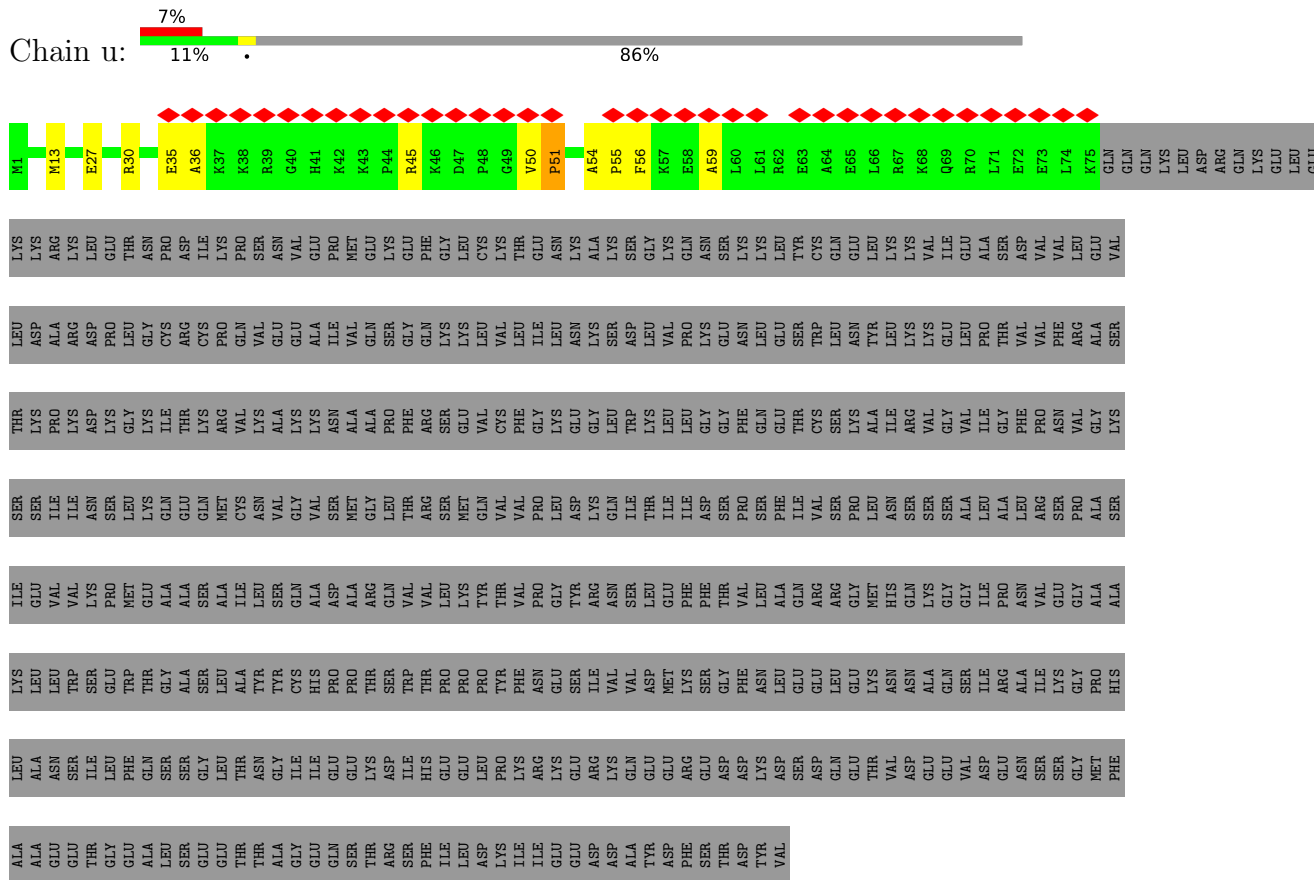


- Molecule 38: Ribosome biogenesis regulatory protein homolog

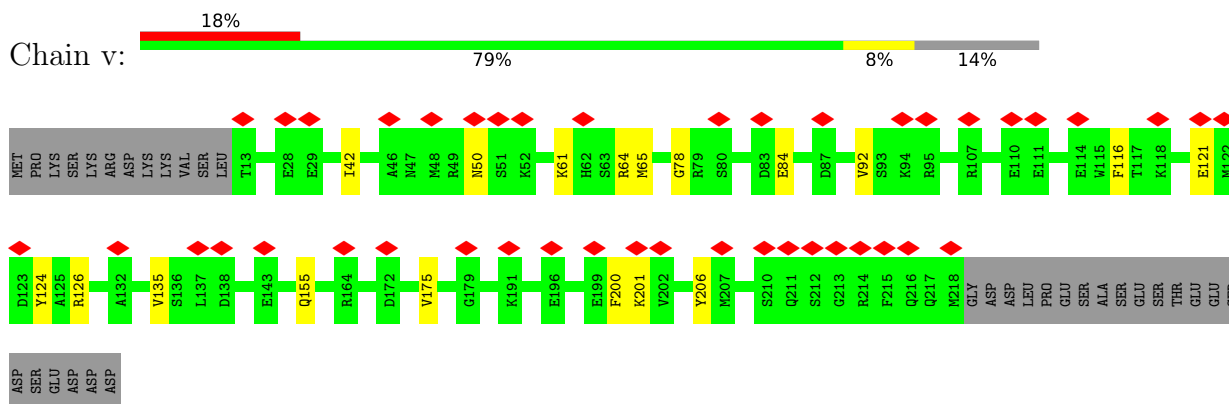




- Molecule 39: Guanine nucleotide-binding protein-like 3

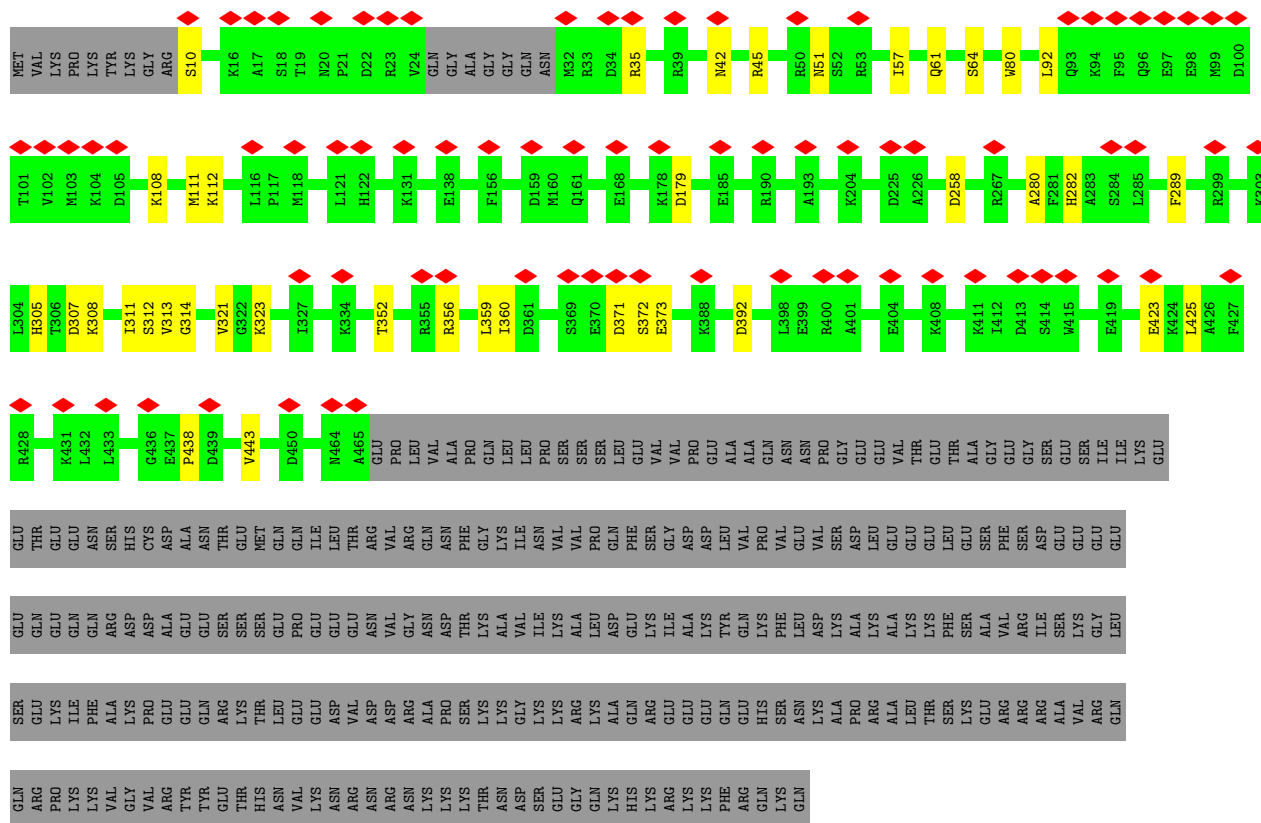


- Molecule 40: mRNA turnover protein 4 homolog

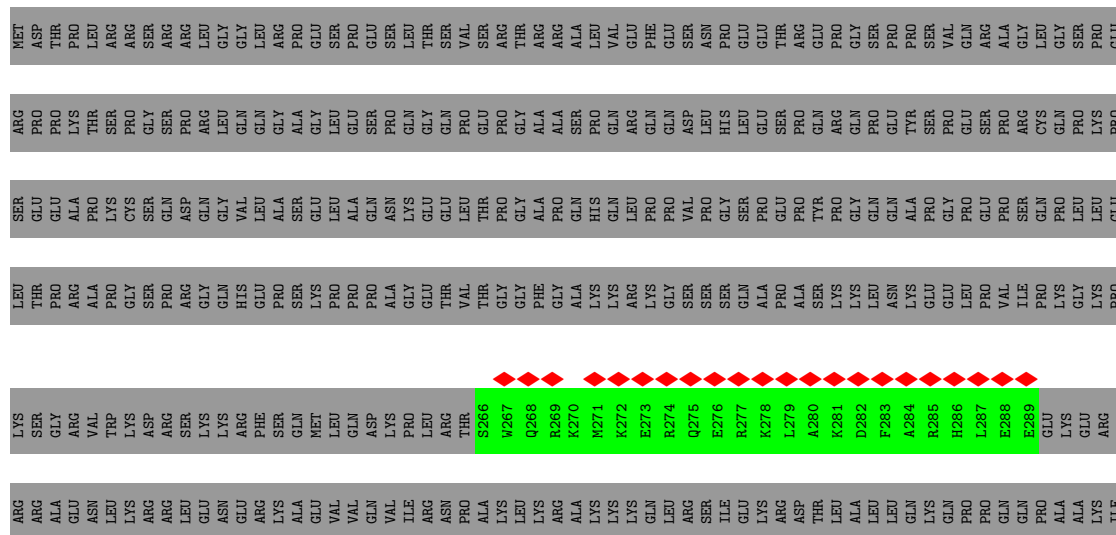


- Molecule 41: G Protein Nucleolar 2



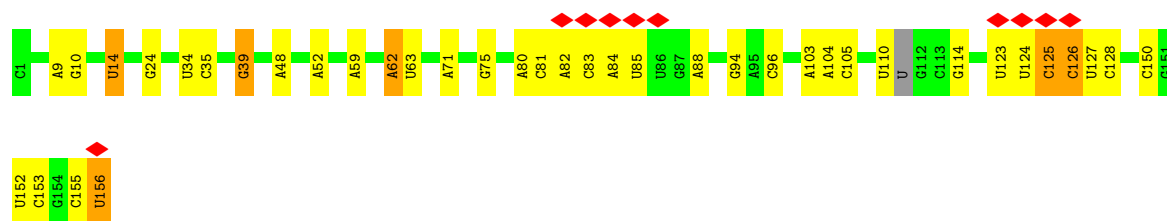


• Molecule 42: Coiled-coil domain-containing protein 86

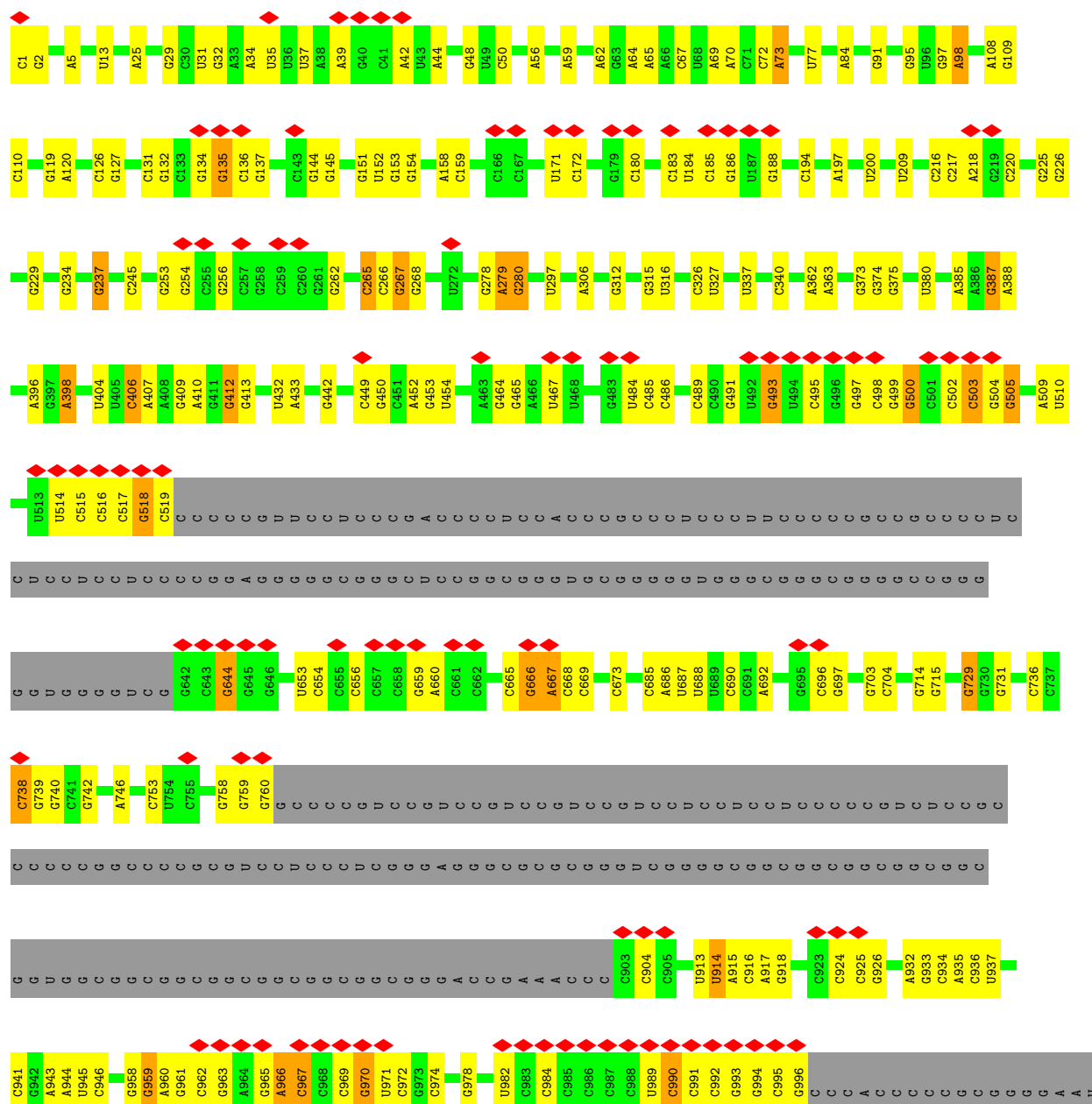
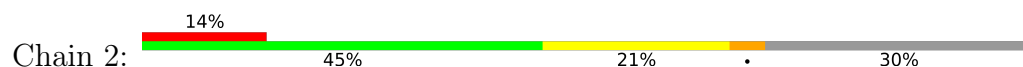


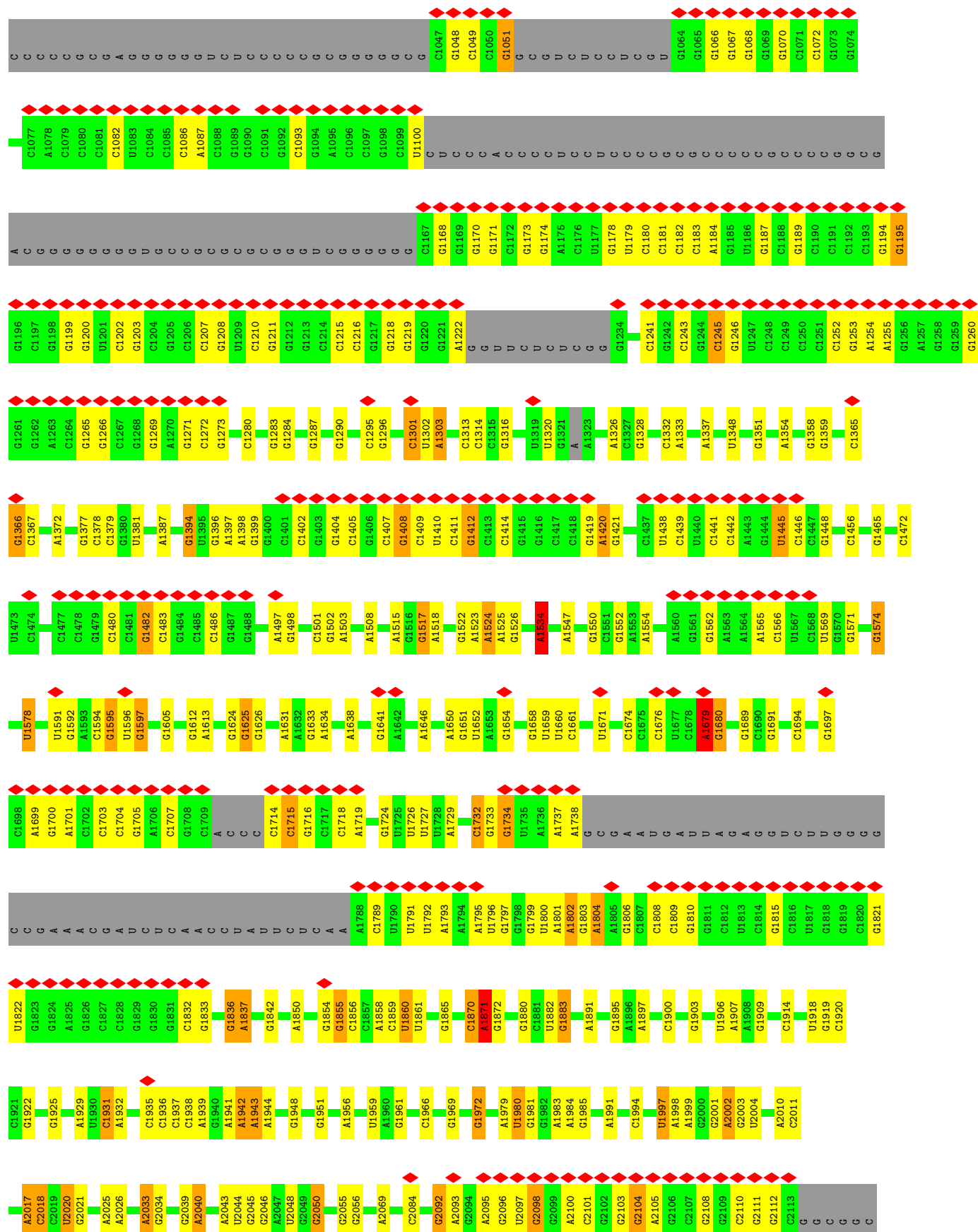
• Molecule 43: 5.8S rRNA



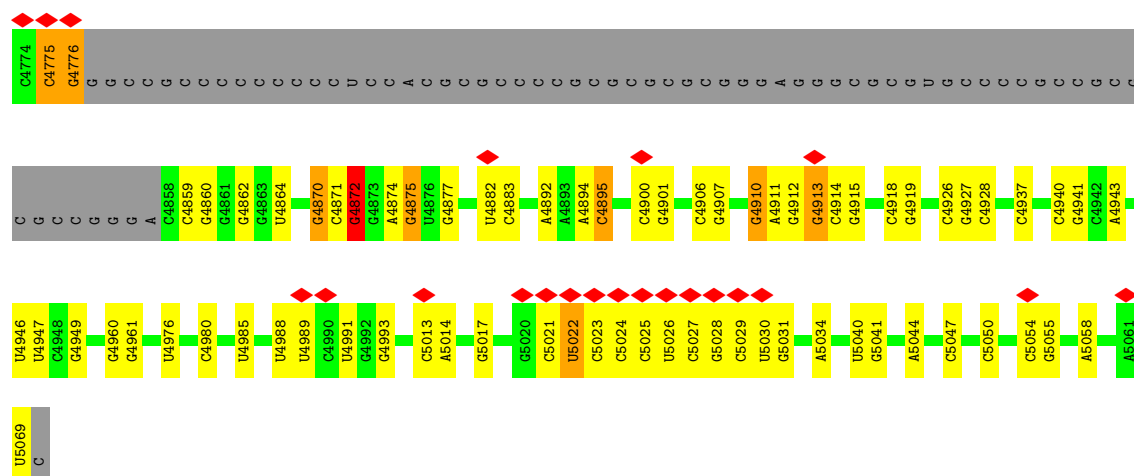


• Molecule 44: 28S rRNA

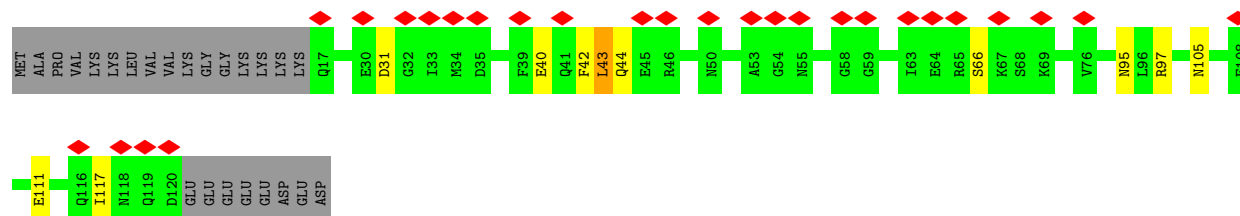




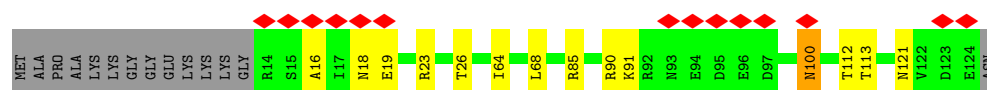
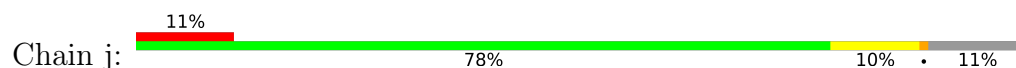




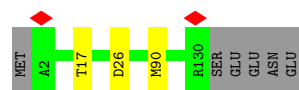
- Molecule 45: 60S ribosomal protein L22



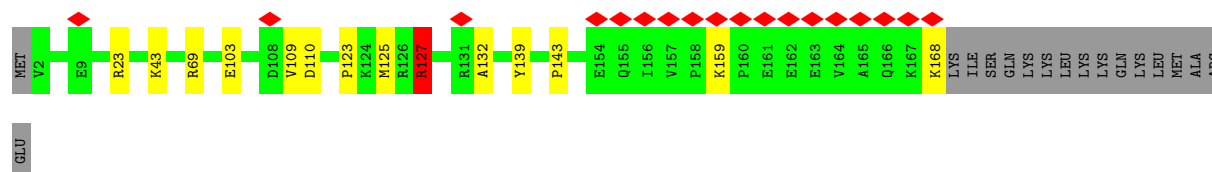
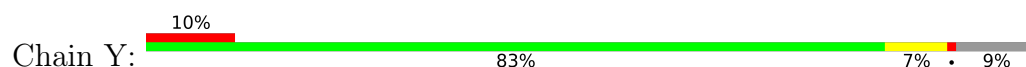
- Molecule 46: 60S ribosomal protein L31



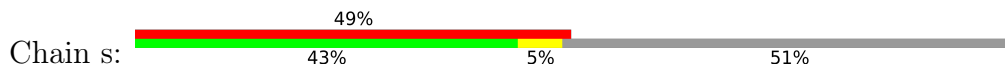
- Molecule 47: 60S ribosomal protein L32



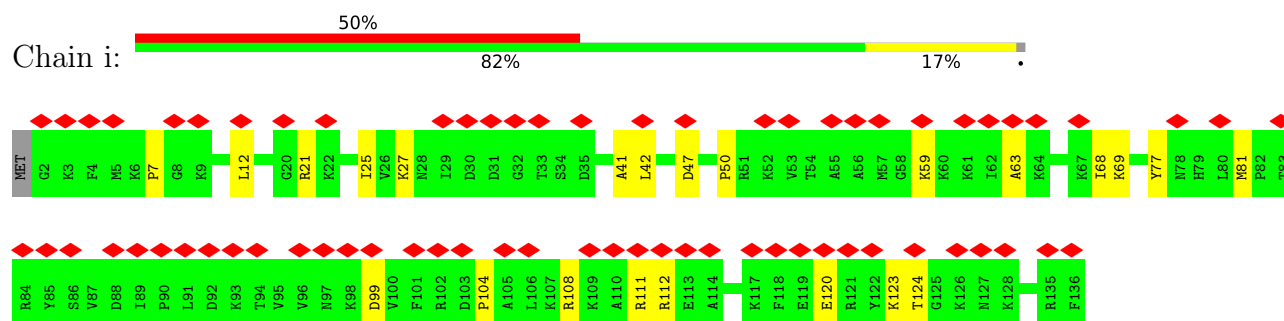
- Molecule 48: 60S ribosomal protein L17



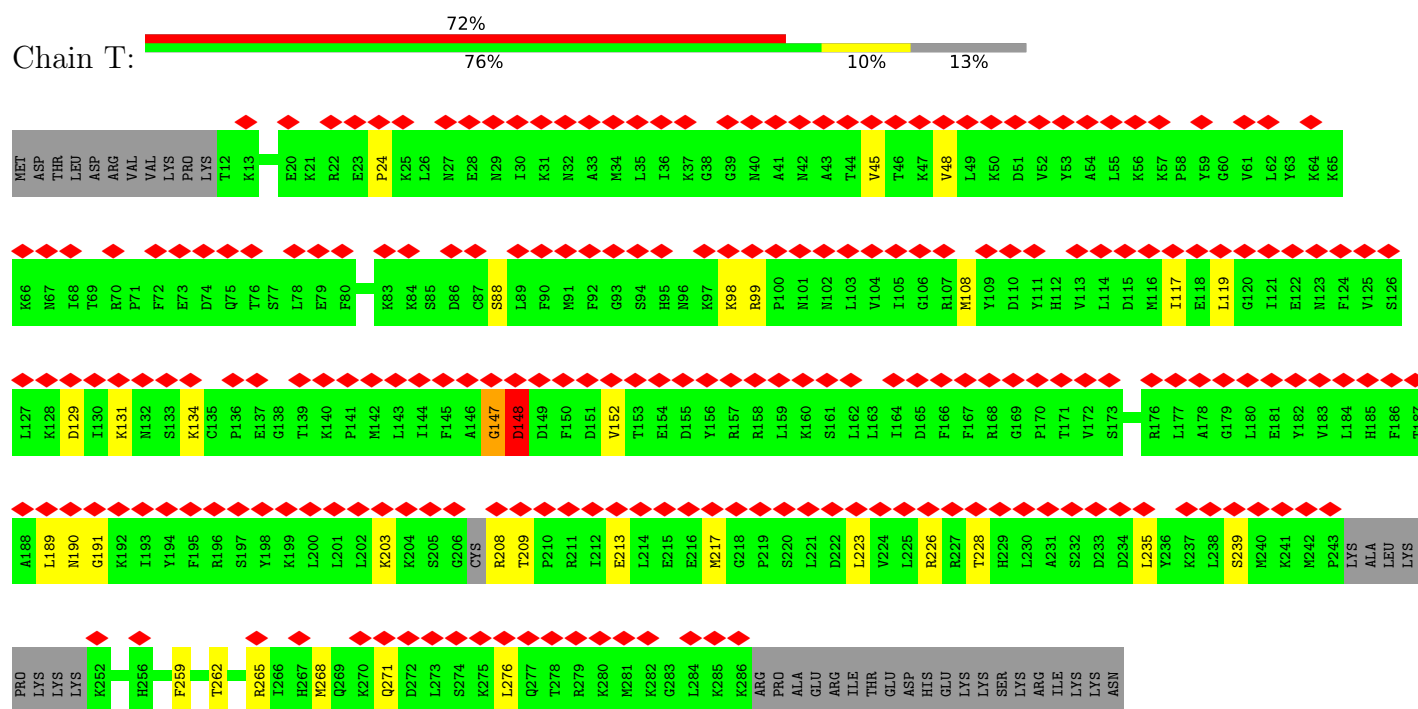
Chain t: 38% 29% 9% 62%



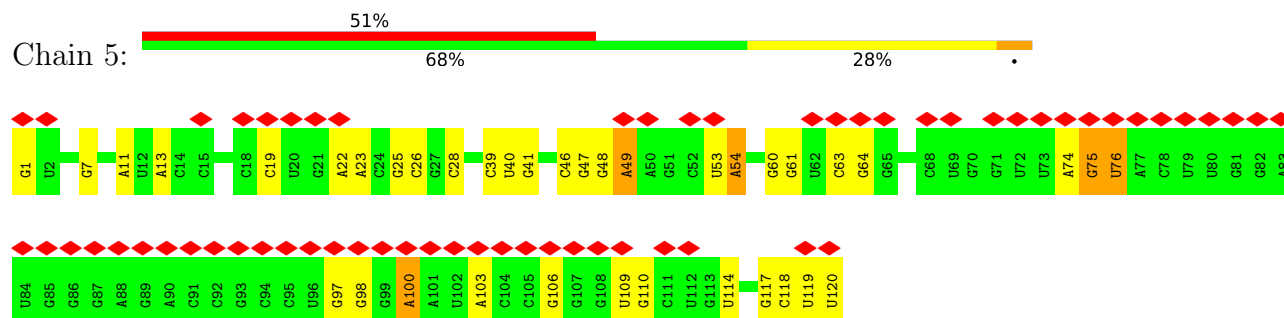
- Molecule 51: 60S ribosomal protein L27



- Molecule 52: Ribosome production factor 2 homolog

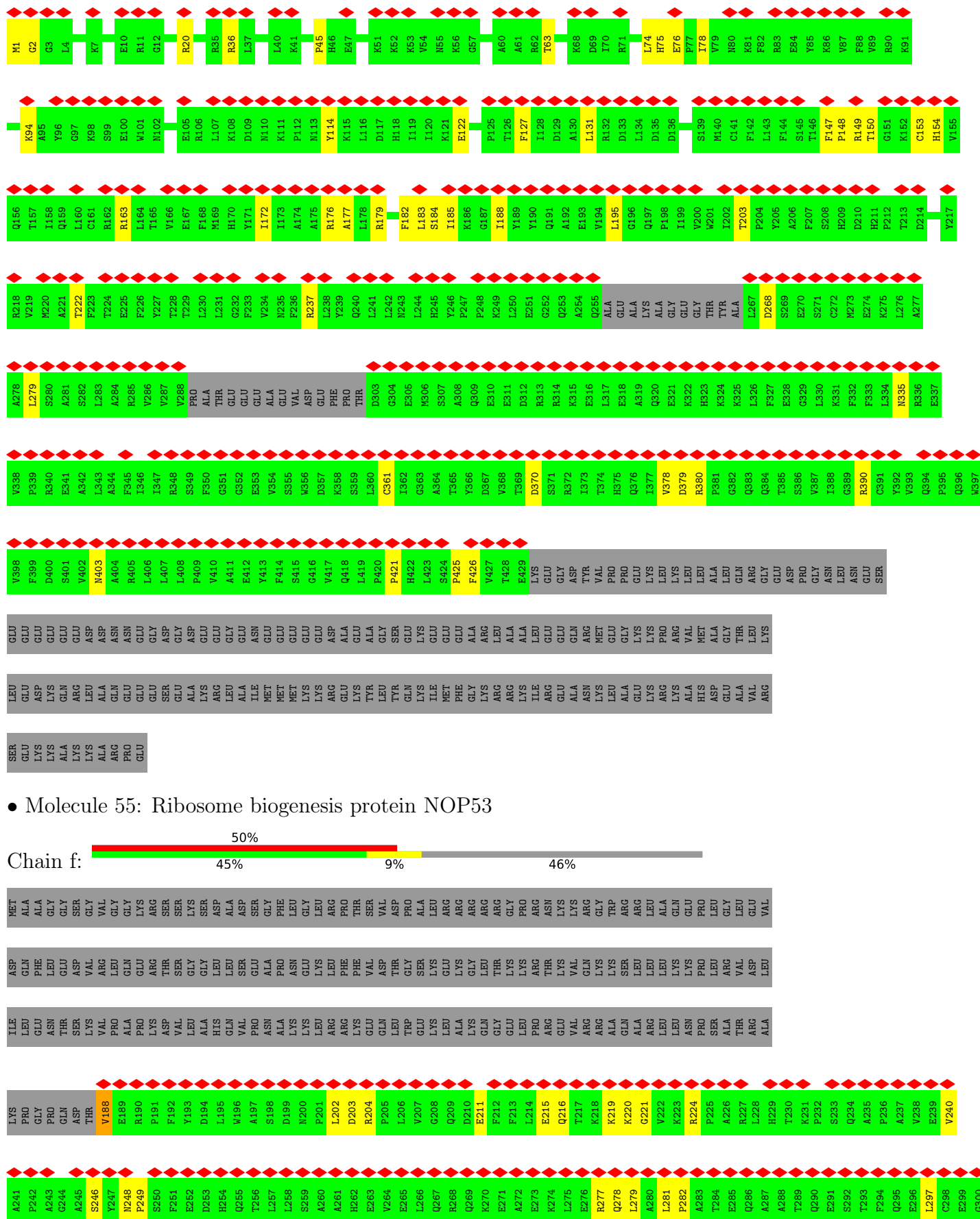


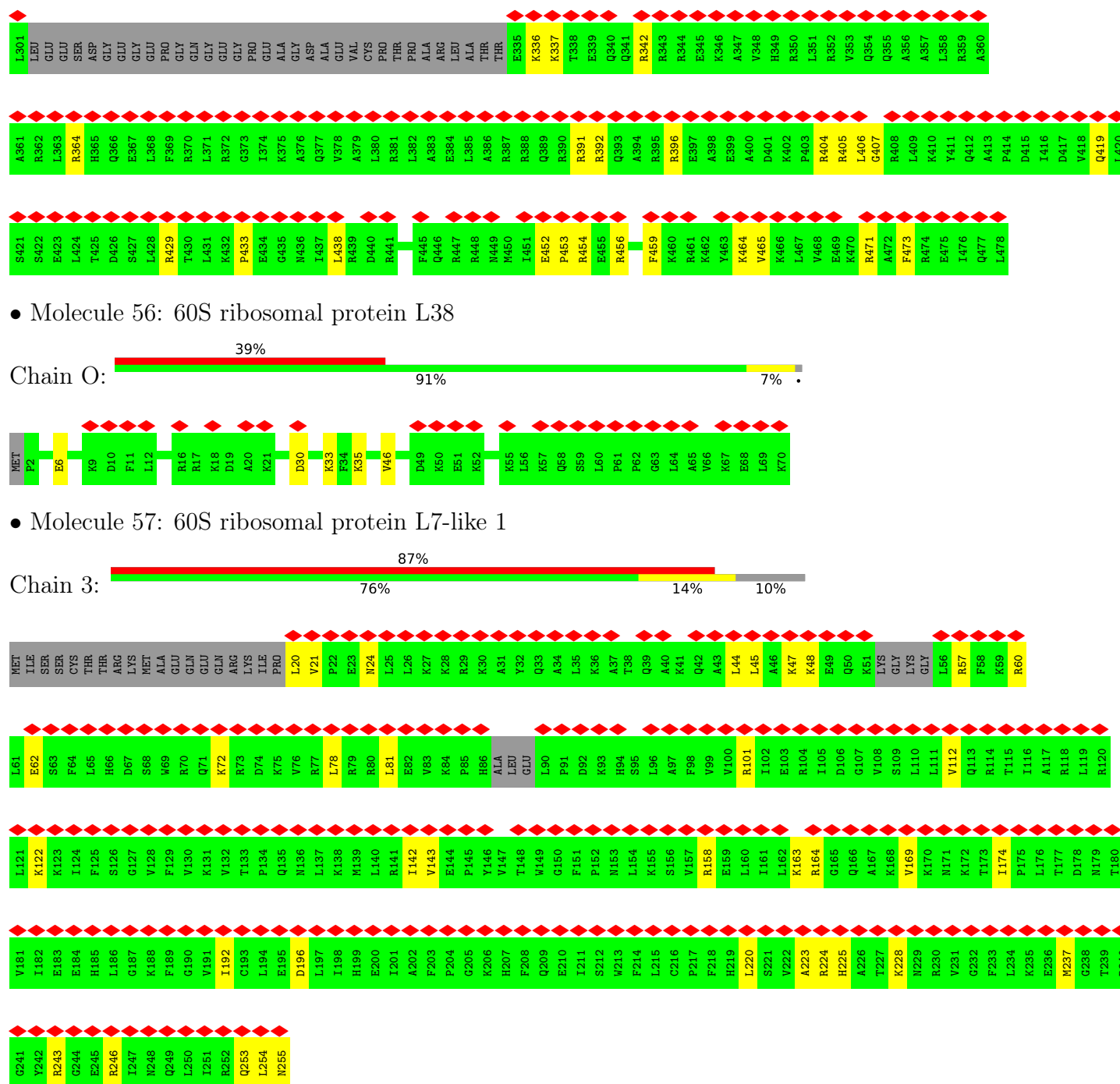
- Molecule 53: 5S RNA



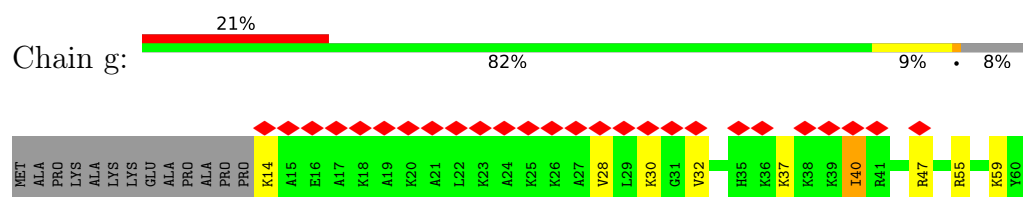
- Molecule 54: Pescadillo homolog

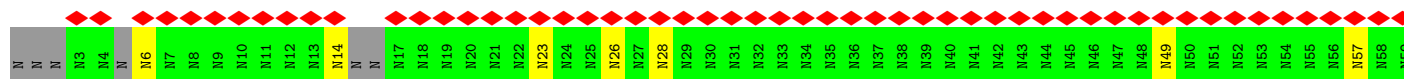






• Molecule 58: 60S ribosomal protein L23a





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18549	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	0.165	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	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: PSU, UR3, B9B, B8W, A2M, E7G, 7MG, B8T, OMG, MG, B9H, OMC, I4U, B8Q, 5MU, P4U, M7A, P7G, OMU, 1MA, B8K, BGH, GTP, 2MG

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	y	0.34	0/1269	0.79	0/1712
2	4	0.38	1/5177 (0.0%)	0.91	24/6942 (0.3%)
3	6	0.34	0/1877	0.74	1/2554 (0.0%)
4	7	0.33	0/1181	0.69	2/1563 (0.1%)
5	9	0.35	0/723	0.84	3/961 (0.3%)
6	B	0.34	1/3315 (0.0%)	0.72	4/4435 (0.1%)
7	D	0.31	0/2907	0.68	3/3905 (0.1%)
8	E	0.34	0/774	0.75	2/1038 (0.2%)
9	F	0.30	0/878	0.63	0/1170
10	G	0.32	0/1971	0.75	4/2651 (0.2%)
11	H	0.31	0/1023	0.60	0/1351
12	I	0.34	0/1537	0.76	2/2066 (0.1%)
13	K	0.30	0/843	0.71	0/1115
14	L	0.27	0/1191	0.62	0/1591
15	M	0.30	0/720	0.68	0/952
16	P	0.30	0/454	0.59	0/599
17	Q	0.32	0/1732	0.67	1/2315 (0.0%)
18	S	0.34	0/1133	0.71	3/1516 (0.2%)
19	U	0.27	0/1746	0.55	0/2338
20	V	0.34	0/1682	0.62	1/2250 (0.0%)
21	X	0.29	0/718	0.72	0/953
22	Z	0.29	0/1537	0.60	1/2052 (0.0%)
23	a	0.30	0/1255	0.76	4/1662 (0.2%)
24	b	0.30	0/1501	0.64	0/2013
25	c	0.33	0/994	0.76	2/1327 (0.2%)
26	e	0.34	0/993	0.74	0/1332
27	h	0.30	0/1132	0.63	0/1504
28	l	0.29	0/1017	0.62	0/1364
29	m	0.33	1/1936 (0.1%)	0.75	0/2596
30	n	0.29	0/895	0.73	3/1198 (0.3%)
31	o	0.32	0/1935	0.73	4/2596 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	p	0.39	1/1916 (0.1%)	0.75	4/2553 (0.2%)
33	z	0.33	0/587	0.80	0/767
34	A	0.32	0/1341	0.81	0/1793
35	C	0.28	0/2068	0.72	2/2767 (0.1%)
36	J	0.30	0/2146	0.66	4/2865 (0.1%)
37	N	0.29	0/3756	0.70	4/5103 (0.1%)
38	R	0.31	0/1668	0.80	4/2255 (0.2%)
39	u	0.40	0/649	0.95	5/851 (0.6%)
40	v	0.30	0/1714	0.69	1/2300 (0.0%)
41	w	0.30	0/3699	0.69	1/4992 (0.0%)
42	r	0.24	0/220	0.72	0/288
43	8	0.30	0/3656	0.47	1/5694 (0.0%)
44	2	0.28	5/83201 (0.0%)	0.49	27/129722 (0.0%)
45	d	0.36	0/864	0.96	6/1160 (0.5%)
46	j	0.32	0/933	0.69	0/1256
47	k	0.32	0/1082	0.68	0/1443
48	Y	0.29	0/1383	0.66	1/1856 (0.1%)
49	t	0.32	0/955	0.77	3/1290 (0.2%)
50	s	0.28	0/1956	0.67	0/2631
51	i	0.32	0/1130	0.75	0/1507
52	T	0.33	0/2204	0.81	4/2944 (0.1%)
53	5	0.23	0/2858	0.41	0/4455
54	q	0.31	0/3395	0.72	1/4578 (0.0%)
55	f	0.49	1/2169 (0.0%)	0.71	5/2902 (0.2%)
56	O	0.38	0/575	0.77	0/761
57	3	0.30	0/1928	0.71	0/2584
58	g	0.39	0/1175	0.69	1/1572 (0.1%)
All	All	0.30	10/175274 (0.0%)	0.61	138/254510 (0.1%)

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	4	0	5
6	B	0	1
7	D	0	1
17	Q	0	1
25	c	0	1
30	n	0	1
39	u	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
48	Y	0	1
49	t	0	1
52	T	0	1
55	f	0	1
All	All	0	17

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	f	188	VAL	C-N	19.48	1.55	1.33
32	p	137	GLU	C-N	8.01	1.40	1.33
44	2	4405	G	C1'-N9	-6.39	1.37	1.47
44	2	4399	U	C1'-N1	5.95	1.56	1.47
44	2	4403	U	C1'-N1	5.94	1.57	1.48
29	m	149	LYS	C-N	-5.71	1.23	1.33
2	4	175	GLY	C-N	-5.42	1.25	1.33
44	2	4404	U	C1'-N1	5.42	1.55	1.47
6	B	240	LEU	C-N	5.18	1.39	1.33
44	2	4523	A2M	O3'-P	5.11	1.61	1.56

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	1871	A2M	OP2-P-O3'	-16.21	69.55	105.20
44	2	1871	A2M	OP1-P-O3'	14.68	137.48	105.20
44	2	1872	G	OP1-P-OP2	-13.46	79.22	119.60
55	f	188	VAL	O-C-N	-10.18	106.72	123.00
2	4	314	GLY	CA-C-N	10.15	134.90	122.42
2	4	314	GLY	C-N-CA	10.15	134.90	122.42
2	4	175	GLY	CA-C-N	9.70	135.43	120.68
2	4	175	GLY	C-N-CA	9.70	135.43	120.68
44	2	1872	G	O5'-P-OP1	-9.35	79.96	108.00
36	J	105	MET	CA-C-N	9.30	138.71	121.97
36	J	105	MET	C-N-CA	9.30	138.71	121.97
2	4	75	ILE	N-CA-C	9.26	119.16	110.74
38	R	23	ARG	CA-C-N	8.94	138.05	121.97
38	R	23	ARG	C-N-CA	8.94	138.05	121.97
55	f	188	VAL	CA-C-N	8.56	137.85	122.62
55	f	188	VAL	C-N-CA	8.56	137.85	122.62
52	T	147	GLY	CA-C-N	8.48	136.97	121.70
52	T	147	GLY	C-N-CA	8.48	136.97	121.70
37	N	266	ASP	CA-C-N	8.04	136.89	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	266	ASP	C-N-CA	8.04	136.89	121.54
44	2	1931	C	C2'-C3'-O3'	7.82	121.23	109.50
2	4	503	THR	CA-C-N	7.41	135.04	121.70
2	4	503	THR	C-N-CA	7.41	135.04	121.70
44	2	1872	G	O5'-P-OP2	6.79	128.36	108.00
55	f	202	LEU	CA-C-N	6.74	134.41	121.54
55	f	202	LEU	C-N-CA	6.74	134.41	121.54
48	Y	127	ARG	CG-CD-NE	6.66	126.65	112.00
30	n	106	TYR	N-CA-C	6.57	124.33	109.81
23	a	76	MET	CA-C-N	6.55	134.25	121.41
23	a	76	MET	C-N-CA	6.55	134.25	121.41
30	n	105	LEU	CA-C-N	6.40	137.42	121.80
30	n	105	LEU	C-N-CA	6.40	137.42	121.80
38	R	151	ASP	CA-C-N	6.36	133.68	121.54
38	R	151	ASP	C-N-CA	6.36	133.68	121.54
2	4	406	GLY	CA-C-N	6.32	133.62	121.54
2	4	406	GLY	C-N-CA	6.32	133.62	121.54
6	B	67	VAL	CB-CA-C	6.29	121.60	111.29
4	7	7	TYR	CA-C-N	6.23	133.44	121.54
4	7	7	TYR	C-N-CA	6.23	133.44	121.54
7	D	318	PRO	CA-C-N	6.15	133.29	121.54
7	D	318	PRO	C-N-CA	6.15	133.29	121.54
32	p	220	MET	CA-C-N	6.14	133.28	121.54
32	p	220	MET	C-N-CA	6.14	133.28	121.54
52	T	147	GLY	CA-C-O	-6.13	115.55	121.06
45	d	43	LEU	CA-CB-CG	6.11	137.67	116.30
37	N	32	PRO	CA-N-CD	-6.07	103.50	112.00
44	2	2470	C	P-O3'-C3'	6.04	129.26	120.20
44	2	914	U	P-O3'-C3'	6.03	129.25	120.20
37	N	59	PRO	CA-N-CD	-6.02	103.58	112.00
23	a	38	ARG	CA-C-N	6.00	133.01	121.54
23	a	38	ARG	C-N-CA	6.00	133.01	121.54
2	4	174	CYS	CA-C-N	-5.97	116.81	121.82
2	4	174	CYS	C-N-CA	-5.97	116.81	121.82
20	V	110	PRO	N-CA-C	5.95	117.96	110.70
43	8	125	C	P-O3'-C3'	5.93	129.10	120.20
10	G	27	VAL	N-CA-C	-5.90	107.54	113.20
8	E	59	GLU	N-CA-CB	5.89	119.40	110.28
2	4	188	VAL	N-CA-C	-5.87	101.28	109.45
44	2	1679	A	P-O3'-C3'	5.82	128.93	120.20
44	2	4555	U	C4'-C3'-O3'	5.76	118.03	109.40
6	B	67	VAL	N-CA-CB	-5.74	101.76	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	4555	U	C2'-C3'-O3'	5.74	118.11	109.50
44	2	2760	G	P-O3'-C3'	5.72	128.78	120.20
44	2	4228	G	P-O3'-C3'	5.71	128.76	120.20
41	w	321	VAL	N-CA-C	-5.65	107.77	113.47
3	6	236	MET	CB-CG-SD	5.62	129.57	112.70
2	4	41	HIS	CA-C-N	5.59	136.35	126.45
2	4	41	HIS	C-N-CA	5.59	136.35	126.45
2	4	12	VAL	CA-CB-CG1	5.57	119.86	110.40
32	p	221	LYS	CA-C-N	5.57	132.17	121.54
32	p	221	LYS	C-N-CA	5.57	132.17	121.54
2	4	391	GLU	CA-C-N	5.54	132.12	121.54
2	4	391	GLU	C-N-CA	5.54	132.12	121.54
2	4	430	PRO	CA-C-N	5.51	132.07	121.54
2	4	430	PRO	C-N-CA	5.51	132.07	121.54
45	d	44	GLN	N-CA-CB	5.51	118.06	110.07
44	2	4269	G	P-O3'-C3'	5.50	128.45	120.20
2	4	72	LEU	N-CA-C	5.47	119.46	112.34
31	o	280	GLY	CA-C-N	5.46	128.76	120.13
31	o	280	GLY	C-N-CA	5.46	128.76	120.13
44	2	406	C	C2'-C3'-O3'	5.44	121.86	113.70
44	2	406	C	P-O3'-C3'	5.43	128.34	120.20
31	o	236	GLU	CA-C-N	5.42	131.89	121.54
31	o	236	GLU	C-N-CA	5.42	131.89	121.54
49	t	50	ARG	CA-C-N	5.42	130.54	122.74
49	t	50	ARG	C-N-CA	5.42	130.54	122.74
17	Q	47	ALA	N-CA-C	5.40	121.75	109.81
35	C	234	ASP	CA-C-N	5.40	131.03	122.61
35	C	234	ASP	C-N-CA	5.40	131.03	122.61
54	q	279	LEU	CA-CB-CG	5.40	135.19	116.30
44	2	4235	G	C2'-C3'-O3'	5.40	121.80	113.70
6	B	294	LYS	N-CA-C	-5.39	107.95	114.75
6	B	360	LEU	CA-CB-CG	5.39	135.18	116.30
39	u	35	GLU	CA-C-N	5.38	131.50	123.05
39	u	35	GLU	C-N-CA	5.38	131.50	123.05
44	2	3905	A	P-O3'-C3'	5.38	128.28	120.20
25	c	111	GLU	N-CA-CB	5.38	118.62	110.28
39	u	13	MET	CA-C-N	5.38	131.81	121.54
39	u	13	MET	C-N-CA	5.38	131.81	121.54
44	2	914	U	C2'-C3'-O3'	5.37	117.56	109.50
44	2	1980	U	P-O3'-C3'	5.33	128.20	120.20
45	d	66	SER	CA-C-N	5.31	131.68	121.54
45	d	66	SER	C-N-CA	5.31	131.68	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	4229	U	P-O3'-C3'	5.29	128.14	120.20
44	2	4913	G	P-O3'-C3'	5.29	128.13	120.20
8	E	40	GLN	CA-CB-CG	5.25	124.60	114.10
44	2	2033	A	P-O3'-C3'	5.24	128.06	120.20
18	S	31	ILE	CA-C-N	5.22	131.50	121.54
18	S	31	ILE	C-N-CA	5.22	131.50	121.54
12	I	60	TRP	CA-C-N	5.20	130.01	122.36
12	I	60	TRP	C-N-CA	5.20	130.01	122.36
2	4	88	ASP	CA-C-N	5.18	131.44	121.54
2	4	88	ASP	C-N-CA	5.18	131.44	121.54
45	d	42	PHE	CA-C-N	-5.18	114.36	122.65
45	d	42	PHE	C-N-CA	-5.18	114.36	122.65
44	2	4572	U	C3'-C2'-O2'	5.17	118.46	110.70
5	9	19	MET	CB-CG-SD	5.16	128.19	112.70
18	S	118	MET	CB-CG-SD	5.16	128.18	112.70
58	g	40	ILE	CA-CB-CG2	5.15	119.26	110.50
10	G	205	THR	CB-CA-C	5.14	120.64	110.42
5	9	4	SER	CA-C-N	5.14	133.14	122.41
5	9	4	SER	C-N-CA	5.14	133.14	122.41
22	Z	83	VAL	CG1-CB-CG2	-5.12	99.54	110.80
44	2	1980	U	C2'-C3'-O3'	5.12	117.18	109.50
44	2	2487	G	P-O3'-C3'	5.11	127.86	120.20
52	T	148	ASP	N-CA-C	5.08	125.23	111.00
39	u	51	PRO	CA-N-CD	-5.08	104.89	112.00
25	c	111	GLU	CB-CG-CD	5.07	121.22	112.60
36	J	100	LYS	CA-C-N	5.07	131.09	121.97
36	J	100	LYS	C-N-CA	5.07	131.09	121.97
40	v	155	GLN	N-CA-CB	5.07	118.92	110.41
44	2	2474	G	P-O3'-C3'	5.06	127.79	120.20
7	D	325	MET	CB-CG-SD	5.06	127.88	112.70
2	4	3	HIS	CA-C-N	5.05	131.18	121.54
2	4	3	HIS	C-N-CA	5.05	131.18	121.54
49	t	130	LEU	CA-CB-CG	5.04	133.96	116.30
10	G	129	PRO	CA-C-N	5.04	129.48	122.08
10	G	129	PRO	C-N-CA	5.04	129.48	122.08

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	4	189	THR	Peptide
2	4	299	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	4	300	SER	Peptide
2	4	503	THR	Peptide
2	4	69	PHE	Peptide
6	B	241	PRO	Peptide
7	D	171	LEU	Peptide
17	Q	154	VAL	Peptide
52	T	190	ASN	Peptide
48	Y	127	ARG	Sidechain
25	c	52	MET	Peptide
55	f	204	ARG	Peptide
30	n	106	TYR	Peptide
49	t	142	SER	Peptide
39	u	36	ALA	Peptide
39	u	50	VAL	Peptide
39	u	54	ALA	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	y	1250	0	1305	10	0
2	4	5093	0	5239	49	0
3	6	1852	0	1828	19	0
4	7	1159	0	1224	9	0
5	9	711	0	724	5	0
6	B	3244	0	3389	16	0
7	D	2853	0	3028	18	0
8	E	764	0	804	6	0
9	F	868	0	963	5	0
10	G	1935	0	2087	30	0
11	H	1015	0	1148	11	0
12	I	1518	0	1601	10	0
13	K	832	0	917	3	0
14	L	1162	0	1213	11	0
15	M	705	0	741	5	0
16	P	444	0	483	6	0
17	Q	1701	0	1818	15	0
18	S	1111	0	1174	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	U	1701	0	1749	13	0
20	V	1650	0	1794	7	0
21	X	708	0	760	8	0
22	Z	1513	0	1628	12	0
23	a	1239	0	1363	13	0
24	b	1461	0	1502	8	0
25	c	975	0	1032	8	0
26	e	979	0	1039	12	0
27	h	1115	0	1205	10	0
28	l	1002	0	1068	9	0
29	m	1898	0	1993	18	0
30	n	876	0	912	9	0
31	o	1897	0	2046	23	0
32	p	1878	0	2009	8	0
33	z	581	0	656	6	0
34	A	1319	0	1358	15	0
35	C	2027	0	2058	53	0
36	J	2106	0	2250	14	0
37	N	3669	0	3614	34	0
38	R	1636	0	1672	16	0
39	u	639	0	718	5	0
40	v	1680	0	1698	12	0
41	w	3623	0	3697	28	0
42	r	217	0	219	0	0
43	8	3295	0	1676	23	0
44	2	75906	0	38197	381	0
45	d	850	0	868	6	0
46	j	918	0	964	8	0
47	k	1064	0	1160	3	0
48	Y	1355	0	1389	10	0
49	t	928	0	906	27	0
50	s	1924	0	2027	20	0
51	i	1107	0	1182	29	0
52	T	2166	0	2262	24	0
53	5	2558	0	1295	46	0
54	q	3317	0	3366	45	0
55	f	2137	0	2202	89	0
56	O	569	0	637	4	0
57	3	1892	0	2024	63	0
58	g	1156	0	1268	28	0
59	x	648	0	432	20	0
60	w	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	w	1	0	0	0	0
All	All	166429	0	129593	1000	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 (1000) 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)
44:2:4083:5MU:C5	44:2:4083:5MU:C4	1.79	1.62
44:2:2484:A:C5	57:3:44:LEU:HD21	1.31	1.61
44:2:2484:A:N7	57:3:44:LEU:HD21	1.36	1.40
44:2:2484:A:N1	57:3:48:LYS:CD	1.82	1.40
51:i:120:GLU:OE1	55:f:282:PRO:CG	1.72	1.38
51:i:120:GLU:OE1	55:f:282:PRO:HG3	1.19	1.36
44:2:2545:U:C2	55:f:396:ARG:NH1	1.82	1.35
51:i:120:GLU:CD	55:f:282:PRO:HG3	1.52	1.35
44:2:2545:U:C5	55:f:396:ARG:HD3	1.56	1.33
44:2:2545:U:N1	55:f:396:ARG:NH1	1.78	1.30
44:2:2484:A:C5	57:3:44:LEU:CD2	2.13	1.30
49:t:54:ASN:CG	59:x:26:N:H4'	1.55	1.29
51:i:123:LYS:NZ	55:f:278:GLN:O	1.62	1.28
44:2:2545:U:C5	55:f:396:ARG:CD	1.97	1.26
50:s:163:ARG:HD2	59:x:6:N:OP2	1.27	1.25
44:2:2484:A:C6	57:3:44:LEU:CD2	2.22	1.23
44:2:2484:A:N1	57:3:48:LYS:HD3	0.90	1.21
35:C:262:LYS:O	53:5:119:U:O2	1.62	1.17
43:8:156:U:O2	57:3:57:ARG:NH1	1.80	1.15
44:2:2484:A:C6	57:3:44:LEU:HD23	1.82	1.13
44:2:2545:U:C6	55:f:396:ARG:HD3	1.82	1.12
44:2:4154:G:H5''	55:f:464:LYS:NZ	1.66	1.09
35:C:262:LYS:HB2	53:5:119:U:H2'	1.12	1.07
44:2:4154:G:H5''	55:f:464:LYS:HZ1	1.16	1.07
44:2:2484:A:C2	57:3:48:LYS:HD3	1.89	1.06
10:G:89:ARG:HH21	58:g:30:LYS:CE	1.69	1.06
51:i:120:GLU:CD	55:f:282:PRO:CG	2.23	1.06
44:2:2484:A:C6	57:3:44:LEU:HD21	1.87	1.05
10:G:89:ARG:NH2	58:g:30:LYS:CE	2.22	1.03
51:i:120:GLU:OE1	55:f:282:PRO:HG2	1.57	1.03
44:2:2678:A:H4'	55:f:336:LYS:HG2	1.40	1.01
49:t:54:ASN:ND2	59:x:26:N:H4'	1.75	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:90:GLN:NE2	57:3:62:GLU:OE2	1.93	1.01
44:2:2545:U:C6	55:f:396:ARG:NH1	1.98	1.01
10:G:89:ARG:NH2	58:g:30:LYS:HE2	1.76	0.99
35:C:262:LYS:HB2	53:5:119:U:C2'	1.92	0.97
44:2:2484:A:C6	57:3:48:LYS:HD3	1.98	0.97
43:8:156:U:H3	58:g:32:VAL:HG11	1.29	0.96
44:2:4310:A:H2'	44:2:4311:A:H8	1.29	0.96
49:t:40:GLU:CD	58:g:14:LYS:HE3	1.90	0.95
44:2:2452:G:H21	44:2:2507:A:H62	1.09	0.94
44:2:2545:U:H5	55:f:396:ARG:CD	1.62	0.94
44:2:2481:G:OP2	54:q:20:ARG:NH2	1.99	0.94
49:t:54:ASN:OD1	59:x:26:N:H4'	1.66	0.94
44:2:2548:C:OP1	55:f:392:ARG:NH1	2.01	0.94
44:2:2484:A:C2	57:3:48:LYS:CD	2.51	0.93
50:s:163:ARG:CD	59:x:6:N:OP2	2.16	0.92
44:2:2484:A:H2	57:3:48:LYS:HG2	1.34	0.90
44:2:2484:A:N7	57:3:44:LEU:CD2	2.29	0.90
44:2:2484:A:N6	57:3:44:LEU:CD2	2.34	0.90
43:8:156:U:O2	57:3:57:ARG:CZ	2.19	0.89
49:t:54:ASN:ND2	59:x:26:N:C4'	2.35	0.89
44:2:2484:A:C2	57:3:48:LYS:CG	2.57	0.87
50:s:176:ARG:NH1	59:x:49:N:OP2	2.08	0.87
51:i:120:GLU:OE2	55:f:282:PRO:HG3	1.75	0.86
44:2:2484:A:C2	57:3:48:LYS:HG2	2.11	0.86
44:2:4310:A:H2'	44:2:4311:A:C8	2.12	0.85
44:2:3717:A:H61	44:2:3933:G:H1'	1.42	0.85
57:3:60:ARG:NH2	58:g:28:VAL:O	2.10	0.84
44:2:3930:U:H3	44:2:4180:G:H1	1.22	0.84
43:8:156:U:O2	57:3:57:ARG:HD3	1.79	0.83
44:2:2452:G:N2	44:2:2507:A:H62	1.77	0.82
10:G:89:ARG:HH21	58:g:30:LYS:HE3	1.44	0.81
35:C:268:ARG:NH2	53:5:19:C:O2	2.14	0.81
44:2:2548:C:OP1	55:f:392:ARG:CZ	2.29	0.81
44:2:2758:G:OP1	55:f:405:ARG:NH1	2.15	0.80
54:q:163:ARG:NH2	55:f:188:VAL:O	2.15	0.79
43:8:156:U:N3	58:g:32:VAL:HG11	1.97	0.79
44:2:4154:G:C5'	55:f:464:LYS:HZ1	1.96	0.78
2:4:20:ASP:OD1	44:2:4405:G:N1	2.16	0.78
44:2:2484:A:N6	57:3:44:LEU:HD23	1.98	0.77
10:G:90:GLN:OE1	57:3:60:ARG:NH1	2.18	0.76
35:C:57:ASN:O	53:5:49:A:N6	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2:3723:A:H2'	44:2:3724:A:H8	1.50	0.76
44:2:2845:A:H61	44:2:3843:C:H42	1.31	0.75
44:2:2452:G:H21	44:2:2507:A:N6	1.84	0.75
44:2:2486:G:OP1	57:3:224:ARG:NE	2.20	0.75
51:i:124:THR:HG23	55:f:282:PRO:HD2	1.69	0.74
51:i:124:THR:CG2	55:f:282:PRO:HD2	2.17	0.74
35:C:225:GLN:NE2	53:5:49:A:P	2.60	0.74
49:t:40:GLU:CD	58:g:14:LYS:CE	2.60	0.74
44:2:2484:A:N1	57:3:48:LYS:CG	2.50	0.73
41:w:323:LYS:N	60:w:801:GTP:O2B	2.21	0.73
35:C:225:GLN:CD	53:5:49:A:P	2.72	0.72
43:8:156:U:C2	57:3:57:ARG:HD3	2.23	0.72
51:i:63:ALA:HB2	55:f:279:LEU:HD21	1.72	0.72
35:C:255:LYS:CD	53:5:117:G:OP1	2.37	0.72
44:2:2544:G:H1	55:f:404:ARG:HH12	1.36	0.72
54:q:380:ARG:HH12	57:3:192:ILE:HB	1.53	0.72
49:t:40:GLU:OE1	58:g:14:LYS:HE3	1.89	0.72
44:2:2483:G:C1'	55:f:459:PHE:HB2	2.20	0.71
55:f:456:ARG:HH12	57:3:44:LEU:HD12	1.54	0.71
35:C:58:ARG:NH2	53:5:25:G:OP2	2.13	0.71
44:2:4298:A:H2'	44:2:4299:U:C6	2.25	0.71
44:2:2483:G:H1'	55:f:459:PHE:HB2	1.72	0.71
49:t:54:ASN:HD21	59:x:26:N:C3'	2.04	0.71
43:8:156:U:H1'	57:3:57:ARG:HH11	1.54	0.70
35:C:270:LYS:HA	53:5:60:G:O3'	1.91	0.70
38:R:50:LEU:HD23	52:T:189:LEU:HD13	1.72	0.70
43:8:156:U:O2	57:3:57:ARG:CD	2.40	0.70
50:s:188:LYS:NZ	59:x:14:N:H3'	2.06	0.70
44:2:493:G:N1	44:2:660:A:C2	2.60	0.69
44:2:2544:G:H1	55:f:404:ARG:NH1	1.91	0.69
49:t:81:ARG:NH2	59:x:28:N:OP2	2.25	0.69
54:q:63:THR:HG22	55:f:407:GLY:HA2	1.73	0.69
35:C:261:VAL:HG12	53:5:119:U:O4	1.90	0.69
44:2:2486:G:OP2	57:3:224:ARG:NH2	2.22	0.68
44:2:3723:A:H2'	44:2:3724:A:C8	2.28	0.68
35:C:158:LYS:NZ	53:5:47:G:OP2	2.26	0.67
35:C:262:LYS:O	53:5:119:U:C2	2.48	0.67
44:2:4154:G:H5''	55:f:464:LYS:HZ2	1.55	0.67
43:8:156:U:H1'	57:3:57:ARG:NH1	2.10	0.66
54:q:380:ARG:NH2	57:3:196:ASP:OD2	2.27	0.66
30:n:2:SER:N	44:2:4946:U:HO2'	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:t:54:ASN:ND2	59:x:26:N:O3'	2.17	0.66
55:f:216:GLN:HE22	58:g:59:LYS:HA	1.61	0.66
44:2:2678:A:C4'	55:f:336:LYS:HG2	2.20	0.66
44:2:4305:G:N2	44:2:4309:G:N7	2.44	0.66
44:2:2557:G:H1	44:2:2570:U:H3	1.43	0.66
44:2:4154:G:C5'	55:f:464:LYS:NZ	2.52	0.66
54:q:45:PRO:HG2	55:f:406:LEU:HD12	1.78	0.66
10:G:89:ARG:HH21	58:g:30:LYS:CD	2.09	0.65
44:2:1858:A:H2'	44:2:1859:C:C6	2.31	0.65
44:2:2548:C:OP1	55:f:392:ARG:NH2	2.29	0.65
35:C:225:GLN:OE1	53:5:49:A:P	2.54	0.65
44:2:1938:C:H5	44:2:4401:G:H22	1.45	0.65
50:s:176:ARG:CZ	59:x:49:N:OP2	2.46	0.64
36:J:193:CYS:HG	44:2:4434:C:HO2'	1.45	0.64
49:t:54:ASN:ND2	59:x:26:N:H5''	2.12	0.64
10:G:90:GLN:CD	57:3:62:GLU:OE2	2.39	0.64
44:2:2484:A:C8	57:3:44:LEU:HD11	2.32	0.64
51:i:63:ALA:CA	55:f:279:LEU:HD21	2.28	0.64
35:C:225:GLN:OE1	53:5:49:A:OP1	2.15	0.64
14:L:43:ILE:O	14:L:47:LYS:HB2	1.99	0.63
44:2:3718:A:H3'	44:2:3719:A:H8	1.64	0.63
10:G:89:ARG:NH2	58:g:30:LYS:HE3	2.04	0.63
10:G:89:ARG:HH22	58:g:30:LYS:HE2	1.64	0.63
41:w:280:ALA:HB3	52:T:271:GLN:HE22	1.64	0.62
54:q:361:CYS:SG	57:3:158:ARG:NH2	2.71	0.62
54:q:380:ARG:NH1	57:3:192:ILE:HD12	2.15	0.62
35:C:256:LYS:NZ	53:5:117:G:H5'	2.14	0.62
44:2:4268:A:N7	44:2:4279:A:N6	2.48	0.62
50:s:77:GLU:OE1	59:x:23:N:O4'	2.17	0.62
44:2:3718:A:H3'	44:2:3719:A:C8	2.35	0.61
52:T:88:SER:HB2	52:T:108:MET:H	1.64	0.61
35:C:158:LYS:HG3	53:5:46:C:OP1	2.00	0.61
44:2:2545:U:H5	55:f:396:ARG:HD2	1.60	0.61
44:2:4309:G:H2'	44:2:4310:A:C8	2.34	0.61
44:2:3722:G:H2'	44:2:3723:A:C8	2.36	0.61
44:2:3724:A:H2'	44:2:3725:G:C8	2.36	0.61
35:C:225:GLN:CD	53:5:49:A:OP2	2.44	0.61
44:2:4306:U:C5	44:2:4309:G:C4	2.88	0.61
35:C:262:LYS:NZ	53:5:120:U:H4'	2.15	0.61
44:2:4740:G:H1'	44:2:4742:G:H5''	1.83	0.61
54:q:380:ARG:HH11	57:3:192:ILE:HD12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:52:CYS:HB2	8:E:57:LYS:HE2	1.82	0.60
44:2:2548:C:P	55:f:392:ARG:CZ	2.89	0.60
54:q:147:PHE:HZ	55:f:438:LEU:HD11	1.66	0.60
35:C:262:LYS:CB	53:5:119:U:H2'	2.07	0.60
12:I:44:GLU:HB3	12:I:58:ASP:HB2	1.84	0.60
25:c:130:ARG:HH22	44:2:1802:A:H1'	1.67	0.60
23:a:39:GLN:HG3	23:a:42:ARG:HH21	1.67	0.60
35:C:197:LYS:HG3	35:C:202:GLN:HB2	1.83	0.60
49:t:54:ASN:ND2	59:x:26:N:C5'	2.65	0.60
36:J:137:ARG:HE	36:J:145:ALA:HB2	1.65	0.59
10:G:180:PRO:HG3	10:G:219:VAL:HG23	1.84	0.59
35:C:262:LYS:HZ1	53:5:120:U:H4'	1.66	0.59
44:2:2678:A:H5'	55:f:336:LYS:HE2	1.83	0.59
44:2:3722:G:H2'	44:2:3723:A:H8	1.67	0.59
14:L:110:LYS:NZ	44:2:1396:G:N7	2.50	0.59
51:i:63:ALA:CB	55:f:279:LEU:HD21	2.32	0.59
40:v:50:ASN:ND2	44:2:1999:A:N1	2.50	0.59
44:2:4297:G:N3	44:2:4297:G:H2'	2.17	0.59
44:2:2679:G:OP1	55:f:337:LYS:N	2.35	0.59
29:m:7:GLY:HA2	29:m:10:LYS:HE2	1.85	0.59
7:D:110:ARG:HB2	19:U:204:ARG:HH21	1.68	0.59
44:2:2488:C:C4	57:3:225:HIS:ND1	2.71	0.58
3:6:10:ASN:HD21	26:e:130:PRO:HG3	1.67	0.58
37:N:16:ARG:HE	37:N:34:ASP:HB3	1.68	0.58
53:5:28:C:H1'	53:5:54:A:H61	1.67	0.58
5:9:87:LYS:HE2	44:2:3617:G:H1	1.68	0.58
44:2:2362:U:H2'	44:2:2363:A2M:H8	1.85	0.58
51:i:124:THR:HG22	55:f:281:LEU:CD1	2.34	0.58
50:s:149:LEU:HD21	50:s:176:ARG:HG3	1.86	0.58
38:R:44:ARG:HG2	52:T:148:ASP:H	1.69	0.57
2:4:138:CYS:O	2:4:142:LYS:HB2	2.03	0.57
35:C:255:LYS:HE2	53:5:117:G:OP1	2.04	0.57
44:2:1445:U:H3	44:2:2103:G:H1	1.51	0.57
7:D:71:ARG:HH21	44:2:3906:A:H2'	1.70	0.57
50:s:188:LYS:HZ2	59:x:14:N:H3'	1.67	0.57
29:m:207:VAL:HG13	29:m:208:GLU:HG3	1.86	0.57
34:A:98:ASN:ND2	34:A:106:GLY:O	2.38	0.56
24:b:1:MET:SD	24:b:43:ARG:NH1	2.78	0.56
26:e:43:LYS:HD2	26:e:62:MET:HE2	1.87	0.56
44:2:2502:G:N1	58:g:47:ARG:NH2	2.51	0.56
10:G:87:LEU:HD22	10:G:184:ILE:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2:2763:U:H3'	55:f:391:ARG:HH21	1.69	0.56
44:2:3717:A:H61	44:2:3933:G:C1'	2.17	0.56
44:2:1207:C:H2'	44:2:1208:G:H8	1.70	0.56
49:t:46:VAL:HG21	49:t:126:VAL:HG21	1.87	0.56
34:A:37:ALA:O	34:A:41:GLU:HB2	2.06	0.56
44:2:3717:A:N6	44:2:3933:G:H1'	2.18	0.56
2:4:400:ASP:HA	2:4:403:LEU:HG	1.87	0.56
27:h:50:ARG:NH2	43:8:83:C:N3	2.54	0.56
44:2:2763:U:O2'	55:f:391:ARG:NE	2.39	0.56
37:N:280:CYS:SG	37:N:281:ARG:NH1	2.79	0.56
10:G:89:ARG:NH1	43:8:155:C:OP2	2.39	0.55
20:V:34:VAL:HG12	20:V:103:LYS:HB2	1.89	0.55
31:o:44:CYS:SG	31:o:45:SER:N	2.77	0.55
44:2:4297:G:H22	44:2:4313:A:H61	1.53	0.55
12:I:120:GLU:OE2	12:I:124:ARG:NH1	2.38	0.55
37:N:291:ASN:ND2	37:N:349:ASP:OD1	2.40	0.55
44:2:2592:U:H3	44:2:4126:C:H42	1.54	0.55
11:H:66:LYS:HD2	43:8:96:C:H5''	1.89	0.55
14:L:16:SER:HB3	14:L:21:ARG:HH11	1.71	0.55
35:C:225:GLN:HE22	53:5:49:A:P	2.28	0.55
12:I:102:ASN:HB3	12:I:115:ARG:HB3	1.89	0.55
50:s:123:ILE:HD11	50:s:191:SER:HA	1.88	0.55
44:2:2845:A:N6	44:2:3843:C:H42	2.03	0.55
2:4:2:ALA:N	41:w:179:ASP:OD2	2.40	0.54
17:Q:78:LEU:HD11	17:Q:88:LYS:HD3	1.88	0.54
29:m:137:ILE:HD11	29:m:149:LYS:HB3	1.89	0.54
36:J:140:LYS:NZ	44:2:4385:A:N1	2.53	0.54
51:i:124:THR:HG22	55:f:281:LEU:HD12	1.88	0.54
7:D:284:MET:HE2	7:D:287:THR:HA	1.89	0.54
35:C:270:LYS:HB3	53:5:60:G:H5''	1.87	0.54
1:y:112:ILE:HG22	1:y:132:ILE:HD13	1.90	0.54
44:2:1552:G:O2'	44:2:1574:B9B:N2	2.40	0.54
29:m:104:VAL:HA	29:m:107:MET:HE1	1.89	0.54
37:N:22:GLN:HB3	37:N:28:LEU:HD13	1.89	0.54
44:2:493:G:O6	44:2:660:A:N1	2.41	0.54
35:C:270:LYS:HB2	53:5:61:G:OP1	2.07	0.54
37:N:180:ILE:HB	37:N:195:LEU:HB2	1.90	0.54
44:2:2482:C:OP1	55:f:454:ARG:HD3	2.07	0.54
10:G:89:ARG:HH21	58:g:30:LYS:HD2	1.72	0.54
35:C:255:LYS:CE	53:5:117:G:OP1	2.56	0.54
35:C:263:LYS:HD2	53:5:1:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:f:452:GLU:OE2	55:f:454:ARG:NH2	2.41	0.54
44:2:2678:A:H4'	55:f:336:LYS:CG	2.28	0.54
54:q:74:LEU:HD13	58:g:55:ARG:HH12	1.73	0.54
17:Q:140:SER:O	17:Q:144:LEU:HB2	2.09	0.53
40:v:124:TYR:HB2	40:v:126:ARG:HH21	1.72	0.53
44:2:1441:C:N4	44:2:2104:G:O6	2.40	0.53
55:f:337:LYS:HD2	55:f:342:ARG:HE	1.73	0.53
35:C:269:PRO:C	53:5:60:G:H4'	2.33	0.53
44:2:2487:G:H22	54:q:154:HIS:CD2	2.23	0.53
7:D:291:ARG:NH1	44:2:667:A:N7	2.55	0.53
41:w:280:ALA:HB3	52:T:271:GLN:NE2	2.23	0.53
2:4:580:LEU:HB3	2:4:585:MET:HG2	1.91	0.53
40:v:116:PHE:O	40:v:201:LYS:NZ	2.42	0.53
50:s:76:LYS:HE3	50:s:78:LEU:HD11	1.90	0.53
10:G:249:ARG:NH2	44:2:4075:U:OP1	2.42	0.53
20:V:7:LEU:HB3	20:V:33:VAL:HG12	1.89	0.53
54:q:148:PRO:HB3	57:3:163:LYS:HB3	1.90	0.53
5:9:21:ALA:HB3	5:9:24:ARG:HG2	1.91	0.53
36:J:148:ARG:NH1	41:w:61:GLN:O	2.41	0.53
41:w:352:THR:HG23	44:2:4539:U:H5''	1.91	0.53
35:C:256:LYS:HZ1	53:5:117:G:H5'	1.74	0.53
39:u:45:ARG:NH1	44:2:4419:U:OP2	2.42	0.53
50:s:36:VAL:HG22	50:s:263:ILE:HD13	1.91	0.53
10:G:89:ARG:NE	58:g:30:LYS:HA	2.24	0.53
50:s:188:LYS:HZ3	59:x:14:N:H3'	1.74	0.53
57:3:45:LEU:HA	57:3:48:LYS:HE2	1.91	0.53
20:V:89:PRO:HD3	44:2:1914:C:H4'	1.91	0.53
24:b:95:ARG:NH2	44:2:1951:G:O2'	2.42	0.53
44:2:245:C:H41	44:2:1366:G:H1	1.56	0.52
6:B:82:PRO:HG3	6:B:328:ASN:HD22	1.74	0.52
25:c:130:ARG:NH2	44:2:1802:A:N3	2.56	0.52
40:v:50:ASN:ND2	44:2:1969:G:O2'	2.42	0.52
2:4:538:HIS:HA	2:4:541:VAL:HG12	1.92	0.52
21:X:51:ALA:H	21:X:54:ILE:HB	1.74	0.52
7:D:110:ARG:NH2	44:2:1508:A:OP1	2.42	0.52
34:A:22:LEU:HB3	34:A:128:LEU:HD11	1.90	0.52
44:2:35:U:O2'	44:2:1651:G:N3	2.42	0.52
44:2:967:C:N4	44:2:2259:G:O2'	2.43	0.52
10:G:217:LYS:NZ	49:t:113:GLU:O	2.40	0.52
19:U:84:PRO:O	19:U:87:HIS:ND1	2.42	0.52
37:N:457:ASP:HB3	37:N:476:LYS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2:493:G:C6	44:2:660:A:N1	2.78	0.52
24:b:15:ARG:HD2	24:b:25:PRO:HG2	1.92	0.52
44:2:4243:C:N4	44:2:4267:G:O6	2.42	0.52
26:e:15:ARG:NH2	44:2:4673:U:OP2	2.42	0.52
44:2:3707:U:H3	44:2:3743:G:H1	1.58	0.52
3:6:49:VAL:HG11	3:6:87:SER:HB3	1.92	0.52
19:U:96:ARG:NH1	44:2:29:G:O2'	2.42	0.52
28:l:98:ARG:NH2	44:2:2262:G:OP2	2.43	0.52
35:C:262:LYS:HG3	53:5:120:U:H5''	1.92	0.52
49:t:127:HIS:CD2	59:x:57:N:O2'	2.63	0.52
52:T:99:ARG:HD3	52:T:226:ARG:HD3	1.92	0.52
20:V:106:ASP:O	44:2:4910:G:N2	2.43	0.52
53:5:76:U:O2	53:5:100:A:N7	2.43	0.52
23:a:97:ARG:NH2	44:2:2725:A:OP2	2.43	0.52
33:z:85:THR:HB	33:z:87:LEU:HD23	1.91	0.52
43:8:156:U:O2	57:3:57:ARG:NE	2.42	0.52
44:2:4418:G:N1	44:2:4421:C:OP2	2.40	0.52
35:C:211:LEU:HB3	35:C:219:TYR:HB2	1.92	0.51
44:2:1972:G:H1	44:2:1994:C:H5	1.58	0.51
50:s:50:ARG:HH21	50:s:257:LYS:HD3	1.75	0.51
6:B:222:VAL:O	6:B:343:ARG:NH1	2.43	0.51
44:2:1732:C:H41	44:2:1796:U:H3	1.58	0.51
44:2:3765:G:O2'	44:2:3766:A:N7	2.42	0.51
10:G:46:GLN:NE2	44:2:4087:G:O6	2.44	0.51
34:A:73:THR:OG1	53:5:39:C:N3	2.41	0.51
35:C:222:GLN:O	35:C:225:GLN:NE2	2.43	0.51
35:C:223:PHE:HB3	35:C:226:TYR:HB2	1.92	0.51
52:T:134:LYS:NZ	52:T:217:MET:O	2.43	0.51
44:2:1858:A:H2'	44:2:1859:C:H6	1.75	0.51
44:2:2486:G:P	57:3:224:ARG:HH21	2.32	0.51
51:i:59:LYS:O	55:f:279:LEU:HD11	2.11	0.51
52:T:117:ILE:HA	52:T:228:THR:HG22	1.93	0.51
54:q:184:SER:OG	54:q:185:ILE:N	2.43	0.51
29:m:54:ARG:NH1	44:2:3680:U:OP1	2.44	0.51
44:2:1398:A:OP2	44:2:1420:A:N6	2.44	0.51
6:B:57:VAL:HG23	6:B:366:LYS:HB3	1.92	0.51
10:G:144:THR:O	10:G:148:GLU:HB2	2.10	0.51
39:u:27:GLU:OE2	39:u:30:ARG:NH1	2.44	0.51
44:2:2706:G:N2	44:2:2708:U:O4'	2.44	0.51
7:D:109:ARG:NH2	44:2:2343:G:OP2	2.43	0.51
19:U:47:LYS:NZ	44:2:280:G:OP1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:10:ILE:HG13	44:2:1554:A:H4'	1.93	0.51
22:Z:29:VAL:O	22:Z:33:ARG:HB2	2.10	0.51
33:z:11:ARG:NH2	44:2:4678:G:N7	2.59	0.51
44:2:4338:G:OP2	44:2:4339:A:N6	2.43	0.51
8:E:81:LEU:HD21	8:E:94:LEU:HD22	1.92	0.51
13:K:30:ARG:NH1	44:2:327:U:O2'	2.44	0.51
44:2:2544:G:C6	55:f:404:ARG:NH1	2.72	0.51
44:2:4140:C:N3	44:2:4145:C:O2'	2.43	0.51
50:s:207:LYS:NZ	59:x:23:N:H5'	2.26	0.51
2:4:194:ASP:OD1	2:4:194:ASP:N	2.44	0.51
7:D:71:ARG:NH2	44:2:3905:A:O5'	2.44	0.51
40:v:64:ARG:NH1	40:v:65:MET:O	2.44	0.51
54:q:149:ARG:NH1	57:3:253:GLN:O	2.44	0.51
3:6:4:ARG:NH1	3:6:210:THR:O	2.44	0.50
34:A:112:HIS:ND1	34:A:126:TYR:O	2.44	0.50
3:6:57:ARG:NH1	26:e:127:ASP:OD1	2.44	0.50
44:2:1595:G:H1'	44:2:1597:G:H21	1.75	0.50
44:2:2544:G:O6	55:f:404:ARG:NH1	2.44	0.50
19:U:165:THR:HG23	19:U:168:GLY:H	1.77	0.50
54:q:185:ILE:HG22	55:f:433:PRO:HA	1.94	0.50
3:6:116:LEU:HD21	3:6:173:LEU:HD11	1.91	0.50
16:P:41:ARG:NH1	44:2:2431:A:OP1	2.40	0.50
27:h:121:ARG:NH1	44:2:194:C:O2	2.45	0.50
32:p:131:ASN:ND2	44:2:1727:U:OP1	2.45	0.50
49:t:107:ASN:HA	49:t:118:CYS:H	1.76	0.50
6:B:57:VAL:HG12	6:B:73:VAL:HG12	1.92	0.50
44:2:2484:A:H61	57:3:48:LYS:NZ	2.08	0.50
44:2:3715:U:H3	44:2:3738:G:H22	1.59	0.50
2:4:510:ARG:NH2	44:2:2625:U:OP2	2.43	0.50
23:a:42:ARG:HA	23:a:45:ILE:HD12	1.93	0.50
31:o:155:GLY:O	31:o:158:ARG:NH1	2.44	0.50
44:2:1086:C:H2'	44:2:1087:A:H8	1.76	0.50
44:2:1245:C:H2'	44:2:1246:G:H8	1.76	0.50
44:2:3772:U:O2'	52:T:268:MET:SD	2.60	0.50
3:6:66:ASN:ND2	3:6:111:ASN:O	2.45	0.50
11:H:86:LYS:NZ	43:8:39:G:OP1	2.45	0.50
37:N:443:VAL:O	37:N:446:GLN:NE2	2.44	0.50
11:H:52:LYS:NZ	43:8:62:A:OP1	2.45	0.50
22:Z:55:ARG:NH2	44:2:1351:G:O6	2.39	0.50
44:2:2678:A:O3'	55:f:336:LYS:HA	2.12	0.50
44:2:2693:G:OP1	56:O:35:LYS:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2:2704:C:H2'	44:2:2705:G:H8	1.77	0.50
10:G:161:VAL:HG11	10:G:200:THR:HG23	1.92	0.50
44:2:32:G:H21	44:2:50:C:H5	1.59	0.50
3:6:24:CYS:HB3	3:6:48:VAL:HG12	1.94	0.49
17:Q:116:ARG:NH2	17:Q:155:MET:O	2.45	0.49
26:e:90:ARG:NH2	26:e:124:GLU:OE1	2.43	0.49
44:2:1597:G:H5''	48:Y:132:ALA:HB2	1.93	0.49
52:T:119:LEU:HB3	52:T:223:LEU:HD12	1.94	0.49
44:2:2020:U:H2'	44:2:2021:G:H8	1.77	0.49
44:2:4310:A:H8	44:2:4310:A:OP2	1.95	0.49
1:y:123:ARG:NH1	40:v:61:LYS:O	2.43	0.49
2:4:588:LYS:NZ	44:2:388:A:OP2	2.44	0.49
22:Z:125:GLN:O	22:Z:129:ASP:HB2	2.13	0.49
25:c:130:ARG:NH1	44:2:1837:A:OP2	2.44	0.49
34:A:158:SER:OG	34:A:159:LYS:N	2.46	0.49
35:C:73:MET:SD	53:5:114:U:H4'	2.52	0.49
38:R:26:VAL:HG11	38:R:67:ASP:HB3	1.94	0.49
40:v:78:GLY:HA3	40:v:84:GLU:HA	1.93	0.49
41:w:10:SER:N	44:2:4378:A:OP2	2.45	0.49
50:s:79:ARG:NH2	50:s:180:PRO:O	2.45	0.49
54:q:188:ILE:HB	54:q:203:THR:HB	1.94	0.49
41:w:35:ARG:NH2	44:2:4302:U:OP1	2.45	0.49
1:y:5:PHE:HE1	1:y:11:LYS:HG3	1.77	0.49
10:G:35:ARG:NH1	44:2:4128:A:O2'	2.44	0.49
44:2:2763:U:H2'	55:f:391:ARG:CZ	2.41	0.49
52:T:203:LYS:HZ1	52:T:213:GLU:H	1.61	0.49
57:3:164:ARG:HH21	57:3:255:ASN:HA	1.77	0.49
2:4:540:ALA:HB1	2:4:544:ARG:HH21	1.78	0.49
23:a:13:SER:OG	23:a:38:ARG:NH2	2.46	0.49
44:2:1411:C:O2'	44:2:1412:G:N7	2.44	0.49
44:2:4244:A:H62	44:2:4264:G:H21	1.60	0.49
9:F:105:LYS:NZ	55:f:297:LEU:HD13	2.28	0.49
11:H:95:LEU:O	44:2:135:G:N2	2.44	0.49
35:C:15:ARG:NH1	44:2:4266:G:OP1	2.46	0.49
44:2:2482:C:OP1	55:f:454:ARG:NH1	2.46	0.49
44:2:2845:A:H61	44:2:3843:C:N4	2.05	0.49
54:q:36:ARG:NH2	54:q:114:TYR:OH	2.46	0.49
10:G:53:ARG:NH1	44:2:4163:U:OP2	2.46	0.49
26:e:92:ASP:N	26:e:92:ASP:OD1	2.45	0.49
29:m:233:ARG:NH1	44:2:4184:G:OP1	2.43	0.49
35:C:255:LYS:HD2	53:5:117:G:OP1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2:1733:G:O6	44:2:1734:G:N2	2.46	0.49
44:2:3641:U:OP2	44:2:3646:A:N6	2.45	0.49
2:4:474:ASP:OD1	2:4:474:ASP:N	2.46	0.49
7:D:140:LYS:O	7:D:204:ARG:NH2	2.46	0.49
28:l:33:LYS:HA	47:k:90:MET:HG3	1.94	0.49
33:z:2:ALA:N	44:2:4593:C:OP2	2.46	0.49
37:N:447:LYS:NZ	37:N:448:LEU:O	2.46	0.49
43:8:150:C:H2'	55:f:471:ARG:HH22	1.78	0.49
2:4:533:ASP:OD1	2:4:533:ASP:N	2.46	0.49
3:6:31:SER:OG	3:6:32:GLU:N	2.44	0.49
18:S:74:ARG:NH1	44:2:736:C:OP1	2.46	0.49
34:A:92:TYR:HB3	34:A:172:GLY:HA2	1.94	0.49
44:2:2418:A:N1	44:2:2429:A:O2'	2.45	0.49
44:2:2543:A:H3'	44:2:2546:G:H21	1.76	0.49
6:B:36:ASP:HB3	6:B:39:LYS:HD2	1.95	0.48
37:N:433:SER:OG	37:N:434:SER:N	2.46	0.48
41:w:51:ASN:HB3	41:w:57:ILE:HD11	1.94	0.48
51:i:47:ASP:HB3	51:i:69:LYS:HB3	1.94	0.48
54:q:172:ILE:HG13	54:q:177:ALA:HB3	1.95	0.48
17:Q:35:ARG:NH2	44:2:337:U:OP1	2.45	0.48
49:t:54:ASN:OD1	59:x:26:N:C4'	2.51	0.48
51:i:120:GLU:CD	55:f:282:PRO:CB	2.85	0.48
37:N:38:ASP:OD1	37:N:38:ASP:N	2.46	0.48
49:t:144:PRO:O	49:t:148:ARG:HB2	2.13	0.48
31:o:123:ARG:NH1	44:2:970:G:OP1	2.46	0.48
37:N:45:GLN:HB3	37:N:62:PHE:HE1	1.75	0.48
44:2:2488:C:C4	57:3:225:HIS:CE1	3.01	0.48
44:2:2488:C:N3	57:3:225:HIS:CE1	2.81	0.48
13:K:28:ARG:NH2	44:2:326:C:OP2	2.44	0.48
37:N:133:SER:OG	37:N:134:GLY:N	2.47	0.48
37:N:303:THR:OG1	37:N:332:ARG:NH1	2.45	0.48
44:2:2624:G:OP2	45:d:97:ARG:NH2	2.46	0.48
44:2:3663:A:N6	44:2:4168:G:O2'	2.46	0.48
44:2:4100:C:N4	44:2:4109:G:OP2	2.45	0.48
51:i:12:LEU:HB2	51:i:81:MET:HB3	1.94	0.48
31:o:222:LEU:HB2	31:o:237:LYS:HD2	1.96	0.48
44:2:2097:U:H5'	44:2:2098:G:H4'	1.95	0.48
30:n:68:ARG:NH1	44:2:442:G:OP1	2.45	0.48
44:2:380:U:H5''	44:2:413:G:H21	1.78	0.48
44:2:2483:G:C2'	55:f:459:PHE:HB2	2.44	0.48
49:t:55:LEU:HD11	57:3:72:LYS:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:3:78:LEU:HD23	57:3:81:LEU:HD13	1.96	0.48
11:H:4:ILE:O	11:H:56:ARG:NH1	2.45	0.48
18:S:3:PHE:H	24:b:175:PHE:HZ	1.61	0.48
31:o:281:ILE:HD12	31:o:286:LEU:HD11	1.96	0.48
44:2:2572:C:O2	51:i:112:ARG:NH2	2.47	0.48
54:q:184:SER:HA	55:f:246:SER:HA	1.96	0.48
55:f:219:LYS:HE3	55:f:221:GLY:HA3	1.96	0.48
7:D:103:ALA:HA	44:2:1517:2MG:HN2	1.78	0.48
28:l:28:GLU:OE1	28:l:31:ASN:ND2	2.47	0.48
38:R:24:ILE:O	38:R:74:ASN:ND2	2.41	0.48
41:w:307:ASP:N	41:w:307:ASP:OD1	2.46	0.48
54:q:421:PRO:HB3	55:f:249:PRO:C	2.39	0.48
1:y:123:ARG:NH2	44:2:1997:U:OP1	2.47	0.48
4:7:66:ASP:OD2	4:7:103:ARG:NH1	2.44	0.48
17:Q:188:ASN:O	17:Q:192:PHE:HB2	2.13	0.48
30:n:2:SER:N	44:2:4946:U:O2'	2.46	0.48
37:N:361:ASP:N	37:N:361:ASP:OD1	2.47	0.48
44:2:1679:A:H1'	44:2:1680:G:H2'	1.95	0.48
4:7:53:LYS:NZ	4:7:62:GLU:OE2	2.45	0.47
41:w:42:ASN:OD1	41:w:45:ARG:NH2	2.46	0.47
46:j:64:ILE:HG23	46:j:68:LEU:HD23	1.96	0.47
19:U:155:VAL:O	19:U:162:ARG:NH2	2.47	0.47
35:C:225:GLN:NE2	53:5:48:G:O3'	2.46	0.47
53:5:75:G:N2	53:5:100:A:OP2	2.46	0.47
55:f:465:VAL:HG22	58:g:37:LYS:HD2	1.96	0.47
4:7:9:CYS:SG	6:B:378:ARG:NH1	2.86	0.47
38:R:103:LYS:HB3	52:T:24:PRO:HB3	1.97	0.47
40:v:50:ASN:OD1	44:2:1998:A:N6	2.47	0.47
44:2:1938:C:H41	44:2:4401:G:H1	1.61	0.47
44:2:3938:G:N2	44:2:4171:C:OP2	2.46	0.47
45:d:40:GLU:HA	45:d:43:LEU:HD23	1.96	0.47
31:o:278:THR:OG1	31:o:279:ASN:N	2.47	0.47
36:J:105:MET:SD	36:J:231:THR:OG1	2.72	0.47
43:8:126:C:O2'	43:8:128:C:N4	2.47	0.47
54:q:421:PRO:HA	55:f:248:ASN:OD1	2.13	0.47
23:a:62:ARG:NH1	44:2:4645:C:OP2	2.48	0.47
28:l:63:VAL:HG12	28:l:79:ARG:HB3	1.97	0.47
33:z:23:PRO:O	33:z:27:SER:OG	2.32	0.47
41:w:314:GLY:HA2	41:w:360:ILE:HB	1.96	0.47
44:2:518:G:H1'	44:2:644:G:H1	1.79	0.47
52:T:98:LYS:HD3	53:5:98:G:H4'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:N:24:GLU:OE1	37:N:93:GLN:NE2	2.47	0.47
44:2:990:C:N4	44:2:1051:G:O2'	2.47	0.47
44:2:1679:A:H8	44:2:1680:G:H8	1.63	0.47
44:2:4092:G:H3'	44:2:4093:G:H21	1.79	0.47
12:I:140:GLN:HB2	12:I:143:GLU:HG2	1.96	0.47
16:P:5:LYS:O	44:2:2512:A:N6	2.48	0.47
17:Q:186:ARG:NH1	44:2:1394:G:OP1	2.48	0.47
22:Z:178:ARG:HB2	22:Z:184:ARG:HB3	1.96	0.47
23:a:105:LEU:HD22	23:a:135:LYS:HG3	1.96	0.47
27:h:4:ASN:HB3	27:h:7:VAL:HG22	1.97	0.47
28:l:66:ARG:HH21	28:l:68:SER:HG	1.60	0.47
29:m:242:ARG:NH1	29:m:244:GLY:O	2.47	0.47
30:n:110:ILE:O	31:o:141:ARG:NH2	2.48	0.47
37:N:200:LYS:HD3	37:N:224:LYS:HD3	1.97	0.47
38:R:35:ASP:HB2	38:R:40:LEU:HB3	1.96	0.47
38:R:74:ASN:HA	52:T:209:THR:HG21	1.96	0.47
38:R:141:ARG:HB2	38:R:149:ALA:HB2	1.96	0.47
41:w:92:LEU:HD22	52:T:259:PHE:CD1	2.50	0.47
43:8:14:OMU:HM23	43:8:14:OMU:H1'	1.68	0.47
44:2:2811:G:N1	44:2:2814:C:OP2	2.40	0.47
57:3:243:ARG:HB3	57:3:246:ARG:HB2	1.96	0.47
2:4:442:ILE:HD13	4:7:89:THR:HG21	1.96	0.47
17:Q:16:LYS:NZ	44:2:97:G:OP1	2.46	0.47
19:U:17:ASP:OD1	19:U:17:ASP:N	2.48	0.47
35:C:21:ARG:HA	35:C:24:ARG:HG2	1.96	0.47
35:C:225:GLN:OE1	53:5:49:A:OP2	2.33	0.47
38:R:71:LEU:HA	38:R:74:ASN:HD22	1.80	0.47
44:2:4212:A:N6	44:2:4219:A:OP2	2.47	0.47
49:t:131:PHE:HB3	49:t:134:TRP:HB3	1.96	0.47
54:q:176:ARG:O	54:q:179:ARG:NH2	2.48	0.47
3:6:150:SER:HA	3:6:194:ALA:HB3	1.97	0.47
14:L:85:GLN:HA	14:L:88:VAL:HG12	1.96	0.47
24:b:85:ASP:OD1	24:b:85:ASP:N	2.47	0.47
31:o:224:LYS:HD3	31:o:227:HIS:HB2	1.97	0.47
22:Z:66:MET:HE1	22:Z:100:VAL:HG13	1.96	0.46
23:a:62:ARG:NH2	44:2:4646:U:OP2	2.48	0.46
30:n:33:VAL:HG23	30:n:38:GLU:HB2	1.98	0.46
2:4:226:LEU:O	2:4:233:ARG:NH2	2.45	0.46
2:4:620:HIS:O	2:4:633:ARG:NH2	2.48	0.46
16:P:2:SER:N	44:2:2407:G:O6	2.49	0.46
30:n:37:ASP:N	30:n:37:ASP:OD1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:R:186:GLU:HA	38:R:189:ARG:HG2	1.96	0.46
44:2:1194:G:N2	44:2:1195:G:O6	2.47	0.46
44:2:1562:G:N2	44:2:1565:A:OP2	2.48	0.46
44:2:2439:G:O2'	54:q:2:GLY:HA3	2.15	0.46
52:T:45:VAL:HA	52:T:48:VAL:HG22	1.98	0.46
2:4:170:THR:HG21	2:4:247:LEU:HD13	1.96	0.46
30:n:87:LYS:NZ	44:2:1903:G:OP1	2.42	0.46
31:o:273:SER:OG	31:o:274:VAL:N	2.48	0.46
51:i:104:PRO:O	51:i:108:ARG:NE	2.47	0.46
22:Z:4:ASP:O	32:p:115:ARG:NH1	2.48	0.46
29:m:19:HIS:ND1	29:m:190:LYS:O	2.42	0.46
29:m:33:ASP:HB3	29:m:36:GLU:HG2	1.96	0.46
41:w:108:LYS:HG2	52:T:265:ARG:HA	1.96	0.46
44:2:4298:A:N6	44:2:4313:A:C6	2.84	0.46
54:q:426:PHE:CD1	55:f:240:VAL:HG11	2.51	0.46
18:S:39:ASP:N	18:S:39:ASP:OD1	2.48	0.46
37:N:62:PHE:HB3	37:N:69:ILE:HD12	1.96	0.46
44:2:184:U:O2'	44:2:253:G:N2	2.49	0.46
44:2:2459:G:N2	44:2:2462:C:OP2	2.47	0.46
44:2:2487:G:H22	54:q:154:HIS:CG	2.33	0.46
54:q:403:ASN:HD22	54:q:425:PRO:HG3	1.81	0.46
11:H:112:ARG:NH2	44:2:265:C:O2	2.46	0.46
31:o:178:PRO:HB2	31:o:181:LEU:HD23	1.98	0.46
37:N:139:ARG:NH1	37:N:151:THR:OG1	2.48	0.46
44:2:1870:C:H2'	44:2:1871:A2M:H8	1.96	0.46
44:2:1942:A:C2	44:2:2039:G:N2	2.79	0.46
44:2:3672:G:OP2	44:2:3672:G:N2	2.45	0.46
44:2:3720:G:H22	44:2:3733:A:H2	1.64	0.46
4:7:19:MET:SD	4:7:19:MET:N	2.89	0.46
17:Q:80:GLU:OE2	17:Q:113:ASN:ND2	2.46	0.46
17:Q:177:LYS:HB3	17:Q:180:ALA:HB3	1.98	0.46
23:a:61:ALA:HA	23:a:64:ARG:HD3	1.98	0.46
31:o:254:ASP:HA	31:o:257:ILE:HG22	1.97	0.46
38:R:43:ASP:O	52:T:147:GLY:N	2.48	0.46
44:2:2877:G:N2	44:2:3824:A:O2'	2.44	0.46
2:4:415:LYS:HA	2:4:425:LYS:HE2	1.98	0.46
10:G:161:VAL:HG23	10:G:164:ILE:HA	1.97	0.46
32:p:32:ARG:HH21	44:2:963:G:H5''	1.81	0.46
37:N:248:SER:HB3	37:N:265:GLN:HG3	1.98	0.46
38:R:77:TRP:CE3	52:T:208:ARG:NH2	2.83	0.46
44:2:1301:C:OP2	44:2:1303:A:N6	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2:1858:A:H2'	44:2:1859:C:C5	2.51	0.46
44:2:4209:G:O6	44:2:4224:A:N6	2.48	0.46
49:t:144:PRO:O	49:t:148:ARG:CB	2.63	0.46
57:3:220:LEU:HB3	57:3:254:LEU:HB3	1.97	0.46
2:4:363:ALA:HB3	3:6:181:LEU:H	1.80	0.46
29:m:230:PRO:HD2	29:m:233:ARG:HD3	1.97	0.46
29:m:233:ARG:HB2	44:2:4184:G:H5'	1.97	0.46
44:2:3616:U:OP2	44:2:3617:G:N2	2.48	0.46
46:j:23:ARG:HG2	46:j:121:ASN:HA	1.98	0.46
7:D:152:LEU:HD23	7:D:251:ILE:HG12	1.98	0.46
13:K:68:ARG:NH1	44:2:3722:G:OP2	2.49	0.46
27:h:11:ARG:NH1	44:2:229:G:OP1	2.49	0.46
31:o:234:ASP:OD1	31:o:234:ASP:N	2.47	0.46
34:A:16:ARG:HH21	34:A:137:PRO:HD3	1.80	0.46
44:2:665:C:H4'	44:2:666:G:H5'	1.97	0.46
48:Y:127:ARG:HD2	48:Y:139:TYR:HD2	1.80	0.46
10:G:160:ASP:OD2	43:8:152:U:O2'	2.34	0.45
37:N:451:ASP:OD1	37:N:451:ASP:N	2.49	0.45
44:2:1860:U:H2'	44:2:1861:U:O2	2.15	0.45
44:2:2039:G:H5''	44:2:2040:A:H5''	1.97	0.45
44:2:3719:A:H2'	44:2:3720:G:O4'	2.16	0.45
52:T:235:LEU:O	52:T:239:SER:HB2	2.17	0.45
2:4:249:ALA:HB1	2:4:283:PRO:HD2	1.98	0.45
6:B:238:LYS:HB2	6:B:238:LYS:HE2	1.79	0.45
7:D:66:SER:HA	7:D:77:PRO:HA	1.98	0.45
21:X:47:MET:HE1	21:X:55:TRP:HB3	1.97	0.45
27:h:74:TYR:OH	43:8:75:G:OP2	2.33	0.45
31:o:164:PHE:HA	31:o:175:VAL:HG12	1.97	0.45
35:C:260:GLU:OE1	35:C:262:LYS:NZ	2.48	0.45
2:4:292:ASP:OD1	2:4:292:ASP:N	2.48	0.45
20:V:188:LYS:NZ	44:2:4892:A:OP1	2.49	0.45
44:2:1943:A:N1	44:2:4414:A:O2'	2.50	0.45
10:G:91:THR:HG22	49:t:110:LEU:HD12	1.96	0.45
14:L:47:LYS:HG3	22:Z:157:GLY:HA3	1.99	0.45
35:C:179:ARG:HA	35:C:179:ARG:HD3	1.80	0.45
44:2:2572:C:OP1	55:f:277:ARG:HD2	2.16	0.45
46:j:26:THR:OG1	46:j:85:ARG:NH1	2.45	0.45
51:i:99:ASP:OD1	51:i:99:ASP:N	2.48	0.45
54:q:182:PHE:HB2	54:q:425:PRO:HD2	1.99	0.45
14:L:76:ASP:OD1	14:L:76:ASP:N	2.47	0.45
44:2:34:A:H1'	44:2:1526:G:H21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2:2502:G:H1	58:g:47:ARG:NH2	2.15	0.45
44:2:4638:U:OP1	44:2:5044:A:O2'	2.34	0.45
50:s:252:PHE:HB3	50:s:260:ALA:HB1	1.99	0.45
52:T:98:LYS:HG3	52:T:99:ARG:HG3	1.98	0.45
3:6:79:GLN:OE1	4:7:1:MET:N	2.50	0.45
26:e:100:ASP:OD1	26:e:100:ASP:N	2.49	0.45
36:J:134:LYS:HB3	36:J:149:MET:HB3	1.98	0.45
44:2:1480:C:O2'	44:2:1482:G:OP2	2.35	0.45
44:2:4080:C:H2'	44:2:4081:G:H8	1.81	0.45
44:2:4305:G:C2	44:2:4309:G:N7	2.85	0.45
50:s:118:LEU:O	50:s:122:GLY:N	2.50	0.45
2:4:385:ARG:HA	2:4:387:ARG:HH11	1.82	0.45
12:I:48:LEU:HD22	12:I:56:ARG:HE	1.81	0.45
14:L:135:GLU:O	14:L:139:SER:HB3	2.17	0.45
15:M:17:THR:OG1	15:M:18:LEU:N	2.49	0.45
15:M:52:LYS:NZ	44:2:375:G:OP2	2.44	0.45
32:p:134:ARG:HH22	44:2:1795:A:H4'	1.82	0.45
37:N:107:THR:HG21	37:N:484:ARG:HD3	1.98	0.45
44:2:1855:G:O6	44:2:1880:G:N2	2.49	0.45
54:q:76:GLU:HB3	54:q:78:ILE:HG22	1.99	0.45
54:q:150:THR:HG23	54:q:153:CYS:H	1.81	0.45
57:3:169:VAL:HB	57:3:174:ILE:HD12	1.99	0.45
12:I:34:LEU:HD11	12:I:149:ASN:HB3	1.97	0.45
31:o:219:LYS:HD2	44:2:1290:G:H5''	1.99	0.45
41:w:423:GLU:HG3	41:w:438:PRO:HG3	1.98	0.45
49:t:65:PHE:HA	49:t:68:PHE:HD2	1.81	0.45
1:y:39:PRO:HA	1:y:42:VAL:HG12	1.98	0.45
4:7:71:PHE:O	4:7:75:ARG:NH2	2.50	0.45
31:o:72:LYS:HA	31:o:72:LYS:HD2	1.87	0.45
34:A:95:ARG:HA	34:A:176:PRO:HG3	1.98	0.45
37:N:273:ARG:NH1	37:N:276:ASP:OD2	2.44	0.45
39:u:30:ARG:NH2	44:2:1859:C:OP1	2.50	0.45
41:w:258:ASP:HA	52:T:276:LEU:HD21	1.98	0.45
44:2:1408:G:O2'	44:2:1412:G:O6	2.35	0.45
44:2:4301:U:H2'	44:2:4309:G:H1	1.82	0.45
46:j:18:ASN:O	46:j:90:ARG:NH2	2.49	0.45
12:I:171:ASP:OD2	12:I:173:ARG:NH1	2.50	0.45
17:Q:155:MET:HA	17:Q:156:PRO:HD3	1.75	0.45
29:m:107:MET:HE3	29:m:107:MET:HB3	1.77	0.45
37:N:209:PRO:HB3	37:N:301:LEU:HD22	1.98	0.45
44:2:1534:A2M:H8	44:2:1534:A2M:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:372:GLU:HG3	2:4:374:PRO:HD3	1.97	0.44
2:4:413:LEU:HD23	6:B:69:LYS:HG3	1.99	0.44
16:P:21:ARG:O	16:P:38:ASN:ND2	2.49	0.44
44:2:2544:G:N1	55:f:404:ARG:NH1	2.44	0.44
44:2:2763:U:C2'	55:f:391:ARG:NE	2.80	0.44
19:U:65:ARG:NH2	44:2:2457:G:OP1	2.49	0.44
22:Z:66:MET:HE2	22:Z:98:LEU:HD13	1.98	0.44
34:A:35:ARG:HH22	34:A:123:ILE:HG22	1.81	0.44
34:A:96:LYS:HA	34:A:96:LYS:HD3	1.83	0.44
36:J:31:GLU:OE2	36:J:35:ARG:NH2	2.50	0.44
41:w:312:SER:HB3	41:w:360:ILE:HD11	1.99	0.44
12:I:152:GLU:O	12:I:156:ASN:HB2	2.17	0.44
17:Q:170:THR:OG1	17:Q:173:GLU:OE1	2.32	0.44
19:U:50:ARG:NH2	44:2:279:A:OP1	2.48	0.44
23:a:60:ARG:NH1	44:2:2808:G:O3'	2.47	0.44
26:e:43:LYS:HG2	44:2:4508:C:H5'	1.99	0.44
44:2:126:C:H2'	44:2:127:G:H8	1.82	0.44
44:2:2548:C:P	55:f:392:ARG:NH2	2.90	0.44
2:4:290:LYS:H	2:4:321:SER:HA	1.83	0.44
36:J:129:GLU:HB2	41:w:64:SER:H	1.83	0.44
40:v:121:GLU:HB2	40:v:200:PHE:HB3	1.99	0.44
46:j:100:ASN:HD22	46:j:100:ASN:HA	1.66	0.44
54:q:20:ARG:NH1	55:f:454:ARG:HH22	2.15	0.44
2:4:373:ARG:NH2	3:6:136:GLU:OE2	2.50	0.44
14:L:60:HIS:NE2	44:2:4354:U:O2	2.51	0.44
15:M:49:TRP:O	44:2:1646:A:O2'	2.32	0.44
19:U:46:ASP:OD1	19:U:46:ASP:N	2.48	0.44
29:m:114:CYS:HB2	29:m:169:VAL:HG13	1.98	0.44
44:2:2521:G:H2'	44:2:2522:7MG:H82	1.98	0.44
44:2:4094:G:N2	44:2:4115:G:OP1	2.45	0.44
44:2:4419:U:O4	44:2:4424:A:N6	2.51	0.44
46:j:16:ALA:HA	46:j:19:GLU:HG3	1.99	0.44
56:O:30:ASP:OD2	56:O:30:ASP:N	2.49	0.44
2:4:257:LEU:HB2	2:4:288:ALA:HB1	1.98	0.44
3:6:129:LEU:O	3:6:133:LEU:HB2	2.17	0.44
6:B:165:HIS:ND1	6:B:166:THR:O	2.50	0.44
10:G:187:LYS:HB3	10:G:187:LYS:HE2	1.85	0.44
21:X:69:TRP:HZ3	29:m:176:ASP:HB2	1.83	0.44
23:a:135:LYS:NZ	44:2:2898:G:OP2	2.47	0.44
28:l:87:ARG:NH1	44:2:690:C:OP1	2.50	0.44
37:N:343:ARG:NH2	37:N:401:GLY:O	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:R:191:ARG:NH1	44:2:4373:G:OP1	2.51	0.44
44:2:2103:G:N7	44:2:2104:G:N1	2.66	0.44
44:2:4298:A:H2'	44:2:4299:U:H6	1.80	0.44
54:q:75:HIS:HB2	55:f:220:LYS:HE2	1.99	0.44
57:3:101:ARG:NH1	57:3:122:LYS:O	2.50	0.44
2:4:151:LEU:HA	2:4:154:VAL:HG12	1.99	0.44
5:9:17:ARG:HD2	44:2:3838:U:H5'	1.99	0.44
44:2:714:G:H2'	44:2:715:G:H8	1.82	0.44
44:2:2483:G:O2'	55:f:459:PHE:N	2.50	0.44
44:2:4572:U:O2'	44:2:4573:G:OP1	2.36	0.44
2:4:66:LEU:HD23	2:4:96:LEU:HD12	1.99	0.44
2:4:296:ILE:HA	2:4:299:LEU:HD23	1.99	0.44
6:B:249:ARG:NH1	44:2:2837:U:OP1	2.46	0.44
32:p:151:ASN:O	32:p:155:TYR:HB2	2.17	0.44
34:A:72:CYS:SG	34:A:73:THR:N	2.91	0.44
35:C:255:LYS:HE2	53:5:117:G:P	2.58	0.44
44:2:1804:A:H62	44:2:1836:G:H1	1.66	0.44
44:2:2848:G:O2'	44:2:3838:U:O4	2.36	0.44
48:Y:23:ARG:HD3	48:Y:125:MET:HE1	2.00	0.44
52:T:129:ASP:O	52:T:131:LYS:NZ	2.47	0.44
14:L:64:LYS:NZ	44:2:70:A:OP2	2.45	0.44
25:c:116:LYS:O	25:c:120:LYS:HB2	2.18	0.44
38:R:68:ASN:HA	38:R:71:LEU:HG	2.00	0.44
41:w:308:LYS:O	41:w:356:ARG:NH2	2.51	0.44
44:2:4894:A:H5''	44:2:4895:C:H2'	1.99	0.44
7:D:186:SER:O	7:D:186:SER:OG	2.36	0.43
11:H:3:LYS:HE2	43:8:81:C:H5'	1.99	0.43
12:I:141:LYS:HE3	12:I:141:LYS:HB2	1.83	0.43
19:U:73:ARG:NH2	44:2:31:U:O2'	2.51	0.43
29:m:128:ARG:NE	44:2:3681:G:OP2	2.50	0.43
35:C:270:LYS:HA	53:5:60:G:H4'	1.99	0.43
44:2:3644:U:O2	44:2:4554:G:O2'	2.33	0.43
44:2:3700:C:O2'	44:2:3746:A:N6	2.48	0.43
44:2:4980:C:N3	48:Y:69:ARG:NH2	2.66	0.43
54:q:183:LEU:HD13	54:q:188:ILE:HD13	1.99	0.43
57:3:78:LEU:HD21	57:3:142:ILE:HG23	2.00	0.43
7:D:204:ARG:NH1	7:D:205:ARG:O	2.49	0.43
8:E:29:LEU:HD12	8:E:91:VAL:HG21	1.99	0.43
10:G:59:ARG:NH1	44:2:2471:G:OP1	2.43	0.43
15:M:36:LYS:O	15:M:45:ARG:NH1	2.51	0.43
27:h:36:LYS:HB3	27:h:36:LYS:HE3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:v:42:ILE:HD11	40:v:92:VAL:HG13	2.00	0.43
41:w:282:HIS:HB3	41:w:289:PHE:HB3	2.00	0.43
44:2:966:A:N6	44:2:2092:G:O4'	2.51	0.43
44:2:1328:G:OP1	44:2:3906:A:N6	2.50	0.43
44:2:2514:G:N2	44:2:2744:A:C2	2.86	0.43
44:2:3758:U:O2'	44:2:3767:C:N4	2.45	0.43
49:t:40:GLU:OE2	58:g:14:LYS:NZ	2.42	0.43
3:6:44:ASP:OD1	3:6:44:ASP:N	2.47	0.43
3:6:85:ARG:HD2	3:6:94:ILE:HD13	1.99	0.43
37:N:302:ARG:HH12	37:N:466:PRO:HG3	1.83	0.43
55:f:364:ARG:HD2	56:O:6:GLU:O	2.18	0.43
25:c:58:HIS:O	44:2:1732:C:O2'	2.36	0.43
31:o:123:ARG:O	44:2:958:G:O2'	2.36	0.43
35:C:38:ILE:O	35:C:48:LYS:NZ	2.51	0.43
1:y:80:LEU:HD23	1:y:112:ILE:HG12	2.01	0.43
1:y:138:SER:OG	44:2:2002:A:N1	2.51	0.43
17:Q:140:SER:O	17:Q:144:LEU:CB	2.65	0.43
20:V:202:LEU:H	44:2:4872:2MG:HM21	1.83	0.43
27:h:1:MET:N	44:2:226:G:OP2	2.44	0.43
27:h:87:ARG:NH2	44:2:404:U:O3'	2.51	0.43
28:l:107:ARG:NH2	44:2:2263:A:OP1	2.52	0.43
48:Y:103:GLU:HG2	48:Y:109:VAL:HG11	2.01	0.43
2:4:62:LEU:HD22	2:4:99:ILE:HG23	1.99	0.43
22:Z:11:ARG:NH2	44:2:1689:G:OP1	2.52	0.43
24:b:66:GLN:O	44:2:729:2MG:N2	2.51	0.43
24:b:138:ARG:HH21	39:u:56:PHE:HA	1.84	0.43
24:b:170:LYS:HE3	44:2:4875:G:H5''	2.01	0.43
25:c:75:VAL:HG22	25:c:88:ARG:HG2	2.01	0.43
40:v:135:VAL:HG23	40:v:175:VAL:HB	1.99	0.43
44:2:959:G:O2'	44:2:2263:A:N6	2.50	0.43
44:2:1906:U:H2'	44:2:1907:A:H8	1.84	0.43
54:q:335:ASN:HD22	54:q:378:VAL:HG13	1.83	0.43
3:6:238:ASP:OD1	3:6:238:ASP:N	2.51	0.43
29:m:158:ILE:HD12	29:m:162:ASN:HD22	1.84	0.43
35:C:255:LYS:HD3	53:5:117:G:OP1	2.18	0.43
41:w:111:MET:O	52:T:262:THR:OG1	2.33	0.43
44:2:1100:U:O2	44:2:1195:G:O6	2.37	0.43
44:2:4297:G:H22	44:2:4313:A:N6	2.15	0.43
44:2:5022:U:O2'	44:2:5025:C:N4	2.50	0.43
54:q:185:ILE:HD13	55:f:419:GLN:HG3	2.01	0.43
35:C:262:LYS:HG3	53:5:120:U:C5'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:v:42:ILE:HD12	40:v:206:TYR:HD1	1.83	0.43
44:2:2484:A:OP1	57:3:47:LYS:HE2	2.18	0.43
2:4:161:LEU:HD12	2:4:162:PRO:HD2	2.01	0.43
2:4:176:TYR:OH	2:4:263:HIS:ND1	2.40	0.43
11:H:32:ARG:HG2	58:g:79:PHE:HB3	2.00	0.43
11:H:97:LYS:HD2	11:H:97:LYS:HA	1.80	0.43
22:Z:20:SER:OG	22:Z:21:GLN:N	2.52	0.43
23:a:4:LEU:HD11	23:a:29:THR:HG23	2.01	0.43
33:z:97:MET:O	33:z:102:ARG:NH1	2.51	0.43
47:k:26:ASP:OD1	47:k:26:ASP:N	2.43	0.43
49:t:108:ASN:H	49:t:117:GLU:HA	1.84	0.43
2:4:527:LEU:HD21	4:7:135:ARG:HD3	2.01	0.43
17:Q:111:GLN:HA	17:Q:114:VAL:HG12	2.01	0.43
35:C:184:ASP:N	35:C:184:ASP:OD1	2.51	0.43
36:J:6:TYR:OH	44:2:4477:A:OP1	2.36	0.43
36:J:25:ARG:NH2	44:2:4697:U:OP1	2.52	0.43
37:N:264:SER:OG	37:N:265:GLN:N	2.51	0.43
44:2:1332:C:H2'	44:2:1333:A:H8	1.84	0.43
44:2:4657:U:O2'	44:2:4659:G:OP2	2.37	0.43
55:f:215:GLU:HG3	58:g:61:PRO:HB3	2.01	0.43
7:D:69:THR:OG1	7:D:70:GLY:N	2.52	0.42
8:E:35:LEU:HB3	8:E:39:ARG:HH21	1.83	0.42
43:8:9:A:H2'	43:8:10:G:H8	1.84	0.42
44:2:4918:C:H2'	44:2:4919:G:H8	1.83	0.42
48:Y:110:ASP:OD2	48:Y:159:LYS:NZ	2.52	0.42
49:t:121:MET:HE2	49:t:125:LYS:HB2	2.01	0.42
51:i:63:ALA:HB2	55:f:279:LEU:CD2	2.45	0.42
57:3:112:VAL:HG13	57:3:143:VAL:HG12	2.00	0.42
15:M:56:ARG:NH2	44:2:374:G:OP2	2.51	0.42
17:Q:106:SER:OG	44:2:73:A:OP1	2.36	0.42
31:o:183:ARG:HD2	31:o:183:ARG:HA	1.90	0.42
44:2:267:G:H2'	44:2:268:G:H8	1.84	0.42
44:2:4297:G:N3	44:2:4297:G:C2'	2.81	0.42
7:D:283:LYS:HE3	7:D:283:LYS:HB2	1.88	0.42
9:F:45:ALA:HB3	9:F:82:MET:HE2	2.02	0.42
14:L:33:GLY:N	44:2:1515:A:OP1	2.48	0.42
36:J:136:ILE:HD11	36:J:149:MET:HB2	2.01	0.42
2:4:432:ILE:HG13	4:7:1:MET:HE3	2.01	0.42
12:I:21:LYS:HE3	12:I:21:LYS:HB2	1.87	0.42
20:V:32:LYS:H	20:V:32:LYS:HG2	1.68	0.42
44:2:1594:C:O2'	44:2:1597:G:O2'	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2:4478:G:O2'	44:2:4602:A:N1	2.46	0.42
5:9:28:LEU:H	5:9:31:ILE:HD12	1.85	0.42
18:S:97:ALA:HA	18:S:100:ARG:HG2	2.02	0.42
44:2:2361:G:O2'	44:2:3859:G:O6	2.37	0.42
44:2:2763:U:H2'	55:f:391:ARG:NE	2.34	0.42
44:2:4537:C:H2'	44:2:4538:G:H8	1.84	0.42
54:q:185:ILE:O	55:f:433:PRO:HB3	2.19	0.42
19:U:195:ARG:NH2	44:2:98:A:O3'	2.52	0.42
23:a:105:LEU:HD13	23:a:135:LYS:HD2	2.02	0.42
30:n:29:LYS:HE2	30:n:83:MET:HE2	2.01	0.42
44:2:4246:G:H2'	44:2:4247:G:H8	1.85	0.42
46:j:112:THR:OG1	46:j:113:THR:N	2.53	0.42
1:y:45:ASP:O	1:y:49:ALA:CB	2.67	0.42
6:B:174:ARG:NH1	44:2:4985:U:O2	2.52	0.42
10:G:207:VAL:HG21	10:G:215:LEU:HD11	2.02	0.42
14:L:26:ARG:HA	14:L:26:ARG:HD3	1.88	0.42
28:l:26:SER:OG	28:l:28:GLU:OE2	2.34	0.42
37:N:18:LEU:HB3	37:N:32:PRO:HB3	2.00	0.42
44:2:3658:C:H2'	44:2:3659:G:H8	1.84	0.42
51:i:124:THR:HG22	55:f:281:LEU:HD11	2.02	0.42
6:B:301:ASN:OD1	6:B:301:ASN:N	2.53	0.42
36:J:259:LEU:HD13	41:w:80:TRP:HB3	2.01	0.42
38:R:30:LEU:HD22	38:R:44:ARG:HB2	2.02	0.42
43:8:14:OMU:H5'	48:Y:123:PRO:HG3	2.01	0.42
44:2:5:A:H5''	54:q:94:LYS:HG3	2.01	0.42
49:t:111:PHE:HB3	49:t:114:ARG:HB3	2.00	0.42
51:i:7:PRO:HA	51:i:25:ILE:HG23	2.02	0.42
9:F:19:LYS:HA	9:F:19:LYS:HD3	1.91	0.42
27:h:47:MET:HE3	27:h:47:MET:HB3	1.88	0.42
37:N:312:SER:OG	37:N:314:ASN:O	2.33	0.42
44:2:2017:A:O2'	44:2:2018:C:O4'	2.37	0.42
44:2:4306:U:C5	44:2:4309:G:C5	3.08	0.42
44:2:5065:U:H5''	48:Y:43:LYS:HE3	2.01	0.42
54:q:131:LEU:HD11	54:q:195:LEU:HD12	2.02	0.42
54:q:379:ASP:OD2	55:f:429:ARG:HB2	2.20	0.42
57:3:20:LEU:HB3	57:3:21:VAL:H	1.73	0.42
57:3:237:MET:HE1	57:3:254:LEU:HD21	2.01	0.42
3:6:214:GLU:HA	3:6:217:VAL:HG12	2.02	0.42
34:A:18:ARG:HB3	34:A:19:LYS:H	1.75	0.42
34:A:35:ARG:NH1	34:A:122:SER:O	2.47	0.42
37:N:434:SER:O	37:N:434:SER:OG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:w:372:SER:OG	41:w:373:GLU:N	2.53	0.42
44:2:67:C:OP2	44:2:312:G:N2	2.52	0.42
44:2:1524:A2M:H2	44:2:1652:U:H3	1.85	0.42
44:2:4429:C:H2'	44:2:4430:G:O4'	2.19	0.42
45:d:105:ASN:ND2	45:d:111:GLU:OE1	2.53	0.42
17:Q:5:ARG:NH1	44:2:1850:A:OP2	2.45	0.41
21:X:2:ALA:N	44:2:1569:U:O4	2.53	0.41
25:c:116:LYS:HB3	25:c:116:LYS:HE2	1.90	0.41
31:o:57:TYR:HB3	31:o:61:ALA:HB3	2.02	0.41
35:C:199:ILE:HG22	35:C:200:MET:HE2	2.01	0.41
35:C:266:TRP:CD2	53:5:22:A:C8	3.08	0.41
44:2:2904:U:N3	44:2:3591:C:C4	2.88	0.41
44:2:3844:U:H2'	44:2:3845:A:H8	1.85	0.41
51:i:21:ARG:NH1	51:i:47:ASP:OD1	2.53	0.41
58:g:101:ASP:OD1	58:g:101:ASP:N	2.48	0.41
5:9:55:LEU:HD12	5:9:56:PRO:HD2	2.01	0.41
6:B:57:VAL:HG22	6:B:367:PHE:HB3	2.02	0.41
16:P:33:ASN:ND2	16:P:35:ILE:O	2.52	0.41
36:J:91:LEU:HD21	37:N:176:LYS:HE3	2.01	0.41
2:4:523:GLU:OE2	45:d:95:ASN:ND2	2.54	0.41
10:G:73:ARG:HH12	44:2:4162:C:H41	1.68	0.41
11:H:102:LEU:HD23	11:H:102:LEU:HA	1.96	0.41
32:p:214:SER:OG	32:p:215:SER:N	2.54	0.41
39:u:56:PHE:HB2	39:u:59:ALA:HB2	2.02	0.41
44:2:2045:G:O6	44:2:3870:C:O2'	2.37	0.41
44:2:2529:A:O2'	44:2:2531:C:OP2	2.38	0.41
44:2:4134:C:OP2	44:2:4144:C:N4	2.53	0.41
51:i:69:LYS:HE2	51:i:111:ARG:HH22	1.86	0.41
54:q:122:GLU:HG3	55:f:224:ARG:HH11	1.86	0.41
2:4:538:HIS:NE2	45:d:117:ILE:O	2.51	0.41
8:E:38:ILE:HG21	8:E:63:TYR:HB3	2.03	0.41
11:H:109:ARG:NH2	44:2:267:G:OP1	2.53	0.41
25:c:43:LYS:HA	25:c:95:HIS:HB3	2.01	0.41
31:o:222:LEU:HD12	31:o:223:ARG:HG2	2.02	0.41
44:2:2544:G:H1	55:f:404:ARG:CZ	2.33	0.41
48:Y:125:MET:HE2	48:Y:143:PRO:HG3	2.01	0.41
55:f:473:PHE:HE1	58:g:30:LYS:HE2	1.85	0.41
56:O:33:LYS:HG2	56:O:46:VAL:HG22	2.03	0.41
58:g:95:THR:HG22	58:g:139:ARG:HG3	2.03	0.41
1:y:16:ARG:NH2	1:y:57:ARG:O	2.53	0.41
2:4:56:GLN:O	2:4:60:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:69:PHE:HA	2:4:70:PRO:HD3	1.83	0.41
2:4:606:LYS:HE3	16:P:46:ARG:HE	1.85	0.41
9:F:108:LYS:HD2	9:F:108:LYS:HA	1.88	0.41
10:G:89:ARG:NH2	58:g:30:LYS:CD	2.78	0.41
19:U:4:TYR:OH	44:2:151:G:OP2	2.34	0.41
21:X:59:SER:O	44:2:2652:G:N2	2.53	0.41
31:o:161:ARG:O	31:o:182:ASN:ND2	2.50	0.41
37:N:43:ARG:HH21	37:N:46:LEU:HD23	1.85	0.41
44:2:2364:OMG:HM23	44:2:2364:OMG:H1'	1.78	0.41
44:2:5025:C:O2	44:2:5028:G:N2	2.53	0.41
51:i:27:LYS:O	51:i:42:LEU:N	2.53	0.41
53:5:23:A:N3	53:5:118:C:O2'	2.46	0.41
1:y:153:ASP:O	1:y:157:SER:HB3	2.21	0.41
2:4:593:MET:HE2	2:4:593:MET:HB3	1.88	0.41
26:e:19:GLY:O	44:2:2846:G:O2'	2.38	0.41
41:w:305:HIS:HB2	41:w:311:ILE:HD11	2.03	0.41
44:2:1:C:H4'	44:2:2:G:H5'	2.01	0.41
44:2:1550:G:H1	44:2:1578:U:H3	1.68	0.41
44:2:2394:G:O2'	44:2:2819:U:O4	2.34	0.41
44:2:3736:A:N6	44:2:4179:G:O2'	2.46	0.41
55:f:452:GLU:HA	55:f:453:PRO:HD3	1.91	0.41
2:4:366:THR:HG21	3:6:178:GLN:HA	2.03	0.41
7:D:335:MET:HE2	7:D:335:MET:HB3	1.96	0.41
21:X:3:LYS:HD2	21:X:3:LYS:HA	1.89	0.41
26:e:123:LYS:HE2	26:e:123:LYS:HB2	1.83	0.41
38:R:18:ALA:HA	38:R:21:LEU:HG	2.01	0.41
44:2:500:G:OP2	44:2:503:C:O2'	2.35	0.41
44:2:1398:A:N6	44:2:1419:G:O2'	2.54	0.41
44:2:2050:OMG:H1'	44:2:2050:OMG:HM23	1.84	0.41
44:2:2484:A:H62	57:3:44:LEU:CD2	2.24	0.41
44:2:4906:C:H2'	44:2:4907:G:H8	1.84	0.41
44:2:62:A:N3	44:2:77:U:O2'	2.49	0.41
44:2:505:G:H1	44:2:653:U:H3	1.68	0.41
44:2:1301:C:H2'	47:k:17:THR:HG21	2.01	0.41
44:2:2295:C:H2'	44:2:2296:G:H8	1.85	0.41
2:4:295:ARG:HA	2:4:295:ARG:HD2	1.89	0.41
2:4:534:LYS:NZ	45:d:31:ASP:OD2	2.54	0.41
3:6:104:LEU:HA	3:6:107:VAL:HG12	2.03	0.41
6:B:297:LYS:HB2	6:B:297:LYS:HE2	1.93	0.41
7:D:328:LEU:HD12	32:p:187:MET:HG3	2.02	0.41
8:E:78:ASN:OD1	8:E:78:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Z:39:THR:HG22	22:Z:41:SER:H	1.85	0.41
23:a:108:ARG:O	23:a:112:SER:HB2	2.20	0.41
29:m:107:MET:SD	29:m:107:MET:N	2.94	0.41
30:n:106:TYR:HB2	31:o:193:PHE:HD1	1.86	0.41
31:o:146:PRO:HB2	31:o:203:ILE:HG21	2.03	0.41
35:C:109:LEU:HD23	35:C:171:LEU:HD21	2.03	0.41
36:J:167:TYR:O	44:2:4303:C:O2'	2.39	0.41
41:w:425:LEU:HD22	41:w:443:VAL:HG13	2.03	0.41
44:2:2375:A:H2'	44:2:2376:A:H8	1.86	0.41
44:2:2439:G:O5'	54:q:1:MET:N	2.53	0.41
44:2:3855:C:H2'	44:2:3856:A:H8	1.86	0.41
44:2:4492:U:O2'	44:2:4512:U:O2	2.36	0.41
46:j:91:LYS:HD3	46:j:91:LYS:HA	1.86	0.41
50:s:238:SER:HB2	50:s:245:TRP:HB2	2.03	0.41
51:i:41:ALA:HB2	51:i:77:TYR:HE1	1.85	0.41
51:i:50:PRO:HD3	51:i:68:ILE:HG13	2.03	0.41
54:q:268:ASP:N	54:q:268:ASP:OD1	2.54	0.41
32:p:43:ARG:NH2	44:2:974:C:O3'	2.54	0.41
33:z:30:LYS:HB3	33:z:30:LYS:HE2	1.89	0.41
44:2:1895:G:O2'	44:2:1907:A:N3	2.49	0.41
44:2:2904:U:C4	44:2:3591:C:N4	2.89	0.41
54:q:370:ASP:O	54:q:390:ARG:NH2	2.50	0.41
2:4:152:GLU:OE2	2:4:156:GLN:NE2	2.54	0.40
2:4:189:THR:OG1	2:4:209:HIS:O	2.36	0.40
2:4:294:LYS:HG3	2:4:299:LEU:HD21	2.02	0.40
18:S:27:ILE:HA	18:S:38:VAL:HG12	2.02	0.40
26:e:131:ARG:HA	26:e:131:ARG:HD2	1.87	0.40
37:N:307:GLU:HA	37:N:308:PRO:HD3	1.85	0.40
41:w:392:ASP:OD1	41:w:392:ASP:N	2.51	0.40
44:2:1714:C:H2'	44:2:1715:C:H4'	2.03	0.40
44:2:1861:U:O2	44:2:1861:U:O4'	2.39	0.40
50:s:82:LEU:HD13	50:s:233:VAL:HA	2.02	0.40
54:q:36:ARG:HG2	54:q:222:THR:HG21	2.02	0.40
2:4:13:PRO:HG2	2:4:18:PHE:HD1	1.86	0.40
2:4:418:ASP:OD1	2:4:418:ASP:N	2.46	0.40
6:B:168:MET:HE2	6:B:168:MET:HB3	1.99	0.40
31:o:99:ASP:OD1	31:o:99:ASP:N	2.51	0.40
37:N:180:ILE:HD12	37:N:205:LEU:HD21	2.02	0.40
48:Y:168:LYS:HD3	48:Y:168:LYS:HA	1.92	0.40
50:s:258:SER:OG	50:s:259:ALA:N	2.55	0.40
55:f:211:GLU:HG2	58:g:64:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:3:228:LYS:H	57:3:228:LYS:HG2	1.73	0.40
2:4:241:ILE:HD13	2:4:241:ILE:HA	1.95	0.40
18:S:71:LYS:NZ	44:2:738:C:O3'	2.52	0.40
21:X:48:LYS:HE2	21:X:48:LYS:HB3	1.80	0.40
27:h:54:GLU:HB2	27:h:108:ARG:HB3	2.02	0.40
29:m:144:LYS:HB3	29:m:160:SER:HB3	2.03	0.40
35:C:58:ARG:NH1	53:5:26:C:OP2	2.53	0.40
44:2:387:G:O2'	44:2:412:G:N1	2.54	0.40
6:B:373:LYS:HE2	44:2:4627:U:H4'	2.02	0.40
7:D:283:LYS:NZ	22:Z:22:ASP:OD2	2.51	0.40
9:F:54:ARG:NH2	44:2:2651:C:O2'	2.52	0.40
37:N:352:THR:HG21	37:N:367:ARG:HH11	1.86	0.40
41:w:313:VAL:HB	41:w:359:LEU:HD23	2.03	0.40
44:2:186:G:O2'	44:2:1366:G:N3	2.49	0.40
44:2:2487:G:OP1	57:3:223:ALA:HA	2.21	0.40
44:2:3776:G:H1'	44:2:3777:G:H2'	2.02	0.40
44:2:4775:C:H2'	44:2:4776:G:H8	1.86	0.40
54:q:127:PHE:O	54:q:237:ARG:NH1	2.55	0.40
57:3:72:LYS:HB3	57:3:72:LYS:HE3	1.90	0.40
26:e:85:ARG:NE	26:e:99:GLU:O	2.47	0.40
28:l:125:MET:N	28:l:125:MET:SD	2.94	0.40
34:A:115:LEU:HA	34:A:116:GLY:HA2	1.74	0.40
35:C:220:LYS:O	35:C:224:SER:HB3	2.22	0.40
41:w:371:ASP:OD1	41:w:371:ASP:N	2.49	0.40
44:2:153:G:H2'	44:2:154:G:H8	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	y	163/165 (99%)	160 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4	616/634 (97%)	555 (90%)	57 (9%)	4 (1%)	21	54
3	6	242/245 (99%)	227 (94%)	15 (6%)	0	100	100
4	7	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
5	9	82/134 (61%)	71 (87%)	10 (12%)	1 (1%)	10	41
6	B	401/403 (100%)	380 (95%)	21 (5%)	0	100	100
7	D	356/427 (83%)	330 (93%)	26 (7%)	0	100	100
8	E	96/115 (84%)	92 (96%)	4 (4%)	0	100	100
9	F	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
10	G	240/266 (90%)	225 (94%)	15 (6%)	0	100	100
11	H	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
12	I	188/192 (98%)	176 (94%)	11 (6%)	1 (0%)	24	57
13	K	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
14	L	145/148 (98%)	131 (90%)	14 (10%)	0	100	100
15	M	84/97 (87%)	74 (88%)	10 (12%)	0	100	100
16	P	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
17	Q	208/211 (99%)	198 (95%)	10 (5%)	0	100	100
18	S	133/215 (62%)	124 (93%)	9 (7%)	0	100	100
19	U	201/204 (98%)	188 (94%)	13 (6%)	0	100	100
20	V	199/203 (98%)	195 (98%)	4 (2%)	0	100	100
21	X	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
22	Z	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
23	a	146/196 (74%)	141 (97%)	5 (3%)	0	100	100
24	b	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
25	c	115/160 (72%)	101 (88%)	12 (10%)	2 (2%)	7	35
26	e	129/140 (92%)	116 (90%)	13 (10%)	0	100	100
27	h	132/145 (91%)	126 (96%)	6 (4%)	0	100	100
28	l	123/137 (90%)	115 (94%)	8 (6%)	0	100	100
29	m	246/257 (96%)	223 (91%)	23 (9%)	0	100	100
30	n	107/110 (97%)	100 (94%)	6 (6%)	1 (1%)	14	47
31	o	231/288 (80%)	214 (93%)	17 (7%)	0	100	100
32	p	224/248 (90%)	215 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	z	63/129 (49%)	61 (97%)	2 (3%)	0	100	100
34	A	163/178 (92%)	151 (93%)	12 (7%)	0	100	100
35	C	244/297 (82%)	226 (93%)	18 (7%)	0	100	100
36	J	257/260 (99%)	244 (95%)	11 (4%)	2 (1%)	16	49
37	N	470/485 (97%)	444 (94%)	23 (5%)	3 (1%)	21	54
38	R	197/365 (54%)	184 (93%)	12 (6%)	1 (0%)	24	57
39	u	73/549 (13%)	63 (86%)	8 (11%)	2 (3%)	4	27
40	v	204/239 (85%)	197 (97%)	7 (3%)	0	100	100
41	w	445/731 (61%)	424 (95%)	20 (4%)	1 (0%)	43	74
42	r	22/360 (6%)	21 (96%)	1 (4%)	0	100	100
45	d	102/128 (80%)	92 (90%)	10 (10%)	0	100	100
46	j	109/125 (87%)	103 (94%)	6 (6%)	0	100	100
47	k	127/135 (94%)	119 (94%)	8 (6%)	0	100	100
48	Y	165/184 (90%)	156 (94%)	9 (6%)	0	100	100
49	t	109/293 (37%)	103 (94%)	6 (6%)	0	100	100
50	s	237/490 (48%)	230 (97%)	7 (3%)	0	100	100
51	i	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
52	T	260/306 (85%)	235 (90%)	22 (8%)	3 (1%)	10	41
54	q	398/588 (68%)	385 (97%)	13 (3%)	0	100	100
55	f	254/478 (53%)	236 (93%)	17 (7%)	1 (0%)	30	62
56	O	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
57	3	223/255 (88%)	209 (94%)	13 (6%)	1 (0%)	30	62
58	g	141/156 (90%)	135 (96%)	5 (4%)	1 (1%)	18	51
All	All	10226/13292 (77%)	9605 (94%)	597 (6%)	24 (0%)	44	74

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	c	53	PRO
36	J	106	ILE
37	N	59	PRO
37	N	267	ARG
38	R	24	ILE
39	u	51	PRO

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Mol	Chain	Res	Type
39	u	55	PRO
52	T	148	ASP
52	T	152	VAL
55	f	203	ASP
57	3	24	ASN
2	4	301	GLU
5	9	99	GLN
36	J	101	VAL
52	T	191	GLY
2	4	427	ASP
41	w	112	LYS
58	g	40	ILE
2	4	4	TYR
2	4	296	ILE
37	N	65	HIS
25	c	43	LYS
30	n	107	PRO
12	I	104	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	y	137/137 (100%)	137 (100%)	0	100	100
2	4	562/574 (98%)	562 (100%)	0	100	100
3	6	212/213 (100%)	212 (100%)	0	100	100
4	7	126/149 (85%)	126 (100%)	0	100	100
5	9	74/114 (65%)	74 (100%)	0	100	100
6	B	349/349 (100%)	349 (100%)	0	100	100
7	D	298/348 (86%)	298 (100%)	0	100	100
8	E	83/97 (86%)	83 (100%)	0	100	100
9	F	94/100 (94%)	94 (100%)	0	100	100
10	G	204/223 (92%)	202 (99%)	2 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	H	109/110 (99%)	109 (100%)	0	100	100
12	I	169/171 (99%)	169 (100%)	0	100	100
13	K	86/89 (97%)	86 (100%)	0	100	100
14	L	120/121 (99%)	120 (100%)	0	100	100
15	M	73/80 (91%)	73 (100%)	0	100	100
16	P	47/48 (98%)	47 (100%)	0	100	100
17	Q	176/177 (99%)	176 (100%)	0	100	100
18	S	115/161 (71%)	115 (100%)	0	100	100
19	U	171/172 (99%)	171 (100%)	0	100	100
20	V	173/174 (99%)	173 (100%)	0	100	100
21	X	74/75 (99%)	74 (100%)	0	100	100
22	Z	164/165 (99%)	164 (100%)	0	100	100
23	a	133/175 (76%)	133 (100%)	0	100	100
24	b	157/157 (100%)	156 (99%)	1 (1%)	78	79
25	c	106/140 (76%)	106 (100%)	0	100	100
26	e	101/107 (94%)	101 (100%)	0	100	100
27	h	124/135 (92%)	124 (100%)	0	100	100
28	l	109/121 (90%)	109 (100%)	0	100	100
29	m	190/199 (96%)	190 (100%)	0	100	100
30	n	88/89 (99%)	88 (100%)	0	100	100
31	o	208/252 (82%)	208 (100%)	0	100	100
32	p	195/215 (91%)	195 (100%)	0	100	100
33	z	61/115 (53%)	61 (100%)	0	100	100
34	A	138/149 (93%)	138 (100%)	0	100	100
35	C	209/250 (84%)	209 (100%)	0	100	100
36	J	227/228 (100%)	227 (100%)	0	100	100
37	N	396/404 (98%)	396 (100%)	0	100	100
38	R	173/300 (58%)	173 (100%)	0	100	100
39	u	68/485 (14%)	68 (100%)	0	100	100
40	v	182/214 (85%)	182 (100%)	0	100	100
41	w	405/654 (62%)	405 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	r	22/312 (7%)	22 (100%)	0	100	100
45	d	94/115 (82%)	94 (100%)	0	100	100
46	j	101/110 (92%)	100 (99%)	1 (1%)	68	75
47	k	115/121 (95%)	115 (100%)	0	100	100
48	Y	147/163 (90%)	147 (100%)	0	100	100
49	t	103/274 (38%)	103 (100%)	0	100	100
50	s	222/437 (51%)	222 (100%)	0	100	100
51	i	117/118 (99%)	117 (100%)	0	100	100
52	T	241/279 (86%)	241 (100%)	0	100	100
54	q	359/509 (70%)	359 (100%)	0	100	100
55	f	222/402 (55%)	222 (100%)	0	100	100
56	O	64/65 (98%)	64 (100%)	0	100	100
57	3	206/228 (90%)	206 (100%)	0	100	100
58	g	124/133 (93%)	124 (100%)	0	100	100
All	All	9023/11502 (78%)	9019 (100%)	4 (0%)	100	100

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

Mol	Chain	Res	Type
10	G	137[A]	ARG
10	G	137[B]	ARG
24	b	77	ASN
46	j	100	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	y	137	GLN
2	4	59	HIS
2	4	84	ASN
3	6	10	ASN
3	6	82	GLN
3	6	86	ASN
3	6	170	GLN
3	6	228	GLN
4	7	76	ASN

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Mol	Chain	Res	Type
4	7	130	ASN
4	7	132	HIS
5	9	61	HIS
6	B	121	ASN
6	B	184	GLN
6	B	289	GLN
6	B	328	ASN
7	D	43	ASN
7	D	178	ASN
7	D	329	ASN
10	G	46	GLN
11	H	62	ASN
12	I	163	GLN
13	K	92	ASN
14	L	28	HIS
14	L	40	HIS
16	P	4	HIS
18	S	20	HIS
19	U	37	HIS
19	U	149	GLN
19	U	182	HIS
20	V	63	ASN
20	V	180	GLN
20	V	199	HIS
23	a	121	HIS
24	b	50	GLN
24	b	117	HIS
25	c	79	GLN
26	e	50	ASN
27	h	14	ASN
27	h	18	HIS
27	h	61	HIS
28	l	6	GLN
28	l	31	ASN
28	l	85	ASN
29	m	132	ASN
29	m	162	ASN
29	m	194	ASN
30	n	21	GLN
31	o	157	HIS
31	o	266	GLN
32	p	24	ASN

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Mol	Chain	Res	Type
32	p	80	ASN
32	p	99	ASN
32	p	119	ASN
32	p	126	ASN
32	p	205	ASN
33	z	21	ASN
33	z	92	GLN
33	z	99	GLN
34	A	155	HIS
35	C	63	GLN
35	C	198	HIS
35	C	222	GLN
36	J	232	GLN
37	N	49	ASN
37	N	177	ASN
38	R	115	GLN
38	R	176	GLN
39	u	28	HIS
40	v	147	HIS
40	v	152	GLN
45	d	119	GLN
46	j	34	HIS
47	k	63	ASN
48	Y	10	ASN
49	t	119	HIS
49	t	127	HIS
51	i	127	ASN
52	T	32	ASN
52	T	101	ASN
54	q	253	GLN
55	f	286	GLN
55	f	341	GLN
58	g	107	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
43	8	153/156 (98%)	28 (18%)	2 (1%)
44	2	3524/5054 (69%)	962 (27%)	33 (0%)
53	5	119/120 (99%)	19 (15%)	0
59	x	0/60	-	-

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3796/5390 (70%)	1009 (26%)	35 (0%)

All (1009) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
43	8	24	G
43	8	34	U
43	8	35	C
43	8	39	G
43	8	48	A
43	8	52	A
43	8	59	A
43	8	62	A
43	8	63	U
43	8	71	A
43	8	80	A
43	8	82	A
43	8	84	A
43	8	85	U
43	8	88	A
43	8	94	G
43	8	103	A
43	8	104	A
43	8	105	C
43	8	110	U
43	8	114	G
43	8	123	U
43	8	124	U
43	8	125	C
43	8	126	C
43	8	127	U
43	8	153	C
43	8	156	U
44	2	13	U
44	2	25	A
44	2	37	U
44	2	39	A
44	2	42	A
44	2	44	A
44	2	48	G
44	2	56	A
44	2	59	A

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Mol	Chain	Res	Type
44	2	64	A
44	2	65	A
44	2	69	A
44	2	72	C
44	2	73	A
44	2	84	A
44	2	91	G
44	2	95	G
44	2	98	A
44	2	108	A
44	2	109	G
44	2	110	C
44	2	119	G
44	2	120	A
44	2	131	C
44	2	132	G
44	2	134	G
44	2	135	G
44	2	136	C
44	2	137	G
44	2	144	G
44	2	145	G
44	2	152	U
44	2	158	A
44	2	159	C
44	2	171	U
44	2	172	C
44	2	180	C
44	2	183	C
44	2	185	C
44	2	188	G
44	2	197	A
44	2	200	U
44	2	209	U
44	2	216	C
44	2	217	C
44	2	218	A
44	2	220	C
44	2	225	G
44	2	234	G
44	2	237	B9B
44	2	254	G

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Mol	Chain	Res	Type
44	2	256	G
44	2	262	G
44	2	265	C
44	2	266	C
44	2	267	G
44	2	278	G
44	2	279	A
44	2	280	G
44	2	297	U
44	2	306	A
44	2	315	G
44	2	316	U
44	2	340	C
44	2	362	A
44	2	363	A
44	2	385	A
44	2	387	G
44	2	396	A
44	2	398	A2M
44	2	407	A
44	2	409	G
44	2	410	A
44	2	412	G
44	2	432	U
44	2	433	A
44	2	449	C
44	2	450	G
44	2	452	A
44	2	453	G
44	2	454	U
44	2	464	G
44	2	465	G
44	2	467	U
44	2	484	U
44	2	485	C
44	2	486	C
44	2	489	C
44	2	491	G
44	2	493	G
44	2	495	C
44	2	497	G
44	2	498	C

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Mol	Chain	Res	Type
44	2	499	G
44	2	500	G
44	2	502	C
44	2	503	C
44	2	504	G
44	2	505	G
44	2	509	A
44	2	510	U
44	2	514	U
44	2	515	C
44	2	516	C
44	2	517	C
44	2	518	G
44	2	519	C
44	2	644	G
44	2	654	C
44	2	656	C
44	2	659	G
44	2	666	G
44	2	667	A
44	2	668	C
44	2	669	C
44	2	673	C
44	2	685	C
44	2	686	A
44	2	687	U
44	2	688	U
44	2	692	A
44	2	696	C
44	2	697	G
44	2	703	G
44	2	704	C
44	2	731	G
44	2	738	C
44	2	739	G
44	2	740	G
44	2	742	G
44	2	746	A
44	2	753	C
44	2	758	G
44	2	759	G
44	2	760	G

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Mol	Chain	Res	Type
44	2	904	C
44	2	913	U
44	2	914	U
44	2	915	A
44	2	916	C
44	2	917	A
44	2	918	G
44	2	924	C
44	2	925	C
44	2	926	G
44	2	932	A
44	2	933	G
44	2	934	C
44	2	935	A
44	2	936	C
44	2	937	U
44	2	941	C
44	2	943	A
44	2	944	A
44	2	945	U
44	2	946	C
44	2	959	G
44	2	960	A
44	2	961	G
44	2	962	C
44	2	965	G
44	2	966	A
44	2	967	C
44	2	969	C
44	2	970	G
44	2	971	U
44	2	972	C
44	2	982	U
44	2	984	C
44	2	989	U
44	2	990	C
44	2	991	C
44	2	992	C
44	2	993	G
44	2	994	G
44	2	995	C
44	2	996	G

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Mol	Chain	Res	Type
44	2	1048	G
44	2	1049	C
44	2	1051	G
44	2	1066	G
44	2	1067	G
44	2	1068	G
44	2	1070	G
44	2	1072	C
44	2	1082	C
44	2	1093	C
44	2	1168	G
44	2	1170	G
44	2	1171	G
44	2	1173	G
44	2	1174	G
44	2	1178	G
44	2	1179	U
44	2	1180	C
44	2	1181	C
44	2	1182	C
44	2	1183	C
44	2	1184	A
44	2	1187	G
44	2	1189	G
44	2	1195	G
44	2	1199	G
44	2	1200	G
44	2	1202	C
44	2	1203	G
44	2	1210	C
44	2	1211	G
44	2	1215	C
44	2	1216	C
44	2	1218	G
44	2	1219	G
44	2	1222	A
44	2	1241	C
44	2	1243	C
44	2	1245	C
44	2	1252	C
44	2	1253	G
44	2	1254	A

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Mol	Chain	Res	Type
44	2	1255	A
44	2	1260	G
44	2	1265	G
44	2	1266	G
44	2	1269	G
44	2	1271	G
44	2	1272	C
44	2	1273	G
44	2	1280	C
44	2	1283	G
44	2	1284	G
44	2	1287	G
44	2	1295	C
44	2	1296	G
44	2	1301	C
44	2	1302	U
44	2	1303	A
44	2	1313	C
44	2	1314	C
44	2	1320	U
44	2	1337	A
44	2	1354	A
44	2	1358	G
44	2	1359	G
44	2	1365	C
44	2	1366	G
44	2	1367	C
44	2	1372	A
44	2	1377	G
44	2	1378	C
44	2	1379	C
44	2	1381	U
44	2	1387	A
44	2	1394	G
44	2	1397	A
44	2	1399	G
44	2	1402	C
44	2	1404	G
44	2	1405	C
44	2	1407	C
44	2	1408	G
44	2	1409	C

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Mol	Chain	Res	Type
44	2	1410	U
44	2	1412	G
44	2	1414	C
44	2	1420	A
44	2	1421	G
44	2	1438	U
44	2	1439	C
44	2	1442	C
44	2	1445	U
44	2	1446	C
44	2	1448	G
44	2	1465	G
44	2	1472	C
44	2	1482	G
44	2	1483	C
44	2	1486	C
44	2	1497	A
44	2	1498	G
44	2	1501	C
44	2	1502	G
44	2	1503	A
44	2	1518	A
44	2	1523	A
44	2	1525	A
44	2	1534	A2M
44	2	1547	A
44	2	1566	C
44	2	1571	G
44	2	1578	U
44	2	1591	U
44	2	1592	G
44	2	1595	G
44	2	1596	U
44	2	1597	G
44	2	1612	G
44	2	1613	A
44	2	1624	G
44	2	1625	OMG
44	2	1626	G
44	2	1631	A
44	2	1633	G
44	2	1634	A

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Mol	Chain	Res	Type
44	2	1638	A
44	2	1641	G
44	2	1650	A
44	2	1654	G
44	2	1658	G
44	2	1660	U
44	2	1661	C
44	2	1671	U
44	2	1674	C
44	2	1676	C
44	2	1679	A
44	2	1680	G
44	2	1691	G
44	2	1694	C
44	2	1697	G
44	2	1699	A
44	2	1700	G
44	2	1701	A
44	2	1703	C
44	2	1704	C
44	2	1705	G
44	2	1707	C
44	2	1715	C
44	2	1716	G
44	2	1718	C
44	2	1719	A
44	2	1724	G
44	2	1726	U
44	2	1729	A
44	2	1732	C
44	2	1734	G
44	2	1737	A
44	2	1738	A
44	2	1789	C
44	2	1791	U
44	2	1792	U
44	2	1793	A
44	2	1799	G
44	2	1800	U
44	2	1801	A
44	2	1802	A
44	2	1803	G

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Mol	Chain	Res	Type
44	2	1804	A
44	2	1806	G
44	2	1809	C
44	2	1810	G
44	2	1815	G
44	2	1821	G
44	2	1822	U
44	2	1832	C
44	2	1833	G
44	2	1836	G
44	2	1837	A
44	2	1842	G
44	2	1854	G
44	2	1855	G
44	2	1856	C
44	2	1860	U
44	2	1865	G
44	2	1870	C
44	2	1871	A2M
44	2	1882	U
44	2	1883	OMG
44	2	1891	A
44	2	1897	A
44	2	1900	C
44	2	1918	U
44	2	1919	G
44	2	1920	C
44	2	1922	G
44	2	1925	G
44	2	1929	A
44	2	1931	C
44	2	1932	A
44	2	1935	C
44	2	1936	C
44	2	1937	C
44	2	1939	A
44	2	1941	A
44	2	1942	A
44	2	1943	A
44	2	1944	A
44	2	1948	G
44	2	1956	A

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Mol	Chain	Res	Type
44	2	1959	U
44	2	1961	G
44	2	1966	C
44	2	1972	G
44	2	1979	A
44	2	1980	U
44	2	1981	G
44	2	1983	A
44	2	1984	A
44	2	1985	G
44	2	1991	A
44	2	1997	U
44	2	2001	G
44	2	2002	A
44	2	2003	G
44	2	2004	U
44	2	2010	A
44	2	2011	C
44	2	2017	A
44	2	2018	C
44	2	2020	U
44	2	2025	A
44	2	2026	A
44	2	2033	A
44	2	2034	G
44	2	2040	A
44	2	2043	A
44	2	2044	U
44	2	2046	G
44	2	2048	U
44	2	2055	G
44	2	2056	G
44	2	2069	A
44	2	2084	C
44	2	2092	G
44	2	2093	A
44	2	2095	A
44	2	2096	G
44	2	2098	G
44	2	2100	A
44	2	2101	C
44	2	2104	G

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Mol	Chain	Res	Type
44	2	2105	A
44	2	2108	G
44	2	2110	C
44	2	2111	G
44	2	2112	G
44	2	2250	C
44	2	2252	G
44	2	2253	A
44	2	2254	G
44	2	2255	C
44	2	2256	C
44	2	2258	C
44	2	2259	G
44	2	2260	C
44	2	2263	A
44	2	2268	A
44	2	2269	C
44	2	2279	A
44	2	2289	C
44	2	2300	A
44	2	2301	G
44	2	2305	U
44	2	2306	G
44	2	2313	A
44	2	2325	C
44	2	2333	G
44	2	2346	C
44	2	2348	G
44	2	2351	C
44	2	2360	A
44	2	2364	OMG
44	2	2395	A
44	2	2416	G
44	2	2417	A
44	2	2422	OMC
44	2	2424	OMG
44	2	2425	U
44	2	2441	C
44	2	2450	G
44	2	2463	G
44	2	2465	C
44	2	2470	C

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Mol	Chain	Res	Type
44	2	2471	G
44	2	2474	G
44	2	2475	G
44	2	2476	G
44	2	2478	C
44	2	2479	G
44	2	2483	G
44	2	2484	A
44	2	2486	G
44	2	2487	G
44	2	2488	C
44	2	2499	C
44	2	2503	G
44	2	2504	C
44	2	2505	C
44	2	2506	G
44	2	2507	A
44	2	2512	A
44	2	2513	A
44	2	2519	U
44	2	2529	A
44	2	2543	A
44	2	2544	G
44	2	2545	U
44	2	2546	G
44	2	2547	G
44	2	2548	C
44	2	2553	A
44	2	2554	U
44	2	2557	G
44	2	2559	G
44	2	2560	C
44	2	2566	G
44	2	2573	A
44	2	2583	C
44	2	2586	G
44	2	2587	A
44	2	2589	C
44	2	2600	A
44	2	2601	A
44	2	2618	G
44	2	2627	C

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Mol	Chain	Res	Type
44	2	2638	G
44	2	2653	C
44	2	2659	A
44	2	2662	G
44	2	2669	C
44	2	2670	C
44	2	2674	A
44	2	2675	G
44	2	2679	G
44	2	2687	U
44	2	2694	G
44	2	2695	A
44	2	2696	A
44	2	2708	U
44	2	2709	C
44	2	2711	G
44	2	2712	G
44	2	2719	C
44	2	2721	G
44	2	2724	G
44	2	2725	A
44	2	2726	G
44	2	2739	C
44	2	2740	U
44	2	2742	G
44	2	2743	A
44	2	2753	G
44	2	2754	B9B
44	2	2761	U
44	2	2763	U
44	2	2769	U
44	2	2770	C
44	2	2787	A
44	2	2788	U
44	2	2790	U
44	2	2799	G
44	2	2814	C
44	2	2815	A
44	2	2826	U
44	2	2827	G
44	2	2840	A
44	2	2842	G

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Mol	Chain	Res	Type
44	2	2855	G
44	2	2857	A
44	2	2875	C
44	2	2876	G
44	2	2902	G
44	2	2904	U
44	2	2905	C
44	2	2906	G
44	2	2908	U
44	2	3585	G
44	2	3588	C
44	2	3591	C
44	2	3594	C
44	2	3595	U
44	2	3596	A
44	2	3597	G
44	2	3611	A
44	2	3615	G
44	2	3616	U
44	2	3619	G
44	2	3626	G
44	2	3630	A
44	2	3635	A
44	2	3644	U
44	2	3662	A
44	2	3664	G
44	2	3678	G
44	2	3680	U
44	2	3691	G
44	2	3692	A
44	2	3695	U
44	2	3696	C
44	2	3698	G
44	2	3700	C
44	2	3701	OMC
44	2	3702	A
44	2	3709	U
44	2	3710	G
44	2	3712	A
44	2	3714	G
44	2	3715	U
44	2	3716	C

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Mol	Chain	Res	Type
44	2	3717	A
44	2	3718	A
44	2	3723	A
44	2	3724	A
44	2	3729	U
44	2	3735	G
44	2	3736	A
44	2	3745	U
44	2	3746	A
44	2	3748	A
44	2	3750	G
44	2	3752	C
44	2	3753	G
44	2	3754	G
44	2	3759	A
44	2	3760	A
44	2	3761	C
44	2	3762	U
44	2	3765	G
44	2	3766	A
44	2	3767	C
44	2	3769	C
44	2	3771	C
44	2	3772	U
44	2	3773	U
44	2	3774	A
44	2	3775	A
44	2	3776	G
44	2	3777	G
44	2	3778	U
44	2	3779	A
44	2	3781	C
44	2	3783	A
44	2	3838	U
44	2	3839	G
44	2	3840	U
44	2	3851	U
44	2	3865	A
44	2	3867	A2M
44	2	3870	C
44	2	3875	G
44	2	3876	A

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Mol	Chain	Res	Type
44	2	3877	A
44	2	3879	G
44	2	3880	P7G
44	2	3897	B8K
44	2	3903	A
44	2	3904	G
44	2	3905	A
44	2	3906	A
44	2	3915	U
44	2	3916	G
44	2	3922	G
44	2	3923	A
44	2	3924	C
44	2	3925	U
44	2	3926	C
44	2	3931	C
44	2	3938	G
44	2	3939	G
44	2	3944	G
44	2	4068	U
44	2	4076	G
44	2	4077	A
44	2	4083	5MU
44	2	4084	G
44	2	4095	G
44	2	4097	G
44	2	4099	G
44	2	4100	C
44	2	4101	C
44	2	4103	C
44	2	4104	G
44	2	4105	A
44	2	4107	G
44	2	4108	G
44	2	4111	U
44	2	4112	C
44	2	4114	C
44	2	4115	G
44	2	4116	C
44	2	4117	U
44	2	4119	C
44	2	4121	G

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Mol	Chain	Res	Type
44	2	4127	A
44	2	4128	A
44	2	4136	G
44	2	4138	C
44	2	4140	C
44	2	4141	G
44	2	4142	C
44	2	4143	G
44	2	4144	C
44	2	4146	G
44	2	4147	G
44	2	4149	C
44	2	4154	G
44	2	4156	G
44	2	4157	A
44	2	4158	C
44	2	4162	C
44	2	4163	U
44	2	4166	G
44	2	4170	A
44	2	4171	C
44	2	4178	A
44	2	4183	G
44	2	4184	G
44	2	4197	G
44	2	4201	G
44	2	4202	U
44	2	4205	A
44	2	4206	C
44	2	4209	G
44	2	4212	A
44	2	4215	C
44	2	4219	A
44	2	4221	C
44	2	4222	G
44	2	4224	A
44	2	4227	U
44	2	4228	G
44	2	4229	U
44	2	4230	C
44	2	4233	A
44	2	4236	G

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Mol	Chain	Res	Type
44	2	4237	C
44	2	4238	G
44	2	4251	A
44	2	4252	C
44	2	4253	A
44	2	4254	G
44	2	4255	A
44	2	4258	C
44	2	4263	C
44	2	4264	G
44	2	4265	U
44	2	4266	G
44	2	4267	G
44	2	4268	A
44	2	4269	G
44	2	4270	C
44	2	4271	A
44	2	4272	G
44	2	4273	A
44	2	4274	A
44	2	4275	G
44	2	4276	G
44	2	4277	G
44	2	4278	C
44	2	4279	A
44	2	4280	A
44	2	4281	A
44	2	4283	G
44	2	4285	U
44	2	4290	U
44	2	4291	G
44	2	4292	A
44	2	4295	U
44	2	4296	U
44	2	4297	G
44	2	4298	A
44	2	4299	U
44	2	4303	C
44	2	4304	A
44	2	4305	G
44	2	4306	U
44	2	4307	A

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Mol	Chain	Res	Type
44	2	4308	C
44	2	4309	G
44	2	4310	A
44	2	4311	A
44	2	4313	A
44	2	4314	C
44	2	4315	A
44	2	4316	G
44	2	4319	C
44	2	4328	G
44	2	4329	G
44	2	4330	G
44	2	4331	G
44	2	4334	U
44	2	4335	C
44	2	4336	A
44	2	4341	C
44	2	4342	C
44	2	4343	U
44	2	4347	G
44	2	4348	A
44	2	4349	C
44	2	4350	C
44	2	4354	U
44	2	4355	G
44	2	4368	G
44	2	4370	G
44	2	4371	G
44	2	4372	U
44	2	4373	G
44	2	4375	C
44	2	4376	A
44	2	4377	G
44	2	4379	A
44	2	4380	A
44	2	4381	A
44	2	4387	C
44	2	4401	G
44	2	4404	U
44	2	4411	G
44	2	4415	1MA
44	2	4420	U

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Mol	Chain	Res	Type
44	2	4421	C
44	2	4422	A
44	2	4423	U
44	2	4424	A
44	2	4425	G
44	2	4426	C
44	2	4427	G
44	2	4428	A
44	2	4437	U
44	2	4440	G
44	2	4446	U
44	2	4447	C
44	2	4449	A
44	2	4450	U
44	2	4451	G
44	2	4452	U
44	2	4453	C
44	2	4454	G
44	2	4464	A
44	2	4465	U
44	2	4466	C
44	2	4475	G
44	2	4476	C
44	2	4480	A
44	2	4484	A
44	2	4499	G
44	2	4501	U
44	2	4502	C
44	2	4503	A
44	2	4510	A
44	2	4512	U
44	2	4513	A
44	2	4518	A
44	2	4519	C
44	2	4520	G
44	2	4522	G
44	2	4523	A2M
44	2	4524	G
44	2	4528	G
44	2	4529	G
44	2	4531	U
44	2	4532	U

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Mol	Chain	Res	Type
44	2	4545	G
44	2	4548	A
44	2	4550	7MG
44	2	4555	U
44	2	4556	U
44	2	4557	U
44	2	4558	U
44	2	4560	C
44	2	4570	G
44	2	4572	U
44	2	4573	G
44	2	4574	U
44	2	4575	G
44	2	4584	A
44	2	4589	A
44	2	4590	A
44	2	4600	G
44	2	4601	U
44	2	4606	G
44	2	4607	A
44	2	4608	G
44	2	4634	U
44	2	4635	A
44	2	4636	PSU
44	2	4637	OMG
44	2	4652	G
44	2	4656	A
44	2	4670	C
44	2	4672	A
44	2	4678	G
44	2	4684	A
44	2	4694	G
44	2	4695	C
44	2	4696	C
44	2	4700	A
44	2	4708	A
44	2	4709	U
44	2	4719	G
44	2	4730	C
44	2	4731	G
44	2	4733	C
44	2	4734	A

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Mol	Chain	Res	Type
44	2	4740	G
44	2	4741	C
44	2	4742	G
44	2	4751	G
44	2	4754	G
44	2	4757	C
44	2	4759	C
44	2	4761	G
44	2	4764	A
44	2	4765	G
44	2	4771	C
44	2	4775	C
44	2	4776	G
44	2	4859	C
44	2	4860	G
44	2	4862	G
44	2	4864	U
44	2	4870	OMG
44	2	4871	C
44	2	4872	2MG
44	2	4874	A
44	2	4875	G
44	2	4877	G
44	2	4882	U
44	2	4883	C
44	2	4895	C
44	2	4900	C
44	2	4901	G
44	2	4910	G
44	2	4911	A
44	2	4912	G
44	2	4914	C
44	2	4915	G
44	2	4926	C
44	2	4927	G
44	2	4928	C
44	2	4937	C
44	2	4940	C
44	2	4941	G
44	2	4943	A
44	2	4947	U
44	2	4949	G

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Mol	Chain	Res	Type
44	2	4960	G
44	2	4961	G
44	2	4976	U
44	2	4988	U
44	2	4989	U
44	2	4991	U
44	2	4993	G
44	2	5013	C
44	2	5014	A
44	2	5017	G
44	2	5021	C
44	2	5022	U
44	2	5023	C
44	2	5024	C
44	2	5026	U
44	2	5027	C
44	2	5029	C
44	2	5030	U
44	2	5031	G
44	2	5034	A
44	2	5040	U
44	2	5041	G
44	2	5047	C
44	2	5050	C
44	2	5054	C
44	2	5055	G
44	2	5058	A
44	2	5062	G
44	2	5069	U
53	5	7	G
53	5	11	A
53	5	13	A
53	5	40	U
53	5	41	G
53	5	49	A
53	5	53	U
53	5	54	A
53	5	63	C
53	5	64	G
53	5	74	A
53	5	75	G
53	5	76	U

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Mol	Chain	Res	Type
53	5	97	G
53	5	100	A
53	5	103	A
53	5	106	G
53	5	109	U
53	5	110	G

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
43	8	124	U
43	8	125	C
44	2	406	C
44	2	914	U
44	2	1633	G
44	2	1679	A
44	2	1808	C
44	2	1931	C
44	2	1980	U
44	2	2033	A
44	2	2470	C
44	2	2474	G
44	2	2475	G
44	2	2477	A
44	2	2487	G
44	2	2498	C
44	2	2546	G
44	2	2760	G
44	2	3596	A
44	2	3701	OMC
44	2	3780	G
44	2	3905	A
44	2	4157	A
44	2	4228	G
44	2	4229	U
44	2	4235	G
44	2	4269	G
44	2	4297	G
44	2	4426	C
44	2	4555	U
44	2	4571	A
44	2	4572	U

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Mol	Chain	Res	Type
44	2	4634	U
44	2	4699	U
44	2	4913	G

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

65 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$
44	7MG	2	1605	44	23,26,27	3.48	11 (47%)	27,39,42	2.05	9 (33%)
44	7MG	2	2522	44	23,26,27	3.41	10 (43%)	27,39,42	2.08	9 (33%)
44	UR3	2	4597	44	19,22,23	2.69	7 (36%)	26,32,35	2.38	5 (19%)
44	B8W	2	2380	44	23,26,27	2.83	5 (21%)	33,38,41	2.85	18 (54%)
44	OMG	2	2424	44	23,26,27	2.68	8 (34%)	32,38,41	2.92	10 (31%)
44	A2M	2	1326	44	22,25,26	3.21	10 (45%)	30,36,39	2.92	10 (33%)
44	A2M	2	2401	44	22,25,26	3.25	10 (45%)	30,36,39	2.91	11 (36%)
44	OMG	2	2364	44	23,26,27	2.60	9 (39%)	32,38,41	2.79	11 (34%)
44	OMC	2	3909	44	19,22,23	3.06	8 (42%)	25,31,34	1.99	7 (28%)
44	OMG	2	373	44	23,26,27	2.64	9 (39%)	32,38,41	2.71	14 (43%)
44	OMG	2	2050	44	23,26,27	2.62	9 (39%)	32,38,41	2.72	11 (34%)
44	OMU	2	4620	44	19,22,23	2.88	7 (36%)	25,31,34	1.79	4 (16%)
44	1MA	2	4415	44	21,25,26	3.00	4 (19%)	30,37,40	1.78	6 (20%)
44	B8K	2	4690	44	24,28,29	3.05	12 (50%)	29,42,45	2.92	11 (37%)
44	I4U	2	1659	44	20,24,25	3.43	8 (40%)	27,34,37	2.09	2 (7%)
44	OMG	2	1316	44	23,26,27	2.62	9 (39%)	32,38,41	2.80	13 (40%)
44	OMC	2	2365	44	19,22,23	2.91	8 (42%)	25,31,34	0.74	0
44	2MG	2	978	44	23,26,27	3.07	9 (39%)	33,38,41	2.12	7 (21%)
44	B8Q	2	1456	44	18,22,23	2.96	5 (27%)	21,32,35	2.28	6 (28%)
44	OMG	2	4870	44	23,26,27	2.67	8 (34%)	32,38,41	2.95	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	A2M	2	1524	44	22,25,26	3.26	9 (40%)	30,36,39	3.16	13 (43%)
44	A2M	2	1534	44	22,25,26	3.23	10 (45%)	30,36,39	3.01	10 (33%)
44	B8K	2	3897	44	24,28,29	3.15	11 (45%)	29,42,45	2.61	11 (37%)
44	OMC	2	2804	44	19,22,23	2.93	8 (42%)	25,31,34	0.79	1 (4%)
44	OMG	2	4637	44	23,26,27	2.64	8 (34%)	32,38,41	2.83	10 (31%)
44	B9B	2	1574	44	25,28,29	1.82	7 (28%)	35,40,43	5.11	13 (37%)
44	A2M	2	1871	44	22,25,26	3.29	10 (45%)	30,36,39	3.13	12 (40%)
44	A2M	2	398	44	22,25,26	3.23	10 (45%)	30,36,39	2.89	10 (33%)
44	A2M	2	2363	44	22,25,26	3.23	9 (40%)	30,36,39	2.94	11 (36%)
44	OMC	2	4536	44	19,22,23	3.00	8 (42%)	25,31,34	0.72	0
44	P7G	2	1909	44	24,28,29	3.62	11 (45%)	25,41,44	1.40	2 (8%)
44	P4U	2	1348	44	21,24,25	3.45	7 (33%)	28,33,36	1.60	4 (14%)
43	OMU	8	14	43,44	19,22,23	2.94	8 (42%)	25,31,34	1.96	6 (24%)
44	OMG	2	1625	44	23,26,27	2.75	8 (34%)	32,38,41	3.21	9 (28%)
44	OMC	2	2422	44	19,22,23	2.97	8 (42%)	25,31,34	1.27	3 (12%)
44	B9B	2	2754	44	25,28,29	1.78	6 (24%)	35,40,43	5.21	13 (37%)
44	OMG	2	2773	44	23,26,27	2.68	8 (34%)	32,38,41	2.86	9 (28%)
44	OMG	2	4494	44	23,26,27	2.68	8 (34%)	32,38,41	2.85	9 (28%)
44	OMC	2	3869	44	19,22,23	2.93	7 (36%)	25,31,34	1.18	3 (12%)
44	A2M	2	4523	44	22,25,26	3.20	10 (45%)	30,36,39	2.96	11 (36%)
44	B8W	2	4185	44	23,26,27	2.83	5 (21%)	33,38,41	2.80	15 (45%)
44	OMG	2	1522	44	23,26,27	2.65	9 (39%)	32,38,41	2.81	10 (31%)
44	P7G	2	3880	44	24,28,29	3.56	11 (45%)	25,41,44	1.24	2 (8%)
44	A2M	2	3867	44	22,25,26	3.19	10 (45%)	30,36,39	2.97	11 (36%)
44	M7A	2	4564	44	19,25,26	1.55	2 (10%)	25,37,40	4.17	6 (24%)
44	E7G	2	1797	44	24,27,28	3.68	12 (50%)	28,40,43	2.26	9 (32%)
44	OMC	2	2861	44	19,22,23	3.00	8 (42%)	25,31,34	1.28	3 (12%)
44	7MG	2	4550	44	23,26,27	3.55	10 (43%)	27,39,42	2.12	9 (33%)
44	OMC	2	3701	44	19,22,23	3.11	8 (42%)	25,31,34	0.99	1 (4%)
44	2MG	2	729	44	23,26,27	2.98	8 (34%)	33,38,41	2.30	10 (30%)
44	OMG	2	1883	44	23,26,27	2.69	8 (34%)	32,38,41	2.78	11 (34%)
44	A2M	2	3825	44	22,25,26	3.20	10 (45%)	30,36,39	2.97	10 (33%)
44	B9H	2	2786	44	21,25,26	3.14	5 (23%)	22,35,38	2.13	6 (27%)
44	B8T	2	4671	44	19,22,23	3.53	8 (42%)	25,31,34	0.96	1 (4%)
44	E7G	2	2297	44	24,27,28	3.49	11 (45%)	28,40,43	2.25	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	PSU	2	4636	44	18,21,22	1.11	1 (5%)	21,30,33	1.96	4 (19%)
44	2MG	2	1517	44	23,26,27	2.99	9 (39%)	33,38,41	2.32	8 (24%)
44	B9B	2	237	44	25,28,29	1.84	6 (24%)	35,40,43	5.31	13 (37%)
44	2MG	2	4872	44	23,26,27	2.89	9 (39%)	33,38,41	2.60	13 (39%)
44	5MU	2	4083	44	19,22,23	7.35	8 (42%)	27,32,35	3.21	11 (40%)
44	B8W	2	4472	44	23,26,27	2.85	5 (21%)	33,38,41	2.83	17 (51%)
44	BGH	2	3899	44	25,29,30	4.50	17 (68%)	30,43,46	2.68	11 (36%)
44	B8T	2	4483	44	19,22,23	3.55	8 (42%)	25,31,34	1.50	5 (20%)
44	OMC	2	3887	44	19,22,23	3.00	8 (42%)	25,31,34	0.96	1 (4%)
44	OMG	2	4623	44	23,26,27	2.61	9 (39%)	32,38,41	2.77	12 (37%)

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
44	7MG	2	1605	44	-	1/7/37/38	0/3/3/3
44	7MG	2	2522	44	-	0/7/37/38	0/3/3/3
44	UR3	2	4597	44	-	0/7/25/26	0/2/2/2
44	B8W	2	2380	44	-	2/9/27/28	0/3/3/3
44	OMG	2	2424	44	-	2/9/27/28	0/3/3/3
44	A2M	2	1326	44	-	0/9/27/28	0/3/3/3
44	A2M	2	2401	44	-	0/9/27/28	0/3/3/3
44	OMG	2	2364	44	-	3/9/27/28	0/3/3/3
44	OMC	2	3909	44	-	2/9/27/28	0/2/2/2
44	OMG	2	373	44	-	1/9/27/28	0/3/3/3
44	OMG	2	2050	44	-	0/9/27/28	0/3/3/3
44	OMU	2	4620	44	-	0/9/27/28	0/2/2/2
44	1MA	2	4415	44	-	2/7/25/26	0/3/3/3
44	B8K	2	4690	44	-	0/11/41/42	0/3/3/3
44	I4U	2	1659	44	-	2/9/29/30	0/2/2/2
44	OMG	2	1316	44	-	0/9/27/28	0/3/3/3
44	OMC	2	2365	44	-	0/9/27/28	0/2/2/2
44	2MG	2	978	44	-	0/9/27/28	0/3/3/3
44	B8Q	2	1456	44	-	0/7/42/43	0/2/2/2
44	OMG	2	4870	44	-	3/9/27/28	0/3/3/3
44	A2M	2	1524	44	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A2M	2	1534	44	-	2/9/27/28	0/3/3/3
44	B8K	2	3897	44	-	2/11/41/42	0/3/3/3
44	OMC	2	2804	44	-	0/9/27/28	0/2/2/2
44	OMG	2	4637	44	-	2/9/27/28	0/3/3/3
44	B9B	2	1574	44	-	5/11/29/30	0/3/3/3
44	A2M	2	1871	44	-	2/9/27/28	0/3/3/3
44	A2M	2	398	44	-	2/9/27/28	0/3/3/3
44	A2M	2	2363	44	-	0/9/27/28	0/3/3/3
44	OMC	2	4536	44	-	0/9/27/28	0/2/2/2
44	P7G	2	1909	44	-	4/10/40/41	0/3/3/3
44	P4U	2	1348	44	-	1/10/29/30	0/2/2/2
43	OMU	8	14	43,44	-	1/9/27/28	0/2/2/2
44	OMG	2	1625	44	-	3/9/27/28	0/3/3/3
44	OMC	2	2422	44	-	1/9/27/28	0/2/2/2
44	B9B	2	2754	44	-	3/11/29/30	0/3/3/3
44	OMG	2	2773	44	-	2/9/27/28	0/3/3/3
44	OMG	2	4494	44	-	0/9/27/28	0/3/3/3
44	OMC	2	3869	44	-	0/9/27/28	0/2/2/2
44	A2M	2	4523	44	-	0/9/27/28	0/3/3/3
44	B8W	2	4185	44	-	0/9/27/28	0/3/3/3
44	OMG	2	1522	44	-	0/9/27/28	0/3/3/3
44	P7G	2	3880	44	-	3/10/40/41	0/3/3/3
44	A2M	2	3867	44	-	2/9/27/28	0/3/3/3
44	M7A	2	4564	44	-	0/7/37/38	0/3/3/3
44	E7G	2	1797	44	-	1/9/39/40	0/3/3/3
44	OMC	2	2861	44	-	0/9/27/28	0/2/2/2
44	7MG	2	4550	44	-	2/7/37/38	0/3/3/3
44	OMC	2	3701	44	-	7/9/27/28	0/2/2/2
44	2MG	2	729	44	-	2/9/27/28	0/3/3/3
44	OMG	2	1883	44	-	2/9/27/28	0/3/3/3
44	A2M	2	3825	44	-	0/9/27/28	0/3/3/3
44	B9H	2	2786	44	-	0/12/47/48	0/2/2/2
44	B8T	2	4671	44	-	0/7/27/28	0/2/2/2
44	E7G	2	2297	44	-	1/9/39/40	0/3/3/3
44	PSU	2	4636	44	-	3/7/25/26	0/2/2/2
44	2MG	2	1517	44	-	2/9/27/28	0/3/3/3
44	B9B	2	237	44	-	4/11/29/30	0/3/3/3
44	2MG	2	4872	44	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	5MU	2	4083	44	-	3/7/25/26	0/2/2/2
44	B8W	2	4472	44	-	2/9/27/28	0/3/3/3
44	BGH	2	3899	44	-	0/13/43/44	0/3/3/3
44	B8T	2	4483	44	-	0/7/27/28	0/2/2/2
44	OMC	2	3887	44	-	1/9/27/28	0/2/2/2
44	OMG	2	4623	44	-	0/9/27/28	0/3/3/3

All (542) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	4083	5MU	C4-C5	21.05	1.79	1.44
44	2	4083	5MU	C6-N1	16.61	1.66	1.38
44	2	4083	5MU	C6-C5	-11.52	1.15	1.34
44	2	4083	5MU	C4-N3	-11.00	1.18	1.38
44	2	1659	I4U	C4-N3	10.77	1.45	1.31
44	2	1348	P4U	C4-N3	10.49	1.44	1.31
44	2	4415	1MA	C2-N3	10.05	1.48	1.30
44	2	4472	B8W	O6-C6	9.46	1.49	1.35
44	2	1871	A2M	C3'-C4'	-9.40	1.29	1.53
44	2	2786	B9H	C2-N3	9.39	1.49	1.37
44	2	3899	BGH	C2'-C1'	-9.26	1.30	1.53
44	2	1524	A2M	C3'-C4'	-9.10	1.29	1.53
44	2	4185	B8W	O6-C6	9.09	1.48	1.35
44	2	2380	B8W	O6-C6	9.07	1.48	1.35
44	2	3867	A2M	C3'-C4'	-8.94	1.30	1.53
44	2	2363	A2M	C3'-C4'	-8.93	1.30	1.53
44	2	1456	B8Q	C6-C5	8.92	1.51	1.33
44	2	3899	BGH	O4'-C1'	8.89	1.62	1.42
44	2	1326	A2M	C3'-C4'	-8.89	1.30	1.53
44	2	2401	A2M	C3'-C4'	-8.89	1.30	1.53
44	2	398	A2M	C3'-C4'	-8.88	1.30	1.53
44	2	1534	A2M	C3'-C4'	-8.88	1.30	1.53
44	2	3825	A2M	C3'-C4'	-8.88	1.30	1.53
44	2	4523	A2M	C3'-C4'	-8.67	1.31	1.53
44	2	1797	E7G	C8-N9	8.50	1.51	1.45
44	2	1797	E7G	C5-N7	8.30	1.46	1.35
44	2	978	2MG	C2-N3	8.27	1.47	1.32
44	2	3880	P7G	C5-N7	8.16	1.45	1.35
44	2	2297	E7G	C5-N7	8.15	1.45	1.35
44	2	1909	P7G	C5-N7	8.13	1.45	1.35
44	2	1909	P7G	C8-N9	8.07	1.51	1.45
44	2	4185	B8W	C2-N2	8.02	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	4550	7MG	C5-N7	7.94	1.45	1.35
44	2	2380	B8W	C2-N2	7.89	1.49	1.33
44	2	4472	B8W	C2-N2	7.85	1.49	1.33
44	2	729	2MG	C2-N3	7.84	1.47	1.32
44	2	3899	BGH	O4'-C4'	-7.81	1.27	1.45
44	2	4550	7MG	C8-N9	7.78	1.50	1.45
44	2	1871	A2M	O4'-C4'	7.74	1.62	1.45
44	2	1517	2MG	C2-N3	7.72	1.46	1.32
44	2	1605	7MG	C5-N7	7.68	1.45	1.35
44	2	1605	7MG	C8-N9	7.65	1.50	1.45
44	2	2522	7MG	C5-N7	7.64	1.45	1.35
44	2	2401	A2M	O4'-C4'	7.64	1.62	1.45
44	2	3897	B8K	C8-N9	7.62	1.50	1.45
44	2	398	A2M	O4'-C4'	7.61	1.61	1.45
44	2	4872	2MG	C2-N3	7.60	1.46	1.32
44	2	1524	A2M	O4'-C4'	7.57	1.61	1.45
44	2	1534	A2M	O4'-C4'	7.57	1.61	1.45
44	2	4523	A2M	O4'-C4'	7.56	1.61	1.45
44	2	2363	A2M	O4'-C4'	7.54	1.61	1.45
44	2	3880	P7G	C8-N9	7.53	1.50	1.45
44	2	1326	A2M	O4'-C4'	7.52	1.61	1.45
44	2	2786	B9H	C6-C5	7.45	1.48	1.33
44	2	3899	BGH	C8-N9	7.45	1.50	1.45
44	2	4483	B8T	C2-N3	7.39	1.51	1.36
44	2	3825	A2M	O4'-C4'	7.38	1.61	1.45
44	2	2297	E7G	C8-N9	7.27	1.50	1.45
44	2	2522	7MG	C8-N9	7.20	1.50	1.45
44	2	4671	B8T	C2-N3	7.18	1.50	1.36
44	2	978	2MG	C2-N2	7.18	1.48	1.33
44	2	1517	2MG	C2-N2	7.11	1.48	1.33
44	2	3867	A2M	O4'-C4'	7.10	1.60	1.45
44	2	4671	B8T	C4-N3	7.00	1.44	1.32
44	2	4483	B8T	C4-N3	6.96	1.44	1.32
44	2	978	2MG	C4-N3	6.93	1.50	1.34
44	2	729	2MG	C2-N2	6.92	1.47	1.33
44	2	4690	B8K	C8-N9	6.92	1.50	1.45
43	8	14	OMU	C2-N1	6.87	1.49	1.38
44	2	729	2MG	C4-N3	6.84	1.49	1.34
44	2	4671	B8T	C6-C5	6.83	1.50	1.35
44	2	4415	1MA	C4-N3	6.80	1.49	1.35
44	2	2786	B9H	C2-N1	6.80	1.47	1.38
44	2	1517	2MG	C4-N3	6.74	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	4620	OMU	C2-N1	6.70	1.49	1.38
44	2	3909	OMC	C6-C5	6.68	1.50	1.35
44	2	4872	2MG	C2-N2	6.65	1.47	1.33
44	2	3701	OMC	C2-N3	6.57	1.49	1.36
44	2	1625	OMG	C4-N3	6.55	1.49	1.34
44	2	4597	UR3	C6-C5	6.54	1.50	1.35
44	2	4690	B8K	C2-N3	6.53	1.49	1.33
44	2	4536	OMC	C2-N3	6.49	1.49	1.36
43	8	14	OMU	C2-N3	6.49	1.49	1.38
44	2	3897	B8K	C2-N3	6.48	1.48	1.33
44	2	3887	OMC	C2-N3	6.43	1.49	1.36
44	2	4620	OMU	C2-N3	6.42	1.49	1.38
44	2	4483	B8T	C6-C5	6.40	1.49	1.35
44	2	1625	OMG	C2-N3	6.36	1.48	1.33
44	2	3869	OMC	C2-N3	6.33	1.48	1.36
44	2	1348	P4U	C2-N3	6.32	1.48	1.36
44	2	2773	OMG	C4-N3	6.31	1.48	1.34
44	2	4494	OMG	C4-N3	6.28	1.48	1.34
44	2	2424	OMG	C4-N3	6.28	1.48	1.34
44	2	1883	OMG	C4-N3	6.28	1.48	1.34
44	2	1659	I4U	C2-N3	6.27	1.48	1.36
44	2	2422	OMC	C2-N3	6.27	1.48	1.36
44	2	1625	OMG	C2-N2	6.25	1.48	1.34
44	2	2365	OMC	C2-N3	6.24	1.48	1.36
44	2	1456	B8Q	C2-N3	6.24	1.46	1.35
44	2	1909	P7G	C4-N3	6.23	1.48	1.37
44	2	2861	OMC	C2-N3	6.22	1.48	1.36
44	2	2804	OMC	C2-N3	6.19	1.48	1.36
44	2	4870	OMG	C4-N3	6.19	1.48	1.34
44	2	2773	OMG	C2-N3	6.17	1.48	1.33
44	2	3880	P7G	C4-N3	6.16	1.48	1.37
44	2	4870	OMG	C2-N2	6.16	1.48	1.34
44	2	2424	OMG	C2-N3	6.12	1.48	1.33
44	2	3701	OMC	C6-C5	6.07	1.49	1.35
44	2	4597	UR3	C2-N3	6.06	1.50	1.39
44	2	2773	OMG	C2-N2	6.06	1.48	1.34
44	2	4483	B8T	C4-N4	6.05	1.48	1.36
44	2	4637	OMG	C4-N3	6.05	1.48	1.34
44	2	1883	OMG	C2-N2	6.04	1.48	1.34
44	2	4494	OMG	C2-N3	6.02	1.47	1.33
44	2	4671	B8T	C4-N4	6.02	1.48	1.36
44	2	1316	OMG	C4-N3	6.00	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	2424	OMG	C2-N2	6.00	1.48	1.34
44	2	4494	OMG	C2-N2	6.00	1.48	1.34
44	2	4870	OMG	C2-N3	5.99	1.47	1.33
44	2	1883	OMG	C2-N3	5.99	1.47	1.33
44	2	1522	OMG	C2-N2	5.99	1.48	1.34
44	2	1522	OMG	C4-N3	5.98	1.47	1.34
44	2	4623	OMG	C4-N3	5.97	1.47	1.34
44	2	2861	OMC	C6-C5	5.94	1.48	1.35
44	2	373	OMG	C2-N2	5.94	1.48	1.34
44	2	1797	E7G	C4-N3	5.94	1.47	1.34
44	2	373	OMG	C4-N3	5.92	1.47	1.34
44	2	1522	OMG	C2-N3	5.92	1.47	1.33
44	2	2365	OMC	C6-C5	5.92	1.48	1.35
44	2	4536	OMC	C6-C5	5.92	1.48	1.35
44	2	4637	OMG	C2-N3	5.89	1.47	1.33
44	2	1909	P7G	C2-N2	5.89	1.48	1.34
44	2	2050	OMG	C4-N3	5.88	1.47	1.34
44	2	4623	OMG	C2-N2	5.88	1.47	1.34
44	2	1348	P4U	C6-C5	5.88	1.48	1.35
44	2	3887	OMC	C6-C5	5.87	1.48	1.35
44	2	2364	OMG	C4-N3	5.87	1.47	1.34
44	2	2050	OMG	C2-N2	5.86	1.47	1.34
44	2	4872	2MG	C4-N3	5.85	1.47	1.34
44	2	2422	OMC	C6-C5	5.84	1.48	1.35
44	2	1316	OMG	C2-N2	5.83	1.47	1.34
44	2	4637	OMG	C2-N2	5.83	1.47	1.34
44	2	3880	P7G	C2-N2	5.81	1.47	1.34
44	2	2804	OMC	C6-C5	5.79	1.48	1.35
44	2	1316	OMG	C2-N3	5.77	1.47	1.33
44	2	1797	E7G	C2-N3	5.76	1.47	1.33
44	2	2364	OMG	C2-N2	5.75	1.47	1.34
44	2	373	OMG	C2-N3	5.75	1.47	1.33
44	2	3869	OMC	C6-C5	5.75	1.48	1.35
44	2	2364	OMG	C2-N3	5.75	1.47	1.33
44	2	2297	E7G	C4-N3	5.74	1.47	1.34
44	2	2754	B9B	C2-N2	5.74	1.45	1.33
44	2	4550	7MG	C2-N3	5.71	1.47	1.33
44	2	4550	7MG	C4-N3	5.70	1.47	1.34
44	2	1909	P7G	C4-N9	5.70	1.44	1.35
44	2	3899	BGH	C4-N3	5.68	1.47	1.34
44	2	237	B9B	C2-N2	5.67	1.45	1.33
44	2	1574	B9B	C2-N2	5.66	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	4623	OMG	C2-N3	5.65	1.46	1.33
44	2	1659	I4U	C6-C5	5.64	1.48	1.35
44	2	2522	7MG	C4-N3	5.57	1.47	1.34
44	2	2050	OMG	C2-N3	5.55	1.46	1.33
44	2	1605	7MG	C4-N3	5.54	1.46	1.34
44	2	1605	7MG	C2-N3	5.54	1.46	1.33
44	2	2297	E7G	C2-N3	5.54	1.46	1.33
44	2	3899	BGH	C2-N3	5.52	1.46	1.33
44	2	2522	7MG	C2-N3	5.49	1.46	1.33
44	2	4597	UR3	C2-N1	5.49	1.46	1.38
44	2	3880	P7G	C4-N9	5.48	1.44	1.35
44	2	3909	OMC	C4-N4	5.47	1.47	1.33
44	2	4620	OMU	C6-C5	5.40	1.47	1.35
43	8	14	OMU	C6-C5	5.38	1.47	1.35
44	2	3909	OMC	C2-N3	5.35	1.47	1.36
44	2	3899	BGH	C4-N9	5.30	1.44	1.37
44	2	3909	OMC	C2-N1	5.28	1.51	1.40
44	2	1797	E7G	C2-N2	5.25	1.46	1.34
44	2	3701	OMC	C4-N3	5.24	1.44	1.34
44	2	4536	OMC	C4-N3	5.19	1.44	1.34
44	2	2297	E7G	C2-N2	5.16	1.46	1.34
44	2	2422	OMC	C2-N1	5.15	1.50	1.40
44	2	2861	OMC	C2-N1	5.12	1.50	1.40
44	2	3880	P7G	C2-N1	5.10	1.45	1.33
44	2	2297	E7G	C4-N9	5.08	1.44	1.37
44	2	1797	E7G	C4-N9	5.08	1.44	1.37
44	2	3867	A2M	O4'-C1'	-5.06	1.30	1.42
44	2	3887	OMC	C4-N3	5.05	1.44	1.34
44	2	2365	OMC	C4-N3	5.00	1.44	1.34
44	2	2804	OMC	C4-N3	4.97	1.44	1.34
44	2	1909	P7G	C2-N1	4.95	1.45	1.33
44	2	3899	BGH	C2-N2	4.94	1.45	1.34
44	2	4483	B8T	C2-N1	4.94	1.50	1.40
44	2	2861	OMC	C4-N3	4.93	1.44	1.34
44	2	3887	OMC	C2-N1	4.91	1.50	1.40
44	2	3701	OMC	C2-N1	4.89	1.50	1.40
44	2	2422	OMC	C4-N3	4.87	1.44	1.34
44	2	1524	A2M	O4'-C1'	-4.87	1.30	1.42
44	2	3869	OMC	C2-N1	4.86	1.50	1.40
44	2	3869	OMC	C4-N3	4.86	1.44	1.34
44	2	3701	OMC	C4-N4	4.85	1.45	1.33
44	2	398	A2M	O4'-C1'	-4.84	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	4550	7MG	C2-N2	4.83	1.45	1.34
44	2	3897	B8K	C4-N9	4.83	1.43	1.37
44	2	1605	7MG	C2-N2	4.82	1.45	1.34
44	2	2401	A2M	O4'-C1'	-4.80	1.30	1.42
44	2	3825	A2M	O4'-C1'	-4.79	1.30	1.42
44	2	1456	B8Q	C2-N1	4.79	1.45	1.38
44	2	2522	7MG	C2-N2	4.78	1.45	1.34
44	2	2861	OMC	C4-N4	4.75	1.45	1.33
44	2	4523	A2M	O4'-C1'	-4.75	1.31	1.42
44	2	1326	A2M	O4'-C1'	-4.75	1.31	1.42
44	2	4550	7MG	C4-N9	4.74	1.43	1.37
44	2	4536	OMC	C4-N4	4.71	1.45	1.33
44	2	2804	OMC	C4-N4	4.70	1.45	1.33
44	2	2363	A2M	O4'-C1'	-4.69	1.31	1.42
44	2	4083	5MU	C2-N3	4.69	1.46	1.38
44	2	4690	B8K	C4-N9	4.69	1.43	1.37
44	2	1605	7MG	C4-N9	4.67	1.43	1.37
44	2	3887	OMC	C4-N4	4.64	1.45	1.33
44	2	2365	OMC	C4-N4	4.64	1.45	1.33
44	2	1534	A2M	O4'-C1'	-4.61	1.31	1.42
44	2	4690	B8K	C4-N3	4.60	1.44	1.34
44	2	3869	OMC	C4-N4	4.58	1.45	1.33
44	2	2522	7MG	C4-N9	4.57	1.43	1.37
44	2	2422	OMC	C4-N4	4.53	1.44	1.33
44	2	4671	B8T	C2-N1	4.53	1.49	1.40
44	2	1871	A2M	O4'-C1'	-4.53	1.31	1.42
44	2	3897	B8K	C4-N3	4.51	1.44	1.34
44	2	1348	P4U	O4-C4	4.50	1.40	1.35
44	2	2804	OMC	C2-N1	4.47	1.49	1.40
44	2	3909	OMC	C4-N3	4.45	1.43	1.34
44	2	4536	OMC	C2-N1	4.44	1.49	1.40
44	2	4523	A2M	C6-N6	4.40	1.45	1.34
44	2	3825	A2M	C6-N6	4.39	1.45	1.34
44	2	1524	A2M	C6-N6	4.35	1.45	1.34
44	2	3899	BGH	C5-C6	4.33	1.54	1.43
44	2	1326	A2M	C6-N6	4.32	1.45	1.34
44	2	3867	A2M	C6-N6	4.31	1.45	1.34
44	2	398	A2M	C6-N6	4.30	1.45	1.34
44	2	1871	A2M	C6-N6	4.30	1.45	1.34
44	2	2401	A2M	C6-N6	4.30	1.45	1.34
44	2	1348	P4U	C2-N1	4.27	1.49	1.40
44	2	3897	B8K	C5-C6	4.25	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1534	A2M	C6-N6	4.25	1.45	1.34
44	2	2363	A2M	C6-N6	4.24	1.45	1.34
44	2	1659	I4U	C2-N1	4.13	1.48	1.40
44	2	4415	1MA	C5-C6	4.10	1.54	1.43
44	2	4872	2MG	C2-N1	4.10	1.43	1.36
44	2	4564	M7A	C6-N6	4.10	1.44	1.34
44	2	2365	OMC	C2-N1	4.08	1.48	1.40
44	2	978	2MG	C2-N1	4.04	1.43	1.36
44	2	1517	2MG	C2-N1	4.03	1.43	1.36
43	8	14	OMU	C4-N3	4.03	1.45	1.38
44	2	729	2MG	C2-N1	3.96	1.43	1.36
44	2	2364	OMG	C5-N7	-3.94	1.31	1.39
44	2	4494	OMG	C5-N7	-3.92	1.31	1.39
44	2	4637	OMG	C5-N7	-3.92	1.31	1.39
44	2	4550	7MG	C5-C6	3.92	1.53	1.43
44	2	4564	M7A	C5-N7	3.90	1.48	1.39
44	2	4620	OMU	C4-N3	3.86	1.45	1.38
44	2	1883	OMG	C5-N7	-3.84	1.31	1.39
44	2	2050	OMG	C5-N7	-3.83	1.31	1.39
44	2	1522	OMG	C5-N7	-3.83	1.31	1.39
44	2	1605	7MG	C5-C6	3.82	1.53	1.43
44	2	1797	E7G	C5-C6	3.81	1.53	1.43
44	2	3899	BGH	C5-N7	3.81	1.47	1.39
44	2	3899	BGH	O2'-C2'	3.77	1.51	1.42
44	2	4690	B8K	C5-C6	3.75	1.52	1.43
44	2	1605	7MG	C2-N1	3.73	1.46	1.37
44	2	2297	E7G	C5-C6	3.73	1.52	1.43
44	2	2773	OMG	C5-N7	-3.72	1.31	1.39
44	2	2424	OMG	C5-N7	-3.71	1.31	1.39
44	2	4483	B8T	C6-N1	3.69	1.46	1.38
44	2	4623	OMG	C5-N7	-3.69	1.31	1.39
44	2	1909	P7G	C2-N3	3.68	1.46	1.37
44	2	1574	B9B	O6-C6	3.67	1.40	1.34
44	2	3897	B8K	C2-N2	3.65	1.42	1.34
44	2	4690	B8K	C71-N7	3.65	1.47	1.39
44	2	2522	7MG	C2-N1	3.65	1.46	1.37
44	2	2522	7MG	C5-C6	3.64	1.52	1.43
44	2	4550	7MG	C2-N1	3.63	1.46	1.37
44	2	373	OMG	C5-N7	-3.63	1.31	1.39
44	2	4671	B8T	C5-C4	3.62	1.49	1.41
44	2	1797	E7G	C2-N1	3.61	1.46	1.37
44	2	1316	OMG	C5-N7	-3.61	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	3880	P7G	C2-N3	3.60	1.46	1.37
44	2	237	B9B	O6-C6	3.59	1.40	1.34
44	2	4870	OMG	C5-N7	-3.59	1.31	1.39
44	2	4083	5MU	C2-N1	3.59	1.44	1.38
44	2	4636	PSU	C6-C5	3.57	1.39	1.35
44	2	3701	OMC	C6-N1	3.55	1.46	1.38
44	2	3909	OMC	C6-N1	3.53	1.46	1.38
44	2	1625	OMG	C5-N7	-3.53	1.32	1.39
44	2	2754	B9B	O6-C6	3.52	1.40	1.34
44	2	4415	1MA	C2-N1	3.50	1.43	1.35
44	2	3899	BGH	C71-N7	3.49	1.47	1.39
44	2	1909	P7G	C6-N1	3.48	1.44	1.38
44	2	3897	B8K	C5-N7	3.48	1.46	1.39
44	2	2297	E7G	C2-N1	3.48	1.46	1.37
44	2	4690	B8K	C2-N2	3.46	1.42	1.34
44	2	4690	B8K	C5-N7	3.39	1.46	1.39
44	2	3897	B8K	C6-N1	3.38	1.45	1.38
44	2	1605	7MG	C6-N1	3.37	1.45	1.38
44	2	3897	B8K	C2-N1	3.37	1.45	1.37
44	2	3899	BGH	C6-N1	3.35	1.45	1.38
44	2	3880	P7G	C6-N1	3.35	1.43	1.38
44	2	3897	B8K	C71-N7	3.34	1.47	1.39
44	2	1883	OMG	O6-C6	-3.33	1.17	1.23
44	2	4637	OMG	O6-C6	-3.33	1.17	1.23
44	2	237	B9B	C5-C4	-3.30	1.33	1.39
44	2	1316	OMG	O6-C6	-3.30	1.17	1.23
44	2	3899	BGH	C2-N1	3.30	1.45	1.37
44	2	2050	OMG	O6-C6	-3.29	1.17	1.23
44	2	4494	OMG	O6-C6	-3.27	1.17	1.23
44	2	1797	E7G	C8-N7	3.27	1.51	1.45
44	2	1574	B9B	C5-C4	-3.26	1.33	1.39
44	2	4623	OMG	O6-C6	-3.26	1.17	1.23
44	2	4550	7MG	C6-N1	3.25	1.44	1.38
44	2	1797	E7G	C6-N1	3.25	1.44	1.38
44	2	2380	B8W	C5-C4	-3.24	1.33	1.39
44	2	1534	A2M	C5-C4	-3.23	1.33	1.39
44	2	2364	OMG	O6-C6	-3.22	1.17	1.23
44	2	2380	B8W	C5-N7	-3.19	1.33	1.39
44	2	2365	OMC	C6-N1	3.18	1.45	1.38
44	2	1348	P4U	C6-N1	3.17	1.45	1.38
44	2	4690	B8K	C6-N1	3.17	1.44	1.38
44	2	1534	A2M	O2'-C2'	-3.16	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1522	OMG	O6-C6	-3.15	1.17	1.23
44	2	3897	B8K	C5-C4	3.14	1.47	1.37
44	2	2297	E7G	C8-N7	3.14	1.51	1.45
44	2	2773	OMG	O6-C6	-3.14	1.17	1.23
44	2	2424	OMG	O6-C6	-3.13	1.17	1.23
44	2	373	OMG	C6-N1	3.13	1.44	1.38
44	2	2522	7MG	C6-N1	3.12	1.44	1.38
44	2	4536	OMC	C6-N1	3.12	1.45	1.38
44	2	2050	OMG	C6-N1	3.11	1.44	1.38
44	2	2297	E7G	C6-N1	3.11	1.44	1.38
44	2	2422	OMC	C6-N1	3.11	1.45	1.38
44	2	1326	A2M	C5-C4	-3.10	1.33	1.39
44	2	1625	OMG	C6-N1	3.10	1.44	1.38
44	2	3887	OMC	C6-N1	3.10	1.45	1.38
44	2	729	2MG	C5-N7	-3.10	1.32	1.39
44	2	1659	I4U	C6-N1	3.09	1.45	1.38
44	2	4870	OMG	O6-C6	-3.09	1.17	1.23
44	2	398	A2M	C5-C4	-3.09	1.33	1.39
44	2	2401	A2M	C5-C4	-3.08	1.33	1.39
44	2	4483	B8T	C5-C4	3.07	1.47	1.41
44	2	3869	OMC	C6-N1	3.06	1.45	1.38
44	2	2754	B9B	C5-C4	-3.05	1.33	1.39
44	2	1871	A2M	C5-C4	-3.05	1.33	1.39
44	2	4472	B8W	C5-C4	-3.05	1.33	1.39
44	2	3880	P7G	C8-N7	3.05	1.51	1.45
44	2	2861	OMC	C6-N1	3.05	1.45	1.38
44	2	373	OMG	O6-C6	-3.04	1.17	1.23
44	2	4523	A2M	O3'-C3'	3.04	1.50	1.43
44	2	2363	A2M	C8-N9	-3.04	1.32	1.37
44	2	1517	2MG	C5-N7	-3.03	1.33	1.39
44	2	4620	OMU	O4-C4	-3.03	1.18	1.24
44	2	1625	OMG	O6-C6	-3.02	1.17	1.23
44	2	2804	OMC	C6-N1	3.02	1.45	1.38
44	2	4671	B8T	C6-N1	3.02	1.45	1.38
43	8	14	OMU	O4-C4	-3.01	1.18	1.24
44	2	4185	B8W	C5-N7	-2.99	1.33	1.39
44	2	978	2MG	C5-N7	-2.99	1.33	1.39
44	2	4690	B8K	C2-N1	2.99	1.44	1.37
44	2	4690	B8K	C5-C4	2.98	1.46	1.37
44	2	3825	A2M	C5-C4	-2.98	1.33	1.39
44	2	4597	UR3	C6-N1	2.97	1.45	1.38
44	2	3867	A2M	C5-C4	-2.96	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	4872	2MG	C5-N7	-2.95	1.33	1.39
44	2	4523	A2M	C5-C4	-2.95	1.33	1.39
44	2	237	B9B	C5-N7	-2.95	1.33	1.39
44	2	2804	OMC	O2-C2	-2.95	1.18	1.23
44	2	1348	P4U	O2-C2	-2.94	1.18	1.23
44	2	4870	OMG	C6-N1	2.94	1.44	1.38
44	2	2363	A2M	O2'-C2'	-2.93	1.35	1.42
44	2	2424	OMG	C6-N1	2.93	1.44	1.38
44	2	3899	BGH	O3'-C3'	-2.92	1.35	1.43
44	2	4671	B8T	O2-C2	-2.92	1.18	1.23
44	2	2363	A2M	C5-C4	-2.92	1.33	1.39
44	2	2364	OMG	C6-N1	2.91	1.44	1.38
44	2	1909	P7G	O6-C6	-2.90	1.18	1.23
44	2	4483	B8T	O2-C2	-2.90	1.18	1.23
44	2	4185	B8W	C5-C4	-2.89	1.33	1.39
44	2	4623	OMG	C6-N1	2.87	1.44	1.38
44	2	4494	OMG	C6-N1	2.87	1.44	1.38
43	8	14	OMU	O2-C2	-2.87	1.18	1.23
44	2	1883	OMG	C6-N1	2.86	1.44	1.38
44	2	2401	A2M	O2'-C2'	-2.85	1.35	1.42
44	2	2422	OMC	O2-C2	-2.84	1.18	1.23
44	2	4637	OMG	C6-N1	2.84	1.44	1.38
44	2	3880	P7G	O6-C6	-2.83	1.18	1.23
44	2	4083	5MU	O4-C4	-2.83	1.18	1.23
44	2	1522	OMG	C6-N1	2.82	1.44	1.38
44	2	2365	OMC	O2-C2	-2.82	1.18	1.23
44	2	1316	OMG	C6-N1	2.82	1.44	1.38
44	2	1909	P7G	C8-N7	2.81	1.50	1.45
44	2	3867	A2M	O2'-C2'	-2.81	1.35	1.42
44	2	1871	A2M	O2'-C2'	-2.81	1.35	1.42
44	2	1659	I4U	O2-C2	-2.81	1.18	1.23
44	2	4472	B8W	C5-N7	-2.80	1.34	1.39
44	2	1524	A2M	O3'-C3'	2.79	1.49	1.43
44	2	4536	OMC	O2-C2	-2.79	1.18	1.23
44	2	1524	A2M	O2'-C2'	-2.79	1.35	1.42
44	2	3701	OMC	O2-C2	-2.78	1.18	1.23
44	2	4872	2MG	C4-N9	-2.78	1.31	1.38
44	2	4083	5MU	O2-C2	-2.77	1.18	1.23
44	2	3899	BGH	O6-C6	-2.77	1.18	1.23
44	2	2754	B9B	C5-N7	-2.77	1.34	1.39
44	2	2773	OMG	C6-N1	2.77	1.44	1.38
44	2	4872	2MG	C5-C6	2.76	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1534	A2M	C8-N9	-2.75	1.32	1.37
44	2	1909	P7G	C5-C4	2.75	1.43	1.36
44	2	2401	A2M	C8-N9	-2.75	1.32	1.37
44	2	3880	P7G	C5-C4	2.74	1.43	1.36
44	2	2861	OMC	O2-C2	-2.74	1.18	1.23
44	2	1574	B9B	C5-N7	-2.73	1.34	1.39
44	2	2401	A2M	C5-N7	-2.73	1.34	1.39
44	2	398	A2M	O2'-C2'	-2.72	1.36	1.42
44	2	1524	A2M	C5-C4	-2.72	1.34	1.39
44	2	3825	A2M	O2'-C2'	-2.71	1.36	1.42
44	2	2401	A2M	O3'-C3'	2.70	1.49	1.43
44	2	2363	A2M	C5-N7	-2.70	1.34	1.39
44	2	1326	A2M	C5-N7	-2.68	1.34	1.39
44	2	1524	A2M	C5-N7	-2.68	1.34	1.39
44	2	3887	OMC	O2-C2	-2.67	1.18	1.23
44	2	3825	A2M	C8-N9	-2.67	1.33	1.37
44	2	4620	OMU	O2-C2	-2.66	1.18	1.23
44	2	1534	A2M	O3'-C3'	2.66	1.49	1.43
44	2	1659	I4U	O4-C41	-2.66	1.41	1.47
44	2	1871	A2M	O3'-C3'	2.65	1.49	1.43
44	2	3869	OMC	O2-C2	-2.65	1.18	1.23
44	2	1326	A2M	O2'-C2'	-2.65	1.36	1.42
44	2	4523	A2M	O2'-C2'	-2.65	1.36	1.42
44	2	1326	A2M	O3'-C3'	2.63	1.49	1.43
44	2	729	2MG	C5-C6	2.62	1.54	1.44
44	2	3825	A2M	O3'-C3'	2.62	1.49	1.43
44	2	2522	7MG	O6-C6	-2.61	1.18	1.23
44	2	3909	OMC	C5-C4	2.61	1.49	1.42
44	2	398	A2M	C8-N9	-2.60	1.33	1.37
44	2	4472	B8W	C8-N9	-2.60	1.33	1.37
44	2	4550	7MG	O6-C6	-2.59	1.18	1.23
44	2	1517	2MG	C5-C6	2.59	1.54	1.44
44	2	398	A2M	O3'-C3'	2.59	1.49	1.43
44	2	1326	A2M	C8-N9	-2.58	1.33	1.37
44	2	398	A2M	C5-N7	-2.58	1.34	1.39
44	2	978	2MG	C5-C6	2.57	1.54	1.44
44	2	4523	A2M	C8-N9	-2.57	1.33	1.37
44	2	2363	A2M	O3'-C3'	2.56	1.49	1.43
44	2	1316	OMG	C5-C6	2.56	1.54	1.44
44	2	2773	OMG	C5-C6	2.55	1.53	1.44
44	2	1625	OMG	C2-N1	2.55	1.43	1.37
43	8	14	OMU	C6-N1	2.55	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1625	OMG	C5-C6	2.53	1.53	1.44
44	2	3867	A2M	O3'-C3'	2.53	1.49	1.43
44	2	3867	A2M	C8-N9	-2.53	1.33	1.37
44	2	1797	E7G	O6-C6	-2.53	1.18	1.23
44	2	2297	E7G	O6-C6	-2.53	1.18	1.23
44	2	373	OMG	C2-N1	2.53	1.43	1.37
44	2	4690	B8K	O6-C6	-2.53	1.18	1.23
44	2	3867	A2M	C5-N7	-2.53	1.34	1.39
44	2	1522	OMG	C2-N1	2.51	1.43	1.37
44	2	373	OMG	C5-C6	2.50	1.53	1.44
44	2	1605	7MG	O6-C6	-2.50	1.18	1.23
44	2	4870	OMG	C5-C6	2.49	1.53	1.44
44	2	2380	B8W	C8-N9	-2.48	1.33	1.37
44	2	2786	B9H	C31-N3	-2.48	1.43	1.46
44	2	1871	A2M	C5-N7	-2.48	1.34	1.39
44	2	1871	A2M	C8-N9	-2.47	1.33	1.37
44	2	2050	OMG	C2-N1	2.46	1.43	1.37
44	2	1524	A2M	C8-N9	-2.45	1.33	1.37
44	2	1522	OMG	C5-C6	2.45	1.53	1.44
44	2	1534	A2M	C5-N7	-2.45	1.34	1.39
44	2	237	B9B	C8-N9	-2.44	1.33	1.37
44	2	3701	OMC	C5-C4	2.44	1.48	1.42
44	2	4620	OMU	C6-N1	2.43	1.43	1.38
44	2	2424	OMG	C5-C6	2.43	1.53	1.44
44	2	4872	2MG	C6-N1	2.42	1.43	1.38
44	2	237	B9B	C5-C6	-2.42	1.37	1.41
44	2	2773	OMG	C2-N1	2.41	1.43	1.37
44	2	2050	OMG	C4-N9	-2.40	1.31	1.38
44	2	4494	OMG	C2-N1	2.40	1.43	1.37
44	2	4623	OMG	C5-C6	2.39	1.53	1.44
44	2	3825	A2M	C5-N7	-2.38	1.34	1.39
44	2	4870	OMG	C2-N1	2.38	1.43	1.37
44	2	1883	OMG	C2-N1	2.38	1.43	1.37
44	2	373	OMG	C4-N9	-2.38	1.32	1.38
44	2	2754	B9B	C8-N9	-2.37	1.33	1.37
44	2	2364	OMG	C5-C6	2.37	1.53	1.44
44	2	4536	OMC	C5-C4	2.36	1.48	1.42
44	2	2424	OMG	C2-N1	2.36	1.43	1.37
44	2	2861	OMC	C5-C4	2.35	1.48	1.42
44	2	1574	B9B	C4-N9	-2.35	1.32	1.37
44	2	4637	OMG	C5-C6	2.34	1.53	1.44
44	2	2364	OMG	C2-N1	2.34	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1316	OMG	C2-N1	2.34	1.43	1.37
44	2	3909	OMC	O2-C2	-2.32	1.19	1.23
44	2	4494	OMG	C5-C6	2.32	1.53	1.44
44	2	4637	OMG	C2-N1	2.32	1.43	1.37
44	2	1883	OMG	C5-C6	2.31	1.53	1.44
44	2	398	A2M	C4-N9	-2.31	1.32	1.37
44	2	4597	UR3	O2-C2	-2.29	1.18	1.22
44	2	2754	B9B	C5-C6	-2.29	1.37	1.41
44	2	1456	B8Q	C6-N1	2.29	1.43	1.38
44	2	2401	A2M	C4-N9	-2.29	1.32	1.37
44	2	4597	UR3	C4-N3	2.29	1.45	1.40
44	2	4623	OMG	C2-N1	2.29	1.43	1.37
44	2	4185	B8W	C8-N9	-2.28	1.33	1.37
44	2	2804	OMC	C5-C4	2.27	1.48	1.42
44	2	2050	OMG	C5-C6	2.27	1.52	1.44
44	2	4523	A2M	C5-N7	-2.26	1.35	1.39
44	2	978	2MG	C6-N1	2.26	1.43	1.38
44	2	1574	B9B	C5-C6	-2.25	1.37	1.41
44	2	3899	BGH	C5-C4	2.23	1.44	1.37
44	2	1534	A2M	C4-N9	-2.21	1.33	1.37
44	2	3887	OMC	C5-C4	2.20	1.48	1.42
44	2	2365	OMC	C5-C4	2.20	1.48	1.42
44	2	1517	2MG	C6-N1	2.19	1.43	1.38
44	2	1574	B9B	C8-N9	-2.19	1.33	1.37
44	2	1659	I4U	C5-C4	2.14	1.48	1.43
44	2	729	2MG	C6-N1	2.12	1.42	1.38
44	2	2422	OMC	C5-C4	2.12	1.47	1.42
44	2	4523	A2M	C4-N9	-2.12	1.33	1.37
43	8	14	OMU	C5-C4	2.12	1.48	1.43
44	2	1456	B8Q	O2-C2	-2.12	1.18	1.22
44	2	3867	A2M	C4-N9	-2.10	1.33	1.37
44	2	4623	OMG	C4-N9	-2.10	1.32	1.38
44	2	729	2MG	O6-C6	-2.10	1.19	1.23
44	2	4597	UR3	C5-C4	2.09	1.49	1.43
44	2	2786	B9H	C6-N1	2.09	1.43	1.38
44	2	3825	A2M	C4-N9	-2.08	1.33	1.37
44	2	1316	OMG	C4-N9	-2.07	1.32	1.38
44	2	978	2MG	C4-N9	-2.07	1.32	1.38
44	2	1517	2MG	O6-C6	-2.06	1.19	1.23
44	2	1326	A2M	C4-N9	-2.05	1.33	1.37
44	2	1517	2MG	C4-N9	-2.05	1.32	1.38
44	2	1522	OMG	C4-N9	-2.04	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1871	A2M	C4-N9	-2.03	1.33	1.37
44	2	2364	OMG	C4-N9	-2.03	1.32	1.38
44	2	4872	2MG	O6-C6	-2.02	1.19	1.23
44	2	1605	7MG	C5-C4	2.02	1.43	1.37
44	2	1797	E7G	C5-C4	2.01	1.43	1.37
44	2	978	2MG	O6-C6	-2.00	1.19	1.23

All (541) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	237	B9B	O6-C6-C5	20.59	143.92	116.73
44	2	1574	B9B	O6-C6-C5	20.44	143.72	116.73
44	2	2754	B9B	O6-C6-C5	19.91	143.03	116.73
44	2	237	B9B	O6-C6-N1	-19.34	94.19	120.02
44	2	2754	B9B	O6-C6-N1	-18.81	94.90	120.02
44	2	1574	B9B	O6-C6-N1	-18.79	94.92	120.02
44	2	4564	M7A	C5-C6-N6	13.93	147.41	123.75
44	2	4564	M7A	N6-C6-N1	-11.77	92.16	118.38
44	2	1625	OMG	C1'-N9-C8	-10.77	96.13	126.73
44	2	1625	OMG	C1'-N9-C4	10.45	157.36	126.49
44	2	4083	5MU	C5-C4-N3	9.48	123.56	115.32
44	2	4870	OMG	C1'-N9-C8	-9.36	100.14	126.73
44	2	4870	OMG	C1'-N9-C4	9.25	153.80	126.49
44	2	4597	UR3	C4-N3-C2	-9.23	117.15	124.58
44	2	2424	OMG	C1'-N9-C4	9.11	153.41	126.49
44	2	2773	OMG	C1'-N9-C4	8.91	152.81	126.49
44	2	2424	OMG	C1'-N9-C8	-8.91	101.43	126.73
44	2	1659	I4U	O4-C4-C5	8.87	121.75	115.45
44	2	1522	OMG	C1'-N9-C4	8.74	152.30	126.49
44	2	4494	OMG	C1'-N9-C4	8.74	152.30	126.49
44	2	1522	OMG	C1'-N9-C8	-8.55	102.45	126.73
44	2	2364	OMG	C1'-N9-C4	8.53	151.67	126.49
44	2	2773	OMG	C1'-N9-C8	-8.47	102.67	126.73
44	2	4494	OMG	C1'-N9-C8	-8.41	102.83	126.73
44	2	4637	OMG	C1'-N9-C4	8.35	151.16	126.49
44	2	4623	OMG	C1'-N9-C4	8.35	151.14	126.49
44	2	4623	OMG	C1'-N9-C8	-8.31	103.13	126.73
44	2	2050	OMG	C1'-N9-C4	8.22	150.76	126.49
44	2	4637	OMG	C1'-N9-C8	-8.14	103.61	126.73
44	2	1883	OMG	C1'-N9-C4	8.09	150.40	126.49
44	2	2050	OMG	C1'-N9-C8	-8.09	103.74	126.73
44	2	2364	OMG	C1'-N9-C8	-8.08	103.78	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	1316	OMG	C1'-N9-C4	8.04	150.23	126.49
44	2	1883	OMG	C1'-N9-C8	-8.01	103.98	126.73
44	2	1316	OMG	C1'-N9-C8	-7.95	104.15	126.73
44	2	373	OMG	C1'-N9-C4	7.77	149.43	126.49
44	2	373	OMG	C1'-N9-C8	-7.75	104.71	126.73
44	2	2754	B9B	C5-C4-N3	-7.40	119.39	127.18
44	2	4690	B8K	C72-C71-N7	7.23	129.47	118.80
44	2	2380	B8W	C5-C4-N3	-7.08	119.72	127.18
44	2	1534	A2M	N6-C6-N1	-7.06	102.66	118.38
44	2	1517	2MG	C2-N3-C4	7.01	120.77	112.00
44	2	4185	B8W	C5-C4-N3	-6.99	119.82	127.18
44	2	237	B9B	C5-C4-N3	-6.95	119.86	127.18
44	2	4185	B8W	N2-C2-N3	6.88	127.54	117.22
44	2	1871	A2M	N3-C2-N1	-6.87	118.19	128.58
44	2	729	2MG	C2-N3-C4	6.85	120.57	112.00
44	2	4523	A2M	N6-C6-N1	-6.80	103.23	118.38
44	2	398	A2M	N6-C6-N1	-6.78	103.27	118.38
44	2	2380	B8W	N2-C2-N3	6.71	127.29	117.22
44	2	1326	A2M	N6-C6-N1	-6.70	103.45	118.38
44	2	1534	A2M	N3-C2-N1	-6.69	118.46	128.58
44	2	2363	A2M	N6-C6-N1	-6.67	103.52	118.38
44	2	3867	A2M	N6-C6-N1	-6.66	103.54	118.38
44	2	4472	B8W	N2-C2-N3	6.66	127.20	117.22
44	2	3825	A2M	N6-C6-N1	-6.65	103.56	118.38
44	2	1326	A2M	N3-C2-N1	-6.64	118.53	128.58
44	2	2401	A2M	N6-C6-N1	-6.61	103.65	118.38
44	2	1871	A2M	N6-C6-N1	-6.59	103.71	118.38
44	2	4872	2MG	C2-N3-C4	6.58	120.23	112.00
44	2	2401	A2M	N3-C2-N1	-6.54	118.68	128.58
44	2	398	A2M	N3-C2-N1	-6.54	118.68	128.58
44	2	4472	B8W	C5-C4-N3	-6.53	120.30	127.18
44	2	3825	A2M	N3-C2-N1	-6.50	118.74	128.58
44	2	1524	A2M	N3-C2-N1	-6.49	118.77	128.58
44	2	3867	A2M	N3-C2-N1	-6.43	118.85	128.58
44	2	4690	B8K	C5-C6-N1	6.41	122.22	110.94
44	2	4083	5MU	C5-C6-N1	-6.39	116.37	123.31
44	2	3897	B8K	C72-C71-N7	6.38	128.22	118.80
44	2	978	2MG	C2-N3-C4	6.38	119.98	112.00
44	2	4523	A2M	N3-C2-N1	-6.36	118.95	128.58
44	2	2363	A2M	N3-C2-N1	-6.32	119.01	128.58
44	2	4083	5MU	C4-N3-C2	-6.29	119.09	127.34
44	2	1524	A2M	N6-C6-N1	-6.25	104.47	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	729	2MG	C5-C4-N3	-6.21	118.51	128.39
44	2	1517	2MG	C5-C4-N3	-6.10	118.68	128.39
44	2	3899	BGH	C72-C71-N7	6.04	127.72	118.80
44	2	4690	B8K	C4-C5-N7	6.03	109.81	104.93
44	2	4564	M7A	N3-C2-N1	-6.01	119.49	128.58
44	2	4872	2MG	N1-C2-N2	6.00	122.69	116.56
44	2	4523	A2M	N9-C8-N7	-5.94	105.51	113.94
44	2	1534	A2M	N9-C8-N7	-5.90	105.57	113.94
44	2	1871	A2M	N9-C8-N7	-5.87	105.61	113.94
44	2	3825	A2M	N9-C8-N7	-5.85	105.63	113.94
44	2	3899	BGH	C5-C6-N1	5.82	121.18	110.94
44	2	978	2MG	C5-C4-N3	-5.72	119.28	128.39
44	2	1574	B9B	C5-C4-N3	-5.71	121.17	127.18
44	2	1348	P4U	O4-C4-C5	5.68	119.48	115.45
44	2	2401	A2M	N9-C8-N7	-5.68	105.88	113.94
44	2	3909	OMC	O2-C2-N3	-5.68	113.38	122.33
44	2	398	A2M	N9-C8-N7	-5.67	105.89	113.94
44	2	4415	1MA	C5-C4-N3	-5.66	118.94	127.27
44	2	2786	B9H	C6-N1-C2	-5.66	117.17	121.80
44	2	4564	M7A	N3-C4-N9	5.65	133.94	126.88
44	2	3867	A2M	N9-C8-N7	-5.65	105.92	113.94
44	2	1326	A2M	N9-C8-N7	-5.64	105.94	113.94
44	2	3897	B8K	C5-C6-N1	5.60	120.80	110.94
43	8	14	OMU	C4-N3-C2	-5.59	119.68	126.61
44	2	1871	A2M	C4-N9-C8	5.54	111.56	105.74
44	2	3825	A2M	C4-N9-C8	5.53	111.55	105.74
44	2	1534	A2M	C4-N9-C8	5.50	111.51	105.74
44	2	2773	OMG	C5-C4-N3	-5.49	119.65	128.39
44	2	4472	B8W	C61-O6-C6	5.43	122.28	117.20
44	2	4523	A2M	C4-N9-C8	5.43	111.44	105.74
44	2	1797	E7G	C4-C5-N7	5.41	109.33	104.94
44	2	1524	A2M	N9-C8-N7	-5.40	106.28	113.94
44	2	4872	2MG	C5-C4-N3	-5.39	119.81	128.39
44	2	4620	OMU	C4-N3-C2	-5.39	119.92	126.61
44	2	2424	OMG	C5-C4-N3	-5.38	119.82	128.39
44	2	1456	B8Q	C6-N1-C2	-5.36	117.42	121.80
44	2	3867	A2M	C4-N9-C8	5.34	111.34	105.74
44	2	4523	A2M	C5-C6-N6	5.33	136.49	123.29
44	2	2401	A2M	C4-N9-C8	5.33	111.33	105.74
44	2	398	A2M	C5-C6-N6	5.32	136.47	123.29
44	2	4494	OMG	C5-C4-N3	-5.32	119.92	128.39
44	2	237	B9B	N2-C2-N3	5.31	125.19	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	3899	BGH	C2-N3-C4	5.31	121.45	112.30
44	2	1534	A2M	C5-C6-N6	5.30	136.42	123.29
44	2	1625	OMG	C5-C4-N3	-5.29	119.96	128.39
44	2	2297	E7G	C4-C5-N7	5.25	109.19	104.94
44	2	1797	E7G	C5-C6-N1	5.23	120.14	110.94
44	2	1326	A2M	C5-C6-N6	5.22	136.20	123.29
44	2	4637	OMG	C5-C4-N3	-5.20	120.11	128.39
44	2	398	A2M	C4-N9-C8	5.20	111.20	105.74
44	2	1871	A2M	C5-C6-N6	5.18	136.12	123.29
44	2	4550	7MG	C5-C6-N1	5.16	120.03	110.94
44	2	3825	A2M	C5-C6-N6	5.16	136.06	123.29
44	2	2297	E7G	C5-C6-N1	5.16	120.02	110.94
44	2	2364	OMG	C5-C4-N3	-5.16	120.19	128.39
44	2	2363	A2M	C5-C6-N6	5.15	136.03	123.29
44	2	3867	A2M	C5-C6-N6	5.13	135.99	123.29
44	2	2363	A2M	N9-C8-N7	-5.12	106.67	113.94
44	2	4083	5MU	N3-C2-N1	5.12	121.55	114.89
44	2	4872	2MG	C2-N1-C6	-5.11	118.38	124.55
44	2	2401	A2M	C5-C6-N6	5.09	135.88	123.29
44	2	1883	OMG	C5-C4-N3	-5.08	120.31	128.39
44	2	2786	B9H	C31-N3-C2	5.07	123.52	117.29
44	2	2754	B9B	N3-C4-N9	5.07	133.42	126.99
44	2	1326	A2M	C4-N9-C8	5.04	111.03	105.74
44	2	1524	A2M	C4-N9-C8	5.02	111.00	105.74
44	2	2754	B9B	N2-C2-N3	5.01	124.73	117.22
44	2	4636	PSU	C4-N3-C2	-4.99	119.50	126.37
44	2	2522	7MG	C5-C6-N1	4.98	119.70	110.94
44	2	1524	A2M	C1'-N9-C8	-4.97	116.07	127.09
44	2	2380	B8W	C4-C5-C6	4.97	120.10	115.22
44	2	4690	B8K	C2-N3-C4	4.96	120.84	112.30
44	2	4870	OMG	C5-C4-N3	-4.95	120.52	128.39
44	2	1316	OMG	C5-C4-N3	-4.93	120.54	128.39
44	2	1522	OMG	C5-C4-N3	-4.92	120.55	128.39
44	2	1524	A2M	C5-C6-N6	4.91	135.46	123.29
44	2	4185	B8W	C4-C5-C6	4.89	120.03	115.22
44	2	2380	B8W	O6-C6-N1	4.87	125.43	118.96
44	2	1605	7MG	C5-C6-N1	4.86	119.50	110.94
44	2	4636	PSU	N1-C2-N3	4.85	120.28	115.17
44	2	1456	B8Q	O2-C2-N3	-4.79	116.23	122.95
44	2	3897	B8K	C2-N3-C4	4.78	120.54	112.30
44	2	2363	A2M	C4-N9-C8	4.78	110.76	105.74
44	2	1456	B8Q	N3-C2-N1	4.76	123.78	117.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	2363	A2M	C1'-N9-C8	-4.74	116.59	127.09
44	2	237	B9B	N3-C4-N9	4.72	132.99	126.99
44	2	4872	2MG	CM2-N2-C2	-4.72	113.52	123.65
44	2	729	2MG	C2-N1-C6	-4.72	118.85	124.55
44	2	4637	OMG	C2-N3-C4	4.71	120.42	112.30
44	2	1524	A2M	C4'-O4'-C1'	-4.67	99.16	109.47
44	2	4494	OMG	C2-N3-C4	4.67	120.33	112.30
44	2	1883	OMG	C2-N3-C4	4.65	120.30	112.30
44	2	4623	OMG	C5-C4-N3	-4.63	121.02	128.39
44	2	2297	E7G	C2-N3-C4	4.62	120.27	112.30
44	2	2424	OMG	C2-N3-C4	4.61	120.25	112.30
44	2	2773	OMG	C2-N3-C4	4.61	120.24	112.30
44	2	4550	7MG	C2-N3-C4	4.61	120.23	112.30
44	2	1517	2MG	C2-N1-C6	-4.59	119.00	124.55
44	2	4870	OMG	C2-N3-C4	4.58	120.19	112.30
44	2	2363	A2M	C5-C4-N3	-4.57	120.43	126.72
44	2	2380	B8W	N3-C4-N9	4.55	132.77	126.99
44	2	1909	P7G	C4-C5-N7	4.54	109.77	106.71
44	2	3867	A2M	C1'-N9-C8	-4.53	117.03	127.09
44	2	1797	E7G	C2-N3-C4	4.52	120.09	112.30
44	2	1625	OMG	C2-N3-C4	4.52	120.08	112.30
44	2	1316	OMG	C2-N3-C4	4.51	120.06	112.30
44	2	3909	OMC	O2-C2-N1	4.46	127.64	118.90
44	2	2364	OMG	C2-N3-C4	4.46	119.98	112.30
44	2	4690	B8K	N9-C8-N7	4.42	109.13	103.31
44	2	373	OMG	C5-C4-N3	-4.41	121.36	128.39
44	2	2050	OMG	C5-C4-N3	-4.40	121.39	128.39
44	2	1659	I4U	C5-C4-N3	-4.38	118.43	124.86
44	2	1605	7MG	C2-N3-C4	4.37	119.83	112.30
44	2	2522	7MG	C2-N3-C4	4.37	119.83	112.30
44	2	3897	B8K	C5-C4-N9	4.32	111.87	106.33
44	2	3899	BGH	C5-C4-N9	4.32	111.87	106.33
44	2	4472	B8W	N9-C8-N7	-4.32	107.80	113.94
44	2	1522	OMG	C2-N3-C4	4.32	119.73	112.30
44	2	4623	OMG	C2-N3-C4	4.32	119.73	112.30
44	2	1574	B9B	N9-C8-N7	-4.30	107.84	113.94
44	2	2050	OMG	C2-N3-C4	4.29	119.68	112.30
44	2	3899	BGH	C4-C5-N7	4.29	108.39	104.93
44	2	978	2MG	C2-N1-C6	-4.28	119.37	124.55
44	2	3867	A2M	C5-C4-N3	-4.26	120.85	126.72
44	2	373	OMG	C2-N3-C4	4.25	119.62	112.30
44	2	4083	5MU	C5M-C5-C6	-4.24	117.11	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	4597	UR3	C5-C4-N3	4.24	120.63	115.04
44	2	1524	A2M	C5-C4-N3	-4.23	120.89	126.72
44	2	4185	B8W	N3-C4-N9	4.22	132.34	126.99
44	2	1326	A2M	C5-C4-N3	-4.21	120.92	126.72
44	2	1534	A2M	C5-C4-N3	-4.19	120.94	126.72
44	2	729	2MG	N9-C4-N3	4.14	134.24	125.95
44	2	3897	B8K	C4-C5-N7	4.13	108.27	104.93
44	2	3825	A2M	C5-C4-N3	-4.12	121.04	126.72
44	2	1871	A2M	C5-C4-N3	-4.12	121.05	126.72
44	2	3825	A2M	C1'-N9-C8	-4.11	117.98	127.09
44	2	4472	B8W	C4-C5-C6	4.10	119.25	115.22
44	2	2380	B8W	N9-C8-N7	-4.03	108.22	113.94
44	2	237	B9B	N9-C8-N7	-4.03	108.22	113.94
44	2	1517	2MG	N9-C4-N3	4.02	134.00	125.95
44	2	4185	B8W	O6-C6-N1	4.02	124.30	118.96
44	2	1871	A2M	C2'-C1'-N9	-4.01	107.15	113.75
44	2	2363	A2M	N3-C4-N9	4.00	133.97	127.17
44	2	3880	P7G	C4-C5-N7	4.00	109.40	106.71
44	2	1574	B9B	N2-C2-N3	3.98	123.19	117.22
44	2	2754	B9B	N9-C8-N7	-3.98	108.29	113.94
44	2	2754	B9B	C4-C5-C6	3.97	119.12	115.22
44	2	4523	A2M	C5-C4-N3	-3.96	121.26	126.72
44	2	2401	A2M	C5-C4-N3	-3.95	121.28	126.72
44	2	398	A2M	C5-C4-N3	-3.93	121.30	126.72
44	2	1326	A2M	C1'-N9-C8	-3.93	118.38	127.09
44	2	3899	BGH	N9-C8-N7	3.91	108.46	103.31
44	2	4185	B8W	N9-C8-N7	-3.88	108.43	113.94
44	2	1524	A2M	N3-C4-N9	3.88	133.76	127.17
44	2	3867	A2M	N3-C4-N9	3.88	133.76	127.17
44	2	1348	P4U	C5-C4-N3	-3.87	119.18	124.86
44	2	2401	A2M	C1'-N9-C8	-3.86	118.53	127.09
44	2	2422	OMC	O2-C2-N3	-3.86	116.25	122.33
44	2	1605	7MG	C5-C4-N9	3.85	111.27	106.33
44	2	2297	E7G	C5-C4-N3	-3.83	120.93	128.13
43	8	14	OMU	N3-C2-N1	3.83	119.88	114.89
44	2	4083	5MU	O4-C4-C5	-3.83	120.53	124.92
44	2	1871	A2M	N3-C4-N9	3.80	133.64	127.17
43	8	14	OMU	C5-C4-N3	3.77	120.08	114.80
44	2	237	B9B	N3-C2-N1	-3.76	119.71	125.48
44	2	4690	B8K	C6-C5-C4	-3.76	115.78	122.40
44	2	1797	E7G	C5-C4-N3	-3.76	121.07	128.13
44	2	978	2MG	N9-C4-N3	3.76	133.47	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	2861	OMC	O2-C2-N3	-3.76	116.41	122.33
44	2	4083	5MU	C5M-C5-C4	3.73	122.77	118.78
44	2	4523	A2M	C1'-N9-C8	-3.72	118.83	127.09
44	2	4415	1MA	N1-C2-N3	-3.72	121.58	126.00
44	2	4597	UR3	C6-N1-C2	-3.72	118.76	121.80
44	2	2522	7MG	C5-C4-N9	3.72	111.10	106.33
44	2	4550	7MG	C5-C4-N3	-3.72	121.15	128.13
44	2	1456	B8Q	C31-N3-C4	3.71	121.19	114.76
44	2	4620	OMU	C5-C4-N3	3.71	120.00	114.80
44	2	4620	OMU	N3-C2-N1	3.71	119.72	114.89
44	2	4472	B8W	N1-C2-N3	-3.71	119.80	125.48
44	2	1534	A2M	C2-N3-C4	3.68	120.81	111.83
44	2	1797	E7G	C5-C4-N9	3.67	111.03	106.33
44	2	1871	A2M	C1'-N9-C8	-3.67	118.95	127.09
44	2	2297	E7G	C5-C4-N9	3.65	111.01	106.33
44	2	3825	A2M	N3-C4-N9	3.64	133.36	127.17
44	2	1326	A2M	N3-C4-N9	3.64	133.35	127.17
44	2	3897	B8K	C6-C5-C4	-3.63	116.01	122.40
44	2	4415	1MA	C2-N3-C4	3.63	119.64	112.53
44	2	1574	B9B	N3-C2-N1	-3.62	119.93	125.48
44	2	4550	7MG	C5-C4-N9	3.62	110.97	106.33
44	2	1534	A2M	C1'-N9-C8	-3.62	119.07	127.09
44	2	4472	B8W	N3-C4-N9	3.61	131.57	126.99
44	2	1534	A2M	N3-C4-N9	3.61	133.30	127.17
44	2	398	A2M	C1'-N9-C8	-3.61	119.09	127.09
44	2	3899	BGH	C5-C4-N3	-3.59	121.39	128.13
44	2	237	B9B	C4-C5-C6	3.59	118.74	115.22
44	2	3897	B8K	N9-C8-N7	3.58	108.03	103.31
44	2	2754	B9B	N3-C2-N1	-3.57	120.00	125.48
44	2	2522	7MG	C5-C4-N3	-3.56	121.46	128.13
44	2	1524	A2M	O4'-C1'-N9	3.55	114.92	108.09
44	2	1517	2MG	N1-C2-N2	3.55	120.19	116.56
44	2	1871	A2M	C2-N3-C4	3.55	120.50	111.83
44	2	4185	B8W	N1-C2-N3	-3.55	120.04	125.48
44	2	2401	A2M	N3-C4-N9	3.53	133.16	127.17
44	2	1326	A2M	C2-N3-C4	3.51	120.41	111.83
44	2	2380	B8W	N1-C2-N3	-3.50	120.11	125.48
44	2	1605	7MG	C5-C4-N3	-3.49	121.58	128.13
44	2	4690	B8K	C5-C4-N9	3.48	110.80	106.33
44	2	2363	A2M	C2-N3-C4	3.48	120.33	111.83
44	2	3825	A2M	C2-N3-C4	3.48	120.32	111.83
44	2	4637	OMG	C2-N1-C6	-3.46	118.83	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	2364	OMG	C2-N1-C6	-3.46	118.84	125.11
44	2	1909	P7G	N9-C8-N7	3.43	108.23	103.37
44	2	4564	M7A	C2-N3-C4	3.43	120.20	111.83
44	2	1316	OMG	C2-N1-C6	-3.43	118.90	125.11
44	2	2401	A2M	C2-N3-C4	3.42	120.19	111.83
44	2	4472	B8W	C2-N1-C6	3.42	120.72	115.96
44	2	3867	A2M	C2-N3-C4	3.42	120.17	111.83
44	2	4872	2MG	N2-C2-N3	-3.42	116.16	120.51
44	2	4523	A2M	C2-N3-C4	3.41	120.16	111.83
44	2	398	A2M	C2-N3-C4	3.40	120.14	111.83
44	2	2786	B9H	C4-N3-C2	-3.39	115.89	122.00
44	2	1524	A2M	C2-N3-C4	3.39	120.10	111.83
44	2	3899	BGH	C6-C5-C4	-3.37	116.47	122.40
44	2	398	A2M	N3-C4-N9	3.37	132.90	127.17
44	2	4523	A2M	C5-N7-C8	3.35	108.71	103.45
44	2	3909	OMC	C4-N3-C2	3.33	125.51	120.26
44	2	4690	B8K	C5-C4-N3	-3.33	121.88	128.13
44	2	4472	B8W	C5-N7-C8	3.32	108.67	103.45
44	2	2522	7MG	C4-C5-N7	3.28	109.25	105.38
44	2	2424	OMG	C2-N1-C6	-3.27	119.17	125.11
44	2	4523	A2M	N3-C4-N9	3.27	132.72	127.17
44	2	373	OMG	C2-N1-C6	-3.24	119.23	125.11
44	2	3825	A2M	C5-N7-C8	3.22	108.51	103.45
44	2	4185	B8W	N2-C2-N1	-3.21	112.41	117.22
44	2	4483	B8T	O3'-C3'-C2'	3.20	122.07	111.82
44	2	1534	A2M	C5-N7-C8	3.19	108.47	103.45
44	2	4550	7MG	C4-C5-N7	3.19	109.15	105.38
43	8	14	OMU	O4-C4-C5	-3.19	119.66	125.16
44	2	2773	OMG	C2-N1-C6	-3.19	119.33	125.11
44	2	2050	OMG	C2-N1-C6	-3.17	119.36	125.11
44	2	3869	OMC	O2-C2-N3	-3.16	117.34	122.33
44	2	1871	A2M	C5-N7-C8	3.15	108.40	103.45
44	2	4494	OMG	C2-N1-C6	-3.14	119.42	125.11
44	2	1326	A2M	C5-N7-C8	3.14	108.38	103.45
44	2	1574	B9B	N3-C4-N9	3.13	130.96	126.99
44	2	1574	B9B	C4-C5-C6	3.11	118.27	115.22
44	2	1883	OMG	C2-N1-C6	-3.10	119.50	125.11
44	2	2380	B8W	N2-C2-N1	-3.08	112.60	117.22
44	2	398	A2M	C5-N7-C8	3.08	108.29	103.45
44	2	3867	A2M	C5-N7-C8	3.07	108.28	103.45
44	2	1522	OMG	C2-N1-C6	-3.07	119.55	125.11
44	2	4185	B8W	C2-N1-C6	3.06	120.22	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	4623	OMG	C2-N1-C6	-3.06	119.56	125.11
44	2	1605	7MG	C4-C5-N7	3.05	108.97	105.38
44	2	2401	A2M	C5-N7-C8	3.04	108.23	103.45
44	2	3909	OMC	C5-C4-N4	3.04	125.96	120.63
44	2	4415	1MA	N9-C4-N3	3.01	133.76	126.90
44	2	1625	OMG	C2-N1-C6	-3.00	119.67	125.11
44	2	3897	B8K	C5-C4-N3	-2.99	122.51	128.13
44	2	4870	OMG	C2-N1-C6	-2.99	119.69	125.11
44	2	1524	A2M	C5-N7-C8	2.98	108.13	103.45
44	2	4597	UR3	C3U-N3-C2	2.95	122.48	117.33
44	2	4620	OMU	O4-C4-C5	-2.94	120.10	125.16
44	2	2363	A2M	C5-N7-C8	2.94	108.06	103.45
44	2	1456	B8Q	C1'-N1-C2	2.92	121.82	117.04
44	2	4472	B8W	C4-N9-C1'	-2.91	119.83	126.63
44	2	4637	OMG	C5-C6-N1	2.91	120.65	113.25
44	2	4872	2MG	N9-C8-N7	-2.90	108.02	113.40
44	2	2364	OMG	C5-C4-N9	2.89	110.83	105.66
44	2	3909	OMC	C5-C4-N3	-2.88	116.47	121.32
44	2	2754	B9B	C61-O6-C6	-2.86	112.69	117.66
44	2	4472	B8W	C5-C6-N1	-2.84	119.69	123.49
44	2	4472	B8W	C4-C5-N7	-2.84	107.33	110.58
44	2	4690	B8K	C2-N1-C6	-2.83	119.97	125.11
43	8	14	OMU	C1'-N1-C2	2.83	122.67	117.59
44	2	4472	B8W	N2-C2-N1	-2.82	113.00	117.22
44	2	1316	OMG	C5-C6-N1	2.80	120.37	113.25
44	2	3899	BGH	O6-C6-N1	-2.79	114.86	120.11
44	2	1316	OMG	C5-C4-N9	2.79	110.65	105.66
44	2	2522	7MG	N9-C8-N7	2.79	107.32	103.37
44	2	1883	OMG	C5-C6-N1	2.77	120.31	113.25
44	2	1883	OMG	O6-C6-C5	-2.76	119.26	126.53
44	2	2754	B9B	C2-N3-C4	2.75	120.88	113.51
44	2	4185	B8W	C5-N7-C8	2.75	107.77	103.45
44	2	1517	2MG	C5-C6-N1	2.74	120.23	113.25
44	2	729	2MG	C5-C6-N1	2.74	120.22	113.25
44	2	2422	OMC	C1'-N1-C2	2.74	124.48	118.44
44	2	373	OMG	C5-C4-N9	2.73	110.55	105.66
44	2	2861	OMC	C1'-N1-C2	2.73	124.47	118.44
44	2	2424	OMG	C5-C6-N1	2.73	120.19	113.25
44	2	4415	1MA	N9-C8-N7	-2.72	108.35	113.40
44	2	4637	OMG	O6-C6-C5	-2.72	119.35	126.53
44	2	4185	B8W	C61-O6-C6	-2.72	114.66	117.20
44	2	2380	B8W	C2-N1-C6	2.72	119.74	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	4494	OMG	C5-C6-N1	2.72	120.17	113.25
44	2	2297	E7G	N9-C8-N7	2.72	107.22	103.37
44	2	4483	B8T	O3'-C3'-C4'	2.72	118.88	111.08
44	2	2050	OMG	C5-C4-N9	2.71	110.51	105.66
44	2	4636	PSU	O2-C2-N1	-2.70	120.00	122.79
44	2	4483	B8T	O2-C2-N3	-2.69	118.08	122.33
44	2	2380	B8W	C4-N9-C1'	-2.69	120.34	126.63
44	2	1524	A2M	C4-N9-C1'	2.69	132.93	126.63
44	2	4671	B8T	C6-C5-C4	2.68	120.23	117.00
44	2	237	B9B	C2-N3-C4	2.68	120.70	113.51
44	2	978	2MG	C5-C6-N1	2.68	120.08	113.25
44	2	1797	E7G	N9-C8-N7	2.68	107.17	103.37
44	2	4637	OMG	O4'-C1'-N9	2.68	114.43	108.36
44	2	1605	7MG	N9-C8-N7	2.68	107.16	103.37
44	2	4870	OMG	C5-C6-N1	2.68	120.06	113.25
44	2	3897	B8K	O6-C6-N1	-2.67	115.09	120.11
44	2	729	2MG	N9-C8-N7	-2.67	108.45	113.40
44	2	2050	OMG	O6-C6-C5	-2.67	119.49	126.53
44	2	4623	OMG	C5-C4-N9	2.67	110.43	105.66
44	2	2773	OMG	C5-C6-N1	2.66	120.03	113.25
44	2	4564	M7A	C5-C4-N3	-2.66	120.41	126.56
44	2	1522	OMG	C5-C4-N9	2.66	110.42	105.66
44	2	2773	OMG	C5-C4-N9	2.66	110.41	105.66
44	2	1456	B8Q	C31-N3-C2	2.65	121.86	117.70
44	2	729	2MG	N1-C2-N2	2.65	119.26	116.56
44	2	4185	B8W	C4-N9-C1'	-2.64	120.45	126.63
44	2	2364	OMG	C5-C6-N1	2.64	119.98	113.25
44	2	2050	OMG	C5-C6-N1	2.64	119.97	113.25
44	2	2786	B9H	O3'-C3'-C4'	2.64	118.66	111.08
44	2	1625	OMG	N9-C4-N3	2.63	131.22	125.95
44	2	373	OMG	C5-C6-N1	2.63	119.94	113.25
44	2	1625	OMG	C5-C6-N1	2.62	119.93	113.25
44	2	4550	7MG	C2-N1-C6	-2.62	120.36	125.11
44	2	4872	2MG	C5-C6-N1	2.62	119.92	113.25
44	2	2786	B9H	C1'-N1-C6	2.61	126.37	120.78
44	2	1797	E7G	C2-N1-C6	-2.61	120.37	125.11
44	2	2380	B8W	C5-N7-C8	2.61	107.56	103.45
44	2	2297	E7G	C2-N1-C6	-2.61	120.38	125.11
44	2	1883	OMG	C2'-C1'-N9	-2.61	109.28	114.24
44	2	2422	OMC	O2-C2-N1	2.61	124.01	118.90
44	2	4185	B8W	C5-C6-N1	-2.61	120.00	123.49
44	2	3880	P7G	N9-C8-N7	2.60	107.05	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	4623	OMG	C5-C6-N1	2.60	119.86	113.25
44	2	978	2MG	N9-C8-N7	-2.60	108.58	113.40
44	2	2754	B9B	C5-N7-C8	2.60	107.53	103.45
44	2	4494	OMG	O6-C6-C5	-2.59	119.68	126.53
43	8	14	OMU	CM2-O2'-C2'	2.59	121.13	114.47
44	2	2861	OMC	O2-C2-N1	2.58	123.96	118.90
44	2	1574	B9B	C5-N7-C8	2.57	107.50	103.45
44	2	1517	2MG	N9-C8-N7	-2.57	108.64	113.40
44	2	1574	B9B	C4-N9-C8	2.57	108.43	105.74
44	2	1517	2MG	O6-C6-C5	-2.56	119.77	126.53
44	2	2363	A2M	C4-N9-C1'	2.56	132.62	126.63
44	2	2364	OMG	O6-C6-C5	-2.56	119.78	126.53
44	2	3899	BGH	C2-N1-C6	-2.55	120.49	125.11
44	2	3887	OMC	O2-C2-N3	-2.55	118.31	122.33
44	2	4083	5MU	C6-C5-C4	2.55	120.12	118.02
44	2	2424	OMG	O6-C6-C5	-2.55	119.81	126.53
44	2	2786	B9H	O2-C2-N1	-2.54	117.11	122.78
44	2	4872	2MG	N9-C4-N3	2.54	131.03	125.95
44	2	4637	OMG	C5-C4-N9	2.54	110.20	105.66
44	2	4690	B8K	O6-C6-C5	-2.53	121.41	127.62
44	2	729	2MG	O6-C6-C5	-2.52	119.87	126.53
44	2	1625	OMG	O6-C6-C5	-2.52	119.88	126.53
44	2	1316	OMG	O4'-C1'-N9	2.52	114.06	108.36
44	2	4494	OMG	C5-C4-N9	2.51	110.14	105.66
44	2	978	2MG	O6-C6-C5	-2.51	119.92	126.53
44	2	2522	7MG	C2-N1-C6	-2.51	120.57	125.11
44	2	1605	7MG	C2-N1-C6	-2.50	120.57	125.11
44	2	4472	B8W	C2-N3-C4	2.50	120.21	113.51
44	2	4083	5MU	O2-C2-N1	-2.49	119.55	122.80
44	2	1522	OMG	C5-C6-N1	2.49	119.60	113.25
44	2	237	B9B	C4-N9-C8	2.49	108.35	105.74
44	2	237	B9B	C5-N7-C8	2.46	107.32	103.45
44	2	4483	B8T	C6-C5-C4	2.46	119.96	117.00
44	2	1574	B9B	C2-N3-C4	2.45	120.08	113.51
44	2	2050	OMG	N2-C2-N1	2.45	121.93	116.76
44	2	4550	7MG	N9-C8-N7	2.45	106.83	103.37
44	2	373	OMG	C2'-C1'-N9	-2.44	109.60	114.24
44	2	1574	B9B	C61-O6-C6	-2.44	113.41	117.66
44	2	373	OMG	O6-C6-C5	-2.43	120.11	126.53
44	2	2380	B8W	C2-N3-C4	2.43	120.02	113.51
44	2	2364	OMG	O4'-C1'-N9	2.42	113.85	108.36
44	2	2380	B8W	C61-O6-C6	-2.42	114.94	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	1316	OMG	C2'-C1'-N9	-2.41	109.66	114.24
44	2	2380	B8W	O6-C6-C5	-2.41	114.26	117.17
44	2	2754	B9B	C4-N9-C8	2.41	108.27	105.74
44	2	373	OMG	O4'-C1'-N9	2.40	113.79	108.36
44	2	2424	OMG	C5-C4-N9	2.39	109.93	105.66
44	2	237	B9B	C61-O6-C6	-2.39	113.50	117.66
44	2	4597	UR3	O2-C2-N1	-2.39	117.45	122.78
44	2	4494	OMG	O4'-C1'-N9	2.38	113.76	108.36
44	2	4185	B8W	C2-N3-C4	2.38	119.89	113.51
44	2	1316	OMG	C4-C5-N7	-2.38	106.90	110.67
44	2	2380	B8W	C5-C6-N1	-2.38	120.31	123.49
44	2	4623	OMG	O4'-C1'-N9	2.38	113.74	108.36
44	2	4870	OMG	O6-C6-C5	-2.37	120.27	126.53
44	2	2773	OMG	O6-C6-C5	-2.37	120.28	126.53
44	2	1316	OMG	O6-C6-C5	-2.37	120.28	126.53
44	2	4623	OMG	O6-C6-C5	-2.37	120.29	126.53
44	2	3899	BGH	N1-C2-N3	-2.36	119.01	123.32
44	2	3869	OMC	C1'-N1-C2	2.35	123.64	118.44
44	2	1883	OMG	O4'-C1'-N9	2.35	113.69	108.36
44	2	4636	PSU	C6-N1-C2	-2.35	120.51	122.69
44	2	3701	OMC	O2-C2-N3	-2.34	118.64	122.33
44	2	4872	2MG	O6-C6-C5	-2.33	120.37	126.53
44	2	1574	B9B	C2-N1-C6	2.32	119.19	115.96
44	2	3909	OMC	C6-N1-C2	-2.32	116.54	120.46
44	2	373	OMG	N9-C8-N7	-2.32	109.09	113.40
44	2	3897	B8K	N1-C2-N3	-2.32	119.08	123.32
44	2	1883	OMG	C5-C4-N9	2.31	109.80	105.66
44	2	4550	7MG	C6-C5-C4	-2.31	118.34	122.40
44	2	4870	OMG	C5-C4-N9	2.30	109.77	105.66
44	2	1316	OMG	N9-C8-N7	-2.29	109.16	113.40
44	2	1522	OMG	O6-C6-C5	-2.28	120.53	126.53
44	2	1797	E7G	C6-C5-C4	-2.27	118.40	122.40
44	2	2401	A2M	C2'-C1'-N9	-2.27	110.01	113.75
44	2	4623	OMG	N9-C8-N7	-2.27	109.18	113.40
44	2	4870	OMG	N9-C8-N7	-2.27	109.19	113.40
44	2	2380	B8W	C6-C5-N7	-2.27	131.16	133.82
44	2	237	B9B	C2-N1-C6	2.26	119.10	115.96
44	2	4472	B8W	C1'-N9-C8	2.25	132.10	127.09
44	2	4523	A2M	C2'-C1'-N9	-2.24	110.06	113.75
44	2	1605	7MG	C6-C5-C4	-2.24	118.46	122.40
44	2	4083	5MU	O4-C4-N3	-2.24	115.90	120.11
44	2	373	OMG	N2-C2-N1	2.24	121.49	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	2522	7MG	C6-C5-C4	-2.24	118.47	122.40
44	2	3897	B8K	C2-N1-C6	-2.24	121.05	125.11
44	2	2297	E7G	C6-C5-C4	-2.22	118.49	122.40
44	2	3869	OMC	O2-C2-N1	2.22	123.24	118.90
44	2	4472	B8W	C4-N9-C8	2.21	108.06	105.74
44	2	373	OMG	C4-C5-N7	-2.20	107.18	110.67
44	2	2804	OMC	O2-C2-N3	-2.20	118.86	122.33
44	2	1625	OMG	N9-C8-N7	-2.20	109.32	113.40
44	2	2050	OMG	O4'-C1'-N9	2.20	113.34	108.36
44	2	4690	B8K	N1-C2-N3	-2.20	119.30	123.32
44	2	2364	OMG	N2-C2-N1	2.19	121.38	116.76
44	2	4185	B8W	C1'-N9-C8	2.18	131.94	127.09
44	2	1522	OMG	O4'-C1'-N9	2.18	113.29	108.36
44	2	2424	OMG	O4'-C1'-N9	2.17	113.28	108.36
44	2	4483	B8T	C6-N1-C2	-2.17	116.79	120.46
44	2	1871	A2M	O4'-C4'-C3'	-2.17	100.85	105.15
44	2	1348	P4U	O2-C2-N3	-2.17	118.92	122.33
44	2	2773	OMG	O4'-C1'-N9	2.16	113.26	108.36
44	2	2754	B9B	C1'-N9-C8	-2.16	122.31	127.09
44	2	4623	OMG	C4-C5-N7	-2.15	107.27	110.67
44	2	4872	2MG	C4-C5-N7	-2.15	107.27	110.67
44	2	2424	OMG	N9-C4-N3	2.14	130.24	125.95
44	2	729	2MG	CM2-N2-C2	-2.14	119.05	123.65
44	2	2380	B8W	C4-N9-C8	2.13	107.98	105.74
44	2	1316	OMG	N2-C2-N1	2.13	121.26	116.76
44	2	4872	2MG	C8-N7-C5	2.13	108.05	104.26
44	2	4472	B8W	C5-C4-N9	2.12	108.12	105.81
44	2	3867	A2M	C4-N9-C1'	2.11	131.56	126.63
44	2	1883	OMG	N9-C8-N7	-2.11	109.49	113.40
44	2	1797	E7G	O6-C6-C5	-2.11	122.45	127.62
44	2	2050	OMG	N9-C8-N7	-2.10	109.50	113.40
44	2	1605	7MG	O6-C6-C5	-2.10	122.46	127.62
44	2	1348	P4U	C41-O4-C4	-2.09	112.96	117.09
44	2	1522	OMG	C4-C5-N7	-2.09	107.36	110.67
44	2	4415	1MA	C8-N7-C5	2.08	107.96	104.26
44	2	4550	7MG	O6-C6-C5	-2.07	122.54	127.62
44	2	4623	OMG	N2-C2-N1	2.07	121.13	116.76
44	2	373	OMG	CM2-O2'-C2'	-2.07	109.17	114.47
44	2	2380	B8W	C1'-N9-C8	2.06	131.68	127.09
44	2	2297	E7G	O6-C6-C5	-2.05	122.59	127.62
44	2	729	2MG	C8-N7-C5	2.04	107.89	104.26
44	2	2364	OMG	C4-C5-N7	-2.03	107.45	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	4083	5MU	C6-N1-C2	-2.03	119.28	121.30
44	2	2522	7MG	O6-C6-C5	-2.02	122.67	127.62
44	2	3909	OMC	C1'-N1-C2	2.01	122.89	118.44
44	2	4872	2MG	C1'-N9-C4	-2.00	120.57	126.49
44	2	4637	OMG	N9-C8-N7	-2.00	109.69	113.40

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	8	14	OMU	C1'-C2'-O2'-CM2
44	2	237	B9B	C5-C6-O6-C61
44	2	237	B9B	N1-C6-O6-C61
44	2	237	B9B	O4'-C4'-C5'-O5'
44	2	398	A2M	O4'-C4'-C5'-O5'
44	2	1348	P4U	N3-C4-O4-C41
44	2	1524	A2M	O4'-C1'-N9-C8
44	2	1524	A2M	O4'-C1'-N9-C4
44	2	1574	B9B	C5-C6-O6-C61
44	2	1574	B9B	N1-C6-O6-C61
44	2	1625	OMG	O4'-C4'-C5'-O5'
44	2	1797	E7G	C72-C71-N7-C8
44	2	1871	A2M	O4'-C4'-C5'-O5'
44	2	1871	A2M	C3'-C4'-C5'-O5'
44	2	1883	OMG	O4'-C4'-C5'-O5'
44	2	2364	OMG	O4'-C4'-C5'-O5'
44	2	2364	OMG	C1'-C2'-O2'-CM2
44	2	2380	B8W	C5-C6-O6-C61
44	2	2424	OMG	O4'-C4'-C5'-O5'
44	2	2754	B9B	C5-C6-O6-C61
44	2	2754	B9B	N1-C6-O6-C61
44	2	3701	OMC	C2'-C1'-N1-C2
44	2	3701	OMC	C2'-C1'-N1-C6
44	2	3867	A2M	O4'-C4'-C5'-O5'
44	2	4083	5MU	O4'-C4'-C5'-O5'
44	2	4415	1MA	O4'-C4'-C5'-O5'
44	2	4415	1MA	C3'-C4'-C5'-O5'
44	2	4472	B8W	C5-C6-O6-C61
44	2	4472	B8W	N1-C6-O6-C61
44	2	4550	7MG	O4'-C4'-C5'-O5'
44	2	4550	7MG	C3'-C4'-C5'-O5'
44	2	4636	PSU	C2'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
44	2	4637	OMG	O4'-C4'-C5'-O5'
44	2	2380	B8W	N1-C6-O6-C61
44	2	237	B9B	C3'-C4'-C5'-O5'
44	2	1625	OMG	C3'-C4'-C5'-O5'
44	2	1883	OMG	C3'-C4'-C5'-O5'
44	2	1909	P7G	O4'-C4'-C5'-O5'
44	2	2424	OMG	C3'-C4'-C5'-O5'
44	2	3867	A2M	C3'-C4'-C5'-O5'
44	2	3897	B8K	O4'-C4'-C5'-O5'
44	2	4083	5MU	C3'-C4'-C5'-O5'
44	2	4636	PSU	C3'-C4'-C5'-O5'
44	2	4637	OMG	C3'-C4'-C5'-O5'
44	2	4872	2MG	O4'-C4'-C5'-O5'
44	2	4636	PSU	O4'-C4'-C5'-O5'
44	2	398	A2M	C3'-C4'-C5'-O5'
44	2	2364	OMG	C3'-C4'-C5'-O5'
44	2	2422	OMC	O4'-C4'-C5'-O5'
44	2	2773	OMG	C3'-C4'-C5'-O5'
44	2	4870	OMG	C3'-C4'-C5'-O5'
44	2	4872	2MG	C3'-C4'-C5'-O5'
44	2	2297	E7G	C72-C71-N7-C8
44	2	3701	OMC	C4'-C5'-O5'-P
44	2	729	2MG	O4'-C4'-C5'-O5'
44	2	3701	OMC	O4'-C4'-C5'-O5'
44	2	3897	B8K	C3'-C4'-C5'-O5'
44	2	1909	P7G	C3'-C4'-C5'-O5'
44	2	1574	B9B	O6-C61-C62-C63
44	2	729	2MG	C3'-C4'-C5'-O5'
44	2	3701	OMC	C3'-C4'-C5'-O5'
44	2	4870	OMG	O4'-C4'-C5'-O5'
44	2	3880	P7G	O4'-C4'-C5'-O5'
44	2	3909	OMC	O4'-C4'-C5'-O5'
44	2	3701	OMC	O4'-C1'-N1-C6
44	2	2773	OMG	O4'-C4'-C5'-O5'
44	2	3880	P7G	N7-C71-C72-C73
44	2	1574	B9B	C62-C61-O6-C6
44	2	1517	2MG	C4'-C5'-O5'-P
44	2	1534	A2M	C4'-C5'-O5'-P
44	2	1625	OMG	C4'-C5'-O5'-P
44	2	4870	OMG	C4'-C5'-O5'-P
44	2	1909	P7G	C72-C71-N7-C8
44	2	1659	I4U	C43-C41-O4-C4

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Mol	Chain	Res	Type	Atoms
44	2	4083	5MU	C4'-C5'-O5'-P
44	2	3887	OMC	C4'-C5'-O5'-P
44	2	1605	7MG	O4'-C4'-C5'-O5'
44	2	3701	OMC	O4'-C1'-N1-C2
44	2	373	OMG	C4'-C5'-O5'-P
44	2	1909	P7G	C72-C71-N7-C5
44	2	1524	A2M	C3'-C2'-O2'-CM'
44	2	1659	I4U	C42-C41-O4-C4
44	2	3880	P7G	C3'-C4'-C5'-O5'
44	2	1574	B9B	C2'-C1'-N9-C8
44	2	2754	B9B	C4'-C5'-O5'-P
44	2	1517	2MG	O4'-C4'-C5'-O5'
44	2	1534	A2M	O4'-C4'-C5'-O5'
44	2	3909	OMC	C2'-C1'-N1-C2

There are no ring outliers.

13 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	2	2522	7MG	1	0
44	2	2364	OMG	1	0
44	2	2050	OMG	1	0
44	2	1524	A2M	1	0
44	2	1534	A2M	1	0
44	2	1574	B9B	1	0
44	2	1871	A2M	1	0
44	2	2363	A2M	1	0
43	8	14	OMU	2	0
44	2	729	2MG	1	0
44	2	1517	2MG	1	0
44	2	4872	2MG	1	0
44	2	4083	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
60	GTP	w	801	61	33,34,34	0.55	0	50,54,54	0.54	0

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
60	GTP	w	801	61	-	1/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	w	801	GTP	C5'-O5'-PA-O1A

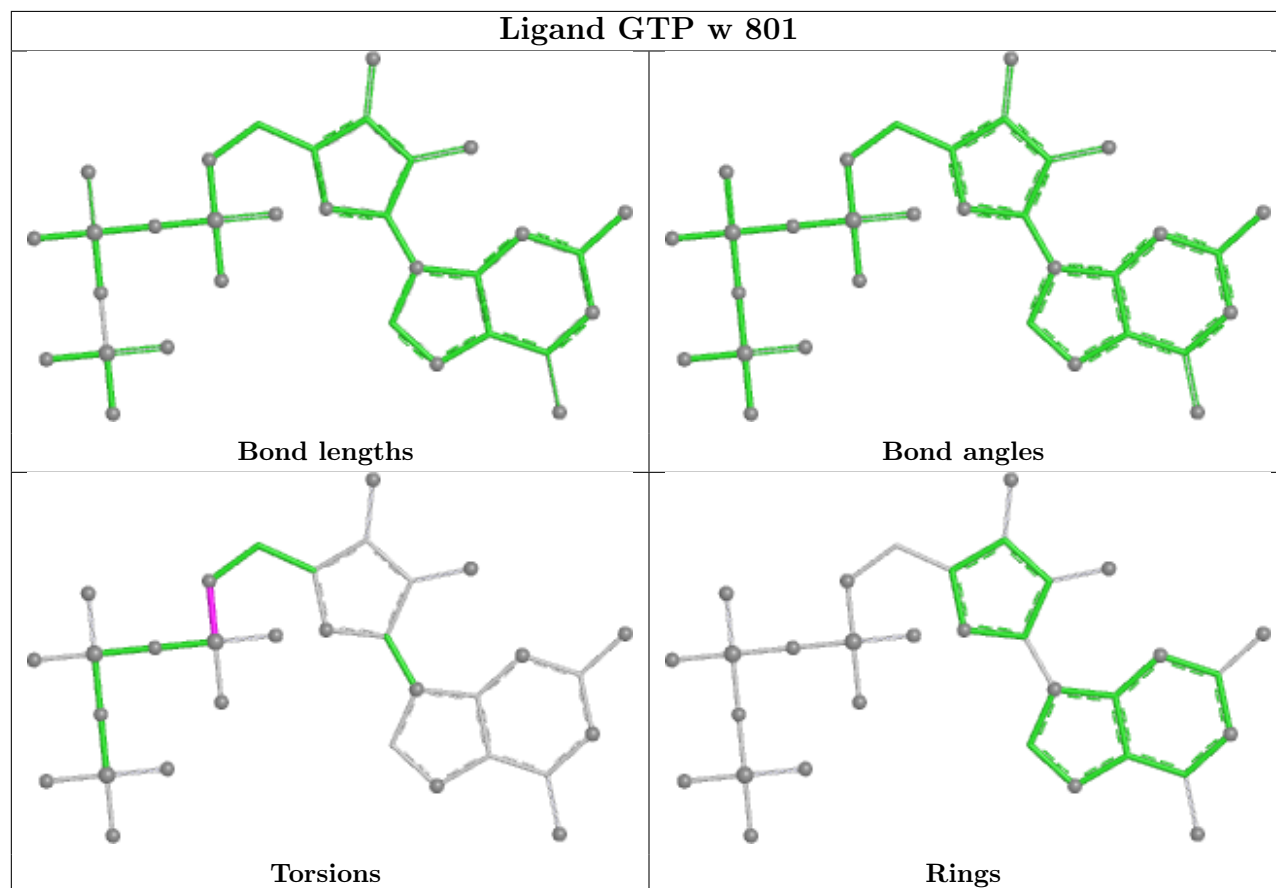
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	w	801	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

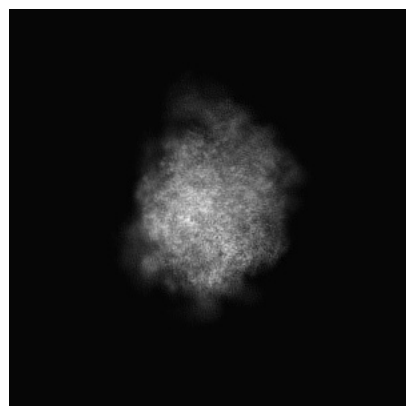
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35673. These allow visual inspection of the internal detail of the map and identification of artifacts.

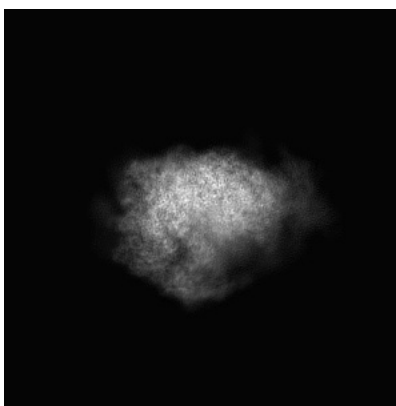
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

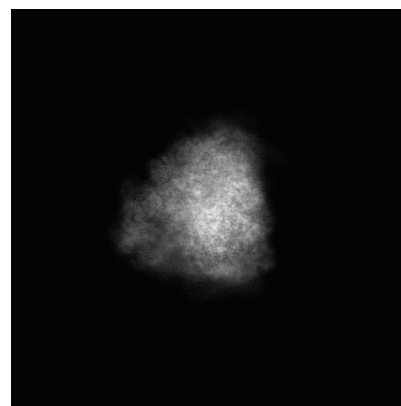
6.1.1 Primary map



X

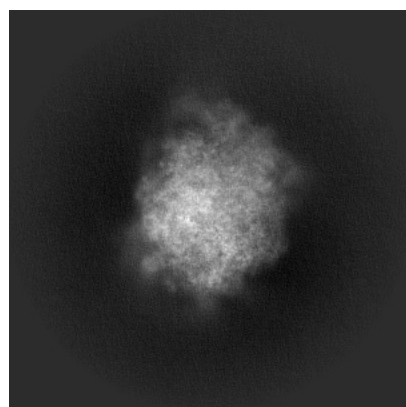


Y

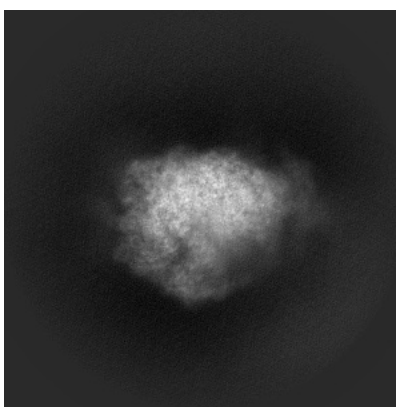


Z

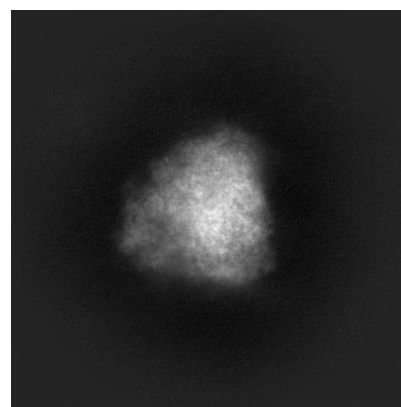
6.1.2 Raw map



X



Y

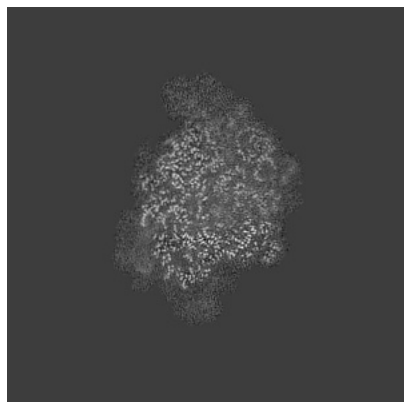


Z

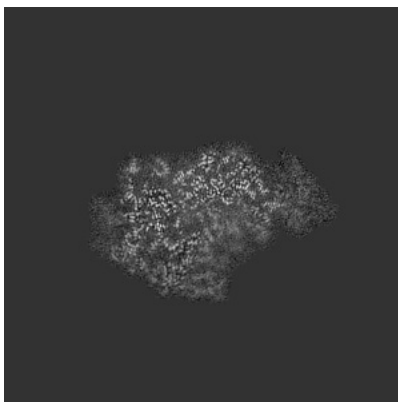
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

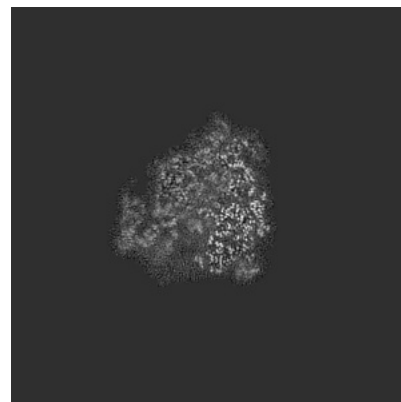
6.2.1 Primary map



X Index: 200

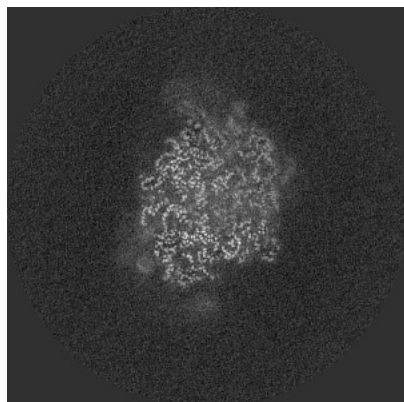


Y Index: 200

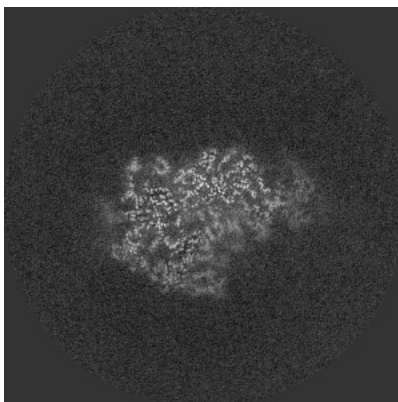


Z Index: 200

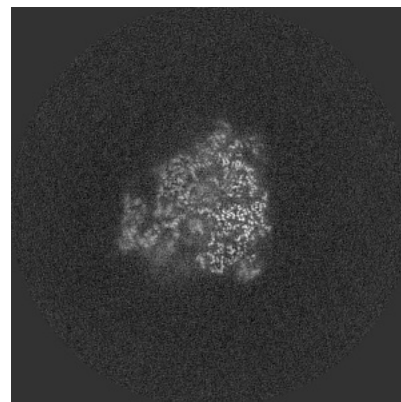
6.2.2 Raw map



X Index: 200



Y Index: 200

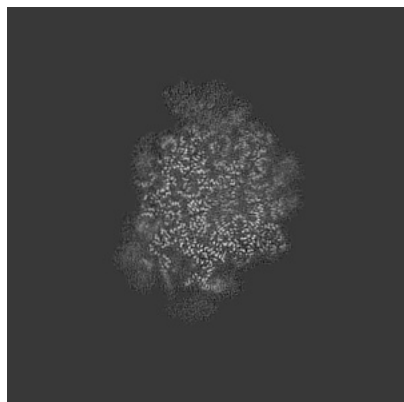


Z Index: 200

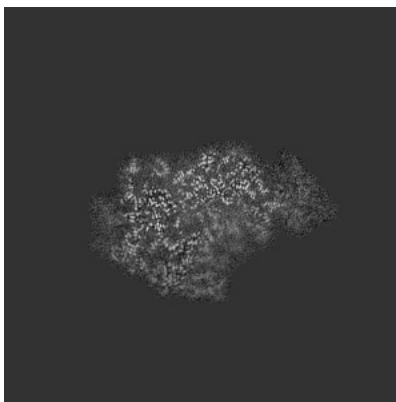
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

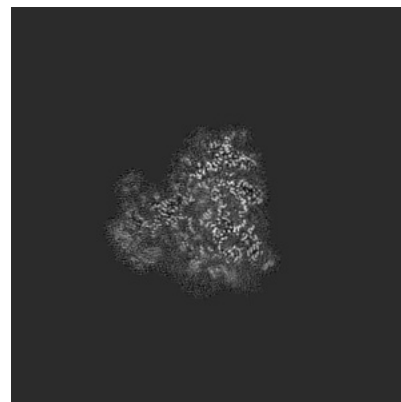
6.3.1 Primary map



X Index: 207

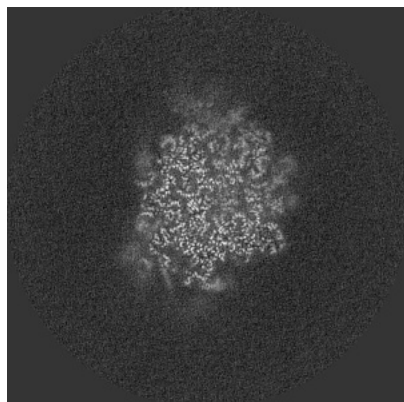


Y Index: 200

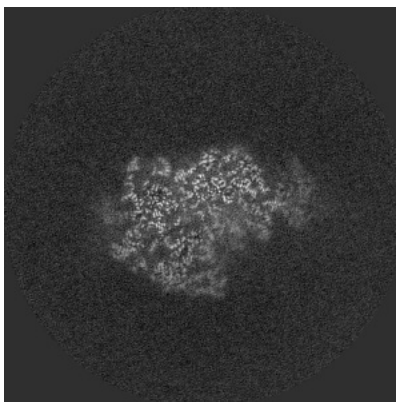


Z Index: 183

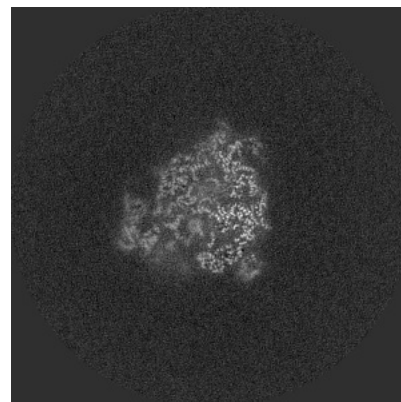
6.3.2 Raw map



X Index: 208



Y Index: 199

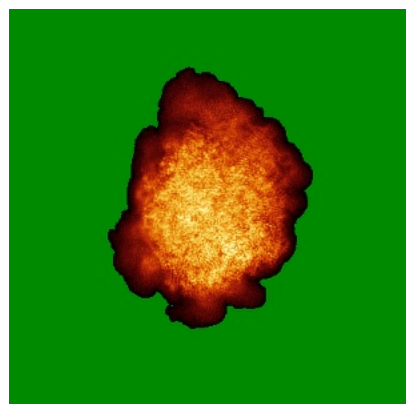


Z Index: 199

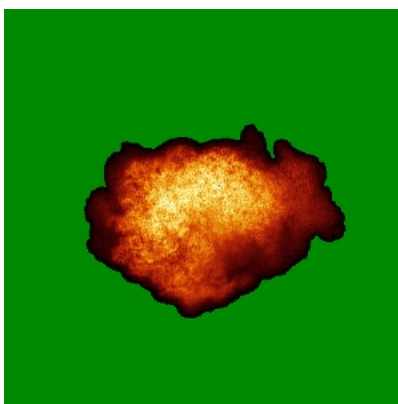
The images above show the largest variance slices of the map in three orthogonal directions.

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

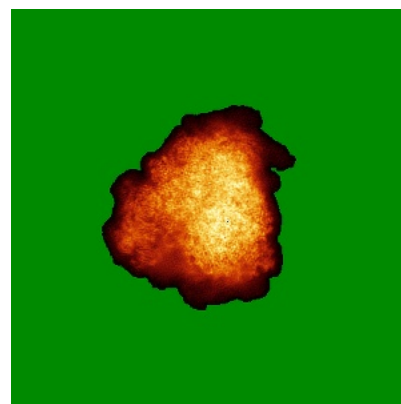
6.4.1 Primary map



X

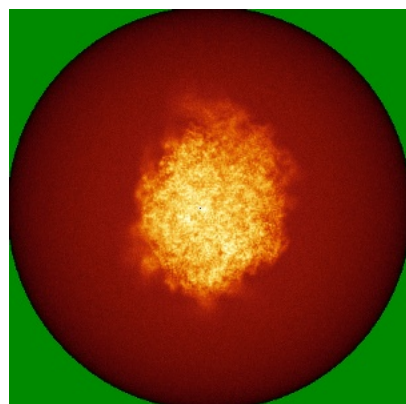


Y

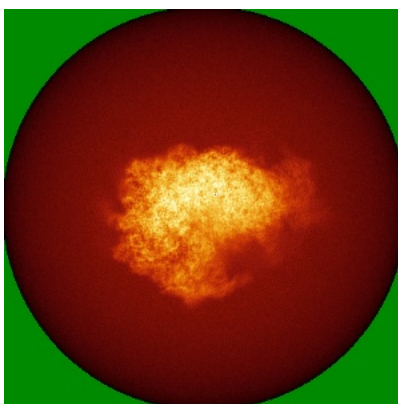


Z

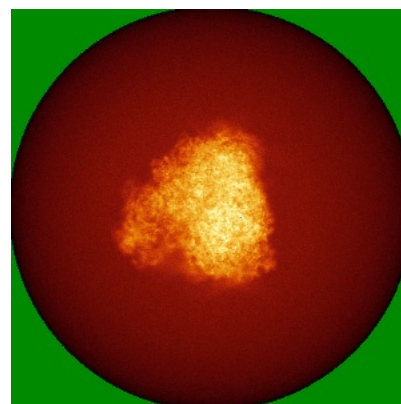
6.4.2 Raw map



X



Y

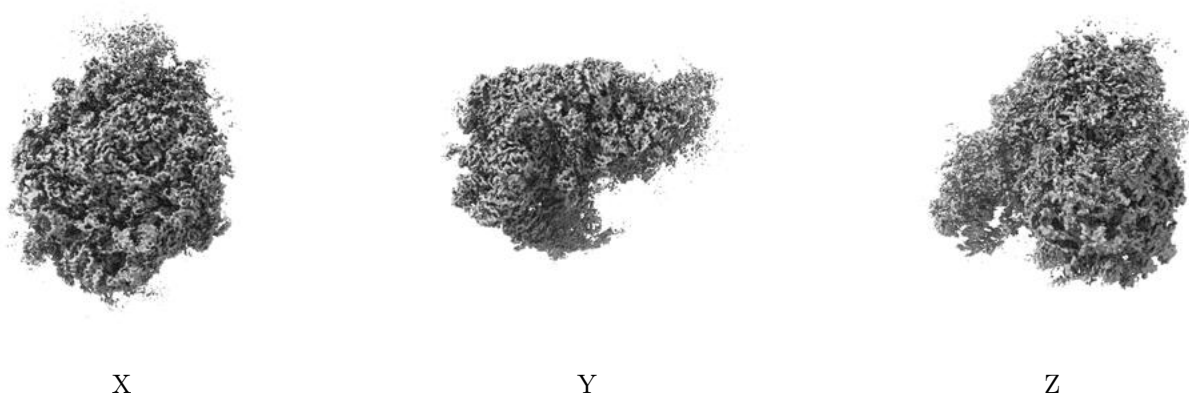


Z

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.

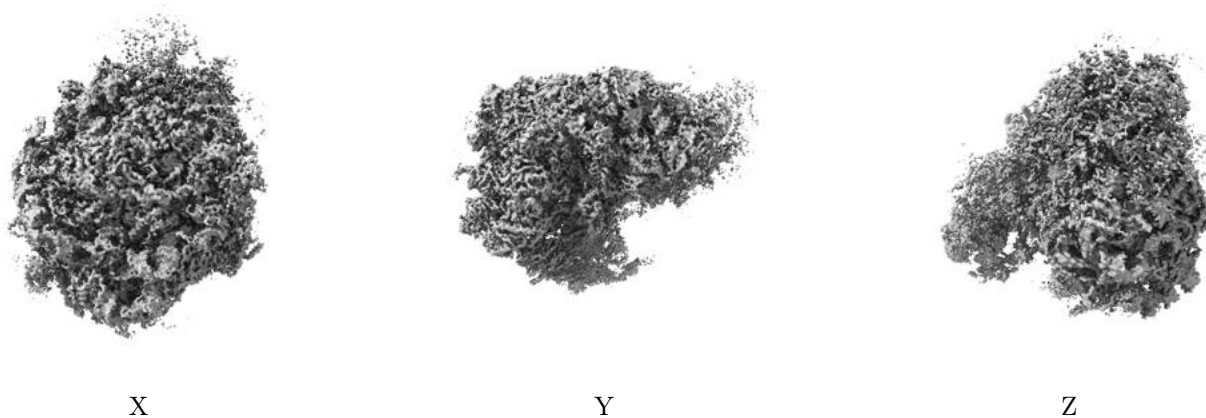
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

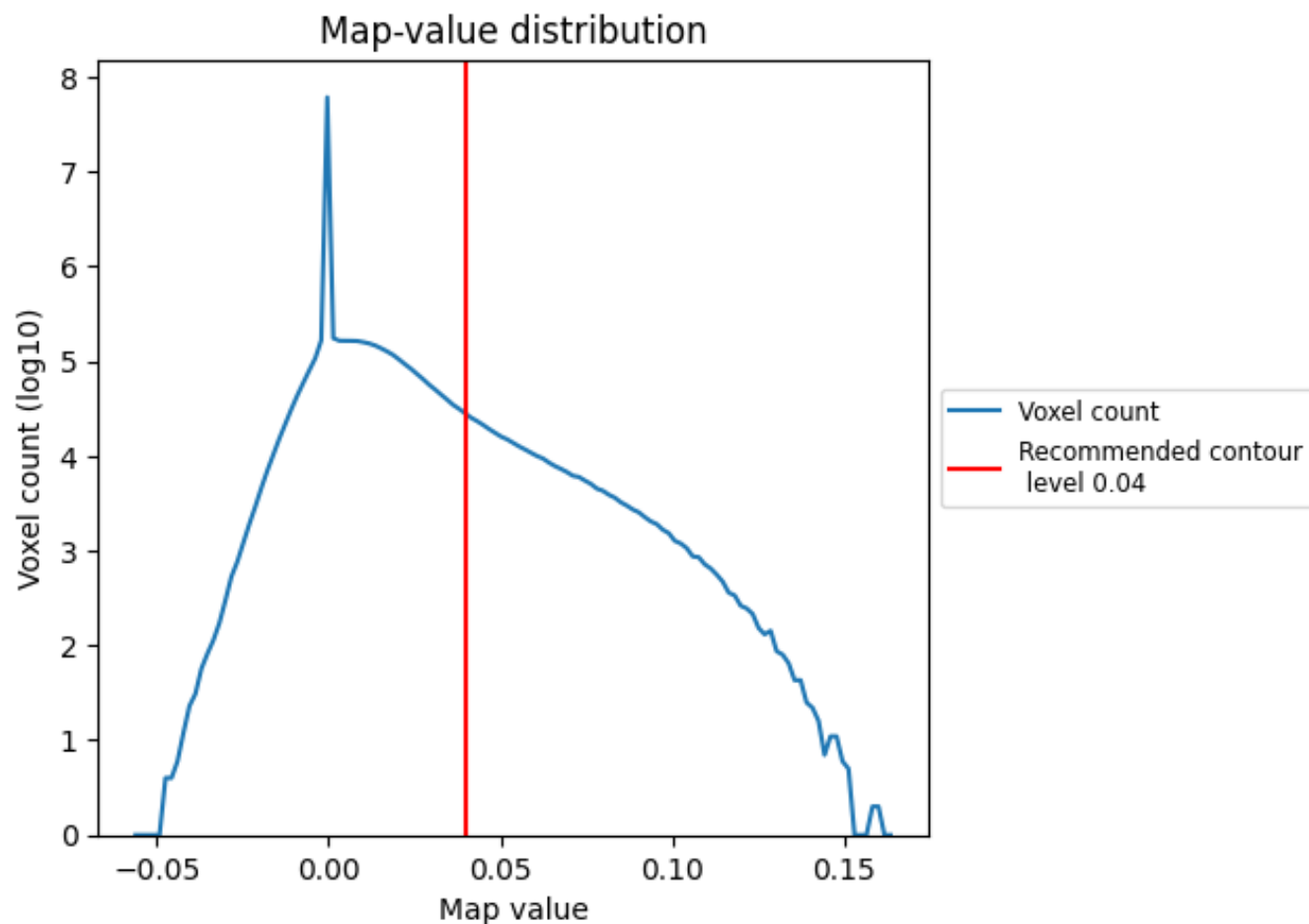
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

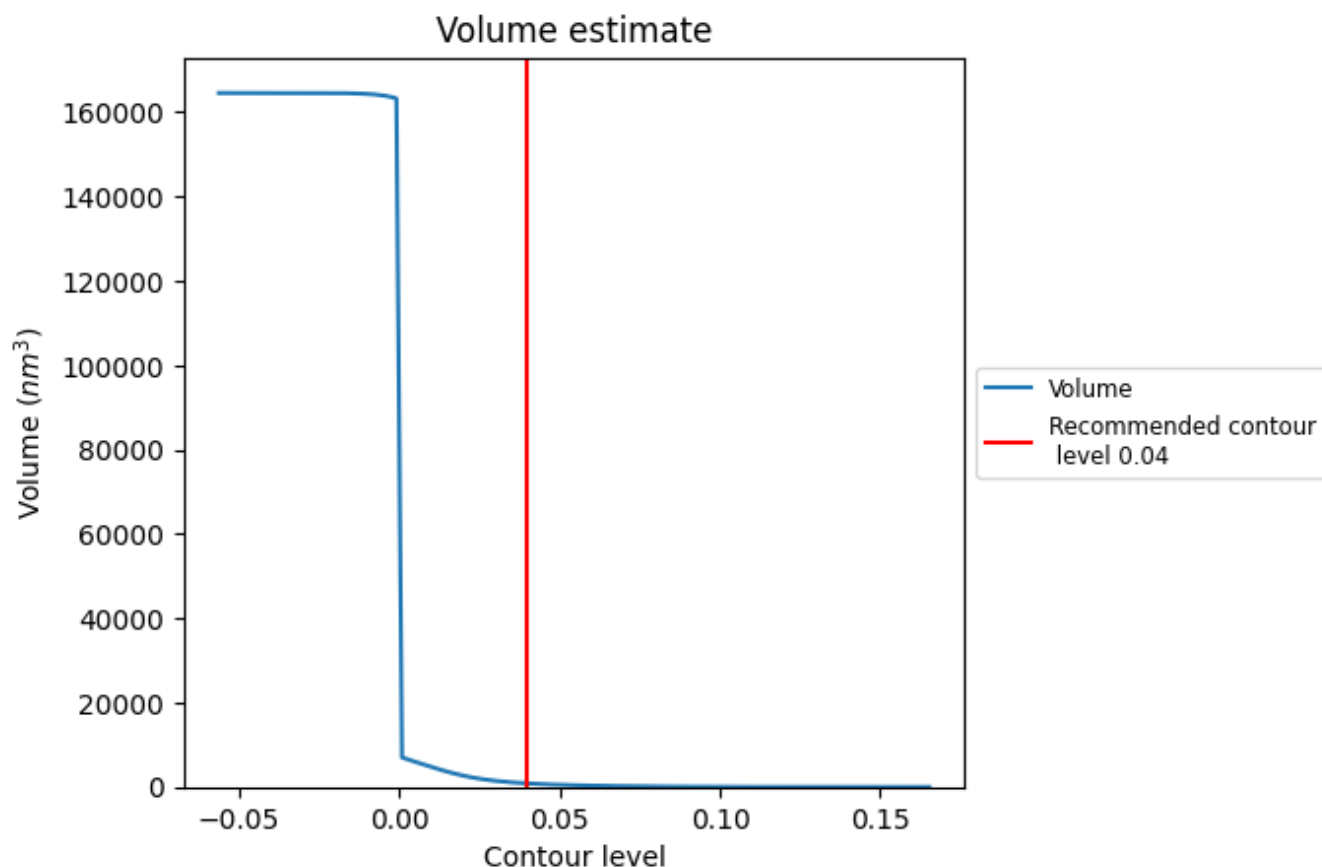
This section contains the results of statistical analysis of the map.

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.

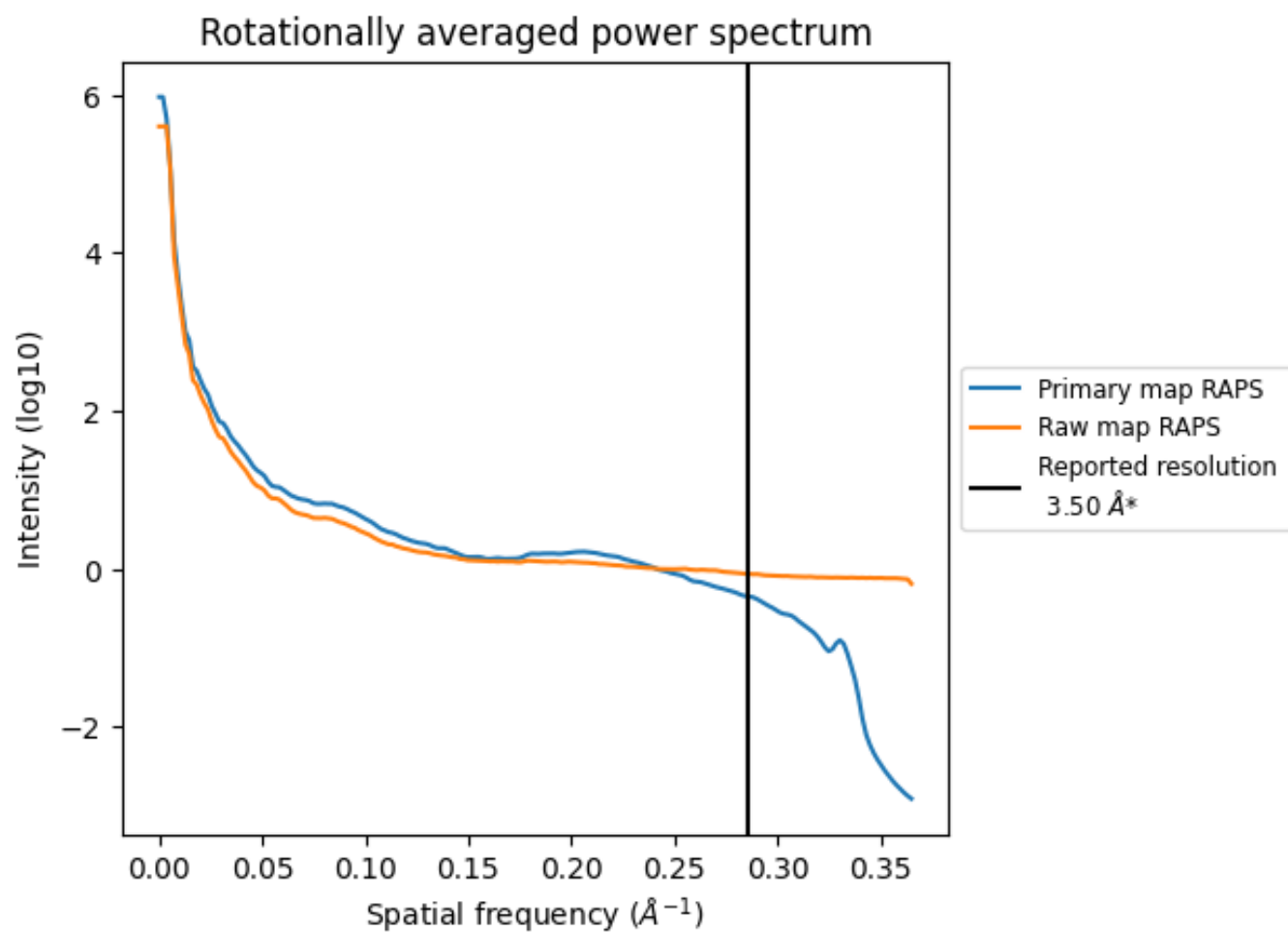
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 849 nm³; this corresponds to an approximate mass of 767 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 ⓘ

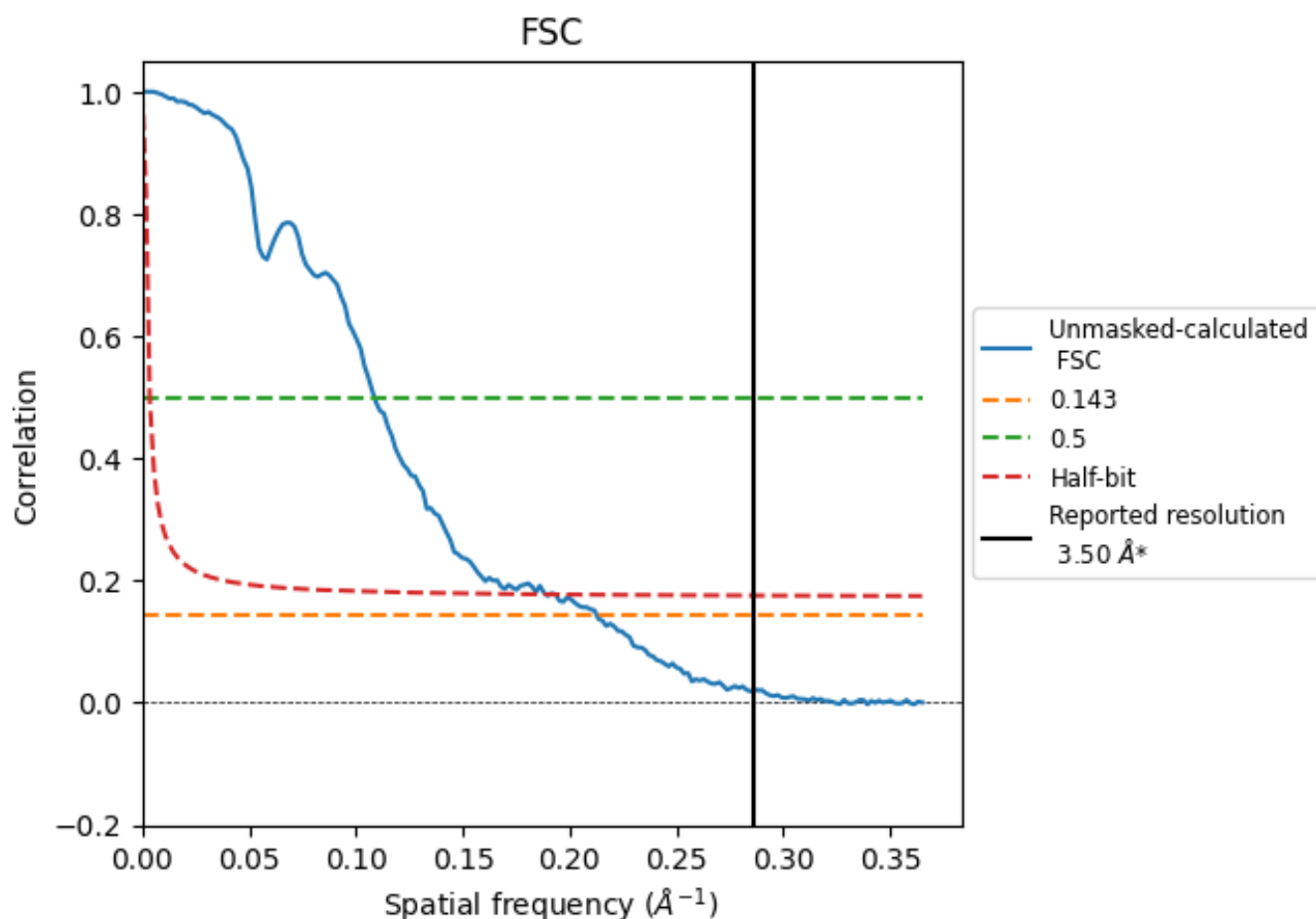


*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

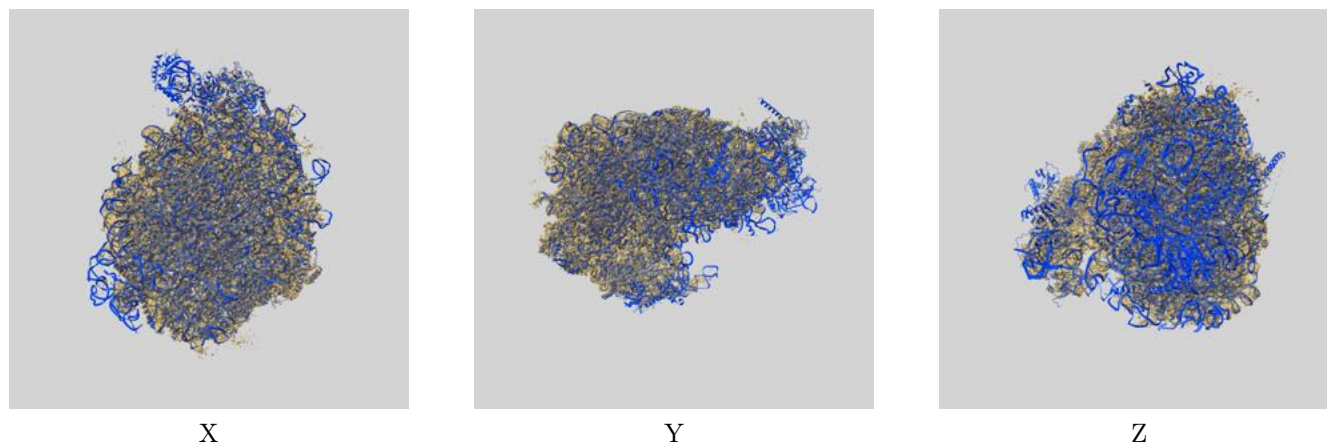
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.70	9.21	5.29

*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 4.70 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

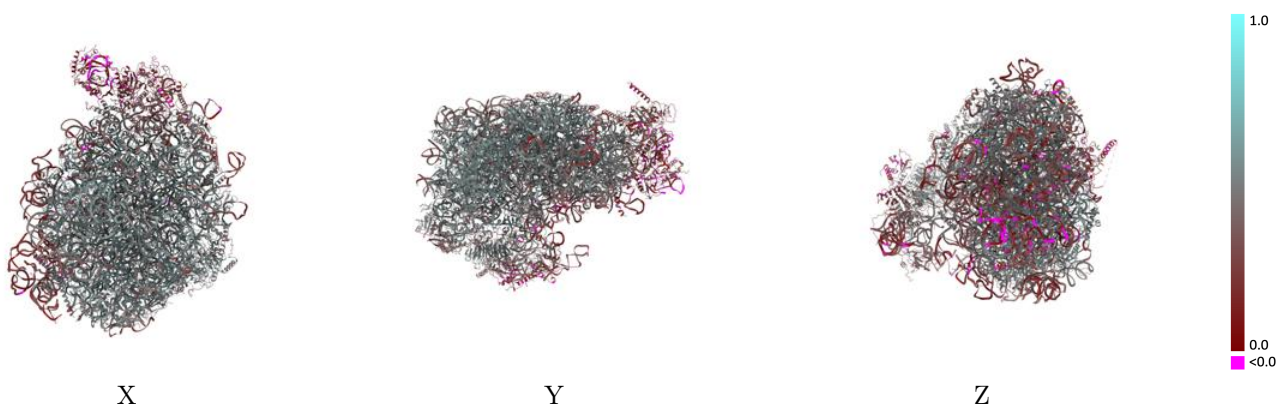
This section contains information regarding the fit between EMDB map EMD-35673 and PDB model 8IR3. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



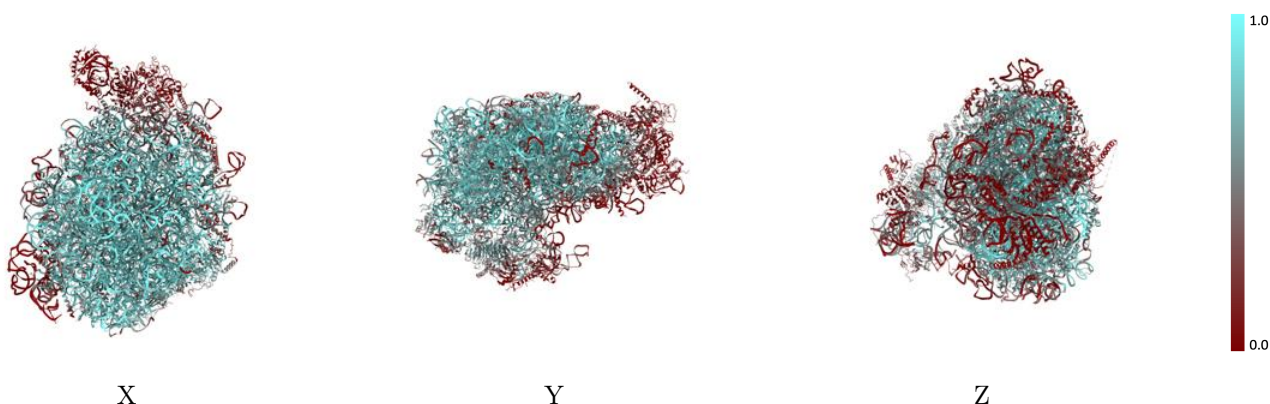
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



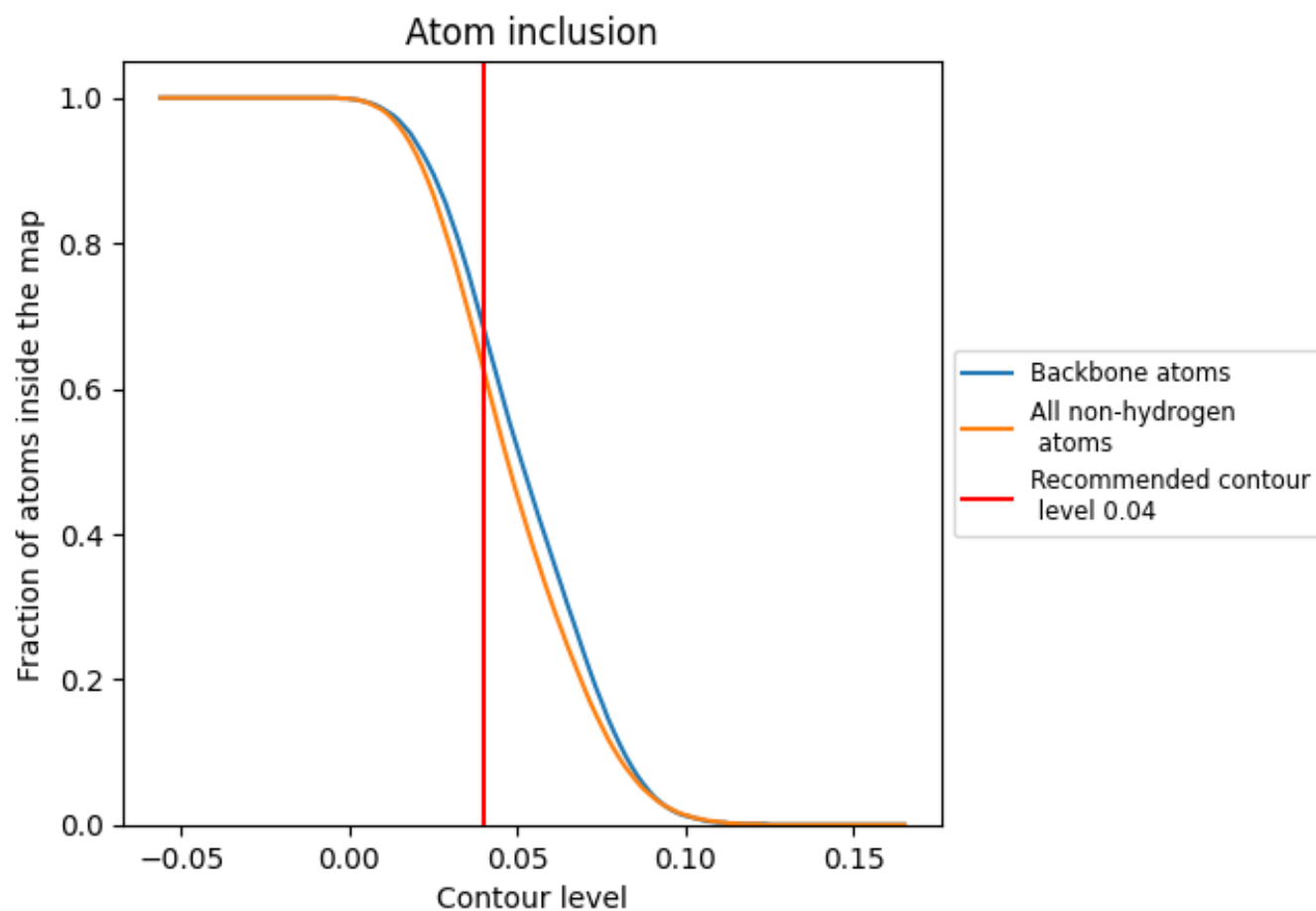
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 62% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6250	 0.4390
2	 0.7200	 0.4400
3	 0.1010	 0.2160
4	 0.5930	 0.4630
5	 0.4090	 0.2530
6	 0.6770	 0.5030
7	 0.6930	 0.5240
8	 0.8810	 0.5140
9	 0.0710	 0.3690
A	 0.1830	 0.3060
B	 0.7890	 0.5400
C	 0.3550	 0.3670
D	 0.7960	 0.5370
E	 0.2930	 0.4090
F	 0.6440	 0.5060
G	 0.4460	 0.4340
H	 0.7220	 0.5130
I	 0.7370	 0.5310
J	 0.7090	 0.5190
K	 0.6100	 0.4640
L	 0.5570	 0.4300
M	 0.8350	 0.5410
N	 0.4720	 0.4280
O	 0.4690	 0.4100
P	 0.8720	 0.5620
Q	 0.6470	 0.4770
R	 0.2940	 0.3390
S	 0.7650	 0.5260
T	 0.2110	 0.3270
U	 0.7560	 0.5130
V	 0.8290	 0.5410
X	 0.4260	 0.4480
Y	 0.7580	 0.5150
Z	 0.6440	 0.4620
a	 0.6110	 0.4990



Continued on next page...

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Chain	Atom inclusion	Q-score
b	 0.7960	 0.5330
c	 0.5210	 0.4360
d	 0.5520	 0.4790
e	 0.7750	 0.5370
f	 0.1460	 0.2800
g	 0.5800	 0.4360
h	 0.7670	 0.5400
i	 0.4100	 0.4440
j	 0.7120	 0.5120
k	 0.8150	 0.5460
l	 0.7910	 0.5380
m	 0.3340	 0.3880
n	 0.8560	 0.5570
o	 0.5640	 0.4720
p	 0.7500	 0.5110
q	 0.2440	 0.3220
r	 0.0670	 0.3300
s	 0.0030	 0.2130
t	 0.0240	 0.2500
u	 0.4720	 0.4030
v	 0.5420	 0.4680
w	 0.6060	 0.4620
x	 0.0000	 0.0260
y	 0.3440	 0.4030
z	 0.5130	 0.4610