



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 03:51 PM JST

PDB ID : 8IPY / pdb_00008ipy
EMDB ID : EMD-35651
Title : human nuclear pre-60S ribosomal particle - State D'
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-03-15
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

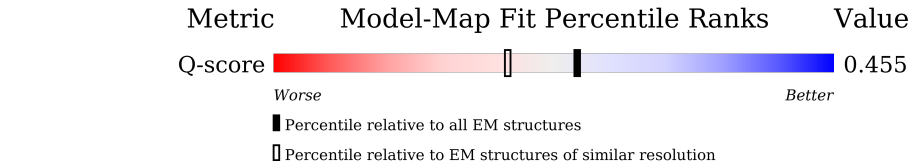
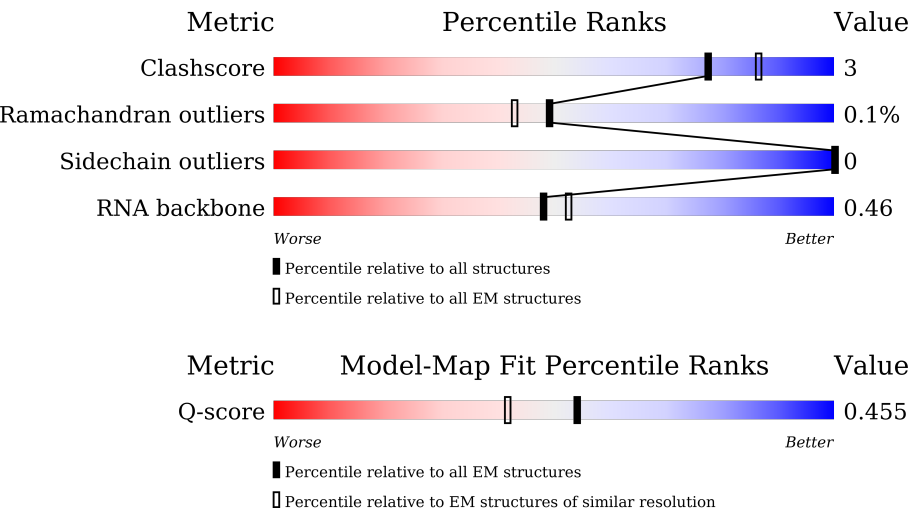
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

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

The reported resolution of this entry is 3.20 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.



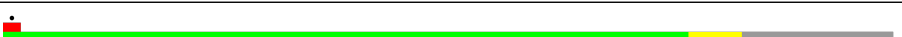
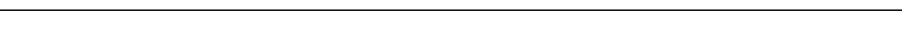
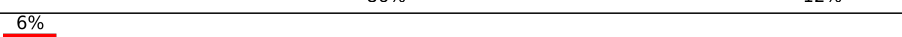
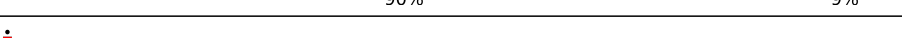
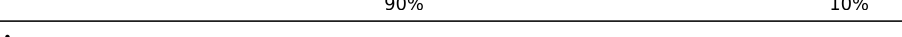
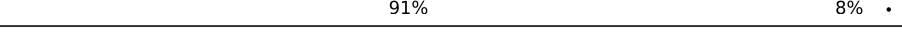
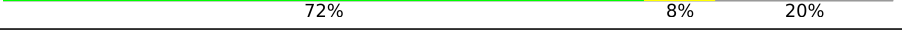
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	N	687	43% 43%5%52%
2	2	5054	6% 47%18%•31%
3	6	245	7% 88%12%

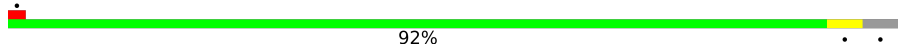
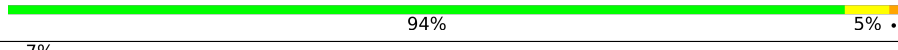
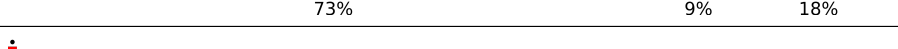
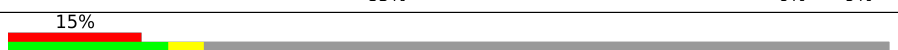
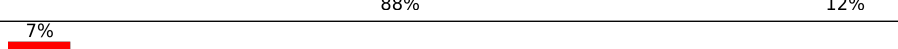
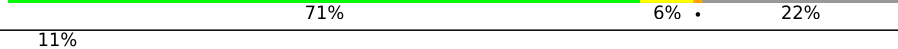
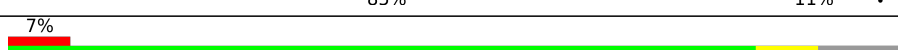
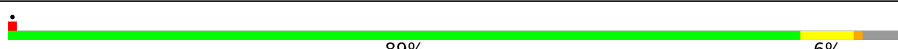
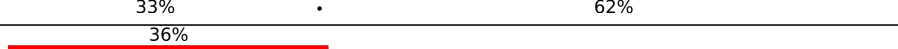
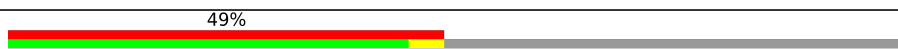
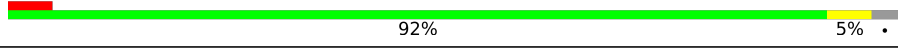
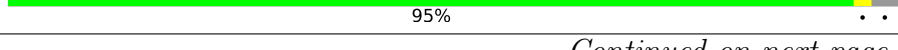
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Mol	Chain	Length	Quality of chain
4	7	163	
5	8	156	
6	9	134	
7	A	159	
8	B	403	
9	D	427	
10	E	115	
11	G	266	
12	H	123	
13	I	192	
14	J	260	
15	L	148	
16	M	97	
17	P	51	
18	Q	211	
19	S	215	
20	U	204	
21	V	203	
22	X	92	
23	Z	188	
24	a	196	
25	b	176	
26	e	140	
27	h	145	
28	l	137	

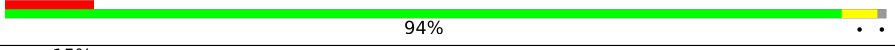
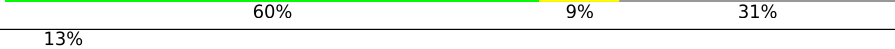
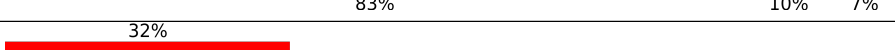
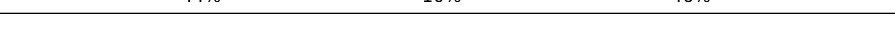
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Mol	Chain	Length	Quality of chain
29	m	257	
30	n	110	
31	o	288	
32	p	248	
33	r	360	
34	u	549	
35	v	239	
36	w	731	
37	y	165	
38	z	129	
39	C	178	
40	R	297	
41	W	485	
42	T	160	
43	4	634	
44	Y	184	
45	k	135	
46	j	125	
47	d	128	
48	t	293	
49	x	160	
50	c	490	
51	1	255	
52	K	105	
53	F	117	

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Mol	Chain	Length	Quality of chain
54	i	136	
55	O	70	
56	3	120	
57	q	588	
58	g	156	
59	f	478	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 163715 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 Protein SDA1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	332	Total	C	N	O	S	0	0
			2719	1762	461	475	21		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3485	Total	C	N	O	P	0	0
			74812	33355	13680	24293	3484		

- 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 RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 6 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	86	Total	C	N	O	S	0	0
			711	433	154	121	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	45	Total	C	N	O	S	0	0
			352	221	76	52	3		

- Molecule 8 is a protein called 60S ribosomal protein L3.

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

- Molecule 9 is a protein called 60S ribosomal protein L4.

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

- Molecule 10 is a protein called 60S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

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

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

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

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

- Molecule 14 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	217	Total	C	N	O	S	0	0
			1772	1134	334	296	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	112	Total	C	N	O	S	0	0
			877	557	172	145	3		

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

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

- Molecule 17 is a protein called 60S ribosomal protein L39.

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

- Molecule 18 is a protein called 60S ribosomal protein L13.

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

- Molecule 19 is a protein called 60S ribosomal protein L14.

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

- Molecule 20 is a protein called 60S ribosomal protein L15.

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

- Molecule 21 is a protein called 60S ribosomal protein L13a.

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

- Molecule 22 is a protein called 60S ribosomal protein L37a.

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

- Molecule 23 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 24 is a protein called 60S ribosomal protein L19.

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

- Molecule 25 is a protein called 60S ribosomal protein L18a.

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

- 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 Coiled-coil domain-containing protein 86.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	r	82	Total	C	N	O	S	0	0
			723	442	158	121	2		

- Molecule 34 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	67	Total	C	N	O	S	0	0
			569	357	119	90	3		

- Molecule 35 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	v	217	Total	C	N	O	S	0	0
			1771	1129	311	320	11		

- Molecule 36 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	w	433	Total	C	N	O	S	0	0
			3472	2201	615	643	13		

- Molecule 37 is a protein called 60S ribosomal protein L12.

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

- Molecule 38 is a protein called Protein LLP homolog.

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

- Molecule 39 is a protein called 60S ribosomal protein L11.

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

- Molecule 40 is a protein called 60S ribosomal protein L5.

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

- Molecule 41 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	W	388	Total	C	N	O	S	0	0
			3018	1889	556	562	11		

- Molecule 42 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	T	124	Total	C	N	O	S	0	0
			1001	632	194	171	4		

- Molecule 43 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	4	611	Total	C	N	O	S	0	0
			5016	3151	918	920	27		

- Molecule 44 is a protein called 60S ribosomal protein L17.

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

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

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

- Molecule 46 is a protein called 60S ribosomal protein 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 L22.

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

- Molecule 48 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

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

- Molecule 49 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	57	Total	C	N	O	P	0	0
			684	285	1	341	57		

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

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

- Molecule 51 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	230	Total	C	N	O	S	0	0
			1897	1226	357	310	4		

- Molecule 52 is a protein called 60S ribosomal protein L36.

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

- Molecule 53 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	F	113	Total	C	N	O	S	0	0
			897	560	185	146	6		

- Molecule 54 is a protein called 60S ribosomal protein L27.

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

- Molecule 55 is a protein called 60S ribosomal protein L38.

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

- Molecule 56 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	3	115	Total	C	N	O	P	0	0
			2453	1093	437	808	115		

- Molecule 57 is a protein called Pescadillo homolog.

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

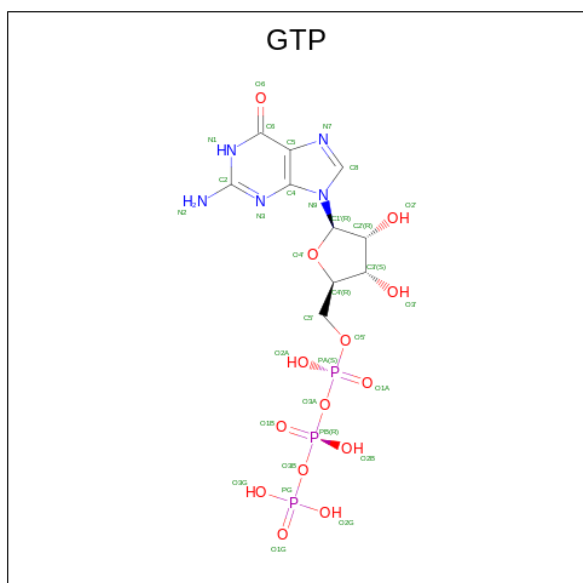
- Molecule 58 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	g	145	Total	C	N	O	S	0	0
			1170	750	222	197	1		

- Molecule 59 is a protein called Ribosome biogenesis protein NOP53.

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

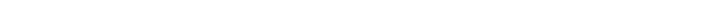
- Molecule 60 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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).

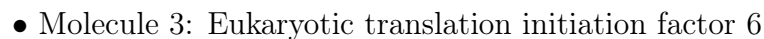
Mol	Chain	Residues	Atoms		AltConf
61	w	1	Total	Mg	0
			1	1	

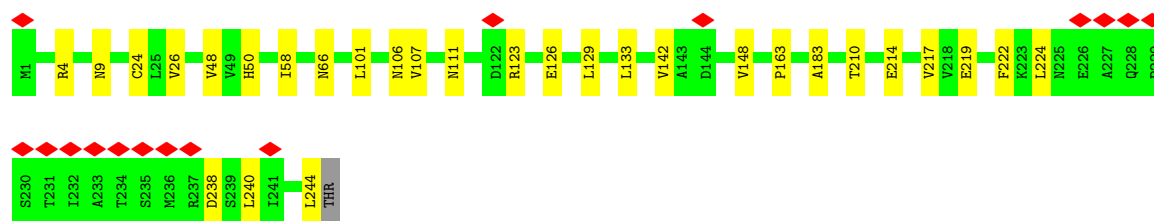
Chain 2: 





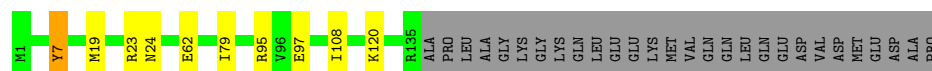


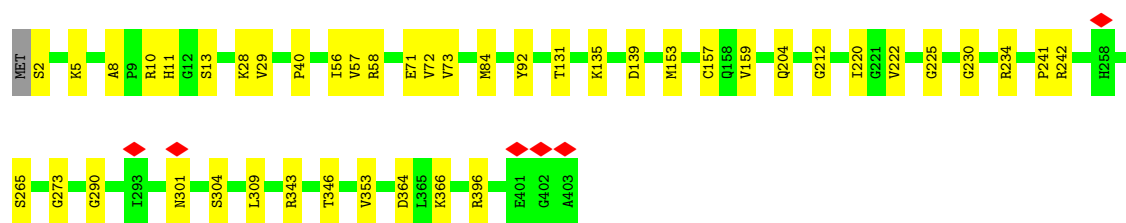




- Molecule 4: Probable ribosome biogenesis protein RLP24

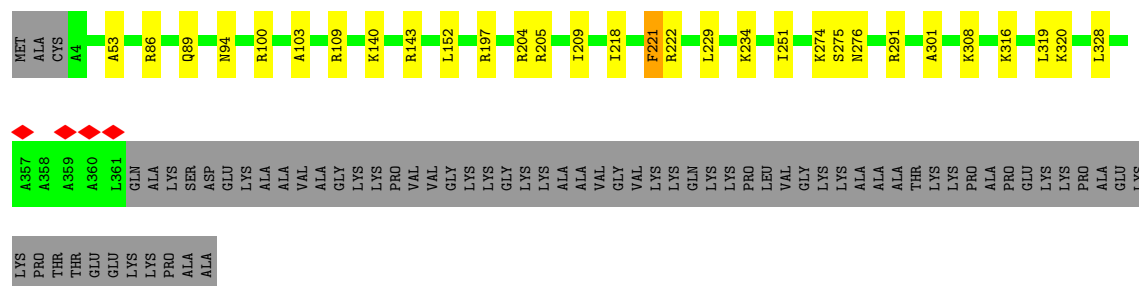
Chain 7: 77% 6% 17%





- Molecule 9: 60S ribosomal protein L4

Chain D: 77% 7% 16%



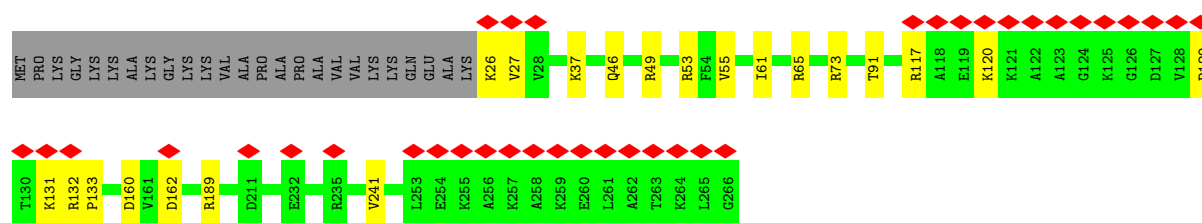
- Molecule 10: 60S ribosomal protein L30

Chain E: 14% 77% 9% 15%



- Molecule 11: 60S ribosomal protein L7a

Chain G: 14% 83% 8% 9%



- Molecule 12: 60S ribosomal protein L35

Chain H: 93% 6%

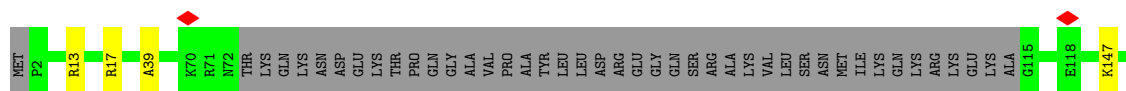
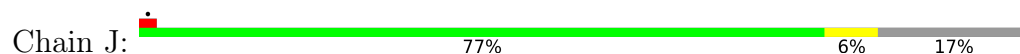


- Molecule 13: 60S ribosomal protein L9

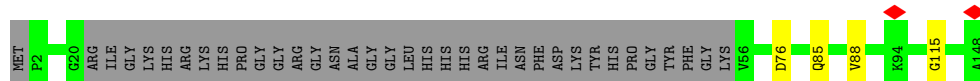
Chain I: 92% 7%



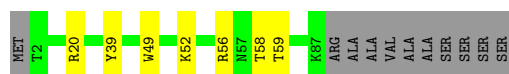
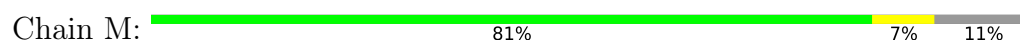
- Molecule 14: Ribosome biogenesis protein NSA2 homolog



- Molecule 15: 60S ribosomal protein L27a



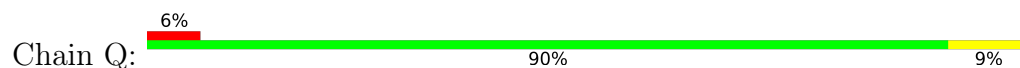
- Molecule 16: 60S ribosomal protein L37



- Molecule 17: 60S ribosomal protein L39

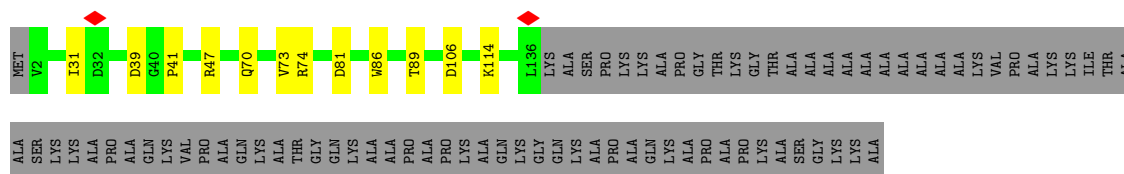


- Molecule 18: 60S ribosomal protein L13

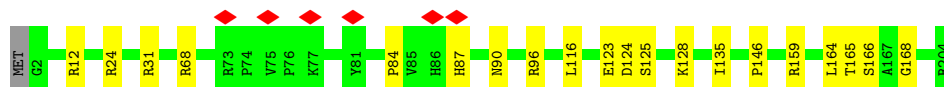
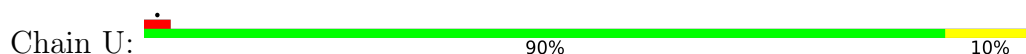


- Molecule 19: 60S ribosomal protein L14





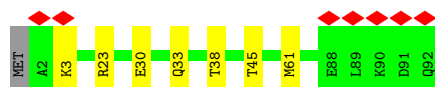
- Molecule 20: 60S ribosomal protein L15



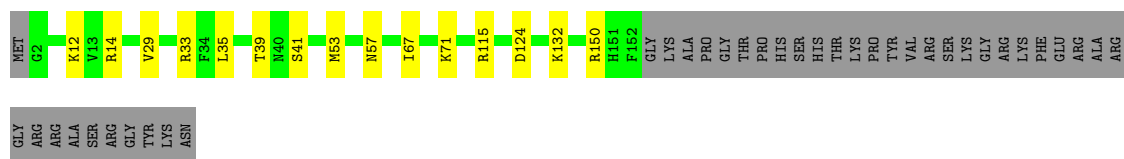
- Molecule 21: 60S ribosomal protein L13a



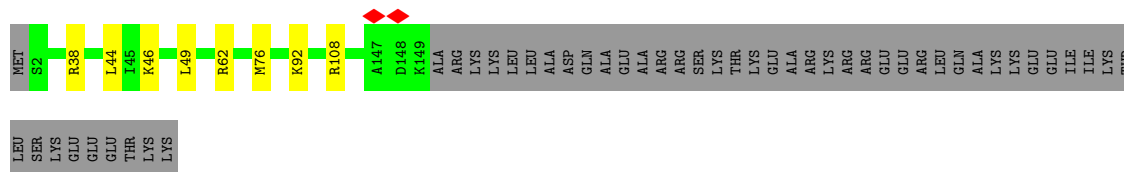
- Molecule 22: 60S ribosomal protein L37a



- Molecule 23: 60S ribosomal protein L18



- Molecule 24: 60S ribosomal protein L19



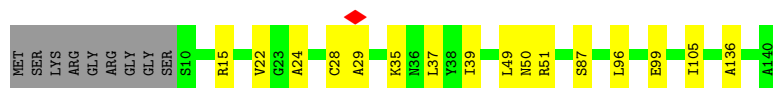
- Molecule 25: 60S ribosomal protein L18a

Chain b:  88% 13%



- Molecule 26: 60S ribosomal protein L23

Chain e:  82% 11% 6%



- Molecule 27: 60S ribosomal protein L26

Chain h:  84% 8% 8%



- Molecule 28: 60S ribosomal protein L28

Chain i:  82% 9% 9%



- Molecule 29: 60S ribosomal protein L8

Chain m:  92%



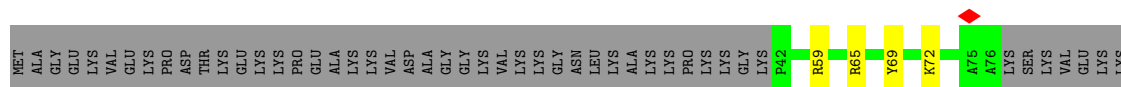
- Molecule 30: 60S ribosomal protein L35a

Chain n:  94% 5% ..

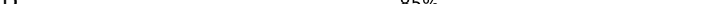


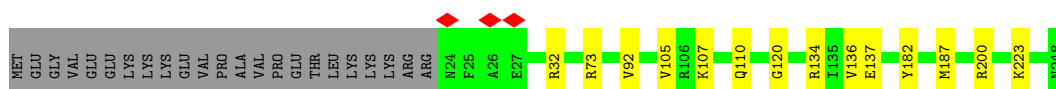
- Molecule 31: 60S ribosomal protein L6

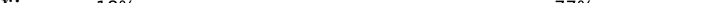
Chain o:  7% 73% 9% 18%

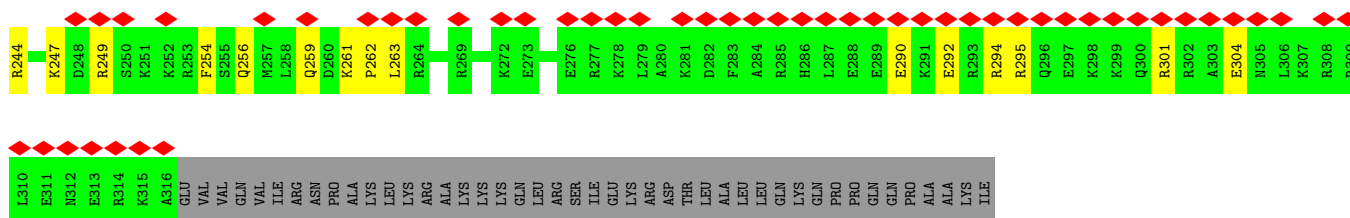
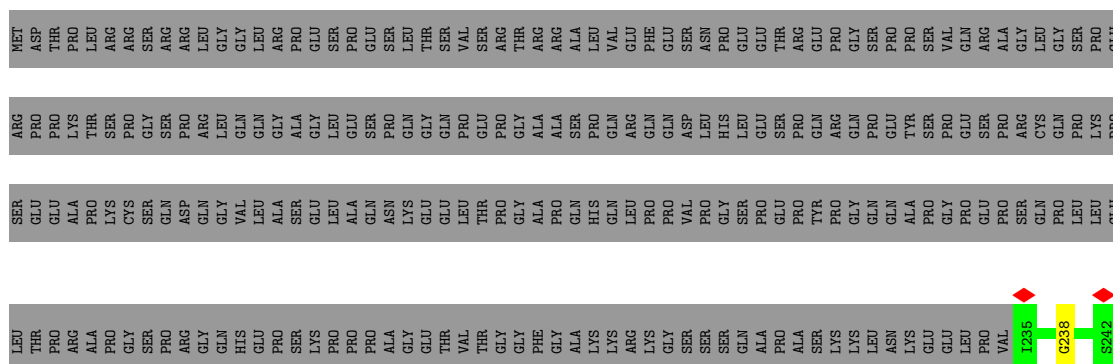


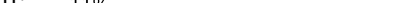


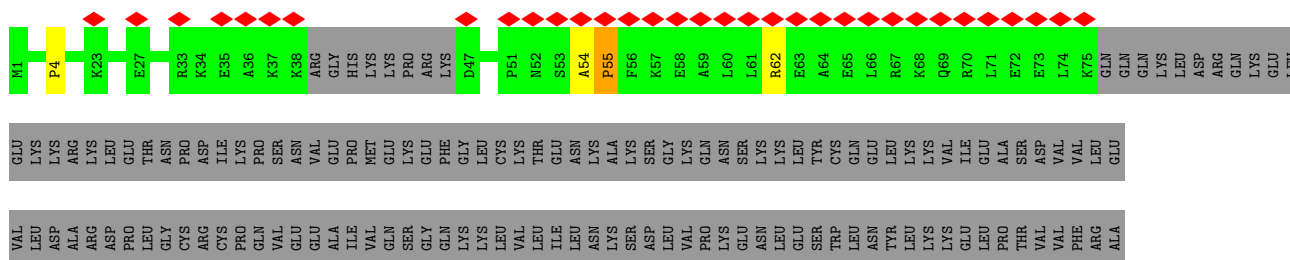
- Chain p:  85% 6% 9%



- Chain r: 

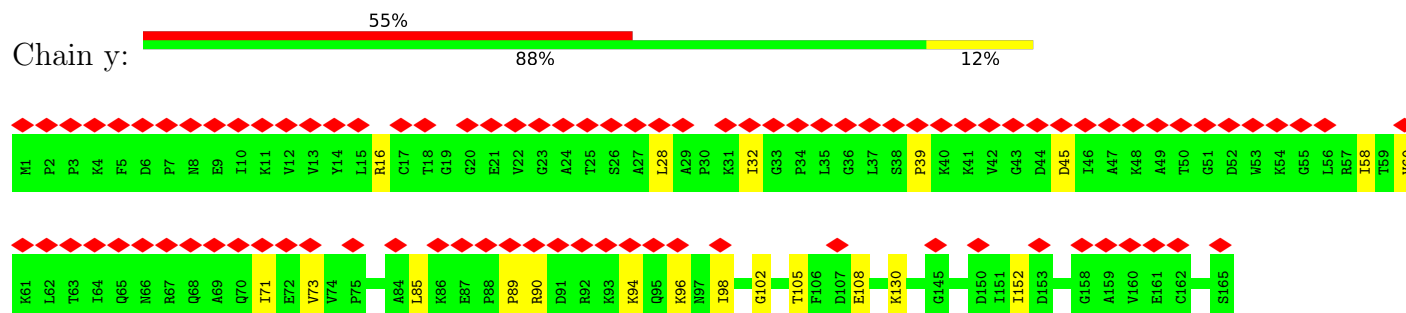


- Chain u:  6% 11% 88%

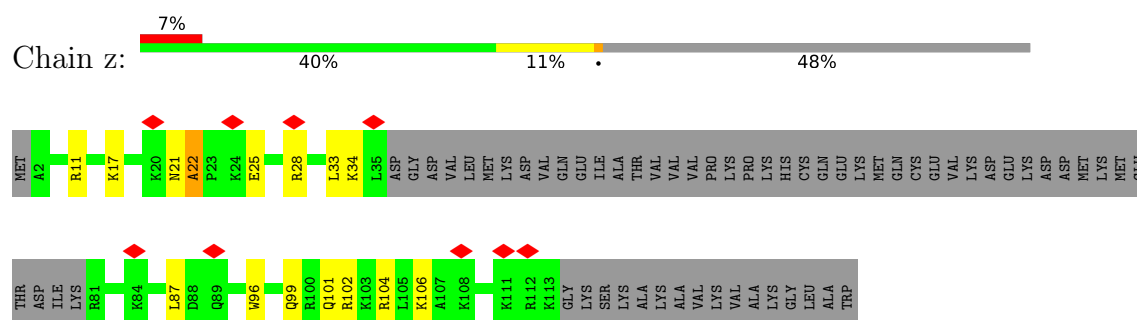




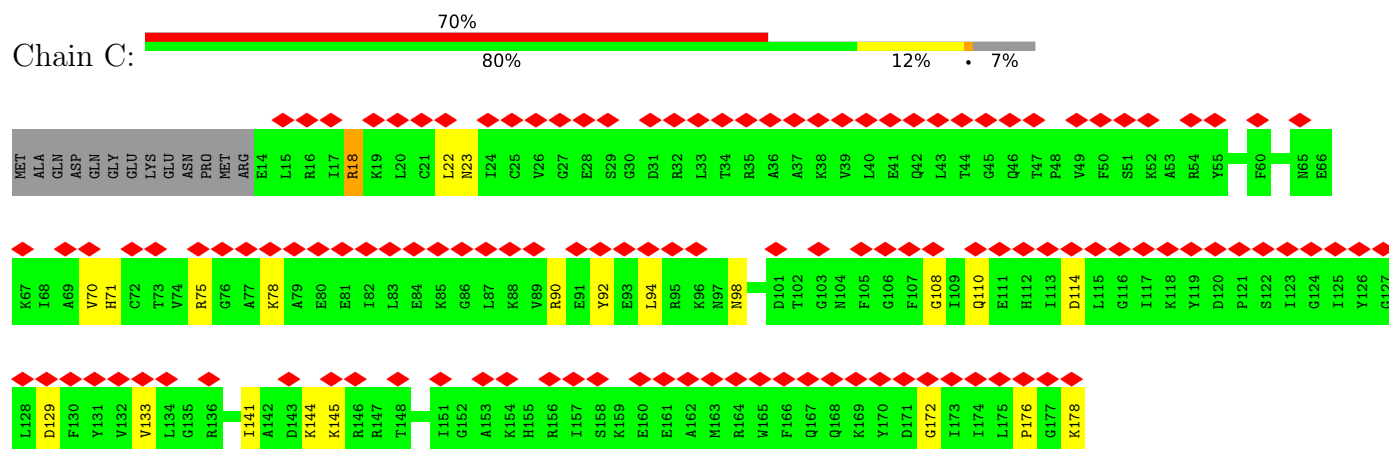
- Molecule 37: 60S ribosomal protein L12



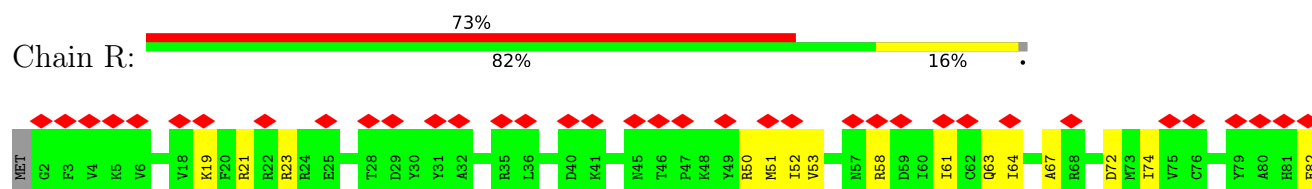
- Molecule 38: Protein LLP homolog

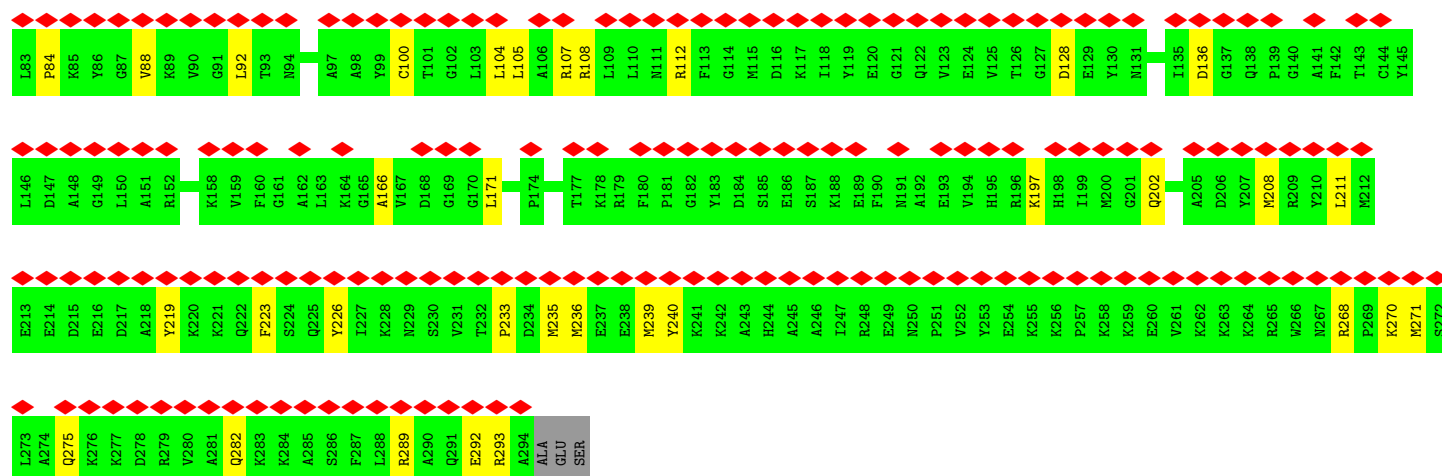


- Molecule 39: 60S ribosomal protein L11

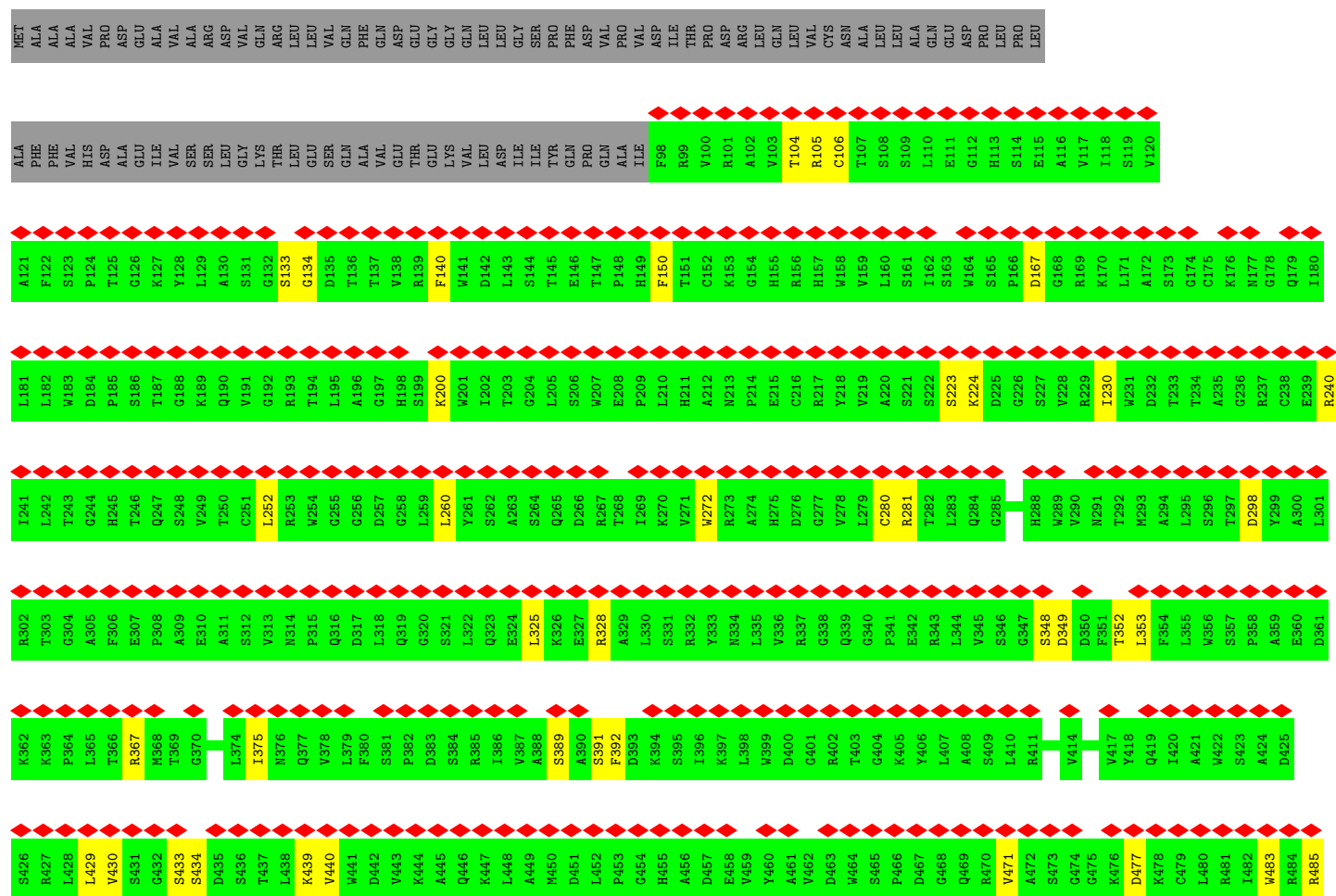
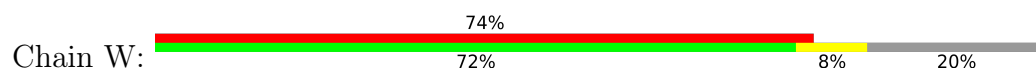


- Molecule 40: 60S ribosomal protein L5



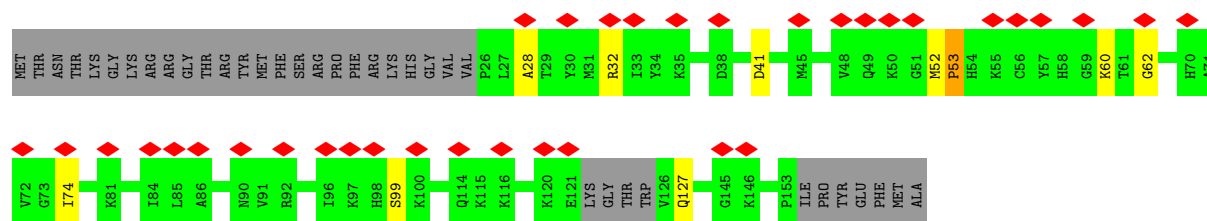


• Molecule 41: Notchless protein homolog 1

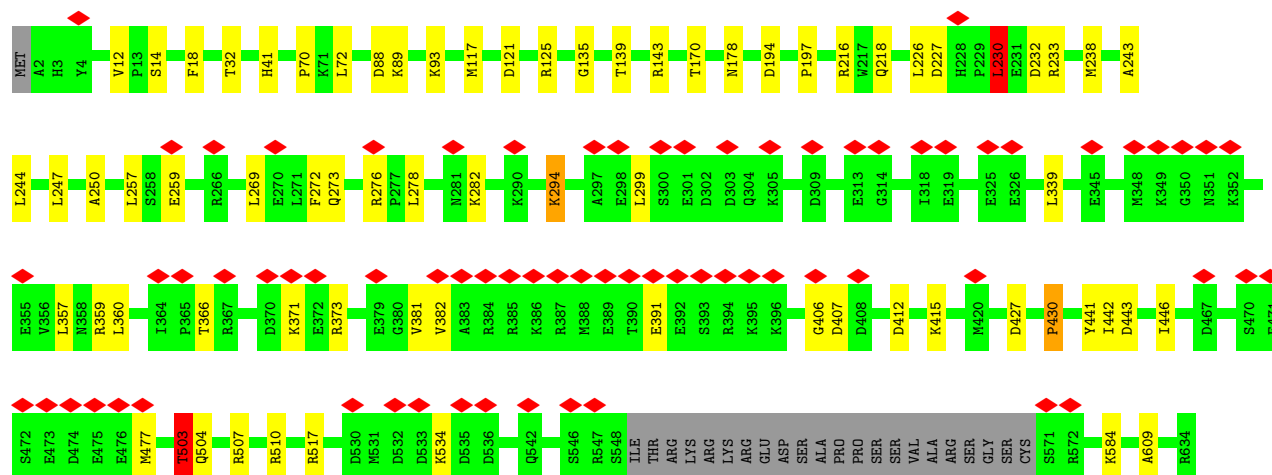
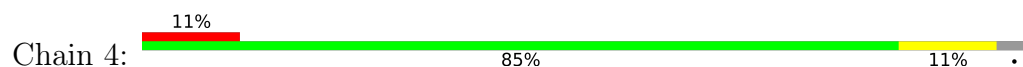


• Molecule 42: 60S ribosomal protein L21

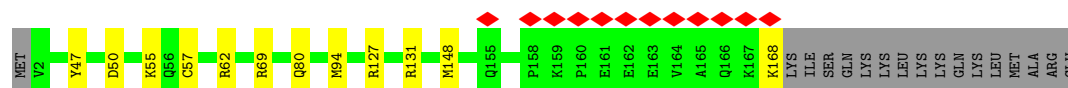
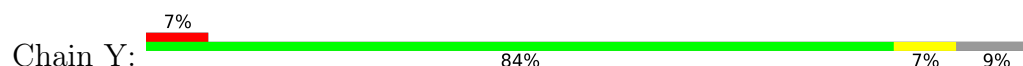




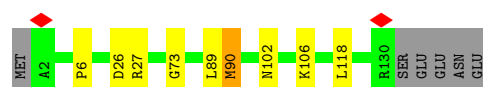
• Molecule 43: GTP-binding protein 4



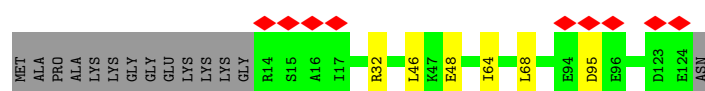
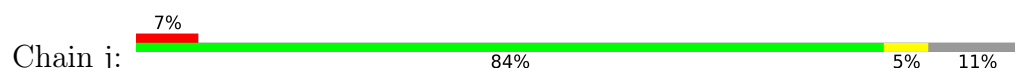
• Molecule 44: 60S ribosomal protein L17



• Molecule 45: 60S ribosomal protein L32

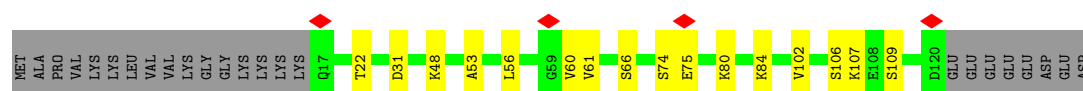


• Molecule 46: 60S ribosomal protein L31



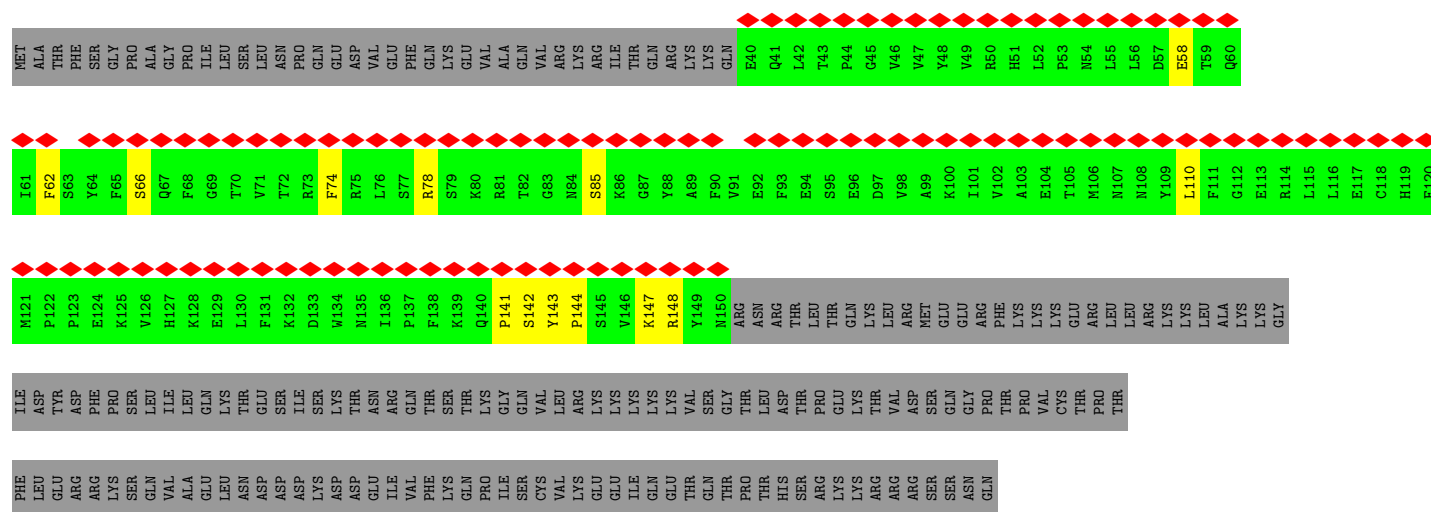
• Molecule 47: 60S ribosomal protein L22

Chain d: 



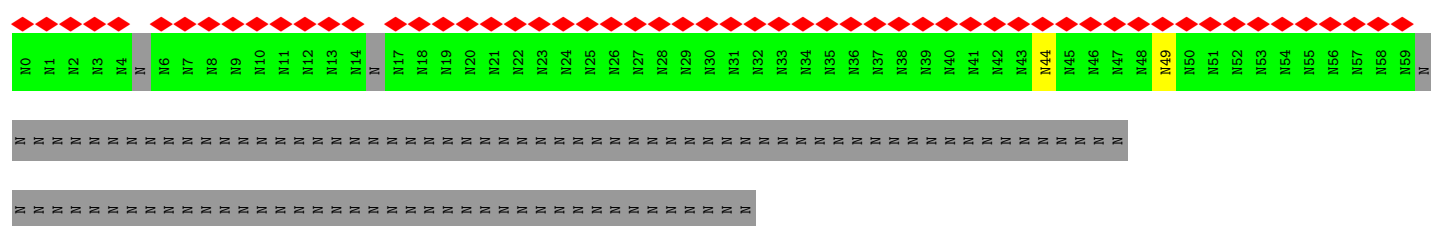
• Molecule 48: MKI67 FHA domain-interacting nucleolar phosphoprotein

Chain t: 



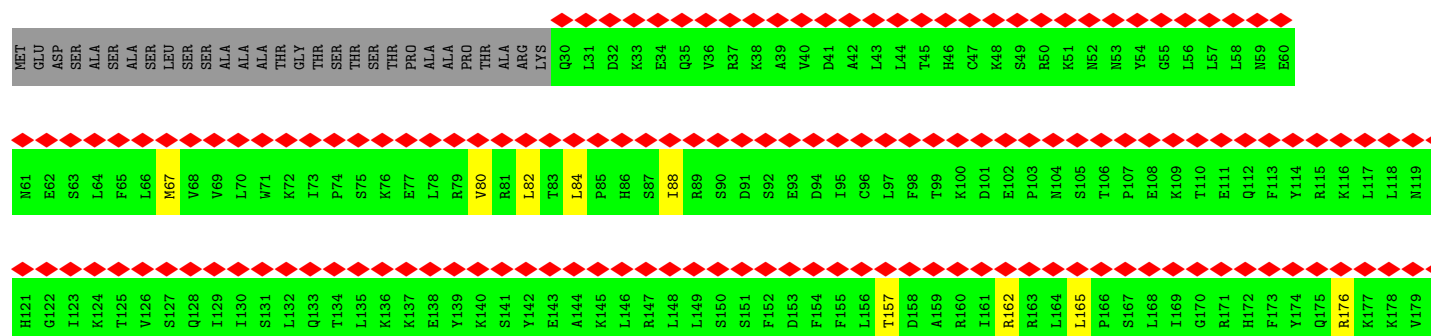
• Molecule 49: ITS2

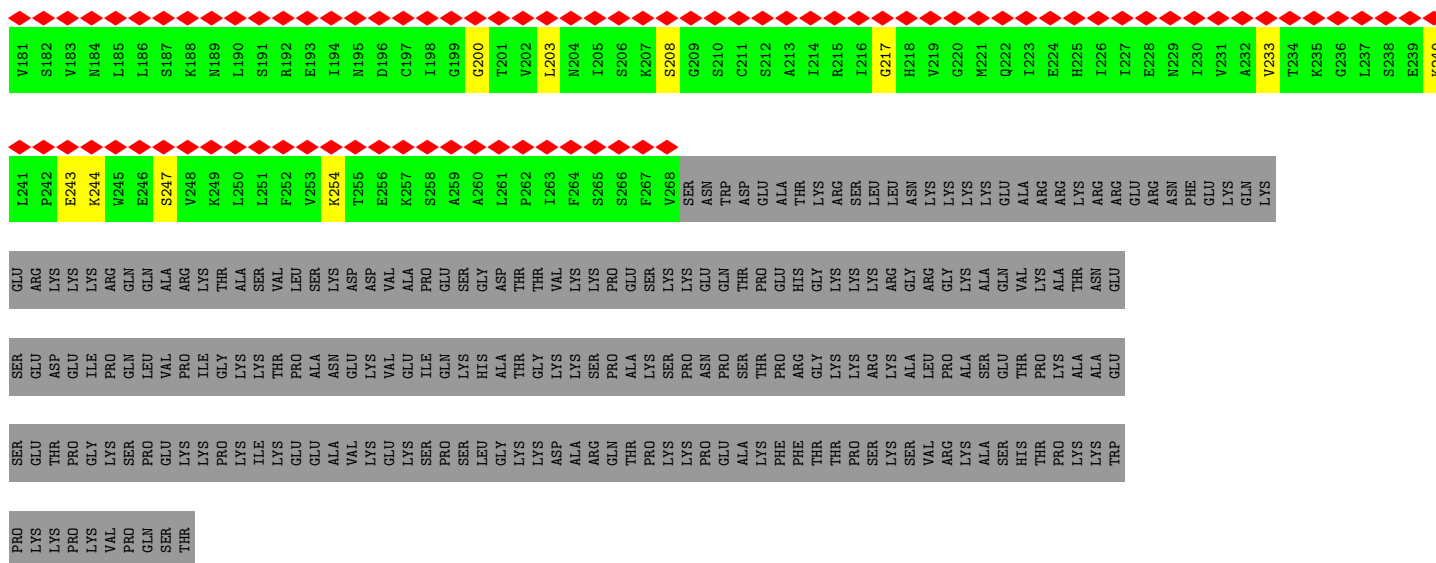
Chain x: 



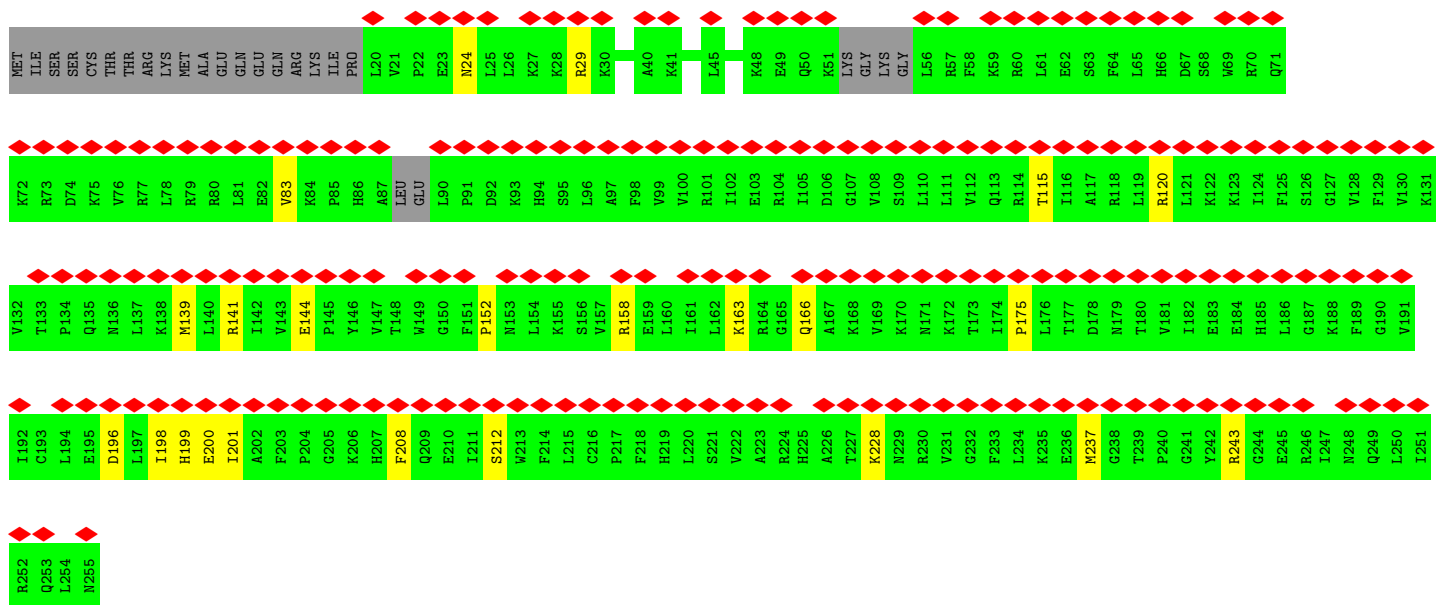
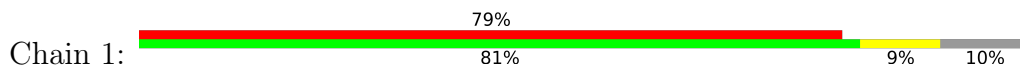
• Molecule 50: Ribosomal L1 domain-containing protein 1

Chain c: 





• Molecule 51: 60S ribosomal protein L7-like 1

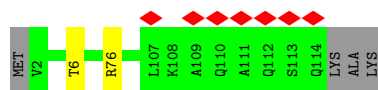


• Molecule 52: 60S ribosomal protein L36

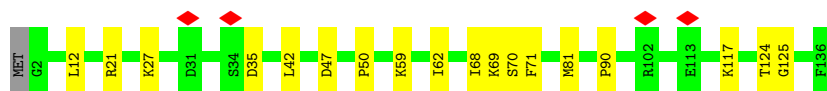
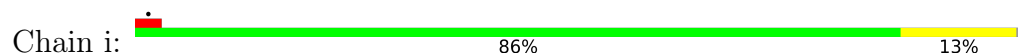


• Molecule 53: 60S ribosomal protein L34





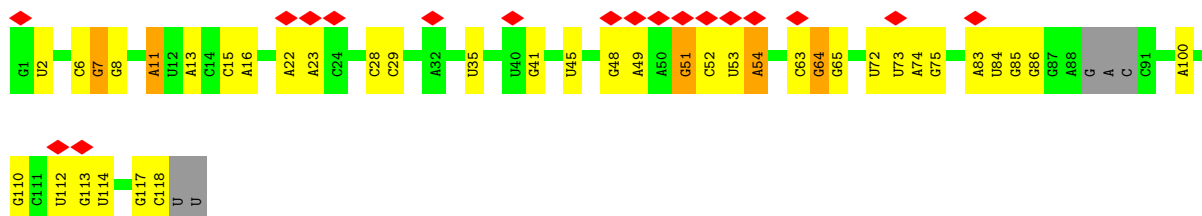
- Molecule 54: 60S ribosomal protein L27



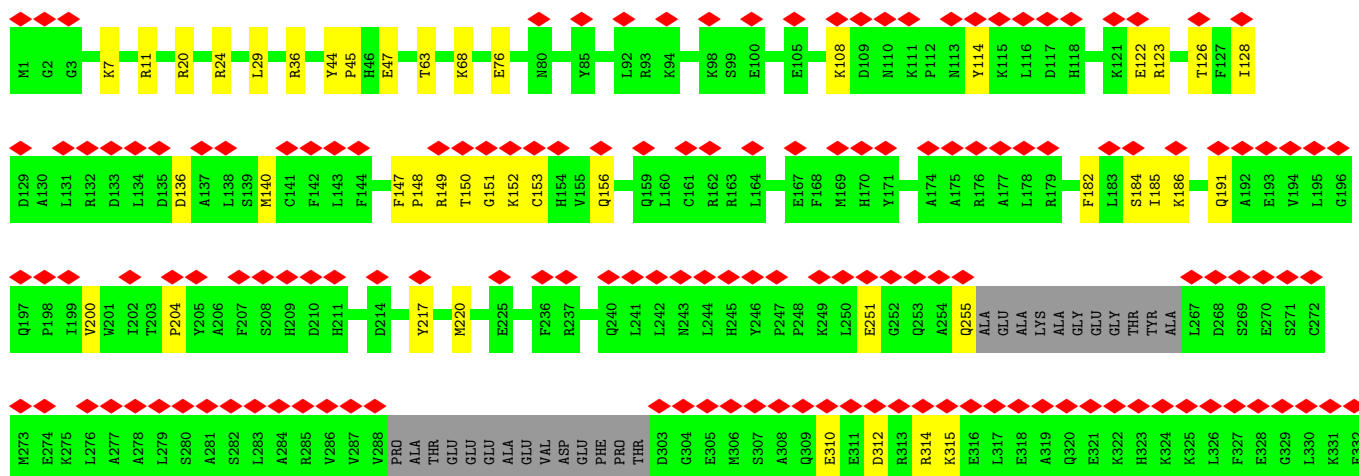
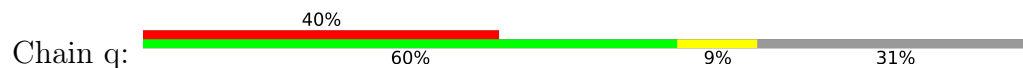
- Molecule 55: 60S ribosomal protein L38

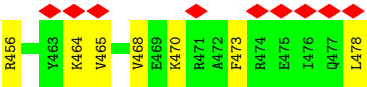


- Molecule 56: 5S rRNA



- Molecule 57: Pescadillo homolog





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26584	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	0.211	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.032	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: OMU, OMC, BGH, 2MG, I4U, M7A, P4U, B8Q, P7G, B9B, B8K, E7G, UR3, 7MG, A2M, 5MU, B8W, B8T, B9H, MG, GTP, OMG

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	N	0.34	0/2772	0.73	1/3738 (0.0%)
2	2	0.23	0/81923	0.44	21/127714 (0.0%)
3	6	0.26	0/1877	0.65	1/2554 (0.0%)
4	7	0.32	0/1181	0.64	2/1563 (0.1%)
5	8	0.23	0/3679	0.41	0/5732
6	9	0.29	0/723	0.75	3/961 (0.3%)
7	A	0.24	0/354	0.63	0/465
8	B	0.26	0/3315	0.63	4/4435 (0.1%)
9	D	0.25	0/2907	0.61	4/3905 (0.1%)
10	E	0.28	0/774	0.69	0/1038
11	G	0.31	0/1960	0.74	4/2637 (0.2%)
12	H	0.27	0/1023	0.57	0/1351
13	I	0.28	0/1537	0.66	1/2066 (0.0%)
14	J	0.20	0/1808	0.48	0/2414
15	L	0.21	0/893	0.52	0/1193
16	M	0.27	0/720	0.61	0/952
17	P	0.27	0/454	0.50	0/599
18	Q	0.28	0/1732	0.58	0/2315
19	S	0.31	0/1133	0.69	2/1516 (0.1%)
20	U	0.23	0/1746	0.55	2/2338 (0.1%)
21	V	0.29	0/1682	0.62	2/2250 (0.1%)
22	X	0.28	0/718	0.69	0/953
23	Z	0.24	0/1239	0.52	0/1658
24	a	0.28	0/1255	0.69	4/1662 (0.2%)
25	b	0.21	0/1501	0.46	0/2013
26	e	0.23	0/993	0.60	0/1332
27	h	0.25	0/1132	0.59	0/1504
28	l	0.26	0/1017	0.57	0/1364
29	m	0.26	0/1936	0.64	0/2596
30	n	0.25	0/895	0.66	3/1198 (0.3%)
31	o	0.27	0/1935	0.67	2/2596 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	p	0.31	0/1916	0.60	0/2553
33	r	0.37	0/732	0.82	1/960 (0.1%)
34	u	0.30	0/576	0.71	2/755 (0.3%)
35	v	0.26	0/1806	0.62	0/2420
36	w	0.26	0/3541	0.59	0/4775
37	y	0.30	0/1269	0.71	0/1712
38	z	0.35	1/587 (0.2%)	0.68	0/767
39	C	0.30	0/1341	0.73	2/1793 (0.1%)
40	R	0.30	0/2428	0.74	3/3252 (0.1%)
41	W	0.25	0/3093	0.63	0/4196
42	T	0.27	0/1018	0.67	1/1357 (0.1%)
43	4	0.33	0/5099	0.80	15/6840 (0.2%)
44	Y	0.25	0/1383	0.57	0/1856
45	k	0.23	0/1082	0.62	1/1443 (0.1%)
46	j	0.25	0/933	0.56	0/1256
47	d	0.27	0/864	0.75	2/1160 (0.2%)
48	t	0.29	0/955	0.68	0/1290
50	c	0.25	0/1956	0.58	1/2631 (0.0%)
51	l	0.28	1/1933 (0.1%)	0.65	2/2591 (0.1%)
52	K	0.29	0/843	0.67	0/1115
53	F	0.25	0/907	0.55	0/1209
54	i	0.27	0/1130	0.61	0/1507
55	O	0.32	0/575	0.79	0/761
56	3	0.24	0/2739	0.49	1/4266 (0.0%)
57	q	0.31	0/3395	0.69	0/4578
58	g	0.29	0/1191	0.61	0/1595
59	f	0.26	0/2169	0.65	2/2902 (0.1%)
All	All	0.25	2/172275 (0.0%)	0.54	89/250152 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	A	0	1
8	B	0	1
11	G	0	2
30	n	0	1
33	r	0	1
34	u	0	1
42	T	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
43	4	0	2
44	Y	0	1
48	t	0	1
51	1	0	1
59	f	0	1
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	z	22	ALA	C-N	5.64	1.40	1.34
51	1	152	PRO	CG-CD	-5.28	1.32	1.50

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1871	A2M	OP2-P-O3'	-15.92	70.18	105.20
2	2	1871	A2M	OP1-P-O3'	14.70	137.55	105.20
2	2	1872	G	OP1-P-OP2	-13.63	78.71	119.60
2	2	1872	G	O5'-P-OP1	-9.23	80.30	108.00
51	1	152	PRO	N-CD-CG	-8.68	90.18	103.20
43	4	406	GLY	CA-C-N	7.77	136.38	121.54
43	4	406	GLY	C-N-CA	7.77	136.38	121.54
43	4	503	THR	CA-C-N	7.75	135.66	121.70
43	4	503	THR	C-N-CA	7.75	135.66	121.70
24	a	38	ARG	CA-C-N	7.27	135.42	121.54
24	a	38	ARG	C-N-CA	7.27	135.42	121.54
2	2	1872	G	O5'-P-OP2	6.89	128.67	108.00
43	4	41	HIS	CA-C-N	6.78	134.49	121.54
43	4	41	HIS	C-N-CA	6.78	134.49	121.54
59	f	202	LEU	CA-C-N	6.70	134.33	121.54
59	f	202	LEU	C-N-CA	6.70	134.33	121.54
24	a	76	MET	CA-C-N	6.68	134.50	121.41
24	a	76	MET	C-N-CA	6.68	134.50	121.41
43	4	70	PRO	N-CA-C	6.60	121.54	114.68
51	1	83	VAL	N-CA-C	-6.53	106.43	112.43
20	U	146	PRO	CA-C-N	6.42	133.81	121.54
20	U	146	PRO	C-N-CA	6.42	133.81	121.54
40	R	82	GLU	CA-C-N	6.39	127.67	120.06
40	R	82	GLU	C-N-CA	6.39	127.67	120.06
1	N	345	PRO	CA-N-CD	-6.34	103.12	112.00
2	2	1678	C	P-O3'-C3'	6.31	129.67	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	31	ILE	CA-C-N	6.17	133.34	121.54
19	S	31	ILE	C-N-CA	6.17	133.34	121.54
2	2	2760	G	P-O3'-C3'	6.14	129.41	120.20
30	n	105	LEU	CA-C-N	6.11	136.72	121.80
30	n	105	LEU	C-N-CA	6.11	136.72	121.80
13	I	188	GLN	CA-CB-CG	6.11	126.31	114.10
43	4	230	LEU	CA-CB-CG	6.00	137.28	116.30
11	G	129	PRO	CA-C-N	5.92	130.80	122.46
11	G	129	PRO	C-N-CA	5.92	130.80	122.46
2	2	4228	G	P-O3'-C3'	5.88	129.02	120.20
43	4	391	GLU	CA-C-N	5.87	132.75	121.54
43	4	391	GLU	C-N-CA	5.87	132.75	121.54
2	2	914	U	P-O3'-C3'	5.86	128.99	120.20
43	4	430	PRO	CA-C-N	5.86	132.72	121.54
43	4	430	PRO	C-N-CA	5.86	132.72	121.54
2	2	3774	A	P-O3'-C3'	5.83	128.94	120.20
2	2	2486	G	P-O3'-C3'	5.72	128.78	120.20
4	7	7	TYR	CA-C-N	5.71	132.44	121.54
4	7	7	TYR	C-N-CA	5.71	132.44	121.54
2	2	406	C	C2'-C3'-O3'	5.70	122.24	113.70
8	B	304	SER	CA-C-N	5.68	132.38	121.54
8	B	304	SER	C-N-CA	5.68	132.38	121.54
6	9	98	SER	CA-C-N	5.60	132.24	121.54
6	9	98	SER	C-N-CA	5.60	132.24	121.54
42	T	127	GLN	CA-CB-CG	5.59	125.27	114.10
2	2	3905	A	P-O3'-C3'	5.57	128.55	120.20
3	6	58	ILE	N-CA-C	5.56	112.16	106.21
39	C	18	ARG	CA-C-N	5.56	128.73	120.90
39	C	18	ARG	C-N-CA	5.56	128.73	120.90
47	d	66	SER	CA-C-N	5.55	132.15	121.54
47	d	66	SER	C-N-CA	5.55	132.15	121.54
2	2	1980	U	P-O3'-C3'	5.55	128.52	120.20
43	4	257	LEU	CA-CB-CG	5.47	135.45	116.30
6	9	99	GLN	CA-CB-CG	5.45	125.00	114.10
56	3	51	G	C2'-C3'-O3'	5.43	121.84	113.70
2	2	2033	A	P-O3'-C3'	5.43	128.34	120.20
43	4	238	MET	CB-CG-SD	5.43	128.98	112.70
9	D	221	PHE	CA-C-N	5.42	131.90	121.54
9	D	221	PHE	C-N-CA	5.42	131.90	121.54
2	2	1931	C	P-O3'-C3'	5.40	128.30	120.20
40	R	235	MET	CA-CB-CG	5.38	124.85	114.10
33	r	261	LYS	CB-CG-CD	5.36	123.62	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	31	ARG	N-CA-C	5.35	117.17	110.91
31	o	127	SER	CA-C-N	5.33	130.93	122.61
31	o	127	SER	C-N-CA	5.33	130.93	122.61
2	2	1808	C	C2'-C3'-O3'	5.33	121.69	113.70
9	D	319	LEU	CA-CB-CG	5.27	134.76	116.30
2	2	406	C	P-O3'-C3'	5.26	128.09	120.20
34	u	4	PRO	CA-C-N	5.26	131.59	121.54
34	u	4	PRO	C-N-CA	5.26	131.59	121.54
43	4	12	VAL	CA-CB-CG1	5.25	119.33	110.40
8	B	29	VAL	CA-C-N	5.23	131.53	121.54
8	B	29	VAL	C-N-CA	5.23	131.53	121.54
2	2	4913	G	P-O3'-C3'	5.21	128.01	120.20
9	D	320	LYS	N-CA-C	-5.20	107.96	114.56
21	V	110	PRO	N-CA-C	5.19	117.03	110.70
50	c	244	LYS	CB-CA-C	5.13	120.64	110.42
11	G	131	LYS	CA-C-N	5.11	134.28	121.80
11	G	131	LYS	C-N-CA	5.11	134.28	121.80
45	k	90	MET	CB-CG-SD	5.10	128.00	112.70
2	2	1931	C	C2'-C3'-O3'	5.03	117.04	109.50
30	n	106	TYR	N-CA-C	5.02	120.91	109.81
2	2	1678	C	C2'-C3'-O3'	5.01	117.02	109.50

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	1	200	GLU	Peptide
43	4	294	LYS	Peptide
43	4	503	THR	Peptide
7	A	107	ARG	Sidechain
8	B	241	PRO	Peptide
11	G	162	ASP	Peptide
11	G	189	ARG	Sidechain
42	T	53	PRO	Peptide
44	Y	131	ARG	Peptide
59	f	204	ARG	Peptide
30	n	106	TYR	Peptide
33	r	254	PHE	Peptide
48	t	142	SER	Peptide
34	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	N	2719	0	2797	17	0
2	2	74812	0	37658	266	0
3	6	1852	0	1828	17	0
4	7	1159	0	1224	9	0
5	8	3315	0	1684	8	0
6	9	711	0	724	7	0
7	A	352	0	398	3	0
8	B	3244	0	3389	28	0
9	D	2853	0	3028	22	0
10	E	764	0	804	5	0
11	G	1927	0	2074	13	0
12	H	1015	0	1148	6	0
13	I	1518	0	1601	8	0
14	J	1772	0	1892	11	0
15	L	877	0	938	3	0
16	M	705	0	741	5	0
17	P	444	0	483	5	0
18	Q	1701	0	1818	16	0
19	S	1111	0	1174	8	0
20	U	1701	0	1749	13	0
21	V	1650	0	1794	8	0
22	X	708	0	760	6	0
23	Z	1223	0	1330	10	0
24	a	1239	0	1363	10	0
25	b	1461	0	1502	17	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	8	0
30	n	876	0	912	3	0
31	o	1897	0	2046	19	0
32	p	1878	0	2009	9	0
33	r	723	0	770	9	0
34	u	569	0	635	2	0
35	v	1771	0	1810	12	0
36	w	3472	0	3527	23	0
37	y	1250	0	1305	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	z	581	0	656	10	0
39	C	1319	0	1358	14	0
40	R	2382	0	2410	31	0
41	W	3018	0	2959	24	0
42	T	1001	0	1064	5	0
43	4	5016	0	5153	45	0
44	Y	1355	0	1389	9	0
45	k	1064	0	1160	7	0
46	j	918	0	964	5	0
47	d	850	0	868	9	0
48	t	928	0	906	9	0
49	x	684	0	456	2	0
50	c	1924	0	2027	12	0
51	l	1897	0	2029	12	0
52	K	832	0	917	3	0
53	F	897	0	989	2	0
54	i	1107	0	1182	19	0
55	O	569	0	635	5	0
56	3	2453	0	1243	15	0
57	q	3317	0	3368	62	0
58	g	1170	0	1283	36	0
59	f	2137	0	2201	111	0
60	w	32	0	12	0	0
61	w	1	0	0	0	0
All	All	163715	0	127449	817	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 3.

All (817) 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)
58:g:30:LYS:HE3	59:f:473:PHE:CE1	1.24	1.70
2:2:4083:5MU:C5	2:2:4083:5MU:C4	1.79	1.68
57:q:186:LYS:NZ	59:f:417:ASP:HB2	1.41	1.34
58:g:37:LYS:HE2	59:f:465:VAL:CG2	1.59	1.33
58:g:33:HIS:HB2	59:f:473:PHE:CZ	1.63	1.32
58:g:30:LYS:CE	59:f:473:PHE:HE1	1.44	1.30
58:g:33:HIS:HB2	59:f:473:PHE:CE2	1.66	1.29
58:g:30:LYS:CE	59:f:473:PHE:CE1	2.17	1.24
55:O:7:GLU:OE1	59:f:364:ARG:NH1	1.76	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:O:49:ASP:OD1	59:f:365:HIS:CE1	2.00	1.15
58:g:37:LYS:HE2	59:f:465:VAL:HG21	1.18	1.13
58:g:37:LYS:CE	59:f:465:VAL:HG21	1.79	1.11
57:q:156:GLN:HG3	59:f:188:VAL:CG2	1.85	1.07
2:2:2763:U:H2'	59:f:391:ARG:NH2	1.71	1.06
24:a:108:ARG:CZ	59:f:339:GLU:OE1	2.03	1.05
2:2:2763:U:H2'	59:f:391:ARG:CZ	1.86	1.04
57:q:204:PRO:HB3	59:f:437:ILE:CD1	1.89	1.03
58:g:33:HIS:CB	59:f:473:PHE:CZ	2.43	1.01
58:g:33:HIS:CB	59:f:473:PHE:CE2	2.45	0.99
57:q:156:GLN:HG3	59:f:188:VAL:HG22	1.42	0.98
2:2:4297:G:N1	2:2:4313:A:H2	1.63	0.95
57:q:186:LYS:HE3	59:f:417:ASP:OD2	1.66	0.95
57:q:186:LYS:HZ2	59:f:417:ASP:HB2	1.21	0.95
2:2:4321:U:H3	2:2:4326:G:H1	0.99	0.94
57:q:186:LYS:HZ1	59:f:417:ASP:HB2	1.11	0.94
58:g:30:LYS:HE3	59:f:473:PHE:CD1	2.03	0.92
55:O:49:ASP:OD1	59:f:365:HIS:NE2	2.01	0.91
2:2:3757:G:H1	2:2:3768:U:H3	1.17	0.90
57:q:20:ARG:NH1	59:f:454:ARG:HH22	1.67	0.90
2:2:4745:G:H1	2:2:4955:A:H61	1.20	0.90
58:g:22:LEU:HD21	59:f:478:LEU:OXT	1.71	0.90
58:g:33:HIS:HB2	59:f:473:PHE:HZ	1.31	0.89
2:2:4297:G:N1	2:2:4313:A:C2	2.36	0.89
57:q:186:LYS:NZ	59:f:417:ASP:CB	2.34	0.88
57:q:68:LYS:HB2	59:f:227:ARG:NH2	1.88	0.87
2:2:2763:U:O2'	59:f:391:ARG:NE	2.09	0.86
54:i:125:GLY:HA3	59:f:288:ALA:HB2	1.58	0.83
2:2:2592:U:H3	2:2:4126:C:H42	1.22	0.83
2:2:2592:U:H3	2:2:4126:C:N4	1.78	0.81
57:q:156:GLN:HG3	59:f:188:VAL:HG23	1.62	0.81
2:2:2763:U:H2'	59:f:391:ARG:NE	1.96	0.80
2:2:2845:A:H61	2:2:3843:C:H42	1.26	0.80
2:2:4297:G:H1	2:2:4313:A:H2	0.89	0.80
58:g:33:HIS:HB2	59:f:473:PHE:HE2	1.39	0.80
54:i:125:GLY:HA3	59:f:288:ALA:CB	2.12	0.80
58:g:33:HIS:CG	59:f:473:PHE:HZ	2.01	0.79
58:g:33:HIS:CB	59:f:473:PHE:HE2	1.95	0.78
58:g:30:LYS:HB3	59:f:473:PHE:CE1	2.19	0.78
54:i:125:GLY:C	59:f:288:ALA:HB2	2.09	0.78
2:2:2007:G:H21	2:2:2012:A:H62	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:g:33:HIS:CB	59:f:473:PHE:HZ	1.90	0.76
24:a:108:ARG:NH1	59:f:339:GLU:CD	2.45	0.75
24:a:108:ARG:NH2	59:f:339:GLU:OE1	2.19	0.75
57:q:186:LYS:HZ1	59:f:417:ASP:CB	1.93	0.75
2:2:2763:U:C2'	59:f:391:ARG:NE	2.51	0.74
54:i:125:GLY:CA	59:f:288:ALA:HB2	2.17	0.74
56:3:7:G:H1	56:3:112:U:H3	1.33	0.74
57:q:184:SER:OG	59:f:245:ALA:O	2.04	0.74
57:q:123:ARG:HG2	59:f:224:ARG:HH12	1.52	0.74
2:2:2452:G:H21	2:2:2507:A:H62	1.34	0.74
57:q:204:PRO:HB3	59:f:437:ILE:HD11	1.71	0.73
58:g:37:LYS:CE	59:f:465:VAL:CG2	2.47	0.72
58:g:59:LYS:HA	59:f:216:GLN:HE22	1.53	0.72
24:a:108:ARG:NH1	59:f:339:GLU:OE1	2.21	0.72
2:2:2763:U:C2'	59:f:391:ARG:HE	2.05	0.69
57:q:20:ARG:HH12	59:f:454:ARG:HH22	1.40	0.69
57:q:63:THR:HG21	59:f:452:GLU:OE1	1.93	0.69
2:2:2763:U:H2'	59:f:391:ARG:HH21	1.55	0.69
57:q:204:PRO:HB3	59:f:437:ILE:HD12	1.75	0.68
58:g:37:LYS:HE2	59:f:465:VAL:HG22	1.69	0.67
23:Z:67:ILE:O	23:Z:71:LYS:HB2	1.94	0.66
57:q:156:GLN:CG	59:f:188:VAL:HG22	2.21	0.65
58:g:22:LEU:O	58:g:26:LYS:HB2	1.97	0.65
2:2:1939:A:N6	2:2:4401:G:N1	2.44	0.65
2:2:2679:G:OP1	59:f:342:ARG:NH2	2.30	0.65
36:w:348:TRP:HA	36:w:361:ASP:O	1.98	0.64
2:2:2763:U:C2'	59:f:391:ARG:NH2	2.58	0.64
57:q:186:LYS:HZ2	59:f:417:ASP:CB	2.04	0.64
1:N:146:LYS:O	1:N:150:ALA:HB2	1.98	0.63
2:2:1098:G:H1	2:2:1197:C:H42	1.44	0.63
2:2:2845:A:N6	2:2:3843:C:H42	1.97	0.63
57:q:45:PRO:HG2	59:f:406:LEU:HD12	1.79	0.63
58:g:22:LEU:CD2	59:f:478:LEU:OXT	2.45	0.63
2:2:2845:A:H61	2:2:3843:C:N4	1.96	0.62
41:W:260:LEU:HB2	41:W:272:TRP:HB2	1.81	0.62
39:C:18:ARG:HB3	39:C:133:VAL:HG23	1.82	0.62
47:d:22:THR:O	47:d:109:SER:HA	2.01	0.61
2:2:2007:G:N2	2:2:2012:A:H62	1.98	0.61
2:2:2557:G:H1	2:2:2570:U:H3	1.48	0.61
54:i:125:GLY:O	59:f:288:ALA:HB2	2.01	0.61
26:e:87:SER:HA	26:e:96:LEU:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:i:59:LYS:HD2	59:f:279:LEU:CD1	2.32	0.60
57:q:63:THR:HG22	59:f:407:GLY:HA2	1.84	0.60
57:q:136:ASP:OD1	59:f:237:ALA:HB1	2.01	0.60
26:e:28:CYS:SG	26:e:29:ALA:N	2.73	0.60
2:2:4745:G:H1	2:2:4955:A:N6	1.95	0.60
2:2:1939:A:H61	2:2:4401:G:H1	1.50	0.59
43:4:371:LYS:HB3	43:4:373:ARG:HE	1.68	0.59
38:z:17:LYS:O	38:z:21:ASN:HB2	2.03	0.59
2:2:4929:C:H5''	19:S:114:LYS:HD2	1.83	0.59
21:V:34:VAL:HG12	21:V:103:LYS:HB2	1.84	0.59
2:2:2362:U:H2'	2:2:2363:A2M:H8	1.84	0.59
42:T:28:ALA:O	42:T:32:ARG:NH1	2.36	0.59
50:c:80:VAL:HB	50:c:203:LEU:HB3	1.85	0.59
1:N:134:ARG:O	1:N:138:TYR:HB2	2.03	0.58
57:q:380:ARG:HD2	59:f:429:ARG:HH12	1.69	0.58
2:2:4235:G:O6	2:2:4288:C:N4	2.37	0.58
5:8:83:C:N3	27:h:50:ARG:NH2	2.52	0.58
37:y:60:VAL:HG22	37:y:73:VAL:HG12	1.86	0.58
41:W:471:VAL:HB	41:W:483:TRP:HB2	1.86	0.57
24:a:108:ARG:NH1	59:f:339:GLU:OE2	2.37	0.57
23:Z:35:LEU:O	23:Z:39:THR:HB	2.03	0.57
33:r:244:ARG:HD3	33:r:247:LYS:HD3	1.86	0.57
31:o:173:LEU:HB2	31:o:189:THR:O	2.04	0.57
2:2:967:C:H2'	31:o:110:ARG:HH22	1.69	0.56
2:2:3776:G:H5'	36:w:292:GLY:H	1.70	0.56
9:D:218:ILE:O	9:D:222:ARG:HB3	2.05	0.56
2:2:2452:G:N2	2:2:2507:A:H62	2.04	0.56
35:v:121:GLU:HB2	35:v:200:PHE:HB3	1.87	0.56
2:2:3697:U:H5''	2:2:3698:G:H5'	1.88	0.56
2:2:4539:U:H5''	36:w:352:THR:HG23	1.86	0.56
39:C:22:LEU:O	39:C:71:HIS:HA	2.05	0.56
56:3:28:C:H1'	56:3:54:A:H61	1.69	0.56
41:W:280:CYS:SG	41:W:281:ARG:NH1	2.78	0.56
57:q:340:ARG:NH1	57:q:361:CYS:SG	2.78	0.56
10:E:47:ILE:HG12	10:E:72:HIS:HB3	1.86	0.56
50:c:157:THR:HG21	50:c:165:LEU:HD11	1.86	0.56
58:g:37:LYS:HE3	59:f:465:VAL:HG21	1.81	0.56
2:2:1939:A:N6	2:2:4401:G:H1	2.01	0.56
58:g:36:LYS:HG3	59:f:470:LYS:HG2	1.87	0.56
2:2:1187:G:N7	40:R:275:GLN:NE2	2.55	0.55
2:2:4434:C:HO2'	14:J:193:CYS:HG	1.51	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:l:163:LYS:HB3	57:q:148:PRO:HB3	1.88	0.55
41:W:375:ILE:HD13	41:W:391:SER:HB2	1.89	0.55
43:4:170:THR:HG22	43:4:218:GLN:HB2	1.89	0.55
50:c:82:LEU:O	50:c:200:GLY:HA3	2.07	0.55
1:N:389:GLU:HG3	1:N:428:VAL:HG22	1.88	0.54
42:T:41:ASP:HA	42:T:60:LYS:O	2.07	0.54
2:2:2020:U:H2'	2:2:2021:G:H8	1.72	0.54
2:2:73:A:N7	18:Q:103:ARG:NH2	2.55	0.54
57:q:20:ARG:HH11	59:f:454:ARG:HH22	1.51	0.54
57:q:333:PHE:HB3	57:q:376:GLN:HG3	1.90	0.54
2:2:1268:G:N7	7:A:111:ARG:NH2	2.55	0.54
2:2:1552:G:O2'	2:2:1574:B9B:N2	2.41	0.54
36:w:210:LEU:HD22	36:w:365:VAL:HG11	1.89	0.54
59:f:452:GLU:OE2	59:f:454:ARG:NH2	2.41	0.54
40:R:268:ARG:NH2	40:R:271:MET:SD	2.81	0.54
46:j:46:LEU:HD11	46:j:64:ILE:HG21	1.90	0.54
57:q:68:LYS:HB2	59:f:227:ARG:HH21	1.72	0.54
4:7:62:GLU:HG3	4:7:108:ILE:HD11	1.90	0.53
59:f:337:LYS:HD2	59:f:342:ARG:HE	1.73	0.53
9:D:328:LEU:HD12	32:p:187:MET:HG3	1.91	0.53
13:I:152:GLU:O	13:I:156:ASN:HB2	2.08	0.53
2:2:2572:C:OP1	59:f:277:ARG:HD2	2.08	0.53
36:w:50:ARG:HG2	36:w:56:ILE:HA	1.89	0.53
2:2:3937:C:H1'	20:U:125:SER:HB2	1.91	0.53
6:9:101:GLU:HA	6:9:104:ARG:HG2	1.91	0.53
54:i:62:ILE:HG22	59:f:279:LEU:HD22	1.90	0.53
50:c:67:MET:HE3	50:c:254:LYS:HD3	1.90	0.53
1:N:38:TYR:HB2	1:N:63:MET:HE1	1.90	0.53
2:2:4472:B8W:N2	2:2:4483:B8T:O2	2.41	0.53
3:6:163:PRO:HA	3:6:183:ALA:HB1	1.91	0.53
28:l:16:PHE:HB3	28:l:27:THR:H	1.74	0.53
57:q:68:LYS:CB	59:f:227:ARG:NH2	2.68	0.53
36:w:219:VAL:HB	36:w:313:VAL:HG22	1.91	0.53
23:Z:12:LYS:HD2	23:Z:14:ARG:HH21	1.73	0.53
2:2:29:G:O2'	20:U:96:ARG:NH1	2.42	0.53
2:2:667:A:N7	9:D:291:ARG:NH1	2.57	0.53
2:2:1702:C:H4'	9:D:308:LYS:HD3	1.91	0.53
8:B:57:VAL:HG12	8:B:73:VAL:HG12	1.91	0.53
21:V:7:LEU:HB3	21:V:33:VAL:HG12	1.89	0.53
28:l:94:ARG:HH12	31:o:112:MET:HE2	1.73	0.53
2:2:4421:C:N4	2:2:4424:A:N7	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:375:G:N7	16:M:56:ARG:NH2	2.56	0.52
2:2:2763:U:C2'	59:f:391:ARG:HH21	2.17	0.52
2:2:3722:G:H2'	2:2:3723:A2M:H8	1.91	0.52
44:Y:50:ASP:HB3	44:Y:55:LYS:HB2	1.91	0.52
2:2:2678:A:H4'	59:f:336:LYS:HG2	1.91	0.52
57:q:63:THR:CG2	59:f:452:GLU:OE1	2.58	0.52
8:B:230:GLY:O	8:B:234:ARG:HB2	2.10	0.52
20:U:165:THR:HG23	20:U:168:GLY:H	1.74	0.52
46:j:32:ARG:HB3	46:j:48:GLU:HG2	1.92	0.52
2:2:2343:G:OP2	9:D:109:ARG:NH2	2.43	0.52
2:2:4236:G:N2	2:2:4289:U:O2	2.42	0.52
13:I:8:GLN:OE1	33:r:256:GLN:NE2	2.43	0.52
8:B:222:VAL:O	8:B:343:ARG:NH1	2.43	0.52
36:w:267:ARG:HH21	36:w:464:ASN:HB3	1.74	0.52
2:2:2420:A:OP2	44:Y:127:ARG:NH1	2.43	0.52
2:2:4602:A:H62	2:2:4609:G:H21	1.58	0.52
36:w:18:SER:HB2	36:w:33:ARG:HH12	1.75	0.52
2:2:4297:G:O6	2:2:4313:A:N1	2.43	0.52
3:6:24:CYS:HB3	3:6:48:VAL:HG12	1.91	0.52
43:4:178:ASN:ND2	43:4:197:PRO:O	2.43	0.52
43:4:269:LEU:O	43:4:273:GLN:NE2	2.43	0.51
32:p:107:LYS:HD2	32:p:110:GLN:HE21	1.74	0.51
40:R:108:ARG:O	40:R:112:ARG:HB2	2.11	0.51
40:R:23:ARG:O	40:R:23:ARG:NH1	2.43	0.51
41:W:140:PHE:HB2	41:W:150:PHE:HB2	1.90	0.51
2:2:4596:C:OP1	3:6:9:ASN:ND2	2.42	0.51
2:2:2549:G:H5'	59:f:388:ARG:NH2	2.25	0.51
23:Z:29:VAL:O	23:Z:33:ARG:HB2	2.10	0.51
25:b:138:ARG:NH2	34:u:55:PRO:O	2.41	0.51
2:2:493:G:O6	2:2:660:A:N1	2.44	0.51
58:g:30:LYS:CB	59:f:473:PHE:CE1	2.92	0.51
2:2:3641:U:OP2	2:2:3646:A:N6	2.44	0.51
7:A:101:HIS:O	7:A:109:ARG:NH2	2.44	0.51
23:Z:124:ASP:OD1	23:Z:124:ASP:N	2.43	0.51
36:w:312:SER:HB2	36:w:360:ILE:HD11	1.93	0.51
43:4:227:ASP:N	43:4:227:ASP:OD1	2.44	0.51
57:q:76:GLU:CD	59:f:220:LYS:HE3	2.35	0.51
57:q:312:ASP:OD1	57:q:315:LYS:NZ	2.42	0.51
3:6:163:PRO:HB3	43:4:359:ARG:HD2	1.92	0.51
8:B:84:MET:O	8:B:204:GLN:HA	2.11	0.51
31:o:157:HIS:HB3	31:o:160:LYS:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:4:443:ASP:HB3	43:4:446:ILE:HB	1.91	0.51
57:q:147:PHE:HZ	59:f:438:LEU:HD11	1.76	0.51
2:2:1708:G:O2'	2:2:1715:C:N4	2.44	0.51
19:S:81:ASP:OD1	19:S:81:ASP:N	2.43	0.51
32:p:92:VAL:O	32:p:120:GLY:HA2	2.10	0.51
57:q:184:SER:OG	57:q:185:ILE:N	2.44	0.51
2:2:2300:A:N7	9:D:143:ARG:NH1	2.59	0.50
51:1:237:MET:O	51:1:243:ARG:NH2	2.44	0.50
2:2:5040:U:OP2	8:B:396:ARG:NH2	2.44	0.50
18:Q:78:LEU:HD11	18:Q:88:LYS:HD3	1.94	0.50
19:S:106:ASP:OD2	31:o:161:ARG:NH2	2.44	0.50
43:4:14:SER:O	43:4:18:PHE:HB2	2.11	0.50
51:1:166:GLN:HA	51:1:175:PRO:HA	1.94	0.50
1:N:41:ASN:HB3	1:N:56:LEU:HD13	1.93	0.50
2:2:1914:C:H4'	21:V:89:PRO:HD3	1.93	0.50
2:2:2391:G:OP2	43:4:504:GLN:NE2	2.45	0.50
31:o:69:TYR:O	31:o:72:LYS:NZ	2.44	0.50
2:2:1374:G:H1'	9:D:234:LYS:HG2	1.93	0.50
2:2:2335:C:H2'	2:2:2336:G:H8	1.77	0.50
40:R:208:MET:HA	40:R:211:LEU:HD23	1.93	0.50
48:t:141:PRO:HG2	48:t:144:PRO:HG3	1.93	0.50
2:2:2856:C:O2	8:B:242:ARG:NH2	2.45	0.50
2:2:4241:C:OP2	39:C:145:LYS:NZ	2.45	0.50
2:2:4769:G:OP1	21:V:176:ARG:NH1	2.44	0.50
43:4:121:ASP:H	43:4:125:ARG:HD3	1.77	0.50
43:4:230:LEU:O	43:4:233:ARG:NH1	2.44	0.50
57:q:122:GLU:HG3	59:f:224:ARG:HH11	1.76	0.50
2:2:264:C:O2	12:H:112:ARG:NH1	2.45	0.50
2:2:4673:U:OP2	26:e:15:ARG:NH2	2.45	0.50
41:W:252:LEU:HD11	41:W:260:LEU:HD12	1.92	0.50
2:2:245:C:H41	2:2:1366:G:H22	1.59	0.50
40:R:50:ARG:NH2	56:3:6:C:O2'	2.45	0.50
57:q:36:ARG:NH2	57:q:114:TYR:OH	2.44	0.50
2:2:1677:U:O2	2:2:1679:A:N6	2.44	0.50
2:2:2562:G:N2	2:2:2565:A:OP2	2.45	0.50
2:2:2583:C:OP2	53:F:76:ARG:NH1	2.45	0.50
2:2:2845:A:O3'	6:9:22:LYS:NZ	2.45	0.50
3:6:219:GLU:HG3	3:6:224:LEU:HD12	1.93	0.50
41:W:430:VAL:HA	41:W:439:LYS:O	2.12	0.50
51:1:115:THR:HB	51:1:139:MET:HE1	1.93	0.50
2:2:3865:A:N3	45:k:27:ARG:NH2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:o:161:ARG:O	31:o:182:ASN:ND2	2.45	0.50
36:w:221:VAL:HG22	36:w:251:ILE:HB	1.94	0.50
25:b:97:TYR:HB3	25:b:108:GLN:HE21	1.76	0.49
43:4:534:LYS:NZ	47:d:31:ASP:O	2.42	0.49
57:q:140:MET:HE1	57:q:220:MET:HG2	1.93	0.49
1:N:375:MET:O	1:N:379:ASN:ND2	2.45	0.49
2:2:4358:U:H4'	18:Q:197:LYS:HD2	1.94	0.49
3:6:238:ASP:OD1	3:6:238:ASP:N	2.45	0.49
39:C:129:ASP:OD1	39:C:129:ASP:N	2.45	0.49
58:g:33:HIS:CG	59:f:473:PHE:CZ	2.86	0.49
2:2:968:C:OP2	31:o:110:ARG:NH1	2.44	0.49
2:2:1393:G:O2'	18:Q:190:ARG:NH2	2.45	0.49
2:2:1853:G:N2	2:2:1853:G:OP2	2.45	0.49
2:2:2400:G:H21	53:F:6:THR:HG22	1.76	0.49
43:4:517:ARG:NH2	43:4:534:LYS:O	2.44	0.49
2:2:194:C:O2	27:h:121:ARG:NH1	2.46	0.49
2:2:994:G:N7	2:2:1050:C:N4	2.61	0.49
2:2:4265:U:O4	40:R:19:LYS:NZ	2.46	0.49
40:R:21:ARG:NH2	56:3:8:G:O6	2.45	0.49
2:2:2483:G:OP2	57:q:20:ARG:NH2	2.44	0.49
2:2:977:C:OP2	31:o:59:ARG:NH2	2.46	0.49
2:2:1517:2MG:HN2	9:D:103:ALA:HA	1.77	0.49
2:2:4088:C:OP1	29:m:37:ARG:NH1	2.45	0.49
2:2:667:A:OP1	28:l:67:ARG:NH2	2.45	0.49
2:2:1378:C:N4	18:Q:159:ASN:OD1	2.45	0.49
33:r:238:GLY:O	33:r:249:ARG:NH2	2.45	0.49
2:2:1445:U:H3	2:2:2103:G:H22	1.60	0.49
2:2:2521:G:H2'	2:2:2522:7MG:H82	1.95	0.49
8:B:58:ARG:O	8:B:71:GLU:HA	2.13	0.49
36:w:425:LEU:HD22	36:w:443:VAL:HG13	1.94	0.49
43:4:503:THR:O	43:4:507:ARG:NH2	2.45	0.49
54:i:21:ARG:NH1	54:i:47:ASP:O	2.45	0.49
57:q:186:LYS:CE	59:f:417:ASP:OD2	2.51	0.49
2:2:970:G:OP1	31:o:123:ARG:NH1	2.46	0.49
9:D:301:ALA:HB1	23:Z:132:LYS:HD3	1.94	0.49
41:W:391:SER:OG	41:W:392:PHE:N	2.46	0.49
57:q:191:GLN:HG2	57:q:200:VAL:HG22	1.95	0.49
2:2:300:A:H2'	2:2:301:G:H8	1.77	0.48
2:2:3620:G:OP1	2:2:3622:C:N4	2.45	0.48
14:J:199:VAL:HA	14:J:220:ILE:HG22	1.94	0.48
54:i:12:LEU:HB2	54:i:81:MET:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:97:G:OP1	18:Q:16:LYS:NZ	2.45	0.48
39:C:114:ASP:OD1	39:C:114:ASP:N	2.46	0.48
48:t:62:PHE:O	48:t:66:SER:HB2	2.13	0.48
50:c:88:ILE:HG23	50:c:217:GLY:HA2	1.94	0.48
2:2:1179:U:O4	40:R:289:ARG:NH1	2.47	0.48
2:2:1521:C:OP1	9:D:100:ARG:NH2	2.46	0.48
2:2:4126:C:OP1	11:G:37:LYS:NZ	2.46	0.48
6:9:36:ARG:HH22	6:9:92:LEU:HD22	1.78	0.48
14:J:238:TRP:HB3	36:w:85:ARG:HB2	1.96	0.48
48:t:148:ARG:NH2	49:x:44:N:O2'	2.46	0.48
56:3:112:U:H2'	56:3:113:G:H8	1.78	0.48
2:2:2875:C:OP1	22:X:23:ARG:NH1	2.46	0.48
5:8:126:C:O2'	5:8:128:C:N4	2.41	0.48
2:2:423:G:OP1	44:Y:62:ARG:NH1	2.47	0.48
2:2:1398:A:N6	2:2:1419:G:O2'	2.47	0.48
2:2:2712:G:O6	24:a:46:LYS:NZ	2.45	0.48
8:B:40:PRO:HB2	38:z:34:LYS:HE3	1.94	0.48
31:o:178:PRO:HB2	31:o:181:LEU:HD23	1.94	0.48
32:p:182:TYR:HB3	32:p:200:ARG:HG3	1.94	0.48
50:c:162:ARG:HA	50:c:165:LEU:HG	1.95	0.48
2:2:382:G:N1	2:2:385:A:OP2	2.45	0.48
2:2:665:C:H4'	2:2:666:G:H5'	1.95	0.48
2:2:2686:G:O2'	2:2:2688:G:N7	2.45	0.48
8:B:92:TYR:HB2	8:B:159:VAL:HB	1.95	0.48
20:U:84:PRO:O	20:U:87:HIS:ND1	2.45	0.48
38:z:101:GLN:HA	38:z:104:ARG:HD3	1.95	0.48
40:R:58:ARG:HH12	56:3:28:C:H41	1.60	0.48
41:W:433:SER:OG	41:W:434:SER:N	2.47	0.48
8:B:131:THR:O	8:B:135:LYS:NZ	2.46	0.48
25:b:144:GLN:HA	33:r:262:PRO:HD3	1.95	0.48
35:v:40:LEU:HD11	35:v:102:LEU:HD22	1.95	0.48
2:2:992:C:N4	2:2:995:C:O2'	2.46	0.48
2:2:1306:C:H2'	2:2:1307:A:H8	1.79	0.48
2:2:3838:U:H5'	6:9:17:ARG:HD2	1.96	0.48
40:R:51:MET:HA	40:R:63:GLN:O	2.14	0.48
59:f:219:LYS:HE3	59:f:221:GLY:HA3	1.96	0.48
3:6:66:ASN:ND2	3:6:111:ASN:O	2.47	0.48
10:E:17:ARG:HD3	10:E:103:ASP:HA	1.94	0.48
19:S:41:PRO:HB3	19:S:70:GLN:HE21	1.78	0.48
37:y:89:PRO:O	37:y:94:LYS:NZ	2.47	0.48
41:W:200:LYS:HB3	41:W:224:LYS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:x:49:N:OP2	50:c:176:ARG:NH1	2.46	0.48
50:c:84:LEU:HD21	50:c:233:VAL:HG23	1.96	0.48
54:i:59:LYS:HD2	59:f:279:LEU:HD13	1.95	0.48
2:2:758:G:H5''	13:I:52:LYS:HG3	1.95	0.47
2:2:4163:U:OP2	11:G:53:ARG:NH1	2.45	0.47
2:2:4516:G:OP2	8:B:2:SER:N	2.47	0.47
55:O:7:GLU:HB2	55:O:10:ASP:HB2	1.96	0.47
2:2:134:G:OP2	12:H:74:LYS:NZ	2.47	0.47
2:2:2625:U:OP2	43:4:510:ARG:NH2	2.47	0.47
21:V:185:VAL:HG12	21:V:189:ILE:HG12	1.96	0.47
23:Z:53:MET:HE3	23:Z:57:ASN:HB3	1.95	0.47
37:y:130:LYS:HG2	37:y:152:ILE:HG12	1.95	0.47
50:c:243:GLU:HB3	50:c:247:SER:HB2	1.96	0.47
57:q:7:LYS:O	57:q:11:ARG:NH2	2.46	0.47
58:g:30:LYS:NZ	59:f:473:PHE:CE1	2.79	0.47
2:2:3855:C:H2'	2:2:3856:A:H8	1.80	0.47
8:B:10:ARG:NH1	8:B:11:HIS:O	2.47	0.47
11:G:26:LYS:HG3	11:G:27:VAL:HG13	1.96	0.47
36:w:164:ILE:HD11	43:4:278:LEU:HA	1.96	0.47
40:R:197:LYS:HG3	40:R:202:GLN:HB2	1.95	0.47
41:W:325:LEU:HD23	41:W:328:ARG:HH11	1.79	0.47
43:4:232:ASP:OD1	43:4:232:ASP:N	2.46	0.47
2:2:4570:G:H2'	2:2:4571:A2M:H8	1.95	0.47
4:7:19:MET:SD	4:7:19:MET:N	2.87	0.47
35:v:208:TRP:HB2	35:v:215:PHE:HD1	1.79	0.47
45:k:26:ASP:OD1	45:k:26:ASP:N	2.44	0.47
57:q:136:ASP:OD1	59:f:441:ARG:NH2	2.48	0.47
2:2:727:C:OP1	32:p:73:ARG:NH2	2.47	0.47
8:B:153:MET:O	8:B:157:CYS:HB2	2.15	0.47
35:v:208:TRP:HA	35:v:214:ARG:O	2.15	0.47
37:y:45:ASP:HB3	37:y:71:ILE:HD11	1.96	0.47
39:C:75:ARG:O	39:C:78:LYS:NZ	2.47	0.47
39:C:92:TYR:HB3	39:C:172:GLY:HA2	1.96	0.47
39:C:141:ILE:HA	39:C:144:LYS:HE2	1.97	0.47
43:4:244:LEU:O	43:4:282:LYS:NZ	2.47	0.47
10:E:38:ILE:HG21	10:E:63:TYR:HB3	1.97	0.47
13:I:94:SER:HB2	13:I:142:ASP:HB3	1.97	0.47
15:L:85:GLN:HA	15:L:88:VAL:HG22	1.97	0.47
38:z:99:GLN:HA	38:z:102:ARG:HD2	1.96	0.47
57:q:68:LYS:CB	59:f:227:ARG:HH21	2.27	0.47
2:2:2092:G:O2'	2:2:2262:G:N2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:2705:G:O6	24:a:46:LYS:NZ	2.48	0.47
2:2:4370:G:N2	2:2:4371:G:N2	2.63	0.47
35:v:125:ALA:HB2	35:v:197:MET:HB3	1.97	0.47
41:W:223:SER:OG	41:W:224:LYS:N	2.47	0.47
50:c:82:LEU:O	50:c:200:GLY:CA	2.63	0.47
2:2:1921:C:N3	25:b:161:ARG:NH2	2.63	0.47
25:b:139:ARG:O	25:b:143:LYS:HB2	2.15	0.47
40:R:74:ILE:O	56:3:114:U:O2'	2.32	0.47
43:4:294:LYS:HG3	43:4:299:LEU:HD22	1.96	0.47
56:3:2:U:H3	56:3:117:G:H1	1.62	0.47
2:2:3688:U:OP2	29:m:198:ARG:NH2	2.48	0.47
14:J:152:LYS:NZ	14:J:249:GLU:OE2	2.46	0.47
2:2:1906:U:H2'	2:2:1907:A:H8	1.79	0.47
2:2:4419:U:H5'	2:2:4424:A:H61	1.79	0.47
12:H:79:LYS:O	12:H:84:ARG:NH2	2.47	0.47
20:U:123:GLU:HG3	20:U:128:LYS:HG3	1.97	0.47
38:z:25:GLU:OE1	38:z:28:ARG:NH2	2.47	0.47
40:R:223:PHE:HB3	40:R:226:TYR:HB2	1.96	0.47
58:g:35:HIS:HB3	59:f:468:VAL:O	2.15	0.47
1:N:187:LEU:HD12	1:N:192:ILE:HD11	1.96	0.46
2:2:962:C:O3'	32:p:32:ARG:NH1	2.48	0.46
2:2:2101:C:H2'	2:2:2102:G:H2'	1.97	0.46
8:B:225:GLY:HA2	8:B:273:GLY:HA3	1.97	0.46
8:B:364:ASP:OD1	8:B:364:ASP:N	2.48	0.46
12:H:82:ASP:OD1	12:H:82:ASP:N	2.47	0.46
19:S:41:PRO:HG3	19:S:73:VAL:HG13	1.96	0.46
32:p:105:VAL:HG13	32:p:136:VAL:HG12	1.97	0.46
37:y:39:PRO:HD2	43:4:259:GLU:HB3	1.95	0.46
43:4:250:ALA:HB2	43:4:339:LEU:HB2	1.96	0.46
2:2:4620:OMU:OP1	26:e:51:ARG:NH1	2.48	0.46
4:7:24:ASN:ND2	26:e:99:GLU:OE2	2.49	0.46
17:P:28:ARG:NH1	17:P:36:ARG:O	2.45	0.46
46:j:64:ILE:HG23	46:j:68:LEU:HD23	1.96	0.46
48:t:148:ARG:NH2	50:c:208:SER:OG	2.48	0.46
2:2:404:U:O3'	27:h:87:ARG:NH2	2.48	0.46
2:2:2476:G:N7	58:g:48:ARG:NH2	2.64	0.46
39:C:94:LEU:HD22	39:C:98:ASN:HD21	1.81	0.46
45:k:6:PRO:HG3	45:k:73:GLY:HA3	1.96	0.46
9:D:86:ARG:NH1	9:D:89:GLN:OE1	2.49	0.46
13:I:180:TYR:OH	14:J:17:ARG:NH1	2.49	0.46
21:V:6:VAL:HG12	21:V:32:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:38:THR:HG22	22:X:45:THR:HG22	1.98	0.46
42:T:41:ASP:H	42:T:99:SER:HB2	1.80	0.46
47:d:56:LEU:HD23	47:d:61:VAL:HB	1.98	0.46
2:2:1573:G:OP1	24:a:92:LYS:NZ	2.44	0.46
2:2:1992:U:H5'	2:2:1993:C:H5'	1.96	0.46
2:2:5024:C:H5	2:2:5028:G:H21	1.64	0.46
12:H:117:ARG:NH2	18:Q:127:PHE:O	2.49	0.46
2:2:1253:G:O2'	2:2:1257:A:N6	2.49	0.46
11:G:117:ARG:HD3	11:G:120:LYS:HD3	1.98	0.46
20:U:116:LEU:HD22	20:U:135:ILE:HD11	1.97	0.46
57:q:310:GLU:OE2	57:q:314:ARG:NH2	2.49	0.46
2:2:1896:A:OP1	32:p:223:LYS:NZ	2.47	0.46
17:P:41:ARG:HG2	43:4:609:ALA:HB2	1.97	0.46
29:m:116:LEU:HB3	29:m:126:LEU:HB2	1.96	0.46
35:v:207:MET:O	35:v:215:PHE:HA	2.16	0.46
43:4:72:LEU:HD13	43:4:89:LYS:HG3	1.98	0.46
2:2:1332:C:H2'	2:2:1333:A:H8	1.80	0.46
2:2:1562:G:N2	2:2:1565:A:OP2	2.49	0.46
13:I:111:LEU:HD21	13:I:125:ARG:HB2	1.98	0.46
40:R:64:ILE:HG23	40:R:105:LEU:HD21	1.97	0.46
40:R:88:VAL:HG13	40:R:239:MET:HE1	1.97	0.46
41:W:477:ASP:OD1	41:W:477:ASP:N	2.47	0.46
43:4:226:LEU:O	43:4:233:ARG:NH2	2.49	0.46
58:g:23:LYS:HD2	59:f:478:LEU:HA	1.98	0.46
2:2:1499:C:OP1	23:Z:150:ARG:NH2	2.49	0.46
8:B:290:GLY:O	8:B:301:ASN:ND2	2.48	0.46
36:w:307:ASP:N	36:w:307:ASP:OD1	2.47	0.46
40:R:211:LEU:HG	40:R:219:TYR:HB2	1.98	0.46
40:R:292:GLU:OE2	40:R:293:ARG:NH1	2.49	0.46
2:2:1951:G:O2'	25:b:95:ARG:NH2	2.49	0.45
2:2:4996:C:OP1	46:j:32:ARG:NH1	2.46	0.45
5:8:47:C:H1'	5:8:61:A:H2'	1.98	0.45
36:w:305:HIS:HB2	36:w:311:ILE:HD11	1.98	0.45
41:W:230:ILE:HB	41:W:240:ARG:HB2	1.98	0.45
43:4:170:THR:HA	43:4:218:GLN:O	2.15	0.45
2:2:4457:U:OP1	26:e:50:ASN:ND2	2.49	0.45
5:8:75:G:OP2	27:h:74:TYR:OH	2.35	0.45
14:J:147:LYS:HD3	14:J:171:ILE:HD11	1.96	0.45
22:X:30:GLU:OE1	22:X:33:GLN:NE2	2.46	0.45
29:m:20:VAL:HA	29:m:23:ARG:HG3	1.98	0.45
48:t:58:GLU:HB2	48:t:74:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1185:G:O4'	40:R:282:GLN:NE2	2.49	0.45
9:D:152:LEU:HD23	9:D:251:ILE:HG12	1.98	0.45
15:L:76:ASP:HB3	15:L:115:GLY:HA3	1.99	0.45
28:l:66:ARG:NH1	28:l:75:THR:O	2.49	0.45
44:Y:94:MET:HG2	44:Y:148:MET:HE2	1.97	0.45
56:3:11:A:O2'	56:3:13:A:OP2	2.34	0.45
1:N:57:ALA:HB1	1:N:99:THR:HG21	1.97	0.45
2:2:95:G:OP2	18:Q:11:LYS:NZ	2.49	0.45
13:I:4:ILE:HB	33:r:259:GLN:HG3	1.98	0.45
56:3:15:C:H2'	56:3:16:A:H8	1.81	0.45
2:2:2562:G:N2	2:2:2566:G:N7	2.65	0.45
14:J:202:ASN:ND2	14:J:213:VAL:O	2.49	0.45
39:C:176:PRO:HG2	39:C:178:LYS:HG2	1.98	0.45
47:d:48:LYS:HG2	47:d:53:ALA:HB2	1.98	0.45
2:2:2112:G:OP1	2:2:2251:G:N1	2.49	0.45
2:2:2431:A:OP1	17:P:41:ARG:NH1	2.48	0.45
2:2:3774:A:N7	2:2:3776:G:N2	2.64	0.45
2:2:4244:A:H62	2:2:4264:G:H21	1.64	0.45
21:V:51:LYS:HE3	21:V:144:GLU:HB3	1.99	0.45
47:d:74:SER:OG	47:d:75:GLU:N	2.50	0.45
48:t:144:PRO:HA	48:t:147:LYS:HB2	1.98	0.45
57:q:44:TYR:CE1	59:f:450:MET:HG2	2.51	0.45
2:2:238:C:O2	27:h:102:SER:OG	2.35	0.45
2:2:969:C:O2'	2:2:970:G:N2	2.50	0.45
2:2:2601:A:N6	2:2:2744:A:OP2	2.45	0.45
9:D:275:SER:OG	9:D:276:ASN:N	2.46	0.45
48:t:143:TYR:HA	48:t:144:PRO:HD3	1.87	0.45
1:N:85:LEU:O	1:N:89:HIS:HB3	2.17	0.45
2:2:990:C:N4	2:2:1051:G:O2'	2.42	0.45
2:2:1282:G:OP2	9:D:316:LYS:NZ	2.49	0.45
8:B:57:VAL:HA	8:B:72:VAL:O	2.17	0.45
54:i:50:PRO:HD3	54:i:68:ILE:HG13	1.99	0.45
1:N:288:HIS:HE2	1:N:327:ILE:HD13	1.82	0.45
2:2:260:C:H2'	2:2:261:G:H8	1.82	0.45
2:2:664:G:N2	2:2:666:G:O6	2.49	0.45
2:2:4496:A:H61	2:2:4504:C:H42	1.65	0.45
57:q:220:MET:HE1	59:f:442:PHE:HB2	1.99	0.45
2:2:1480:C:O2'	2:2:1482:G:OP2	2.35	0.44
2:2:3928:A:OP1	20:U:90:ASN:ND2	2.46	0.44
10:E:79:ILE:HG22	10:E:90:ARG:HB3	1.97	0.44
18:Q:96:ILE:HD12	18:Q:117:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:130:GLU:OE2	34:u:62:ARG:NH2	2.50	0.44
26:e:37:LEU:HD21	26:e:105:ILE:HD11	1.99	0.44
30:n:36:ARG:NH1	30:n:79:GLY:O	2.50	0.44
36:w:25:GLN:HB3	36:w:32:MET:HG2	1.97	0.44
2:2:375:G:OP2	16:M:52:LYS:NZ	2.45	0.44
2:2:989:U:O2	2:2:1064:G:O6	2.34	0.44
2:2:4741:C:OP1	2:2:4900:C:N4	2.45	0.44
4:7:97:GLU:OE2	43:4:441:TYR:OH	2.35	0.44
36:w:210:LEU:HB2	36:w:365:VAL:HG21	1.99	0.44
1:N:119:LEU:HD22	1:N:141:ILE:HG12	1.98	0.44
11:G:61:ILE:HG22	11:G:65:ARG:HE	1.81	0.44
11:G:160:ASP:OD1	11:G:160:ASP:N	2.47	0.44
33:r:290:GLU:HB3	33:r:294:ARG:HH12	1.82	0.44
42:T:62:GLY:HA3	42:T:74:ILE:HG23	1.99	0.44
2:2:85:G:N2	2:2:98:A:OP2	2.44	0.44
2:2:2459:G:N2	2:2:2462:C:OP2	2.47	0.44
2:2:4105:A:N3	2:2:4106:G:N1	2.64	0.44
3:6:240:LEU:O	3:6:244:LEU:HB2	2.18	0.44
6:9:28:LEU:O	6:9:32:HIS:ND1	2.50	0.44
9:D:140:LYS:O	9:D:204:ARG:NH2	2.50	0.44
37:y:28:LEU:HB3	37:y:32:ILE:HD12	1.99	0.44
39:C:23:ASN:HA	39:C:70:VAL:O	2.17	0.44
40:R:100:CYS:O	40:R:104:LEU:HB2	2.18	0.44
2:2:1988:G:OP1	36:w:147:LYS:NZ	2.47	0.44
2:2:4302:U:O2'	2:2:4308:C:N4	2.51	0.44
2:2:4670:C:O2'	2:2:4672:A:OP2	2.34	0.44
26:e:35:LYS:HD2	26:e:35:LYS:HA	1.84	0.44
51:1:228:LYS:H	51:1:228:LYS:HG2	1.62	0.44
2:2:1732:C:H42	2:2:1797:G:H1	1.65	0.44
2:2:1939:A:N1	2:2:4401:G:C2	2.85	0.44
2:2:3892:U:O2'	44:Y:80:GLN:OE1	2.35	0.44
8:B:212:GLY:HA3	38:z:33:LEU:HD11	2.00	0.44
40:R:166:ALA:HB1	40:R:171:LEU:HD12	1.98	0.44
41:W:352:THR:HG21	41:W:367:ARG:HH11	1.81	0.44
43:4:381:VAL:HG23	43:4:382:VAL:HG23	2.00	0.44
2:2:4251:A:H5''	39:C:108:GLY:HA3	2.00	0.44
7:A:55:LYS:HA	7:A:58:GLN:HG2	2.00	0.44
25:b:74:ARG:O	25:b:76:LYS:NZ	2.49	0.44
40:R:53:VAL:HA	40:R:61:ILE:O	2.18	0.44
43:4:243:ALA:O	43:4:247:LEU:HB2	2.18	0.44
51:1:196:ASP:OD2	57:q:380:ARG:NH1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:i:27:LYS:HB3	54:i:42:LEU:HB3	2.00	0.44
2:2:952:G:H4'	30:n:75:THR:HG23	2.00	0.44
8:B:353:VAL:HG11	38:z:22:ALA:HB2	1.98	0.44
54:i:47:ASP:HB3	54:i:69:LYS:HB3	2.00	0.44
55:O:49:ASP:OD1	59:f:365:HIS:HE1	1.84	0.44
57:q:150:THR:HG23	57:q:153:CYS:H	1.83	0.44
2:2:35:U:H4'	2:2:1525:A:H2	1.83	0.44
24:a:44:LEU:HD22	24:a:49:LEU:HD22	2.00	0.44
36:w:136:ASP:OD1	36:w:136:ASP:N	2.48	0.44
40:R:67:ALA:HA	40:R:72:ASP:HA	2.00	0.44
43:4:503:THR:H	43:4:507:ARG:HH21	1.66	0.44
54:i:62:ILE:HG22	59:f:279:LEU:CD2	2.48	0.44
2:2:2295:C:H2'	2:2:2296:G:H8	1.83	0.43
8:B:10:ARG:NH2	8:B:265:SER:O	2.51	0.43
29:m:30:ARG:NH1	29:m:36:GLU:OE2	2.50	0.43
43:4:135:GLY:O	43:4:139:THR:OG1	2.35	0.43
57:q:47:GLU:OE2	59:f:404:ARG:HB3	2.17	0.43
2:2:1994:C:H4'	37:y:130:LYS:HB3	1.99	0.43
2:2:2592:U:N3	2:2:4126:C:N4	2.51	0.43
2:2:4980:C:N3	44:Y:69:ARG:NH2	2.63	0.43
8:B:139:ASP:OD2	38:z:96:TRP:NE1	2.46	0.43
9:D:209:ILE:HB	9:D:229:LEU:HD13	2.00	0.43
41:W:200:LYS:HD2	41:W:200:LYS:HA	1.79	0.43
2:2:1646:A:O2'	16:M:49:TRP:O	2.36	0.43
2:2:4077:A:H62	2:2:4169:G:H21	1.66	0.43
2:2:4236:G:HO2'	2:2:4328:G:HO2'	1.63	0.43
11:G:73:ARG:NH1	11:G:241:VAL:O	2.46	0.43
18:Q:111:GLN:HA	18:Q:114:VAL:HG12	2.00	0.43
23:Z:39:THR:HG22	23:Z:41:SER:H	1.83	0.43
31:o:150:LEU:O	31:o:161:ARG:HA	2.19	0.43
56:3:35:U:O2	56:3:45:U:O2'	2.32	0.43
28:l:94:ARG:HG3	28:l:111:ILE:HD11	1.99	0.43
31:o:153:LEU:HD11	31:o:195:ILE:HG13	2.01	0.43
45:k:106:LYS:HB3	45:k:106:LYS:HE2	1.85	0.43
2:2:327:U:O2'	52:K:30:ARG:NH1	2.51	0.43
3:6:129:LEU:O	3:6:133:LEU:HB2	2.18	0.43
9:D:94:ASN:OD1	9:D:94:ASN:N	2.52	0.43
32:p:134:ARG:HA	32:p:137:GLU:HG3	2.00	0.43
41:W:348:SER:OG	41:W:349:ASP:N	2.52	0.43
52:K:22:SER:OG	52:K:23:LYS:N	2.51	0.43
54:i:35:ASP:OD1	54:i:35:ASP:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:79:ILE:HD12	43:4:442:ILE:HG22	1.99	0.43
27:h:10:ASP:HB3	27:h:13:LYS:HB2	2.00	0.43
40:R:52:ILE:HD13	56:3:6:C:H4'	2.00	0.43
47:d:106:SER:OG	47:d:107:LYS:N	2.51	0.43
51:1:120:ARG:NH2	51:1:212:SER:O	2.50	0.43
51:1:199:HIS:CE1	57:q:336:ARG:HE	2.36	0.43
57:q:381:PRO:HD3	59:f:429:ARG:HH22	1.82	0.43
4:7:120:LYS:HG3	43:4:477:MET:HE1	2.00	0.43
11:G:91:THR:HG22	48:t:110:LEU:HD13	2.00	0.43
31:o:277:LEU:HA	31:o:281:ILE:HD11	2.01	0.43
40:R:84:PRO:HG3	40:R:92:LEU:HD11	2.01	0.43
40:R:136:ASP:OD1	40:R:136:ASP:N	2.49	0.43
2:2:1375:C:OP1	9:D:274:LYS:NZ	2.47	0.43
2:2:2262:G:OP2	28:l:98:ARG:NH2	2.47	0.43
2:2:2489:C:H41	57:q:149:ARG:HG3	1.83	0.43
2:2:3917:A:H2'	2:2:3918:G:H8	1.84	0.43
2:2:4162:C:H5	11:G:73:ARG:HH12	1.67	0.43
8:B:220:ILE:HB	8:B:346:THR:HB	1.99	0.43
1:N:395:ILE:HB	1:N:435:LEU:HD11	2.01	0.43
2:2:702:U:H5'	31:o:121:VAL:HG11	2.01	0.43
2:2:1945:G:N2	14:J:39:ALA:O	2.47	0.43
2:2:2026:A:H5''	33:r:263:LEU:HD13	2.01	0.43
2:2:4078:C:OP1	20:U:31:ARG:NH1	2.52	0.43
5:8:39:G:OP1	12:H:86:LYS:NZ	2.46	0.43
11:G:132:ARG:HA	11:G:133:PRO:HD3	1.85	0.43
14:J:13:ARG:NH2	43:4:194:ASP:OD1	2.52	0.43
16:M:20:ARG:NH2	16:M:39:TYR:OH	2.50	0.43
35:v:27:ILE:HG12	35:v:76:ALA:HB2	1.99	0.43
42:T:52:MET:HA	42:T:53:PRO:HD3	1.87	0.43
52:K:12:ASN:O	52:K:16:LYS:NZ	2.49	0.43
54:i:124:THR:HG23	59:f:282:PRO:HD2	2.01	0.43
2:2:4266:G:O2'	2:2:4269:G:O6	2.36	0.43
44:Y:94:MET:HE3	44:Y:94:MET:HB2	1.97	0.43
48:t:78:ARG:HA	48:t:85:SER:HA	2.00	0.43
51:1:141:ARG:HA	51:1:144:GLU:HG3	2.00	0.43
57:q:126:THR:HG22	57:q:128:ILE:H	1.84	0.43
2:2:4092:G:H3'	2:2:4093:G:H21	1.84	0.42
2:2:4464:A:H62	43:4:32:THR:HB	1.84	0.42
8:B:56:ILE:O	8:B:73:VAL:HA	2.19	0.42
17:P:33:ASN:ND2	17:P:35:ILE:O	2.52	0.42
41:W:133:SER:OG	41:W:134:GLY:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1500:A:H5''	2:2:1501:C:H5''	2.02	0.42
2:2:3870:C:H2'	2:2:3871:A:H8	1.84	0.42
3:6:123:ARG:HA	3:6:126:GLU:HG2	2.00	0.42
13:I:86:LEU:HD23	13:I:186:THR:HG21	2.02	0.42
21:V:55:LEU:HD23	21:V:58:LEU:HD12	2.00	0.42
38:z:87:LEU:HD21	38:z:106:LYS:HZ3	1.85	0.42
1:N:374:LEU:HD21	1:N:402:THR:HB	2.02	0.42
2:2:279:A:N7	20:U:12:ARG:NH1	2.67	0.42
2:2:2045:G:N2	2:2:2046:G:N7	2.67	0.42
2:2:2764:A:H2'	2:2:2765:A:H8	1.83	0.42
8:B:309:LEU:HD11	43:4:430:PRO:HB3	2.01	0.42
9:D:218:ILE:O	9:D:221:PHE:C	2.61	0.42
20:U:24:ARG:HE	20:U:24:ARG:HB3	1.64	0.42
41:W:105:ARG:HE	41:W:106:CYS:H	1.66	0.42
41:W:167:ASP:OD1	41:W:167:ASP:N	2.46	0.42
25:b:161:ARG:HH11	25:b:164:LYS:HD3	1.84	0.42
35:v:164:ARG:HA	35:v:164:ARG:HD3	1.84	0.42
40:R:236:MET:HA	40:R:239:MET:HG3	2.01	0.42
57:q:337:GLU:HG3	57:q:379:ASP:HB2	2.01	0.42
58:g:101:ASP:OD1	58:g:101:ASP:N	2.46	0.42
2:2:958:G:O2'	31:o:123:ARG:O	2.35	0.42
2:2:2406:G:O2'	17:P:48:LYS:NZ	2.52	0.42
2:2:4265:U:O5'	2:2:4279:A:N6	2.52	0.42
16:M:58:THR:OG1	16:M:59:THR:N	2.53	0.42
25:b:11:LYS:HE3	25:b:11:LYS:HB2	1.89	0.42
2:2:1069:G:OP2	31:o:65:ARG:NH2	2.51	0.42
2:2:2418:A:N1	2:2:2429:A:O2'	2.51	0.42
2:2:2621:A:OP1	47:d:80:LYS:NZ	2.52	0.42
2:2:3717:A:H2'	2:2:3718:A2M:H8	2.01	0.42
2:2:4476:C:O2'	2:2:4478:G:OP2	2.36	0.42
2:2:4761:G:H2'	2:2:4762:A:H8	1.84	0.42
43:4:584:LYS:HB3	43:4:584:LYS:HE3	1.86	0.42
56:3:23:A:N3	56:3:118:C:O2'	2.50	0.42
58:g:33:HIS:HB3	59:f:473:PHE:CE2	2.46	0.42
2:2:2519:U:O2'	2:2:2530:U:O2	2.35	0.42
2:2:4467:A:O2'	2:2:4510:A:N3	2.46	0.42
2:2:4678:G:H5''	38:z:11:ARG:HD3	2.02	0.42
5:8:131:G:H5''	58:g:108:GLN:HE21	1.85	0.42
35:v:96:LEU:HD23	35:v:96:LEU:HA	1.94	0.42
57:q:347:ILE:O	57:q:352:GLY:N	2.52	0.42
1:N:65:GLN:O	1:N:110:LYS:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:4606:G:O3'	43:4:216:ARG:NH2	2.49	0.42
18:Q:70:VAL:H	18:Q:159:ASN:HD21	1.66	0.42
19:S:86:TRP:O	19:S:89:THR:OG1	2.38	0.42
54:i:70:SER:OG	54:i:71:PHE:N	2.53	0.42
2:2:351:C:OP2	9:D:197:ARG:NH1	2.45	0.42
2:2:1408:G:O2'	2:2:1412:G:O6	2.37	0.42
2:2:4321:U:O4	2:2:4326:G:O6	2.37	0.42
35:v:69:LYS:HD3	35:v:69:LYS:HA	1.82	0.42
25:b:139:ARG:HB2	25:b:142:VAL:HG22	2.01	0.42
28:l:7:TRP:O	28:l:11:ARG:HB2	2.20	0.42
2:2:653:U:OP1	23:Z:115:ARG:NH1	2.53	0.41
2:2:2411:C:H2'	2:2:2412:A:H8	1.84	0.41
2:2:4100:C:N4	2:2:4109:G:OP2	2.47	0.41
2:2:4494:OMG:HM21	26:e:22:VAL:HG11	2.02	0.41
37:y:105:THR:OG1	37:y:108:GLU:OE1	2.35	0.41
40:R:107:ARG:HA	40:R:107:ARG:HD2	1.89	0.41
41:W:429:LEU:O	41:W:440:VAL:HA	2.20	0.41
54:i:90:PRO:O	54:i:117:LYS:NZ	2.53	0.41
54:i:125:GLY:HA3	59:f:288:ALA:HB3	1.97	0.41
2:2:385:A:OP1	27:h:77:LYS:NZ	2.52	0.41
2:2:1952:G:H4'	25:b:93:MET:HE3	2.02	0.41
10:E:98:ASP:HA	10:E:99:PRO:HD3	1.93	0.41
14:J:162:ARG:HB3	36:w:216:SER:HA	2.02	0.41
36:w:37:THR:HG23	36:w:40:ARG:HH21	1.85	0.41
40:R:236:MET:O	40:R:240:TYR:CB	2.68	0.41
44:Y:168:LYS:HA	44:Y:168:LYS:HD3	1.92	0.41
2:2:1086:C:H2'	2:2:1087:A:H8	1.86	0.41
2:2:1810:G:H2'	2:2:1811:G:H8	1.85	0.41
2:2:4498:U:H4'	2:2:4500:U:H4'	2.03	0.41
2:2:4912:G:N7	2:2:4913:G:N2	2.69	0.41
3:6:214:GLU:HA	3:6:217:VAL:HG12	2.01	0.41
20:U:159:ARG:HB3	20:U:164:LEU:HB2	2.03	0.41
27:h:47:MET:HE3	27:h:47:MET:HB3	1.91	0.41
41:W:298:ASP:OD1	41:W:298:ASP:N	2.52	0.41
43:4:357:LEU:HD23	43:4:360:LEU:HD12	2.03	0.41
2:2:736:C:OP1	19:S:74:ARG:NH1	2.47	0.41
2:2:4940:C:OP1	31:o:156:ARG:NH1	2.49	0.41
3:6:4:ARG:NH1	3:6:210:THR:O	2.54	0.41
5:8:27:U:H4'	9:D:53:ALA:HB3	2.03	0.41
14:J:153:VAL:HG11	14:J:248:PRO:HB2	2.00	0.41
37:y:16:ARG:HA	37:y:58:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C:90:ARG:HD2	39:C:90:ARG:HA	1.90	0.41
43:4:117:MET:HE2	43:4:117:MET:HB2	1.96	0.41
2:2:667:A:H5''	2:2:668:C:H5''	2.03	0.41
2:2:2111:G:N7	2:2:2251:G:O2'	2.49	0.41
2:2:3687:A:O2'	29:m:236:GLY:N	2.53	0.41
2:2:4394:A:N6	2:2:4395:U:O4	2.54	0.41
2:2:4645:C:OP2	24:a:62:ARG:NH1	2.54	0.41
11:G:46:GLN:OE1	11:G:49:ARG:NH2	2.54	0.41
29:m:27:ALA:O	29:m:128:ARG:NH2	2.43	0.41
29:m:116:LEU:O	29:m:126:LEU:N	2.53	0.41
40:R:128:ASP:OD1	40:R:128:ASP:N	2.54	0.41
46:j:95:ASP:OD1	46:j:95:ASP:N	2.52	0.41
59:f:452:GLU:HA	59:f:453:PRO:HD3	1.91	0.41
2:2:729:2MG:N2	25:b:66:GLN:O	2.41	0.41
2:2:2611:A:H5'	2:2:2688:G:H4'	2.03	0.41
2:2:4582:C:OP2	8:B:28:LYS:NZ	2.49	0.41
11:G:117:ARG:HA	11:G:120:LYS:HG2	2.03	0.41
25:b:147:ASP:HB3	25:b:150:ILE:HB	2.03	0.41
26:e:24:ALA:HB3	26:e:39:ILE:HD12	2.02	0.41
33:r:292:GLU:HA	33:r:295:ARG:HG2	2.03	0.41
37:y:90:ARG:HG3	37:y:98:ILE:HD11	2.02	0.41
57:q:24:ARG:NH1	57:q:29:LEU:O	2.53	0.41
57:q:150:THR:OG1	57:q:151:GLY:N	2.53	0.41
1:N:399:LYS:HG3	1:N:439:PHE:HD1	1.85	0.41
2:2:1168:G:O6	2:2:1194:G:N2	2.48	0.41
2:2:2490:U:OP2	57:q:108:LYS:NZ	2.45	0.41
2:2:4251:A:H1'	39:C:110:GLN:HG3	2.03	0.41
3:6:106:ASN:ND2	26:e:136:ALA:O	2.53	0.41
5:8:14:OMU:H1'	5:8:14:OMU:HM23	1.68	0.41
33:r:301:ARG:HH21	33:r:304:GLU:HG2	1.86	0.41
43:4:357:LEU:HA	43:4:360:LEU:HD12	2.02	0.41
47:d:84:LYS:HE3	47:d:102:VAL:HB	2.03	0.41
2:2:73:A:H62	18:Q:103:ARG:HH22	1.69	0.41
2:2:153:G:H2'	2:2:154:G:H8	1.85	0.41
2:2:323:C:H2'	2:2:324:A:H8	1.86	0.41
2:2:1595:G:H1'	2:2:1597:G:H21	1.85	0.41
2:2:1884:C:H2'	2:2:1885:G:H8	1.84	0.41
4:7:95:ARG:HD2	4:7:95:ARG:HA	1.86	0.41
8:B:8:ALA:HB2	26:e:49:LEU:HD22	2.03	0.41
18:Q:80:GLU:OE2	18:Q:104:ASN:ND2	2.54	0.41
22:X:3:LYS:HD2	22:X:3:LYS:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:230:G:OP1	27:h:15:ARG:NH1	2.48	0.41
2:2:1479:G:H21	18:Q:184:MET:HE1	1.86	0.41
15:L:76:ASP:OD1	15:L:76:ASP:N	2.54	0.41
19:S:39:ASP:HB3	19:S:47:ARG:HG2	2.02	0.41
20:U:68:ARG:NH1	20:U:124:ASP:O	2.51	0.41
36:w:213:VAL:HG21	36:w:362:CYS:HB3	2.02	0.41
36:w:431:LYS:HA	36:w:431:LYS:HD3	1.95	0.41
37:y:96:LYS:H	37:y:96:LYS:HG2	1.58	0.41
41:W:353:LEU:HD11	41:W:389:SER:HB3	2.02	0.41
47:d:60:VAL:HG23	47:d:61:VAL:HG23	2.01	0.41
51:l:29:ARG:NH1	59:f:265:GLU:OE2	2.54	0.41
57:q:251:GLU:OE2	57:q:255:GLN:NE2	2.48	0.41
1:N:52:PRO:HA	1:N:96:LEU:HD11	2.03	0.41
2:2:2652:G:N2	22:X:61:MET:SD	2.91	0.41
2:2:3664:G:H2'	2:2:3665:G:H8	1.86	0.41
2:2:4439:U:H1'	43:4:93:LYS:HB3	2.02	0.41
3:6:26:VAL:O	3:6:50:HIS:HA	2.21	0.41
3:6:142:VAL:HG23	3:6:148:VAL:HG12	2.03	0.41
20:U:165:THR:OG1	20:U:166:SER:N	2.53	0.41
22:X:38:THR:HA	22:X:45:THR:HA	2.03	0.41
28:l:105:ASP:OD1	28:l:105:ASP:N	2.46	0.41
35:v:39:TYR:O	35:v:104:PHE:HA	2.20	0.41
51:l:201:ILE:HA	51:l:208:PHE:HE1	1.86	0.41
1:N:293:PRO:HG2	1:N:330:LEU:HD11	2.04	0.40
2:2:1699:A:OP1	2:2:2085:G:O2'	2.37	0.40
2:2:2017:A:O2'	2:2:2018:C:O4'	2.38	0.40
2:2:2486:G:OP2	59:f:456:ARG:HD3	2.21	0.40
2:2:4154:G:H5''	59:f:464:LYS:HZ1	1.86	0.40
4:7:23:ARG:HH11	6:9:28:LEU:HD12	1.86	0.40
25:b:76:LYS:HE2	25:b:76:LYS:HB2	1.91	0.40
25:b:83:ARG:HG2	25:b:92:ASN:HB3	2.03	0.40
27:h:35:SER:OG	27:h:36:LYS:N	2.55	0.40
28:l:33:LYS:HA	45:k:90:MET:HG3	2.03	0.40
35:v:96:LEU:HD21	35:v:102:LEU:HD21	2.03	0.40
37:y:85:LEU:HD11	37:y:102:GLY:HA3	2.03	0.40
56:3:64:G:H2'	56:3:65:G:H8	1.85	0.40
2:2:2302:C:O2'	45:k:102:ASN:O	2.37	0.40
2:2:2763:U:C3'	59:f:391:ARG:HH21	2.33	0.40
2:2:4432:C:H2'	2:2:4433:G:H8	1.86	0.40
3:6:101:LEU:HD13	3:6:107:VAL:HG21	2.04	0.40
3:6:219:GLU:O	3:6:222:PHE:O	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:7:TYR:HD2	6:9:99:GLN:HG2	1.87	0.40
8:B:57:VAL:HG23	8:B:366:LYS:HB3	2.03	0.40
31:o:245:GLN:NE2	31:o:249:ASP:OD2	2.49	0.40
45:k:89:LEU:HD13	45:k:118:LEU:HD22	2.02	0.40
56:3:7:G:O6	56:3:112:U:O4	2.39	0.40
57:q:152:LYS:HD2	57:q:217:TYR:HD2	1.86	0.40
2:2:4436:U:H5	43:4:143:ARG:HD3	1.85	0.40
25:b:7:LEU:HD12	25:b:106:VAL:HG12	2.03	0.40
40:R:208:MET:HE2	40:R:233:PRO:HG3	2.03	0.40
41:W:104:THR:OG1	41:W:485:ARG:O	2.39	0.40
43:4:247:LEU:HD23	43:4:247:LEU:HA	1.96	0.40
43:4:272:PHE:O	43:4:276:ARG:HB2	2.22	0.40
2:2:907:C:H2'	2:2:908:G:H8	1.87	0.40
2:2:1328:G:O2'	2:2:2349:A:OP1	2.39	0.40
2:2:1870:C:H2'	2:2:1871:A2M:H8	2.04	0.40
2:2:4622:A:H4'	8:B:13:SER:HB2	2.03	0.40
9:D:204:ARG:NH1	9:D:205:ARG:O	2.54	0.40
11:G:55:VAL:HG21	58:g:41:ARG:HD2	2.02	0.40
18:Q:83:VAL:HG12	18:Q:114:VAL:HG21	2.04	0.40
44:Y:47:TYR:OH	44:Y:57:CYS:O	2.38	0.40
50:c:240:LYS:HD3	50:c:240:LYS:HA	1.89	0.40
51:1:158:ARG:HG2	51:1:198:ILE:HD13	2.03	0.40
57:q:182:PHE:CZ	59:f:246:SER:HB3	2.56	0.40
58:g:73:HIS:HD2	58:g:112:ALA:HA	1.86	0.40
2:2:142:G:O2'	2:2:144:G:OP1	2.35	0.40
2:2:4753:U:OP1	30:n:100:ARG:NH1	2.54	0.40
18:Q:202:ALA:O	18:Q:206:ASP:HB2	2.21	0.40
43:4:412:ASP:HB3	43:4:415:LYS:HE3	2.03	0.40
59:f:235:ALA:HB3	59:f:448:ARG:HG2	2.03	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	N	324/687 (47%)	309 (95%)	15 (5%)	0	100	100
3	6	242/245 (99%)	227 (94%)	15 (6%)	0	100	100
4	7	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
6	9	82/134 (61%)	71 (87%)	11 (13%)	0	100	100
7	A	41/159 (26%)	39 (95%)	2 (5%)	0	100	100
8	B	401/403 (100%)	382 (95%)	18 (4%)	1 (0%)	43	73
9	D	356/427 (83%)	334 (94%)	22 (6%)	0	100	100
10	E	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
11	G	239/266 (90%)	225 (94%)	14 (6%)	0	100	100
12	H	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
13	I	188/192 (98%)	179 (95%)	9 (5%)	0	100	100
14	J	213/260 (82%)	207 (97%)	6 (3%)	0	100	100
15	L	108/148 (73%)	101 (94%)	7 (6%)	0	100	100
16	M	84/97 (87%)	80 (95%)	4 (5%)	0	100	100
17	P	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
18	Q	208/211 (99%)	200 (96%)	8 (4%)	0	100	100
19	S	133/215 (62%)	127 (96%)	6 (4%)	0	100	100
20	U	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
21	V	199/203 (98%)	192 (96%)	7 (4%)	0	100	100
22	X	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
23	Z	149/188 (79%)	147 (99%)	2 (1%)	0	100	100
24	a	146/196 (74%)	142 (97%)	4 (3%)	0	100	100
25	b	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
26	e	129/140 (92%)	118 (92%)	11 (8%)	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%)	221 (90%)	25 (10%)	0	100	100
30	n	107/110 (97%)	102 (95%)	5 (5%)	0	100	100
31	o	231/288 (80%)	220 (95%)	11 (5%)	0	100	100
32	p	224/248 (90%)	216 (96%)	8 (4%)	0	100	100
33	r	80/360 (22%)	77 (96%)	3 (4%)	0	100	100
34	u	63/549 (12%)	58 (92%)	4 (6%)	1 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	v	215/239 (90%)	206 (96%)	9 (4%)	0	100	100
36	w	427/731 (58%)	406 (95%)	19 (4%)	2 (0%)	24	59
37	y	163/165 (99%)	155 (95%)	8 (5%)	0	100	100
38	z	63/129 (49%)	60 (95%)	3 (5%)	0	100	100
39	C	163/178 (92%)	145 (89%)	18 (11%)	0	100	100
40	R	291/297 (98%)	273 (94%)	17 (6%)	1 (0%)	36	68
41	W	386/485 (80%)	365 (95%)	21 (5%)	0	100	100
42	T	120/160 (75%)	112 (93%)	8 (7%)	0	100	100
43	4	607/634 (96%)	555 (91%)	47 (8%)	5 (1%)	16	50
44	Y	165/184 (90%)	158 (96%)	7 (4%)	0	100	100
45	k	127/135 (94%)	120 (94%)	7 (6%)	0	100	100
46	j	109/125 (87%)	103 (94%)	6 (6%)	0	100	100
47	d	102/128 (80%)	95 (93%)	7 (7%)	0	100	100
48	t	109/293 (37%)	105 (96%)	4 (4%)	0	100	100
50	c	237/490 (48%)	231 (98%)	6 (2%)	0	100	100
51	l	224/255 (88%)	216 (96%)	7 (3%)	1 (0%)	30	62
52	K	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
53	F	111/117 (95%)	109 (98%)	2 (2%)	0	100	100
54	i	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
55	O	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
57	q	398/588 (68%)	382 (96%)	16 (4%)	0	100	100
58	g	143/156 (92%)	135 (94%)	8 (6%)	0	100	100
59	f	254/478 (53%)	236 (93%)	17 (7%)	1 (0%)	30	62
All	All	10023/13467 (74%)	9493 (95%)	518 (5%)	12 (0%)	49	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	u	55	PRO
51	l	24	ASN
59	f	203	ASP
40	R	270	LYS
43	4	88	ASP
36	w	132	VAL

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Mol	Chain	Res	Type
43	4	230	LEU
43	4	407	ASP
36	w	323	LYS
43	4	427	ASP
43	4	366	THR
8	B	5	LYS

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	N	308/629 (49%)	308 (100%)	0	100	100
3	6	212/213 (100%)	212 (100%)	0	100	100
4	7	126/149 (85%)	126 (100%)	0	100	100
6	9	74/114 (65%)	74 (100%)	0	100	100
7	A	34/126 (27%)	34 (100%)	0	100	100
8	B	349/349 (100%)	349 (100%)	0	100	100
9	D	298/348 (86%)	298 (100%)	0	100	100
10	E	83/97 (86%)	83 (100%)	0	100	100
11	G	203/223 (91%)	203 (100%)	0	100	100
12	H	109/110 (99%)	109 (100%)	0	100	100
13	I	169/171 (99%)	169 (100%)	0	100	100
14	J	191/228 (84%)	191 (100%)	0	100	100
15	L	94/121 (78%)	94 (100%)	0	100	100
16	M	73/80 (91%)	73 (100%)	0	100	100
17	P	47/48 (98%)	47 (100%)	0	100	100
18	Q	176/177 (99%)	176 (100%)	0	100	100
19	S	115/161 (71%)	115 (100%)	0	100	100
20	U	171/172 (99%)	171 (100%)	0	100	100
21	V	173/174 (99%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	X	74/75 (99%)	74 (100%)	0	100	100
23	Z	136/165 (82%)	136 (100%)	0	100	100
24	a	133/175 (76%)	133 (100%)	0	100	100
25	b	157/157 (100%)	157 (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	r	76/312 (24%)	76 (100%)	0	100	100
34	u	61/485 (13%)	61 (100%)	0	100	100
35	v	194/214 (91%)	194 (100%)	0	100	100
36	w	385/654 (59%)	385 (100%)	0	100	100
37	y	137/137 (100%)	137 (100%)	0	100	100
38	z	61/115 (53%)	61 (100%)	0	100	100
39	C	138/149 (93%)	138 (100%)	0	100	100
40	R	246/250 (98%)	246 (100%)	0	100	100
41	W	322/404 (80%)	322 (100%)	0	100	100
42	T	109/140 (78%)	109 (100%)	0	100	100
43	4	554/574 (96%)	554 (100%)	0	100	100
44	Y	147/163 (90%)	147 (100%)	0	100	100
45	k	115/121 (95%)	115 (100%)	0	100	100
46	j	101/110 (92%)	101 (100%)	0	100	100
47	d	94/115 (82%)	94 (100%)	0	100	100
48	t	103/274 (38%)	103 (100%)	0	100	100
50	c	222/437 (51%)	222 (100%)	0	100	100
51	l	206/228 (90%)	206 (100%)	0	100	100
52	K	86/89 (97%)	86 (100%)	0	100	100
53	F	97/100 (97%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	i	117/118 (99%)	117 (100%)	0	100	100
55	O	64/65 (98%)	64 (100%)	0	100	100
57	q	359/509 (70%)	359 (100%)	0	100	100
58	g	126/133 (95%)	126 (100%)	0	100	100
59	f	222/402 (55%)	222 (100%)	0	100	100
All	All	8862/11678 (76%)	8862 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	41	ASN
1	N	111	ASN
1	N	149	ASN
1	N	155	ASN
1	N	158	ASN
1	N	379	ASN
3	6	82	GLN
3	6	86	ASN
3	6	156	ASN
4	7	24	ASN
4	7	130	ASN
4	7	132	HIS
6	9	99	GLN
8	B	121	ASN
8	B	167	GLN
9	D	60	HIS
9	D	310	HIS
9	D	317	ASN
9	D	329	ASN
10	E	15	ASN
10	E	72	HIS
13	I	8	GLN
13	I	98	HIS
13	I	116	ASN
13	I	138	GLN
14	J	4	ASN
14	J	55	HIS
14	J	247	ASN

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Mol	Chain	Res	Type
17	P	17	GLN
18	Q	15	HIS
18	Q	149	GLN
18	Q	205	GLN
19	S	20	HIS
19	S	66	HIS
19	S	70	GLN
19	S	78	GLN
19	S	120	ASN
20	U	37	HIS
20	U	149	GLN
20	U	156	HIS
21	V	180	GLN
21	V	184	ASN
23	Z	7	HIS
24	a	39	GLN
24	a	134	ASN
24	a	141	HIS
26	e	108	ASN
28	l	21	ASN
29	m	187	HIS
29	m	216	HIS
30	n	99	HIS
31	o	157	HIS
32	p	110	GLN
33	r	256	GLN
33	r	312	ASN
35	v	62	HIS
35	v	106	ASN
35	v	186	GLN
36	w	149	GLN
36	w	222	GLN
36	w	255	ASN
37	y	66	ASN
37	y	149	HIS
38	z	89	GLN
38	z	92	GLN
38	z	98	ASN
39	C	98	ASN
40	R	63	GLN
40	R	111	ASN
40	R	225	GLN

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Mol	Chain	Res	Type
41	W	469	GLN
42	T	77	ASN
43	4	41	HIS
43	4	84	ASN
43	4	196	GLN
43	4	538	HIS
45	k	57	ASN
45	k	63	ASN
46	j	34	HIS
48	t	67	GLN
51	1	94	HIS
51	1	185	HIS
51	1	229	ASN
52	K	20	ASN
57	q	197	GLN
57	q	211	HIS
57	q	240	GLN
57	q	335	ASN
57	q	403	ASN
57	q	422	HIS
58	g	33	HIS
59	f	216	GLN
59	f	248	ASN
59	f	286	GLN
59	f	341	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	3461/5054 (68%)	820 (23%)	21 (0%)
49	x	0/160	-	-
5	8	155/156 (99%)	29 (18%)	0
56	3	113/120 (94%)	23 (20%)	2 (1%)
All	All	3729/5490 (67%)	872 (23%)	23 (0%)

All (872) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	25	A
2	2	39	A
2	2	42	A

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Mol	Chain	Res	Type
2	2	44	A
2	2	48	G
2	2	56	A
2	2	59	A
2	2	64	A
2	2	65	A
2	2	69	A
2	2	72	C
2	2	73	A
2	2	76	A
2	2	84	A
2	2	91	G
2	2	98	A
2	2	108	A
2	2	109	G
2	2	110	C
2	2	112	C
2	2	119	G
2	2	120	A
2	2	122	U
2	2	131	C
2	2	132	G
2	2	134	G
2	2	135	G
2	2	137	G
2	2	144	G
2	2	152	U
2	2	159	C
2	2	169	G
2	2	170	C
2	2	172	C
2	2	175	C
2	2	183	C
2	2	185	C
2	2	188	G
2	2	197	A
2	2	200	U
2	2	209	U
2	2	217	C
2	2	218	A
2	2	234	G
2	2	237	B9B

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Mol	Chain	Res	Type
2	2	254	G
2	2	256	G
2	2	262	G
2	2	265	C
2	2	266	C
2	2	279	A
2	2	280	G
2	2	297	U
2	2	306	A
2	2	315	G
2	2	316	U
2	2	340	C
2	2	345	C
2	2	349	A
2	2	363	A
2	2	373	OMG
2	2	387	G
2	2	398	A2M
2	2	407	A
2	2	409	G
2	2	410	A
2	2	412	G
2	2	432	U
2	2	433	A
2	2	449	C
2	2	450	G
2	2	452	A
2	2	453	G
2	2	454	U
2	2	465	G
2	2	467	U
2	2	483	G
2	2	484	U
2	2	485	C
2	2	486	C
2	2	489	C
2	2	491	G
2	2	493	G
2	2	495	C
2	2	496	G
2	2	497	G
2	2	499	G

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Mol	Chain	Res	Type
2	2	500	G
2	2	501	C
2	2	502	C
2	2	503	C
2	2	504	G
2	2	505	G
2	2	509	A
2	2	510	U
2	2	511	C
2	2	513	U
2	2	514	U
2	2	515	C
2	2	516	C
2	2	518	G
2	2	519	C
2	2	653	U
2	2	654	C
2	2	657	C
2	2	659	G
2	2	666	G
2	2	667	A
2	2	668	C
2	2	673	C
2	2	685	C
2	2	686	A
2	2	692	A
2	2	696	C
2	2	703	G
2	2	704	C
2	2	731	G
2	2	738	C
2	2	739	G
2	2	740	G
2	2	742	G
2	2	746	A
2	2	759	G
2	2	904	C
2	2	905	C
2	2	906	C
2	2	913	U
2	2	914	U
2	2	915	A

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Mol	Chain	Res	Type
2	2	916	C
2	2	917	A
2	2	918	G
2	2	924	C
2	2	925	C
2	2	926	G
2	2	932	A
2	2	933	G
2	2	936	C
2	2	941	C
2	2	943	A
2	2	944	A
2	2	945	U
2	2	956	A
2	2	959	G
2	2	960	A
2	2	961	G
2	2	962	C
2	2	965	G
2	2	966	A
2	2	967	C
2	2	968	C
2	2	969	C
2	2	970	G
2	2	977	C
2	2	982	U
2	2	984	C
2	2	989	U
2	2	990	C
2	2	991	C
2	2	992	C
2	2	993	G
2	2	994	G
2	2	995	C
2	2	1048	G
2	2	1049	C
2	2	1051	G
2	2	1066	G
2	2	1067	G
2	2	1068	G
2	2	1070	G
2	2	1072	C

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Mol	Chain	Res	Type
2	2	1082	C
2	2	1170	G
2	2	1173	G
2	2	1177	U
2	2	1178	G
2	2	1179	U
2	2	1180	C
2	2	1181	C
2	2	1182	C
2	2	1183	C
2	2	1184	A
2	2	1185	G
2	2	1187	G
2	2	1189	G
2	2	1194	G
2	2	1195	G
2	2	1198	G
2	2	1200	G
2	2	1202	C
2	2	1203	G
2	2	1211	G
2	2	1215	C
2	2	1216	C
2	2	1219	G
2	2	1222	A
2	2	1241	C
2	2	1243	C
2	2	1245	C
2	2	1252	C
2	2	1253	G
2	2	1255	A
2	2	1256	G
2	2	1260	G
2	2	1265	G
2	2	1266	G
2	2	1269	G
2	2	1271	G
2	2	1272	C
2	2	1275	G
2	2	1280	C
2	2	1283	G
2	2	1284	G

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Mol	Chain	Res	Type
2	2	1287	G
2	2	1294	A
2	2	1296	G
2	2	1301	C
2	2	1302	U
2	2	1303	A
2	2	1314	C
2	2	1315	C
2	2	1323	A
2	2	1337	A
2	2	1354	A
2	2	1358	G
2	2	1359	G
2	2	1365	C
2	2	1366	G
2	2	1367	C
2	2	1370	G
2	2	1377	G
2	2	1378	C
2	2	1379	C
2	2	1381	U
2	2	1387	A
2	2	1394	G
2	2	1398	A
2	2	1399	G
2	2	1402	C
2	2	1404	G
2	2	1405	C
2	2	1407	C
2	2	1408	G
2	2	1409	C
2	2	1410	U
2	2	1412	G
2	2	1420	A
2	2	1439	C
2	2	1442	C
2	2	1444	G
2	2	1446	C
2	2	1448	G
2	2	1449	C
2	2	1465	G
2	2	1472	C

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Mol	Chain	Res	Type
2	2	1482	G
2	2	1483	C
2	2	1486	C
2	2	1497	A
2	2	1498	G
2	2	1503	A
2	2	1518	A
2	2	1525	A
2	2	1534	A2M
2	2	1547	A
2	2	1564	A
2	2	1566	C
2	2	1574	B9B
2	2	1578	U
2	2	1592	G
2	2	1595	G
2	2	1596	U
2	2	1612	G
2	2	1613	A
2	2	1624	G
2	2	1625	OMG
2	2	1626	G
2	2	1631	A
2	2	1633	G
2	2	1634	A
2	2	1638	A
2	2	1641	G
2	2	1649	U
2	2	1650	A
2	2	1654	G
2	2	1661	C
2	2	1671	U
2	2	1672	U
2	2	1673	U
2	2	1674	C
2	2	1675	C
2	2	1676	C
2	2	1677	U
2	2	1679	A
2	2	1680	G
2	2	1681	G
2	2	1691	G

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Mol	Chain	Res	Type
2	2	1697	G
2	2	1699	A
2	2	1700	G
2	2	1701	A
2	2	1703	C
2	2	1704	C
2	2	1705	G
2	2	1715	C
2	2	1717	C
2	2	1718	C
2	2	1719	A
2	2	1724	G
2	2	1731	C
2	2	1732	C
2	2	1796	U
2	2	1797	G
2	2	1803	G
2	2	1804	A
2	2	1806	G
2	2	1809	C
2	2	1810	G
2	2	1815	G
2	2	1816	C
2	2	1821	G
2	2	1822	U
2	2	1832	C
2	2	1834	U
2	2	1836	G
2	2	1837	A
2	2	1842	G
2	2	1854	G
2	2	1855	G
2	2	1856	C
2	2	1861	U
2	2	1862	U
2	2	1865	G
2	2	1869	G
2	2	1870	C
2	2	1871	A2M
2	2	1882	U
2	2	1883	OMG
2	2	1888	A

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Mol	Chain	Res	Type
2	2	1897	A
2	2	1916	G
2	2	1918	U
2	2	1919	G
2	2	1920	C
2	2	1921	C
2	2	1922	G
2	2	1931	C
2	2	1932	A
2	2	1935	C
2	2	1939	A
2	2	1940	G
2	2	1942	A
2	2	1943	A
2	2	1944	A
2	2	1948	G
2	2	1956	A
2	2	1959	U
2	2	1960	A
2	2	1966	C
2	2	1972	G
2	2	1974	U
2	2	1979	A
2	2	1980	U
2	2	1981	G
2	2	1984	A
2	2	1985	G
2	2	1990	A
2	2	1997	U
2	2	2001	G
2	2	2002	A
2	2	2003	G
2	2	2004	U
2	2	2010	A
2	2	2011	C
2	2	2017	A
2	2	2018	C
2	2	2025	A
2	2	2026	A
2	2	2033	A
2	2	2034	G
2	2	2040	A

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Mol	Chain	Res	Type
2	2	2044	U
2	2	2046	G
2	2	2048	U
2	2	2055	G
2	2	2056	G
2	2	2069	A
2	2	2084	C
2	2	2085	G
2	2	2092	G
2	2	2093	A
2	2	2095	A
2	2	2096	G
2	2	2098	G
2	2	2101	C
2	2	2102	G
2	2	2104	G
2	2	2105	A
2	2	2110	C
2	2	2111	G
2	2	2112	G
2	2	2113	C
2	2	2252	G
2	2	2253	A
2	2	2255	C
2	2	2256	C
2	2	2258	C
2	2	2259	G
2	2	2260	C
2	2	2263	A
2	2	2268	A
2	2	2289	C
2	2	2300	A
2	2	2301	G
2	2	2306	G
2	2	2313	A
2	2	2331	G
2	2	2333	G
2	2	2348	G
2	2	2351	C
2	2	2360	A
2	2	2364	OMG
2	2	2395	A

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Mol	Chain	Res	Type
2	2	2410	C
2	2	2416	G
2	2	2417	A
2	2	2418	A
2	2	2422	OMC
2	2	2424	OMG
2	2	2425	U
2	2	2439	G
2	2	2441	C
2	2	2450	G
2	2	2465	C
2	2	2471	G
2	2	2474	G
2	2	2475	G
2	2	2476	G
2	2	2477	A
2	2	2478	C
2	2	2484	A
2	2	2486	G
2	2	2487	G
2	2	2488	C
2	2	2489	C
2	2	2490	U
2	2	2497	C
2	2	2507	A
2	2	2511	A
2	2	2512	A
2	2	2513	A
2	2	2518	G
2	2	2519	U
2	2	2529	A
2	2	2543	A
2	2	2544	G
2	2	2545	U
2	2	2546	G
2	2	2547	G
2	2	2554	U
2	2	2555	G
2	2	2559	G
2	2	2560	C
2	2	2566	G
2	2	2567	G

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Mol	Chain	Res	Type
2	2	2583	C
2	2	2587	A
2	2	2589	C
2	2	2601	A
2	2	2618	G
2	2	2627	C
2	2	2638	G
2	2	2653	C
2	2	2661	U
2	2	2662	G
2	2	2669	C
2	2	2670	C
2	2	2675	G
2	2	2687	U
2	2	2694	G
2	2	2695	A
2	2	2696	A
2	2	2707	U
2	2	2708	U
2	2	2709	C
2	2	2710	C
2	2	2711	G
2	2	2719	C
2	2	2721	G
2	2	2723	U
2	2	2724	G
2	2	2725	A
2	2	2726	G
2	2	2739	C
2	2	2742	G
2	2	2743	A
2	2	2753	G
2	2	2754	B9B
2	2	2758	G
2	2	2761	U
2	2	2763	U
2	2	2769	U
2	2	2770	C
2	2	2772	C
2	2	2787	A
2	2	2788	U
2	2	2790	U

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Mol	Chain	Res	Type
2	2	2799	G
2	2	2814	C
2	2	2815	A
2	2	2826	U
2	2	2827	G
2	2	2842	G
2	2	2855	G
2	2	2875	C
2	2	2901	G
2	2	2902	G
2	2	2904	U
2	2	2905	C
2	2	2906	G
2	2	2908	U
2	2	2909	C
2	2	3585	G
2	2	3588	C
2	2	3591	C
2	2	3594	C
2	2	3595	U
2	2	3596	A
2	2	3597	G
2	2	3606	U
2	2	3615	G
2	2	3616	U
2	2	3626	G
2	2	3635	A
2	2	3644	U
2	2	3662	A
2	2	3663	A
2	2	3672	G
2	2	3673	C
2	2	3679	U
2	2	3680	U
2	2	3682	A
2	2	3691	G
2	2	3696	C
2	2	3702	A
2	2	3710	G
2	2	3711	A
2	2	3712	A
2	2	3713	U

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Mol	Chain	Res	Type
2	2	3714	G
2	2	3722	G
2	2	3729	U
2	2	3735	G
2	2	3736	A
2	2	3748	A
2	2	3750	G
2	2	3753	G
2	2	3771	C
2	2	3772	U
2	2	3773	U
2	2	3775	A
2	2	3776	G
2	2	3833	C
2	2	3838	U
2	2	3839	G
2	2	3840	U
2	2	3867	A2M
2	2	3875	G
2	2	3876	A
2	2	3877	A
2	2	3879	G
2	2	3897	B8K
2	2	3903	A
2	2	3904	G
2	2	3905	A
2	2	3906	A
2	2	3914	U
2	2	3915	U
2	2	3924	C
2	2	3938	G
2	2	4076	G
2	2	4084	G
2	2	4085	A
2	2	4095	G
2	2	4097	G
2	2	4099	G
2	2	4100	C
2	2	4101	C
2	2	4102	C
2	2	4103	C
2	2	4104	G

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Mol	Chain	Res	Type
2	2	4105	A
2	2	4107	G
2	2	4108	G
2	2	4111	U
2	2	4112	C
2	2	4114	C
2	2	4115	G
2	2	4116	C
2	2	4117	U
2	2	4119	C
2	2	4121	G
2	2	4127	A
2	2	4133	C
2	2	4139	G
2	2	4140	C
2	2	4141	G
2	2	4142	C
2	2	4143	G
2	2	4144	C
2	2	4146	G
2	2	4147	G
2	2	4149	C
2	2	4157	A
2	2	4158	C
2	2	4162	C
2	2	4163	U
2	2	4170	A
2	2	4183	G
2	2	4184	G
2	2	4207	C
2	2	4211	C
2	2	4223	C
2	2	4226	G
2	2	4228	G
2	2	4229	U
2	2	4230	C
2	2	4231	C
2	2	4233	A
2	2	4234	A
2	2	4235	G
2	2	4236	G
2	2	4242	U

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Mol	Chain	Res	Type
2	2	4251	A
2	2	4254	G
2	2	4255	A
2	2	4258	C
2	2	4265	U
2	2	4266	G
2	2	4267	G
2	2	4268	A
2	2	4271	A
2	2	4273	A
2	2	4274	A
2	2	4275	G
2	2	4278	C
2	2	4279	A
2	2	4280	A
2	2	4281	A
2	2	4286	C
2	2	4288	C
2	2	4290	U
2	2	4291	G
2	2	4292	A
2	2	4297	G
2	2	4302	U
2	2	4313	A
2	2	4315	A
2	2	4319	C
2	2	4321	U
2	2	4323	A
2	2	4329	G
2	2	4330	G
2	2	4332	C
2	2	4340	U
2	2	4341	C
2	2	4342	C
2	2	4343	U
2	2	4347	G
2	2	4348	A
2	2	4349	C
2	2	4350	C
2	2	4368	G
2	2	4370	G
2	2	4371	G

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Mol	Chain	Res	Type
2	2	4372	U
2	2	4387	C
2	2	4395	U
2	2	4396	A
2	2	4401	G
2	2	4413	C
2	2	4414	A
2	2	4416	G
2	2	4417	C
2	2	4418	G
2	2	4419	U
2	2	4420	U
2	2	4421	C
2	2	4422	A
2	2	4423	U
2	2	4424	A
2	2	4425	G
2	2	4426	C
2	2	4427	G
2	2	4428	A
2	2	4433	G
2	2	4436	U
2	2	4437	U
2	2	4438	U
2	2	4440	G
2	2	4441	A
2	2	4446	U
2	2	4447	C
2	2	4449	A
2	2	4450	U
2	2	4451	G
2	2	4452	U
2	2	4453	C
2	2	4464	A
2	2	4466	C
2	2	4475	G
2	2	4476	C
2	2	4484	A
2	2	4498	U
2	2	4499	G
2	2	4500	U
2	2	4502	C

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Mol	Chain	Res	Type
2	2	4503	A
2	2	4512	U
2	2	4513	A
2	2	4518	A
2	2	4519	C
2	2	4524	G
2	2	4529	B8W
2	2	4543	G
2	2	4545	G
2	2	4548	A
2	2	4550	7MG
2	2	4555	U
2	2	4556	U
2	2	4557	U
2	2	4558	U
2	2	4560	C
2	2	4567	G
2	2	4584	A
2	2	4589	A
2	2	4590	A
2	2	4599	A
2	2	4600	G
2	2	4601	U
2	2	4607	A
2	2	4608	G
2	2	4635	A
2	2	4636	U
2	2	4637	OMG
2	2	4656	A
2	2	4670	C
2	2	4672	A
2	2	4678	G
2	2	4684	A
2	2	4694	G
2	2	4695	C
2	2	4708	A
2	2	4709	U
2	2	4719	G
2	2	4730	C
2	2	4731	G
2	2	4732	G
2	2	4733	C

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Mol	Chain	Res	Type
2	2	4734	A
2	2	4740	G
2	2	4741	C
2	2	4742	G
2	2	4745	G
2	2	4751	G
2	2	4754	G
2	2	4757	C
2	2	4759	C
2	2	4761	G
2	2	4765	G
2	2	4771	C
2	2	4773	C
2	2	4776	G
2	2	4870	OMG
2	2	4871	C
2	2	4872	2MG
2	2	4875	G
2	2	4877	G
2	2	4882	U
2	2	4883	C
2	2	4889	G
2	2	4893	A
2	2	4895	C
2	2	4896	G
2	2	4899	G
2	2	4900	C
2	2	4901	G
2	2	4910	G
2	2	4912	G
2	2	4914	C
2	2	4916	G
2	2	4927	G
2	2	4928	C
2	2	4938	A
2	2	4940	C
2	2	4941	G
2	2	4943	A
2	2	4949	G
2	2	4976	U
2	2	4988	U
2	2	4989	U

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Mol	Chain	Res	Type
2	2	4991	U
2	2	5013	C
2	2	5014	A
2	2	5017	G
2	2	5022	U
2	2	5025	C
2	2	5026	U
2	2	5027	C
2	2	5028	G
2	2	5030	U
2	2	5031	G
2	2	5034	A
2	2	5041	G
2	2	5047	C
2	2	5050	C
2	2	5054	C
2	2	5058	A
2	2	5062	G
2	2	5069	U
5	8	25	G
5	8	34	U
5	8	35	C
5	8	39	G
5	8	48	A
5	8	52	A
5	8	59	A
5	8	62	A
5	8	63	U
5	8	80	A
5	8	82	A
5	8	84	A
5	8	85	U
5	8	103	A
5	8	104	A
5	8	105	C
5	8	108	A
5	8	110	U
5	8	114	G
5	8	123	U
5	8	124	U
5	8	125	C
5	8	126	C

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Mol	Chain	Res	Type
5	8	127	U
5	8	128	C
5	8	147	G
5	8	150	C
5	8	151	G
5	8	156	U
56	3	7	G
56	3	11	A
56	3	22	A
56	3	29	C
56	3	41	G
56	3	48	G
56	3	49	A
56	3	51	G
56	3	52	C
56	3	53	U
56	3	54	A
56	3	63	C
56	3	64	G
56	3	72	U
56	3	73	U
56	3	74	A
56	3	75	G
56	3	83	A
56	3	84	U
56	3	85	G
56	3	86	G
56	3	100	A
56	3	110	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	406	C
2	2	914	U
2	2	1184	A
2	2	1633	G
2	2	1678	C
2	2	1808	C
2	2	1931	C
2	2	1980	U
2	2	2033	A

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Mol	Chain	Res	Type
2	2	2486	G
2	2	2487	G
2	2	2496	G
2	2	2760	G
2	2	3701	OMC
2	2	3774	A
2	2	3875	G
2	2	3905	A
2	2	4228	G
2	2	4555	U
2	2	4636	U
2	2	4913	G
56	3	51	G
56	3	72	U

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

67 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
2	P7G	2	3880	2	24,28,29	4.19	11 (45%)	27,41,44	1.37	2 (7%)
2	BGH	2	3899	2	25,29,30	4.60	17 (68%)	31,43,46	2.58	11 (35%)
2	OMC	2	4536	2	19,22,23	3.04	8 (42%)	26,31,34	1.12	3 (11%)
2	B9B	2	1574	2	25,28,29	1.73	5 (20%)	35,40,43	5.15	11 (31%)
2	OMG	2	373	2	23,26,27	2.68	8 (34%)	33,38,41	2.71	13 (39%)
2	B9H	2	2786	2	20,25,26	3.24	3 (15%)	22,35,38	1.95	5 (22%)
2	B8W	2	4472	2	23,26,27	2.74	5 (21%)	33,38,41	2.47	15 (45%)
2	7MG	2	1605	2	22,26,27	3.87	10 (45%)	29,39,42	2.00	8 (27%)
2	5MU	2	4083	2	19,22,23	7.22	8 (42%)	28,32,35	3.37	10 (35%)
2	B8K	2	4690	2	24,28,29	3.30	12 (50%)	30,42,45	2.67	11 (36%)
2	OMG	2	4870	2	23,26,27	2.70	8 (34%)	33,38,41	3.00	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	7MG	2	2522	2	22,26,27	3.76	10 (45%)	29,39,42	1.97	10 (34%)
2	A2M	2	1534	2	22,25,26	3.18	9 (40%)	31,36,39	2.99	10 (32%)
2	OMG	2	2773	2	23,26,27	2.70	8 (34%)	33,38,41	2.78	9 (27%)
2	A2M	2	3825	2	22,25,26	3.19	9 (40%)	31,36,39	3.01	10 (32%)
2	A2M	2	2401	2	22,25,26	3.20	9 (40%)	31,36,39	3.03	11 (35%)
2	OMC	2	3887	2	19,22,23	3.05	8 (42%)	26,31,34	1.01	1 (3%)
2	B8W	2	4529	2	23,26,27	2.78	5 (21%)	33,38,41	2.58	13 (39%)
2	OMG	2	1522	2	23,26,27	2.68	8 (34%)	33,38,41	2.81	10 (30%)
2	A2M	2	3723	2	22,25,26	3.17	9 (40%)	31,36,39	3.01	10 (32%)
2	A2M	2	1524	2	22,25,26	3.20	9 (40%)	31,36,39	2.99	11 (35%)
2	OMU	2	4620	2	19,22,23	2.97	8 (42%)	26,31,34	1.74	5 (19%)
2	M7A	2	4564	2	20,25,26	2.02	3 (15%)	28,37,40	3.91	7 (25%)
2	B9B	2	2754	2	25,28,29	1.73	5 (20%)	35,40,43	5.23	11 (31%)
2	2MG	2	4872	2	23,26,27	2.93	8 (34%)	32,38,41	2.27	11 (34%)
2	B8Q	2	1456	2	17,22,23	2.96	5 (29%)	22,32,35	2.21	6 (27%)
2	B8W	2	2380	2	23,26,27	2.71	5 (21%)	33,38,41	2.57	14 (42%)
2	OMG	2	2424	2	23,26,27	2.72	8 (34%)	33,38,41	2.91	10 (30%)
2	B8T	2	4671	2	19,22,23	3.61	8 (42%)	26,31,34	0.93	1 (3%)
2	UR3	2	4597	2	19,22,23	2.82	6 (31%)	26,32,35	1.88	3 (11%)
2	OMC	2	2861	2	19,22,23	3.04	8 (42%)	26,31,34	1.10	3 (11%)
2	OMG	2	4623	2	23,26,27	2.67	8 (34%)	33,38,41	2.76	12 (36%)
2	2MG	2	1517	2	23,26,27	2.99	8 (34%)	32,38,41	2.35	8 (25%)
2	A2M	2	4523	2	22,25,26	3.16	9 (40%)	31,36,39	3.00	10 (32%)
2	7MG	2	4550	2	22,26,27	3.85	10 (45%)	29,39,42	1.98	7 (24%)
2	A2M	2	2363	2	22,25,26	3.19	9 (40%)	31,36,39	2.98	11 (35%)
2	OMC	2	3869	2	19,22,23	3.02	8 (42%)	26,31,34	0.90	1 (3%)
2	OMG	2	4494	2	23,26,27	2.71	8 (34%)	33,38,41	2.81	10 (30%)
2	OMC	2	2804	2	19,22,23	2.98	8 (42%)	26,31,34	0.76	0
2	OMC	2	2422	2	19,22,23	3.03	8 (42%)	26,31,34	1.00	2 (7%)
2	OMG	2	2050	2	23,26,27	2.65	8 (34%)	33,38,41	2.72	11 (33%)
2	A2M	2	398	2	22,25,26	3.20	9 (40%)	31,36,39	2.94	10 (32%)
2	P7G	2	1909	2	24,28,29	4.09	11 (45%)	27,41,44	1.55	3 (11%)
2	OMG	2	4637	2	23,26,27	2.66	8 (34%)	33,38,41	2.74	11 (33%)
2	OMG	2	1625	2	23,26,27	2.71	8 (34%)	33,38,41	2.76	10 (30%)
2	OMC	2	3909	2	19,22,23	3.13	8 (42%)	26,31,34	1.85	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	B8W	2	4185	2	23,26,27	2.75	6 (26%)	33,38,41	2.61	13 (39%)
2	2MG	2	729	2	23,26,27	2.97	8 (34%)	32,38,41	2.31	8 (25%)
2	I4U	2	1659	2	21,24,25	3.56	9 (42%)	27,34,37	1.11	2 (7%)
2	2MG	2	978	2	23,26,27	3.03	8 (34%)	32,38,41	2.20	9 (28%)
2	B9B	2	237	2	25,28,29	1.74	6 (24%)	35,40,43	5.18	12 (34%)
2	P4U	2	1348	2	21,24,25	3.61	8 (38%)	27,33,36	1.06	2 (7%)
2	A2M	2	3867	2	22,25,26	3.16	9 (40%)	31,36,39	2.98	10 (32%)
2	OMG	2	1316	2	23,26,27	2.68	8 (34%)	33,38,41	2.74	11 (33%)
5	OMU	8	14	2,5	19,22,23	2.96	8 (42%)	26,31,34	1.79	6 (23%)
2	OMC	2	3701	2	19,22,23	3.01	8 (42%)	26,31,34	0.74	0
2	UR3	2	4530	2	19,22,23	2.89	6 (31%)	26,32,35	1.26	2 (7%)
2	OMC	2	2365	2	19,22,23	2.99	8 (42%)	26,31,34	0.74	0
2	A2M	2	4571	2	22,25,26	3.16	9 (40%)	31,36,39	2.94	11 (35%)
2	A2M	2	1871	2	22,25,26	3.19	10 (45%)	31,36,39	2.97	11 (35%)
2	OMG	2	2364	2	23,26,27	2.66	8 (34%)	33,38,41	2.73	11 (33%)
2	B8K	2	3897	2	24,28,29	3.44	11 (45%)	30,42,45	2.53	11 (36%)
2	B8T	2	4483	2	19,22,23	3.66	8 (42%)	26,31,34	1.37	6 (23%)
2	A2M	2	3718	2	22,25,26	3.20	9 (40%)	31,36,39	2.92	10 (32%)
2	OMG	2	1883	2	23,26,27	2.72	8 (34%)	33,38,41	2.75	11 (33%)
2	E7G	2	2297	2	24,27,28	4.04	11 (45%)	30,40,43	2.12	9 (30%)
2	A2M	2	1326	2	22,25,26	3.18	9 (40%)	31,36,39	2.95	10 (32%)

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
2	P7G	2	3880	2	-	2/10/40/41	0/3/3/3
2	BGH	2	3899	2	-	1/13/43/44	0/3/3/3
2	OMC	2	4536	2	-	0/9/27/28	0/2/2/2
2	B9B	2	1574	2	-	3/11/29/30	0/3/3/3
2	OMG	2	373	2	-	1/9/27/28	0/3/3/3
2	B9H	2	2786	2	-	1/12/47/48	0/2/2/2
2	B8W	2	4472	2	-	2/9/27/28	0/3/3/3
2	7MG	2	1605	2	-	0/7/37/38	0/3/3/3
2	5MU	2	4083	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B8K	2	4690	2	-	0/11/41/42	0/3/3/3
2	OMG	2	4870	2	-	3/9/27/28	0/3/3/3
2	7MG	2	2522	2	-	0/7/37/38	0/3/3/3
2	A2M	2	1534	2	-	2/9/27/28	0/3/3/3
2	OMG	2	2773	2	-	0/9/27/28	0/3/3/3
2	A2M	2	3825	2	-	0/9/27/28	0/3/3/3
2	A2M	2	2401	2	-	0/9/27/28	0/3/3/3
2	OMC	2	3887	2	-	1/9/27/28	0/2/2/2
2	B8W	2	4529	2	-	2/9/27/28	0/3/3/3
2	OMG	2	1522	2	-	0/9/27/28	0/3/3/3
2	A2M	2	3723	2	-	0/9/27/28	0/3/3/3
2	A2M	2	1524	2	-	2/9/27/28	0/3/3/3
2	OMU	2	4620	2	-	0/9/27/28	0/2/2/2
2	M7A	2	4564	2	-	0/7/37/38	0/3/3/3
2	B9B	2	2754	2	-	4/11/29/30	0/3/3/3
2	2MG	2	4872	2	-	2/9/27/28	0/3/3/3
2	B8Q	2	1456	2	-	0/7/42/43	0/2/2/2
2	B8W	2	2380	2	-	2/9/27/28	0/3/3/3
2	OMG	2	2424	2	-	2/9/27/28	0/3/3/3
2	B8T	2	4671	2	-	0/7/27/28	0/2/2/2
2	UR3	2	4597	2	-	0/7/25/26	0/2/2/2
2	OMC	2	2861	2	-	0/9/27/28	0/2/2/2
2	OMG	2	4623	2	-	0/9/27/28	0/3/3/3
2	2MG	2	1517	2	-	1/9/27/28	0/3/3/3
2	A2M	2	4523	2	-	1/9/27/28	0/3/3/3
2	7MG	2	4550	2	-	2/7/37/38	0/3/3/3
2	A2M	2	2363	2	-	0/9/27/28	0/3/3/3
2	OMC	2	3869	2	-	0/9/27/28	0/2/2/2
2	OMG	2	4494	2	-	0/9/27/28	0/3/3/3
2	OMC	2	2804	2	-	0/9/27/28	0/2/2/2
2	OMC	2	2422	2	-	1/9/27/28	0/2/2/2
2	OMG	2	2050	2	-	0/9/27/28	0/3/3/3
2	A2M	2	398	2	-	2/9/27/28	0/3/3/3
2	P7G	2	1909	2	-	3/10/40/41	0/3/3/3
2	OMG	2	4637	2	-	4/9/27/28	0/3/3/3
2	OMG	2	1625	2	-	3/9/27/28	0/3/3/3
2	OMC	2	3909	2	-	2/9/27/28	0/2/2/2
2	B8W	2	4185	2	-	2/9/27/28	0/3/3/3
2	2MG	2	729	2	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	I4U	2	1659	2	-	1/9/29/30	0/2/2/2
2	2MG	2	978	2	-	0/9/27/28	0/3/3/3
2	B9B	2	237	2	-	6/11/29/30	0/3/3/3
2	P4U	2	1348	2	-	1/10/29/30	0/2/2/2
2	A2M	2	3867	2	-	3/9/27/28	0/3/3/3
2	OMG	2	1316	2	-	0/9/27/28	0/3/3/3
5	OMU	8	14	2,5	-	1/9/27/28	0/2/2/2
2	OMC	2	3701	2	-	2/9/27/28	0/2/2/2
2	UR3	2	4530	2	-	0/7/25/26	0/2/2/2
2	OMC	2	2365	2	-	0/9/27/28	0/2/2/2
2	A2M	2	4571	2	-	0/9/27/28	0/3/3/3
2	A2M	2	1871	2	-	2/9/27/28	0/3/3/3
2	OMG	2	2364	2	-	3/9/27/28	0/3/3/3
2	B8K	2	3897	2	-	3/11/41/42	0/3/3/3
2	B8T	2	4483	2	-	0/7/27/28	0/2/2/2
2	A2M	2	3718	2	-	0/9/27/28	0/3/3/3
2	OMG	2	1883	2	-	2/9/27/28	0/3/3/3
2	E7G	2	2297	2	-	1/9/39/40	0/3/3/3
2	A2M	2	1326	2	-	0/9/27/28	0/3/3/3

All (546) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4083	5MU	C4-C5	20.78	1.79	1.44
2	2	4083	5MU	C6-N1	16.00	1.65	1.38
2	2	4083	5MU	C6-C5	-11.45	1.15	1.34
2	2	4083	5MU	C4-N3	-11.05	1.18	1.38
2	2	1659	I4U	C4-N3	10.65	1.45	1.31
2	2	1348	P4U	C4-N3	10.59	1.45	1.31
2	2	2786	B9H	C2-N3	9.82	1.49	1.37
2	2	2297	E7G	C5-N7	9.67	1.46	1.35
2	2	3880	P7G	C5-N7	9.64	1.46	1.35
2	2	3880	P7G	C8-N9	9.43	1.51	1.46
2	2	1909	P7G	C5-N7	9.38	1.46	1.35
2	2	1909	P7G	C8-N9	9.28	1.51	1.46
2	2	3897	B8K	C8-N9	9.27	1.51	1.46
2	2	1605	7MG	C8-N9	9.11	1.51	1.46
2	2	2297	E7G	C8-N9	9.07	1.51	1.46
2	2	4550	7MG	C8-N9	9.03	1.51	1.46
2	2	3899	BGH	O4'-C1'	8.98	1.63	1.42
2	2	4472	B8W	O6-C6	8.90	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1871	A2M	C3'-C4'	-8.89	1.30	1.53
2	2	1524	A2M	C3'-C4'	-8.86	1.30	1.53
2	2	3825	A2M	C3'-C4'	-8.81	1.30	1.53
2	2	1326	A2M	C3'-C4'	-8.81	1.30	1.53
2	2	3723	A2M	C3'-C4'	-8.81	1.30	1.53
2	2	398	A2M	C3'-C4'	-8.78	1.30	1.53
2	2	1605	7MG	C5-N7	8.77	1.45	1.35
2	2	4529	B8W	O6-C6	8.77	1.49	1.35
2	2	2363	A2M	C3'-C4'	-8.76	1.30	1.53
2	2	2401	A2M	C3'-C4'	-8.75	1.30	1.53
2	2	3899	BGH	C2'-C1'	-8.75	1.30	1.53
2	2	1534	A2M	C3'-C4'	-8.75	1.30	1.53
2	2	2522	7MG	C5-N7	8.73	1.45	1.35
2	2	3718	A2M	C3'-C4'	-8.72	1.30	1.53
2	2	4571	A2M	C3'-C4'	-8.72	1.30	1.53
2	2	4550	7MG	C5-N7	8.70	1.45	1.35
2	2	3867	A2M	C3'-C4'	-8.70	1.30	1.53
2	2	4523	A2M	C3'-C4'	-8.63	1.30	1.53
2	2	4185	B8W	O6-C6	8.59	1.48	1.35
2	2	2522	7MG	C8-N9	8.57	1.50	1.46
2	2	2380	B8W	O6-C6	8.47	1.48	1.35
2	2	4690	B8K	C8-N9	8.38	1.50	1.46
2	2	1456	B8Q	C6-C5	8.37	1.52	1.33
2	2	3899	BGH	C8-N9	8.36	1.50	1.46
2	2	978	2MG	C2-N3	8.10	1.47	1.31
2	2	4185	B8W	C2-N2	8.05	1.50	1.33
2	2	4529	B8W	C2-N2	8.02	1.49	1.33
2	2	2380	B8W	C2-N2	7.95	1.49	1.33
2	2	729	2MG	C2-N3	7.88	1.47	1.31
2	2	1517	2MG	C2-N3	7.88	1.47	1.31
2	2	4472	B8W	C2-N2	7.84	1.49	1.33
2	2	4872	2MG	C2-N3	7.79	1.46	1.31
2	2	398	A2M	O4'-C4'	7.74	1.62	1.45
2	2	3718	A2M	O4'-C4'	7.73	1.62	1.45
2	2	1871	A2M	O4'-C4'	7.69	1.62	1.45
2	2	2401	A2M	O4'-C4'	7.66	1.62	1.45
2	2	2363	A2M	O4'-C4'	7.65	1.62	1.45
2	2	3825	A2M	O4'-C4'	7.64	1.62	1.45
2	2	1534	A2M	O4'-C4'	7.63	1.62	1.45
2	2	1326	A2M	O4'-C4'	7.61	1.62	1.45
2	2	4523	A2M	O4'-C4'	7.58	1.61	1.45
2	2	4571	A2M	O4'-C4'	7.52	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3723	A2M	O4'-C4'	7.51	1.61	1.45
2	2	4483	B8T	C2-N3	7.50	1.51	1.36
2	2	3899	BGH	O4'-C4'	-7.48	1.28	1.45
2	2	1524	A2M	O4'-C4'	7.47	1.61	1.45
2	2	3867	A2M	O4'-C4'	7.42	1.61	1.45
2	2	4671	B8T	C2-N3	7.27	1.51	1.36
2	2	4671	B8T	C4-N3	7.10	1.45	1.32
2	2	2786	B9H	C2-N1	7.07	1.48	1.38
2	2	4483	B8T	C4-N3	7.04	1.45	1.32
5	8	14	OMU	C2-N1	7.04	1.49	1.38
2	2	2786	B9H	C6-C5	6.99	1.49	1.33
2	2	4620	OMU	C2-N1	6.94	1.49	1.38
2	2	4671	B8T	C6-C5	6.92	1.51	1.35
2	2	978	2MG	C2-N2	6.86	1.48	1.33
2	2	1517	2MG	C2-N2	6.84	1.48	1.33
2	2	4530	UR3	C6-C5	6.84	1.51	1.35
2	2	729	2MG	C4-N3	6.84	1.50	1.34
2	2	4530	UR3	C2-N1	6.82	1.48	1.38
2	2	4483	B8T	C6-C5	6.82	1.50	1.35
2	2	4597	UR3	C6-C5	6.81	1.50	1.35
2	2	978	2MG	C4-N3	6.69	1.50	1.34
2	2	1517	2MG	C4-N3	6.67	1.50	1.34
2	2	1456	B8Q	C2-N3	6.66	1.46	1.35
2	2	4690	B8K	C2-N3	6.66	1.49	1.33
2	2	729	2MG	C2-N2	6.65	1.48	1.33
2	2	3897	B8K	C2-N3	6.62	1.49	1.33
2	2	4620	OMU	C2-N3	6.60	1.49	1.38
5	8	14	OMU	C2-N3	6.58	1.49	1.38
2	2	3909	OMC	C6-C5	6.55	1.50	1.35
2	2	2297	E7G	C8-N7	6.54	1.52	1.45
2	2	4872	2MG	C2-N2	6.53	1.47	1.33
2	2	3880	P7G	C8-N7	6.43	1.51	1.45
2	2	1909	P7G	C4-N9	6.43	1.44	1.35
2	2	3869	OMC	C2-N3	6.42	1.49	1.36
2	2	4536	OMC	C2-N3	6.42	1.49	1.36
2	2	2424	OMG	C2-N3	6.39	1.48	1.33
2	2	3880	P7G	C4-N9	6.39	1.44	1.35
2	2	3899	BGH	C4-N9	6.37	1.45	1.37
2	2	3887	OMC	C2-N3	6.37	1.49	1.36
2	2	2422	OMC	C2-N3	6.35	1.49	1.36
2	2	3880	P7G	C4-N3	6.35	1.48	1.37
2	2	4483	B8T	C4-N4	6.34	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2861	OMC	C2-N3	6.34	1.49	1.36
2	2	2365	OMC	C2-N3	6.32	1.49	1.36
2	2	1625	OMG	C2-N3	6.31	1.48	1.33
2	2	4671	B8T	C4-N4	6.31	1.48	1.35
2	2	4597	UR3	C2-N3	6.30	1.51	1.39
2	2	1909	P7G	C4-N3	6.30	1.48	1.37
2	2	1883	OMG	C2-N3	6.30	1.48	1.33
2	2	3701	OMC	C2-N3	6.30	1.49	1.36
2	2	4494	OMG	C2-N3	6.29	1.48	1.33
2	2	1659	I4U	C2-N3	6.25	1.49	1.36
2	2	1625	OMG	C4-N3	6.25	1.49	1.34
2	2	2424	OMG	C4-N3	6.25	1.49	1.34
2	2	4870	OMG	C4-N3	6.24	1.49	1.34
2	2	1883	OMG	C4-N3	6.23	1.49	1.34
2	2	2804	OMC	C2-N3	6.23	1.49	1.36
2	2	2773	OMG	C2-N3	6.23	1.48	1.33
2	2	4870	OMG	C2-N3	6.22	1.48	1.33
2	2	4872	2MG	C4-N3	6.22	1.49	1.34
2	2	1348	P4U	C2-N3	6.22	1.49	1.36
2	2	4494	OMG	C4-N3	6.20	1.49	1.34
2	2	2773	OMG	C4-N3	6.17	1.48	1.34
2	2	1348	P4U	C6-C5	6.14	1.49	1.35
2	2	1316	OMG	C4-N3	6.12	1.48	1.34
2	2	373	OMG	C2-N3	6.11	1.47	1.33
2	2	1316	OMG	C2-N3	6.11	1.47	1.33
2	2	1659	I4U	C6-C5	6.11	1.49	1.35
2	2	1522	OMG	C2-N3	6.09	1.47	1.33
2	2	1883	OMG	C2-N2	6.07	1.48	1.34
2	2	2424	OMG	C2-N2	6.07	1.48	1.34
2	2	1522	OMG	C4-N3	6.07	1.48	1.34
2	2	2364	OMG	C4-N3	6.06	1.48	1.34
2	2	4870	OMG	C2-N2	6.06	1.48	1.34
2	2	373	OMG	C4-N3	6.05	1.48	1.34
2	2	3701	OMC	C6-C5	6.05	1.49	1.35
2	2	1522	OMG	C2-N2	6.04	1.48	1.34
2	2	2364	OMG	C2-N3	6.04	1.47	1.33
2	2	4597	UR3	C2-N1	6.03	1.47	1.38
2	2	2773	OMG	C2-N2	6.03	1.48	1.34
2	2	1625	OMG	C2-N2	6.02	1.48	1.34
2	2	373	OMG	C2-N2	6.02	1.48	1.34
2	2	4494	OMG	C2-N2	6.00	1.48	1.34
2	2	3887	OMC	C6-C5	6.00	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2365	OMC	C6-C5	6.00	1.49	1.35
2	2	2050	OMG	C4-N3	5.99	1.48	1.34
2	2	4623	OMG	C2-N3	5.98	1.47	1.33
2	2	2050	OMG	C2-N3	5.98	1.47	1.33
2	2	4623	OMG	C2-N2	5.97	1.48	1.34
2	2	2861	OMC	C6-C5	5.97	1.48	1.35
2	2	2422	OMC	C6-C5	5.96	1.48	1.35
2	2	4637	OMG	C2-N3	5.96	1.47	1.33
2	2	4623	OMG	C4-N3	5.96	1.48	1.34
2	2	4536	OMC	C6-C5	5.95	1.48	1.35
2	2	1316	OMG	C2-N2	5.95	1.48	1.34
2	2	4637	OMG	C4-N3	5.95	1.48	1.34
2	2	3880	P7G	C2-N2	5.93	1.48	1.34
2	2	1909	P7G	C2-N2	5.93	1.48	1.34
2	2	2050	OMG	C2-N2	5.92	1.48	1.34
2	2	4637	OMG	C2-N2	5.92	1.48	1.34
2	2	2804	OMC	C6-C5	5.91	1.48	1.35
2	2	3869	OMC	C6-C5	5.89	1.48	1.35
2	2	2364	OMG	C2-N2	5.88	1.48	1.34
2	2	4564	M7A	C4-N9	5.86	1.49	1.38
2	2	4550	7MG	C2-N3	5.82	1.47	1.33
2	2	3897	B8K	C4-N9	5.81	1.44	1.37
2	2	3899	BGH	C4-N3	5.79	1.48	1.34
2	2	1605	7MG	C2-N3	5.77	1.47	1.33
2	2	3899	BGH	C2-N3	5.74	1.47	1.33
2	2	4530	UR3	C2-N3	5.74	1.50	1.39
2	2	2297	E7G	C4-N9	5.73	1.44	1.37
2	2	237	B9B	C2-N2	5.73	1.45	1.33
2	2	2754	B9B	C2-N2	5.73	1.45	1.33
2	2	3909	OMC	C2-N3	5.70	1.47	1.36
2	2	2297	E7G	C4-N3	5.68	1.47	1.34
2	2	2522	7MG	C2-N3	5.67	1.46	1.33
2	2	1909	P7G	C8-N7	5.67	1.51	1.45
2	2	2297	E7G	C2-N3	5.66	1.46	1.33
2	2	1574	B9B	C2-N2	5.62	1.45	1.33
2	2	4550	7MG	C4-N3	5.61	1.47	1.34
2	2	1605	7MG	C4-N3	5.57	1.47	1.34
2	2	3909	OMC	C2-N1	5.56	1.52	1.40
2	2	4620	OMU	C6-C5	5.54	1.47	1.35
2	2	4550	7MG	C4-N9	5.52	1.44	1.37
2	2	1605	7MG	C4-N9	5.48	1.44	1.37
2	2	2522	7MG	C4-N3	5.48	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3909	OMC	C4-N4	5.44	1.46	1.33
2	2	4690	B8K	C4-N9	5.34	1.43	1.37
2	2	3880	P7G	C2-N1	5.33	1.46	1.33
5	8	14	OMU	C6-C5	5.30	1.47	1.35
2	2	1909	P7G	C2-N1	5.24	1.45	1.33
2	2	2522	7MG	C4-N9	5.24	1.43	1.37
2	2	3701	OMC	C4-N3	5.16	1.44	1.34
2	2	2297	E7G	C2-N2	5.16	1.46	1.34
2	2	4536	OMC	C4-N3	5.14	1.44	1.34
2	2	4483	B8T	C2-N1	5.13	1.51	1.40
2	2	3869	OMC	C4-N3	5.12	1.44	1.34
2	2	3887	OMC	C4-N3	5.12	1.44	1.34
2	2	2365	OMC	C4-N3	5.11	1.44	1.34
2	2	2804	OMC	C4-N3	5.10	1.44	1.34
2	2	2861	OMC	C2-N1	5.08	1.51	1.40
2	2	2422	OMC	C4-N3	5.06	1.44	1.34
2	2	2861	OMC	C4-N3	5.06	1.44	1.34
2	2	3887	OMC	C2-N1	4.98	1.50	1.40
2	2	4536	OMC	C2-N1	4.97	1.50	1.40
2	2	3701	OMC	C4-N4	4.89	1.45	1.33
2	2	2861	OMC	C4-N4	4.89	1.45	1.33
2	2	3887	OMC	C4-N4	4.88	1.45	1.33
2	2	2422	OMC	C2-N1	4.88	1.50	1.40
2	2	3899	BGH	C2-N2	4.87	1.45	1.34
2	2	2422	OMC	C4-N4	4.87	1.45	1.33
2	2	4536	OMC	C4-N4	4.87	1.45	1.33
2	2	3867	A2M	O4'-C1'	-4.86	1.30	1.42
2	2	2804	OMC	C4-N4	4.84	1.45	1.33
2	2	2365	OMC	C4-N4	4.84	1.45	1.33
2	2	3869	OMC	C4-N4	4.83	1.45	1.33
2	2	1605	7MG	C2-N2	4.79	1.45	1.34
2	2	2522	7MG	C2-N2	4.77	1.45	1.34
2	2	3869	OMC	C2-N1	4.76	1.50	1.40
2	2	4550	7MG	C2-N2	4.76	1.45	1.34
2	2	1456	B8Q	C2-N1	4.73	1.45	1.38
2	2	1348	P4U	O4-C4	4.71	1.40	1.35
2	2	1326	A2M	O4'-C1'	-4.61	1.31	1.42
2	2	1524	A2M	O4'-C1'	-4.61	1.31	1.42
2	2	4671	B8T	C2-N1	4.61	1.50	1.40
2	2	398	A2M	O4'-C1'	-4.60	1.31	1.42
2	2	3909	OMC	C4-N3	4.58	1.43	1.34
2	2	1659	I4U	C5-C4	4.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4523	A2M	C6-N6	4.57	1.45	1.34
2	2	3825	A2M	C6-N6	4.57	1.45	1.34
2	2	3718	A2M	O4'-C1'	-4.56	1.31	1.42
2	2	1524	A2M	C6-N6	4.56	1.45	1.34
2	2	1871	A2M	C6-N6	4.55	1.45	1.34
2	2	3899	BGH	C5-N7	4.55	1.47	1.39
2	2	3718	A2M	C6-N6	4.55	1.45	1.34
2	2	2401	A2M	O4'-C1'	-4.54	1.31	1.42
2	2	1326	A2M	C6-N6	4.53	1.45	1.34
2	2	3723	A2M	C6-N6	4.53	1.45	1.34
2	2	4571	A2M	C6-N6	4.52	1.45	1.34
2	2	2401	A2M	C6-N6	4.52	1.45	1.34
2	2	4523	A2M	O4'-C1'	-4.52	1.31	1.42
2	2	4571	A2M	O4'-C1'	-4.52	1.31	1.42
2	2	2363	A2M	O4'-C1'	-4.52	1.31	1.42
2	2	2804	OMC	C2-N1	4.52	1.49	1.40
2	2	3723	A2M	O4'-C1'	-4.52	1.31	1.42
2	2	2363	A2M	C6-N6	4.51	1.45	1.34
2	2	3825	A2M	O4'-C1'	-4.51	1.31	1.42
2	2	1534	A2M	O4'-C1'	-4.50	1.31	1.42
2	2	3867	A2M	C6-N6	4.50	1.45	1.34
2	2	398	A2M	C6-N6	4.49	1.45	1.34
2	2	4083	5MU	C2-N3	4.49	1.46	1.38
2	2	1534	A2M	C6-N6	4.48	1.45	1.34
2	2	1348	P4U	C5-C4	4.47	1.48	1.43
2	2	4690	B8K	C4-N3	4.45	1.44	1.34
2	2	1348	P4U	C2-N1	4.45	1.49	1.40
2	2	3701	OMC	C2-N1	4.42	1.49	1.40
2	2	3897	B8K	C4-N3	4.41	1.44	1.34
2	2	1659	I4U	C2-N1	4.40	1.49	1.40
2	2	2365	OMC	C2-N1	4.36	1.49	1.40
2	2	4564	M7A	C6-N6	4.36	1.45	1.34
2	2	1871	A2M	O4'-C1'	-4.34	1.31	1.42
2	2	3897	B8K	C5-C6	4.33	1.54	1.43
2	2	3899	BGH	C5-C6	4.31	1.54	1.43
2	2	978	2MG	C2-N1	4.30	1.43	1.36
2	2	3897	B8K	C5-N7	4.29	1.47	1.39
2	2	4872	2MG	C2-N1	4.29	1.43	1.36
2	2	1517	2MG	C2-N1	4.27	1.43	1.36
2	2	729	2MG	C2-N1	4.15	1.43	1.36
2	2	4690	B8K	C5-N7	4.10	1.46	1.39
5	8	14	OMU	C4-N3	4.02	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4671	B8T	C5-C4	3.93	1.49	1.40
2	2	4620	OMU	C4-N3	3.93	1.45	1.38
2	2	4564	M7A	C5-N7	3.90	1.48	1.39
2	2	4690	B8K	C5-C6	3.90	1.53	1.43
2	2	1625	OMG	C5-N7	-3.90	1.31	1.39
2	2	1605	7MG	C5-C6	3.88	1.53	1.43
2	2	4494	OMG	C5-N7	-3.87	1.31	1.39
2	2	4550	7MG	C5-C6	3.86	1.53	1.43
2	2	1883	OMG	C5-N7	-3.83	1.31	1.39
2	2	2297	E7G	C5-C6	3.81	1.53	1.43
2	2	3880	P7G	C2-N3	3.81	1.47	1.37
2	2	1909	P7G	C2-N3	3.79	1.47	1.37
2	2	2424	OMG	C5-N7	-3.78	1.31	1.39
2	2	2364	OMG	C5-N7	-3.77	1.31	1.39
2	2	3880	P7G	C6-N1	3.77	1.44	1.38
2	2	4637	OMG	C5-N7	-3.76	1.31	1.39
2	2	1522	OMG	C5-N7	-3.75	1.31	1.39
2	2	1316	OMG	C5-N7	-3.73	1.31	1.39
2	2	3899	BGH	O2'-C2'	3.71	1.52	1.42
2	2	2773	OMG	C5-N7	-3.68	1.31	1.39
2	2	2050	OMG	C5-N7	-3.68	1.31	1.39
2	2	1605	7MG	C2-N1	3.67	1.46	1.37
2	2	4483	B8T	C5-C4	3.63	1.48	1.40
2	2	3909	OMC	C6-N1	3.62	1.46	1.38
2	2	3897	B8K	C6-N1	3.62	1.45	1.38
2	2	4690	B8K	C6-N1	3.62	1.45	1.38
2	2	2522	7MG	C5-C6	3.61	1.52	1.43
2	2	4550	7MG	C2-N1	3.61	1.46	1.37
2	2	373	OMG	C5-N7	-3.60	1.32	1.39
2	2	4870	OMG	C5-N7	-3.60	1.32	1.39
2	2	3899	BGH	C71-N7	3.58	1.47	1.39
2	2	4623	OMG	C5-N7	-3.57	1.32	1.39
2	2	2754	B9B	O6-C6	3.57	1.40	1.35
2	2	2297	E7G	C2-N1	3.57	1.46	1.37
2	2	3897	B8K	C2-N2	3.56	1.42	1.34
2	2	2522	7MG	C2-N1	3.54	1.46	1.37
2	2	1909	P7G	C6-N1	3.53	1.44	1.38
2	2	4690	B8K	C71-N7	3.51	1.47	1.39
2	2	4690	B8K	C2-N2	3.50	1.42	1.34
2	2	3897	B8K	C71-N7	3.49	1.47	1.39
2	2	1574	B9B	O6-C6	3.47	1.40	1.35
2	2	4530	UR3	C6-N1	3.46	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4483	B8T	C6-N1	3.44	1.46	1.38
2	2	3869	OMC	C6-N1	3.39	1.46	1.38
2	2	237	B9B	O6-C6	3.39	1.40	1.35
2	2	1348	P4U	C6-N1	3.39	1.46	1.38
2	2	4083	5MU	C2-N1	3.37	1.43	1.38
2	2	3899	BGH	C6-N1	3.34	1.45	1.38
2	2	1909	P7G	C5-C4	3.34	1.44	1.37
2	2	2522	7MG	C6-N1	3.33	1.45	1.38
2	2	3897	B8K	C2-N1	3.33	1.45	1.37
2	2	3887	OMC	C6-N1	3.33	1.46	1.38
2	2	1605	7MG	C6-N1	3.32	1.45	1.38
2	2	4550	7MG	C6-N1	3.32	1.45	1.38
2	2	4690	B8K	C2-N1	3.31	1.45	1.37
2	2	1659	I4U	C6-N1	3.28	1.45	1.38
2	2	2297	E7G	C6-N1	3.27	1.44	1.38
2	2	4623	OMG	C6-N1	3.27	1.44	1.38
2	2	3880	P7G	C5-C4	3.27	1.43	1.37
2	2	2422	OMC	C6-N1	3.27	1.45	1.38
2	2	4536	OMC	C6-N1	3.27	1.45	1.38
2	2	3899	BGH	C2-N1	3.27	1.45	1.37
2	2	2365	OMC	C6-N1	3.25	1.45	1.38
2	2	2861	OMC	C6-N1	3.24	1.45	1.38
2	2	4671	B8T	C6-N1	3.22	1.45	1.38
2	2	1316	OMG	C6-N1	3.22	1.44	1.38
2	2	4637	OMG	C6-N1	3.20	1.44	1.38
2	2	4597	UR3	C6-N1	3.20	1.45	1.38
2	2	1909	P7G	O6-C6	-3.19	1.18	1.23
2	2	2364	OMG	C6-N1	3.19	1.44	1.38
2	2	1883	OMG	C6-N1	3.19	1.44	1.38
2	2	2773	OMG	C6-N1	3.18	1.44	1.38
2	2	3701	OMC	C6-N1	3.15	1.45	1.38
2	2	373	OMG	C6-N1	3.14	1.44	1.38
2	2	1883	OMG	O6-C6	-3.12	1.17	1.23
2	2	4623	OMG	O6-C6	-3.12	1.17	1.23
2	2	4637	OMG	O6-C6	-3.12	1.17	1.23
2	2	1625	OMG	C6-N1	3.12	1.44	1.38
2	2	4870	OMG	O6-C6	-3.11	1.17	1.23
2	2	1316	OMG	O6-C6	-3.11	1.17	1.23
2	2	4494	OMG	C6-N1	3.10	1.44	1.38
2	2	1522	OMG	C6-N1	3.10	1.44	1.38
2	2	373	OMG	O6-C6	-3.10	1.17	1.23
2	2	2050	OMG	O6-C6	-3.09	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2364	OMG	O6-C6	-3.09	1.17	1.23
2	2	4870	OMG	C6-N1	3.08	1.44	1.38
2	2	2050	OMG	C6-N1	3.08	1.44	1.38
2	2	2424	OMG	C6-N1	3.07	1.44	1.38
2	2	2804	OMC	C6-N1	3.07	1.45	1.38
2	2	4494	OMG	O6-C6	-3.07	1.17	1.23
2	2	3880	P7G	O6-C6	-3.06	1.18	1.23
2	2	2424	OMG	O6-C6	-3.05	1.17	1.23
2	2	1522	OMG	O6-C6	-3.04	1.17	1.23
2	2	4529	B8W	C5-N7	-3.03	1.33	1.39
2	2	1517	2MG	C5-N7	-3.02	1.33	1.39
2	2	2773	OMG	O6-C6	-3.01	1.17	1.23
2	2	729	2MG	C5-N7	-2.99	1.33	1.39
2	2	1574	B9B	C5-C4	-2.96	1.33	1.39
5	8	14	OMU	O4-C4	-2.96	1.18	1.24
2	2	4620	OMU	O4-C4	-2.96	1.18	1.24
2	2	2401	A2M	O3'-C3'	2.95	1.49	1.43
2	2	1625	OMG	O6-C6	-2.95	1.18	1.23
2	2	3867	A2M	O3'-C3'	2.95	1.49	1.43
2	2	3718	A2M	O3'-C3'	2.92	1.49	1.43
2	2	1524	A2M	O3'-C3'	2.92	1.49	1.43
2	2	4083	5MU	O4-C4	-2.92	1.18	1.23
2	2	1534	A2M	O3'-C3'	2.91	1.49	1.43
2	2	398	A2M	O3'-C3'	2.90	1.49	1.43
2	2	3897	B8K	C5-C4	2.90	1.47	1.38
2	2	2380	B8W	C5-C4	-2.87	1.33	1.39
2	2	3899	BGH	O3'-C3'	-2.87	1.36	1.43
2	2	1659	I4U	O4-C41	-2.86	1.40	1.47
2	2	4571	A2M	O3'-C3'	2.86	1.49	1.43
2	2	3825	A2M	O3'-C3'	2.86	1.49	1.43
2	2	2363	A2M	O3'-C3'	2.85	1.49	1.43
2	2	978	2MG	C5-N7	-2.84	1.33	1.39
2	2	4523	A2M	O3'-C3'	2.83	1.49	1.43
2	2	1326	A2M	O3'-C3'	2.83	1.49	1.43
2	2	1871	A2M	O3'-C3'	2.82	1.49	1.43
2	2	3723	A2M	O3'-C3'	2.82	1.49	1.43
2	2	4690	B8K	C5-C4	2.82	1.47	1.38
2	2	4185	B8W	C5-N7	-2.82	1.33	1.39
2	2	4185	B8W	C5-C4	-2.79	1.33	1.39
2	2	4483	B8T	O2-C2	-2.79	1.18	1.23
2	2	4872	2MG	C5-N7	-2.79	1.33	1.39
2	2	4872	2MG	C5-C6	2.79	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	237	B9B	C5-C4	-2.78	1.33	1.39
2	2	237	B9B	C5-N7	-2.78	1.33	1.39
2	2	2754	B9B	C5-C4	-2.77	1.33	1.39
2	2	2380	B8W	C5-N7	-2.77	1.33	1.39
2	2	4671	B8T	O2-C2	-2.75	1.18	1.23
2	2	4620	OMU	C6-N1	2.75	1.44	1.38
2	2	978	2MG	C5-C6	2.74	1.54	1.44
2	2	3909	OMC	C5-C4	2.74	1.49	1.42
2	2	2804	OMC	O2-C2	-2.73	1.18	1.23
2	2	2422	OMC	O2-C2	-2.73	1.18	1.23
2	2	729	2MG	C5-C6	2.73	1.54	1.44
2	2	4529	B8W	C5-C4	-2.73	1.33	1.39
2	2	1659	I4U	O2-C2	-2.72	1.18	1.23
2	2	2365	OMC	O2-C2	-2.72	1.18	1.23
2	2	1517	2MG	C5-C6	2.71	1.54	1.44
2	2	1348	P4U	O2-C2	-2.71	1.18	1.23
2	2	2401	A2M	C5-C4	-2.71	1.33	1.39
5	8	14	OMU	C6-N1	2.69	1.44	1.38
2	2	2363	A2M	O2'-C2'	-2.69	1.35	1.42
2	2	3899	BGH	O6-C6	-2.69	1.18	1.23
2	2	1534	A2M	C5-C4	-2.69	1.34	1.39
2	2	3867	A2M	C5-C4	-2.68	1.34	1.39
2	2	1524	A2M	O2'-C2'	-2.68	1.35	1.42
2	2	4472	B8W	C5-C4	-2.68	1.34	1.39
2	2	3723	A2M	C5-C4	-2.67	1.34	1.39
2	2	3825	A2M	C5-C4	-2.67	1.34	1.39
2	2	1534	A2M	O2'-C2'	-2.66	1.35	1.42
2	2	2363	A2M	C5-C4	-2.66	1.34	1.39
2	2	398	A2M	C5-C4	-2.65	1.34	1.39
2	2	1574	B9B	C5-N7	-2.65	1.34	1.39
2	2	2773	OMG	C5-C6	2.64	1.54	1.44
2	2	1326	A2M	C5-C4	-2.64	1.34	1.39
2	2	4872	2MG	C6-N1	2.64	1.43	1.38
2	2	1871	A2M	C5-C4	-2.63	1.34	1.39
2	2	2754	B9B	C5-N7	-2.62	1.34	1.39
2	2	1524	A2M	C5-C4	-2.62	1.34	1.39
2	2	3718	A2M	C5-C4	-2.62	1.34	1.39
2	2	4571	A2M	C5-C4	-2.62	1.34	1.39
2	2	2401	A2M	O2'-C2'	-2.62	1.35	1.42
2	2	2363	A2M	C8-N9	-2.62	1.32	1.37
2	2	4083	5MU	O2-C2	-2.62	1.18	1.23
2	2	4523	A2M	O2'-C2'	-2.61	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	398	A2M	O2'-C2'	-2.61	1.35	1.42
2	2	3869	OMC	O2-C2	-2.61	1.18	1.23
2	2	4523	A2M	C5-C4	-2.61	1.34	1.39
2	2	3701	OMC	O2-C2	-2.60	1.18	1.23
2	2	1316	OMG	C5-C6	2.60	1.54	1.44
2	2	2050	OMG	C5-C6	2.60	1.54	1.44
2	2	1625	OMG	C5-C6	2.60	1.54	1.44
2	2	3825	A2M	O2'-C2'	-2.60	1.36	1.42
2	2	3718	A2M	O2'-C2'	-2.59	1.36	1.42
2	2	4623	OMG	C5-C6	2.59	1.54	1.44
2	2	4472	B8W	C5-N7	-2.59	1.34	1.39
2	2	3701	OMC	C5-C4	2.59	1.48	1.42
2	2	4637	OMG	C5-C6	2.57	1.53	1.44
2	2	2522	7MG	O6-C6	-2.57	1.18	1.23
2	2	1659	I4U	O4-C4	2.57	1.40	1.35
2	2	4870	OMG	C5-C6	2.56	1.53	1.44
2	2	2861	OMC	O2-C2	-2.56	1.19	1.23
2	2	1522	OMG	C5-C6	2.55	1.53	1.44
2	2	4536	OMC	O2-C2	-2.55	1.19	1.23
2	2	4494	OMG	C5-C6	2.54	1.53	1.44
2	2	3887	OMC	O2-C2	-2.54	1.19	1.23
2	2	1517	2MG	C6-N1	2.54	1.43	1.38
2	2	2424	OMG	C5-C6	2.54	1.53	1.44
2	2	2364	OMG	C5-C6	2.54	1.53	1.44
2	2	373	OMG	C5-C6	2.53	1.53	1.44
2	2	978	2MG	C6-N1	2.53	1.43	1.38
2	2	4637	OMG	C2-N1	2.52	1.43	1.37
2	2	373	OMG	C2-N1	2.52	1.43	1.37
2	2	1605	7MG	O6-C6	-2.51	1.18	1.23
2	2	2773	OMG	C2-N1	2.51	1.43	1.37
2	2	4623	OMG	C2-N1	2.51	1.43	1.37
2	2	3723	A2M	O2'-C2'	-2.50	1.36	1.42
2	2	4550	7MG	O6-C6	-2.50	1.18	1.23
2	2	4529	B8W	C8-N9	-2.50	1.33	1.37
2	2	1871	A2M	O2'-C2'	-2.50	1.36	1.42
2	2	3867	A2M	O2'-C2'	-2.50	1.36	1.42
2	2	2050	OMG	C2-N1	2.49	1.43	1.37
2	2	1522	OMG	C2-N1	2.49	1.43	1.37
2	2	4494	OMG	C2-N1	2.49	1.43	1.37
2	2	2424	OMG	C2-N1	2.49	1.43	1.37
2	2	1625	OMG	C2-N1	2.49	1.43	1.37
2	2	2364	OMG	C2-N1	2.48	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4870	OMG	C2-N1	2.47	1.43	1.37
2	2	1316	OMG	C2-N1	2.47	1.43	1.37
2	2	4571	A2M	O2'-C2'	-2.47	1.36	1.42
2	2	1883	OMG	C2-N1	2.46	1.43	1.37
2	2	4571	A2M	C8-N9	-2.46	1.33	1.37
2	2	2297	E7G	O6-C6	-2.45	1.18	1.23
5	8	14	OMU	O2-C2	-2.45	1.18	1.23
2	2	2401	A2M	C8-N9	-2.43	1.33	1.37
2	2	1883	OMG	C5-C6	2.43	1.53	1.44
2	2	2861	OMC	C5-C4	2.43	1.48	1.42
2	2	3718	A2M	C8-N9	-2.43	1.33	1.37
2	2	2422	OMC	C5-C4	2.42	1.48	1.42
2	2	1456	B8Q	C6-N1	2.41	1.43	1.38
2	2	3887	OMC	C5-C4	2.41	1.48	1.42
2	2	2804	OMC	C5-C4	2.41	1.48	1.42
2	2	4523	A2M	C8-N9	-2.41	1.33	1.37
2	2	1534	A2M	C8-N9	-2.40	1.33	1.37
2	2	4620	OMU	O2-C2	-2.39	1.18	1.23
2	2	2365	OMC	C5-C4	2.39	1.48	1.42
2	2	3723	A2M	C8-N9	-2.39	1.33	1.37
2	2	3825	A2M	C8-N9	-2.38	1.33	1.37
2	2	4872	2MG	C4-N9	-2.37	1.31	1.38
2	2	4571	A2M	C5-N7	-2.37	1.34	1.39
2	2	1326	A2M	O2'-C2'	-2.36	1.36	1.42
2	2	1326	A2M	C8-N9	-2.36	1.33	1.37
2	2	4620	OMU	C5-C4	2.36	1.48	1.43
5	8	14	OMU	C5-C4	2.35	1.48	1.43
2	2	729	2MG	C6-N1	2.34	1.43	1.38
2	2	4530	UR3	C4-N3	2.34	1.46	1.40
2	2	1524	A2M	C8-N9	-2.33	1.33	1.37
2	2	4597	UR3	C5-C4	2.33	1.49	1.43
2	2	3718	A2M	C5-N7	-2.33	1.34	1.39
2	2	398	A2M	C8-N9	-2.32	1.33	1.37
2	2	1524	A2M	C5-N7	-2.30	1.34	1.39
2	2	3869	OMC	C5-C4	2.30	1.48	1.42
2	2	3867	A2M	C8-N9	-2.29	1.33	1.37
2	2	4536	OMC	C5-C4	2.29	1.48	1.42
2	2	2363	A2M	C5-N7	-2.28	1.34	1.39
2	2	3909	OMC	O2-C2	-2.28	1.19	1.23
2	2	1326	A2M	C5-N7	-2.28	1.34	1.39
2	2	398	A2M	C5-N7	-2.25	1.34	1.39
2	2	4530	UR3	C5-C4	2.24	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3867	A2M	C5-N7	-2.21	1.34	1.39
2	2	2401	A2M	C5-N7	-2.20	1.34	1.39
2	2	4597	UR3	C4-N3	2.19	1.45	1.40
2	2	3899	BGH	C5-C4	2.18	1.45	1.38
2	2	237	B9B	C5-C6	-2.18	1.37	1.41
2	2	1871	A2M	C5-N7	-2.17	1.34	1.39
2	2	237	B9B	C8-N9	-2.17	1.33	1.37
2	2	3825	A2M	C5-N7	-2.17	1.34	1.39
2	2	2380	B8W	C8-N9	-2.14	1.33	1.37
2	2	1871	A2M	C8-N9	-2.13	1.33	1.37
2	2	4185	B8W	C4-N3	2.12	1.37	1.34
2	2	3723	A2M	C5-N7	-2.12	1.35	1.39
2	2	1534	A2M	C5-N7	-2.12	1.35	1.39
2	2	4523	A2M	C5-N7	-2.11	1.35	1.39
2	2	4185	B8W	C8-N9	-2.11	1.33	1.37
2	2	4690	B8K	O6-C6	-2.08	1.19	1.23
2	2	4472	B8W	C8-N9	-2.08	1.33	1.37
2	2	978	2MG	C4-N9	-2.07	1.32	1.38
2	2	1574	B9B	C8-N9	-2.07	1.33	1.37
2	2	2754	B9B	C8-N9	-2.03	1.33	1.37
2	2	1456	B8Q	O2-C2	-2.02	1.18	1.22
2	2	1871	A2M	O5'-C5'	-2.01	1.39	1.44
2	2	729	2MG	O6-C6	-2.01	1.19	1.23
2	2	1517	2MG	O6-C6	-2.01	1.19	1.23

All (543) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2754	B9B	O6-C6-C5	21.33	143.58	116.57
2	2	1574	B9B	O6-C6-C5	21.25	143.47	116.57
2	2	237	B9B	O6-C6-C5	20.95	143.10	116.57
2	2	2754	B9B	O6-C6-N1	-18.29	94.52	120.00
2	2	1574	B9B	O6-C6-N1	-18.08	94.82	120.00
2	2	237	B9B	O6-C6-N1	-18.04	94.87	120.00
2	2	4564	M7A	C5-C6-N6	13.86	147.40	123.74
2	2	4564	M7A	N6-C6-N1	-11.73	92.66	118.35
2	2	4083	5MU	C5-C4-N3	10.26	124.07	115.31
2	2	4870	OMG	C1'-N9-C8	-10.01	98.21	126.70
2	2	4870	OMG	C1'-N9-C4	9.74	155.45	126.50
2	2	2424	OMG	C1'-N9-C4	9.29	154.10	126.50
2	2	2424	OMG	C1'-N9-C8	-9.04	100.95	126.70
2	2	1522	OMG	C1'-N9-C4	8.82	152.71	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4494	OMG	C1'-N9-C4	8.78	152.57	126.50
2	2	2773	OMG	C1'-N9-C4	8.70	152.35	126.50
2	2	1522	OMG	C1'-N9-C8	-8.64	102.09	126.70
2	2	1625	OMG	C1'-N9-C4	8.63	152.12	126.50
2	2	2050	OMG	C1'-N9-C4	8.47	151.66	126.50
2	2	2364	OMG	C1'-N9-C4	8.45	151.60	126.50
2	2	2773	OMG	C1'-N9-C8	-8.43	102.70	126.70
2	2	4494	OMG	C1'-N9-C8	-8.33	102.98	126.70
2	2	4637	OMG	C1'-N9-C4	8.31	151.18	126.50
2	2	1316	OMG	C1'-N9-C4	8.29	151.13	126.50
2	2	1883	OMG	C1'-N9-C4	8.27	151.07	126.50
2	2	4623	OMG	C1'-N9-C4	8.23	150.96	126.50
2	2	4623	OMG	C1'-N9-C8	-8.23	103.28	126.70
2	2	2050	OMG	C1'-N9-C8	-8.22	103.29	126.70
2	2	1625	OMG	C1'-N9-C8	-8.13	103.56	126.70
2	2	1883	OMG	C1'-N9-C8	-8.12	103.59	126.70
2	2	1316	OMG	C1'-N9-C8	-8.08	103.69	126.70
2	2	4637	OMG	C1'-N9-C8	-8.08	103.69	126.70
2	2	2364	OMG	C1'-N9-C8	-8.06	103.75	126.70
2	2	4083	5MU	C5-C6-N1	-7.94	115.17	123.34
2	2	373	OMG	C1'-N9-C4	7.87	149.87	126.50
2	2	373	OMG	C1'-N9-C8	-7.87	104.30	126.70
2	2	4597	UR3	C4-N3-C2	-7.43	117.57	124.56
2	2	1517	2MG	C2-N3-C4	7.31	121.10	112.04
2	2	729	2MG	C2-N3-C4	7.12	120.87	112.04
2	2	237	B9B	C5-C4-N3	-7.11	119.19	127.19
2	2	4185	B8W	C5-C4-N3	-7.01	119.30	127.19
2	2	1534	A2M	N6-C6-N1	-6.99	103.05	118.35
2	2	4083	5MU	C4-N3-C2	-6.99	118.31	127.35
2	2	4529	B8W	C5-C4-N3	-6.87	119.46	127.19
2	2	2363	A2M	N6-C6-N1	-6.87	103.30	118.35
2	2	1871	A2M	N6-C6-N1	-6.87	103.31	118.35
2	2	2754	B9B	C5-C4-N3	-6.84	119.50	127.19
2	2	3825	A2M	N6-C6-N1	-6.84	103.37	118.35
2	2	4523	A2M	N6-C6-N1	-6.83	103.40	118.35
2	2	4472	B8W	C5-C4-N3	-6.80	119.54	127.19
2	2	3723	A2M	N6-C6-N1	-6.79	103.47	118.35
2	2	398	A2M	N6-C6-N1	-6.79	103.49	118.35
2	2	2401	A2M	N6-C6-N1	-6.78	103.51	118.35
2	2	3867	A2M	N6-C6-N1	-6.74	103.60	118.35
2	2	1326	A2M	N6-C6-N1	-6.72	103.64	118.35
2	2	4571	A2M	N6-C6-N1	-6.71	103.66	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	3718	A2M	N6-C6-N1	-6.69	103.69	118.35
2	2	1524	A2M	N6-C6-N1	-6.68	103.72	118.35
2	2	978	2MG	C2-N3-C4	6.64	120.28	112.04
2	2	4690	B8K	C72-C71-N7	6.55	128.72	118.86
2	2	2380	B8W	C5-C4-N3	-6.51	119.86	127.19
2	2	4872	2MG	C2-N3-C4	6.43	120.02	112.04
2	2	4185	B8W	N2-C2-N3	6.41	127.22	117.25
2	2	1574	B9B	C5-C4-N3	-6.35	120.05	127.19
2	2	2380	B8W	N2-C2-N3	6.35	127.12	117.25
2	2	3723	A2M	N3-C2-N1	-6.32	118.72	128.60
2	2	2401	A2M	N3-C2-N1	-6.29	118.77	128.60
2	2	1534	A2M	N3-C2-N1	-6.28	118.78	128.60
2	2	1871	A2M	N3-C2-N1	-6.28	118.78	128.60
2	2	3825	A2M	N3-C2-N1	-6.27	118.79	128.60
2	2	398	A2M	N3-C2-N1	-6.26	118.82	128.60
2	2	4523	A2M	N3-C2-N1	-6.24	118.83	128.60
2	2	1326	A2M	N3-C2-N1	-6.22	118.87	128.60
2	2	729	2MG	C5-C4-N3	-6.20	118.41	128.46
2	2	3867	A2M	N3-C2-N1	-6.18	118.93	128.60
2	2	2401	A2M	N9-C8-N7	-6.16	105.49	113.91
2	2	1524	A2M	N3-C2-N1	-6.16	118.97	128.60
2	2	4571	A2M	N3-C2-N1	-6.15	118.98	128.60
2	2	2363	A2M	N3-C2-N1	-6.13	119.01	128.60
2	2	4564	M7A	N3-C2-N1	-6.13	119.01	128.60
2	2	3718	A2M	N3-C2-N1	-6.12	119.03	128.60
2	2	4529	B8W	N2-C2-N3	6.12	126.77	117.25
2	2	1517	2MG	C5-C4-N3	-6.10	118.57	128.46
2	2	3899	BGH	C72-C71-N7	6.07	127.99	118.86
2	2	3825	A2M	N9-C8-N7	-6.06	105.62	113.91
2	2	3723	A2M	N9-C8-N7	-6.05	105.63	113.91
2	2	3897	B8K	C72-C71-N7	6.02	127.92	118.86
2	2	4690	B8K	C5-C6-N1	6.02	121.59	110.99
2	2	1534	A2M	N9-C8-N7	-5.99	105.72	113.91
2	2	4523	A2M	N9-C8-N7	-5.97	105.75	113.91
2	2	1534	A2M	C5-C6-N6	5.93	136.34	123.43
2	2	1871	A2M	C5-C6-N6	5.92	136.31	123.43
2	2	4523	A2M	C5-C6-N6	5.89	136.24	123.43
2	2	3867	A2M	N9-C8-N7	-5.87	105.89	113.91
2	2	398	A2M	N9-C8-N7	-5.86	105.90	113.91
2	2	3825	A2M	C5-C6-N6	5.85	136.16	123.43
2	2	398	A2M	C5-C6-N6	5.84	136.15	123.43
2	2	1524	A2M	N9-C8-N7	-5.84	105.92	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2363	A2M	C5-C6-N6	5.84	136.13	123.43
2	2	1871	A2M	N9-C8-N7	-5.83	105.94	113.91
2	2	3723	A2M	C5-C6-N6	5.83	136.11	123.43
2	2	4472	B8W	N2-C2-N3	5.79	126.26	117.25
2	2	2401	A2M	C5-C6-N6	5.79	136.02	123.43
2	2	1524	A2M	C5-C6-N6	5.78	136.01	123.43
2	2	3718	A2M	C5-C6-N6	5.78	136.01	123.43
2	2	3867	A2M	C5-C6-N6	5.78	136.00	123.43
2	2	1326	A2M	N9-C8-N7	-5.77	106.02	113.91
2	2	4571	A2M	C5-C6-N6	5.74	135.92	123.43
2	2	1326	A2M	C5-C6-N6	5.73	135.91	123.43
2	2	3718	A2M	N9-C8-N7	-5.73	106.07	113.91
2	2	3899	BGH	C5-C6-N1	5.72	121.06	110.99
2	2	2363	A2M	N9-C8-N7	-5.71	106.10	113.91
2	2	3897	B8K	C5-C6-N1	5.67	120.98	110.99
2	2	1456	B8Q	N3-C2-N1	5.63	123.75	117.13
2	2	4529	B8W	O6-C6-N1	5.60	126.74	119.01
2	2	2786	B9H	C31-N3-C2	5.57	124.17	117.21
2	2	4571	A2M	N9-C8-N7	-5.57	106.30	113.91
2	2	3909	OMC	O2-C2-N3	-5.53	113.34	122.33
2	2	1625	OMG	C5-C4-N3	-5.52	119.50	128.46
2	2	2424	OMG	C5-C4-N3	-5.52	119.51	128.46
2	2	4494	OMG	C5-C4-N3	-5.51	119.52	128.46
2	2	2401	A2M	C4-N9-C8	5.48	111.67	105.73
2	2	978	2MG	C5-C4-N3	-5.41	119.68	128.46
2	2	1909	P7G	C4-C5-N7	5.40	109.52	106.67
5	8	14	OMU	C4-N3-C2	-5.38	119.48	126.58
2	2	3723	A2M	C4-N9-C8	5.36	111.54	105.73
2	2	4523	A2M	C4-N9-C8	5.28	111.45	105.73
2	2	1534	A2M	C4-N9-C8	5.23	111.40	105.73
2	2	4620	OMU	C4-N3-C2	-5.23	119.68	126.58
2	2	1883	OMG	C5-C4-N3	-5.22	120.00	128.46
2	2	3825	A2M	C4-N9-C8	5.21	111.38	105.73
2	2	2773	OMG	C5-C4-N3	-5.19	120.04	128.46
2	2	4872	2MG	C5-C4-N3	-5.19	120.04	128.46
2	2	1524	A2M	C4-N9-C8	5.16	111.32	105.73
2	2	2364	OMG	C5-C4-N3	-5.14	120.12	128.46
2	2	3899	BGH	C2-N3-C4	5.12	121.43	112.30
2	2	3867	A2M	C4-N9-C8	5.12	111.28	105.73
2	2	2754	B9B	N2-C2-N3	5.11	125.20	117.25
2	2	1316	OMG	C5-C4-N3	-5.10	120.19	128.46
2	2	1522	OMG	C5-C4-N3	-5.10	120.19	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1456	B8Q	C31-N3-C4	5.09	121.91	114.25
2	2	398	A2M	C4-N9-C8	5.08	111.23	105.73
2	2	2297	E7G	C5-C6-N1	5.06	119.90	110.99
2	2	4870	OMG	C5-C4-N3	-5.04	120.28	128.46
2	2	237	B9B	N2-C2-N3	5.02	125.06	117.25
2	2	1605	7MG	C5-C6-N1	4.98	119.77	110.99
2	2	4564	M7A	N3-C4-N9	4.98	133.16	126.87
2	2	2363	A2M	C4-N9-C8	4.97	111.11	105.73
2	2	2050	OMG	C5-C4-N3	-4.97	120.40	128.46
2	2	4637	OMG	C5-C4-N3	-4.95	120.44	128.46
2	2	4690	B8K	C4-C5-N7	4.94	109.30	104.91
2	2	1326	A2M	C4-N9-C8	4.93	111.07	105.73
2	2	2297	E7G	C4-C5-N7	4.93	109.29	104.91
2	2	4872	2MG	C2-N1-C6	-4.92	118.81	124.48
2	2	237	B9B	N3-C4-N9	4.92	133.81	126.99
2	2	3897	B8K	C2-N3-C4	4.92	121.06	112.30
2	2	3718	A2M	C4-N9-C8	4.90	111.03	105.73
2	2	1871	A2M	C4-N9-C8	4.88	111.01	105.73
2	2	2522	7MG	C5-C6-N1	4.87	119.58	110.99
2	2	4550	7MG	C5-C6-N1	4.87	119.57	110.99
2	2	3880	P7G	C4-C5-N7	4.85	109.23	106.67
2	2	1517	2MG	C2-N1-C6	-4.83	118.92	124.48
2	2	373	OMG	C5-C4-N3	-4.80	120.67	128.46
2	2	4571	A2M	C4-N9-C8	4.80	110.93	105.73
2	2	2786	B9H	C6-N1-C2	-4.79	117.50	121.79
2	2	4083	5MU	N3-C2-N1	4.77	121.22	114.89
2	2	4623	OMG	C5-C4-N3	-4.76	120.73	128.46
2	2	4690	B8K	C2-N3-C4	4.76	120.78	112.30
2	2	2363	A2M	C5-C4-N3	-4.70	120.62	126.75
2	2	4571	A2M	C5-C4-N3	-4.67	120.65	126.75
2	2	729	2MG	C2-N1-C6	-4.63	119.16	124.48
2	2	4083	5MU	C5M-C5-C6	-4.62	116.68	122.85
2	2	1326	A2M	C5-C4-N3	-4.62	120.73	126.75
2	2	1456	B8Q	O2-C2-N3	-4.59	116.20	122.95
2	2	1625	OMG	C2-N3-C4	4.59	120.48	112.30
2	2	4530	UR3	C4-N3-C2	-4.59	120.24	124.56
2	2	4690	B8K	N9-C8-N7	4.58	109.47	103.33
2	2	4494	OMG	C2-N3-C4	4.57	120.44	112.30
2	2	3718	A2M	C5-C4-N3	-4.57	120.79	126.75
2	2	2424	OMG	C2-N3-C4	4.56	120.43	112.30
2	2	3867	A2M	C5-C4-N3	-4.55	120.82	126.75
2	2	3825	A2M	C5-C4-N3	-4.54	120.82	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2773	OMG	C2-N3-C4	4.52	120.36	112.30
2	2	4529	B8W	N3-C4-N9	4.52	133.26	126.99
2	2	1883	OMG	C2-N3-C4	4.51	120.34	112.30
2	2	4185	B8W	N3-C4-N9	4.50	133.23	126.99
2	2	1316	OMG	C2-N3-C4	4.49	120.30	112.30
2	2	2364	OMG	C2-N3-C4	4.48	120.28	112.30
2	2	1534	A2M	C5-C4-N3	-4.47	120.92	126.75
2	2	2297	E7G	C2-N3-C4	4.47	120.26	112.30
2	2	1522	OMG	C2-N3-C4	4.47	120.25	112.30
2	2	373	OMG	C2-N3-C4	4.46	120.25	112.30
2	2	1605	7MG	C2-N3-C4	4.46	120.25	112.30
2	2	3723	A2M	C5-C4-N3	-4.46	120.94	126.75
2	2	4623	OMG	C2-N3-C4	4.46	120.24	112.30
2	2	1574	B9B	N2-C2-N3	4.45	124.18	117.25
2	2	4637	OMG	C2-N3-C4	4.43	120.20	112.30
2	2	2754	B9B	N3-C4-N9	4.43	133.13	126.99
2	2	4550	7MG	C2-N3-C4	4.41	120.16	112.30
2	2	2401	A2M	C5-C4-N3	-4.38	121.03	126.75
2	2	4870	OMG	C2-N3-C4	4.37	120.09	112.30
2	2	398	A2M	C5-C4-N3	-4.35	121.07	126.75
2	2	1871	A2M	C5-C4-N3	-4.34	121.09	126.75
2	2	3897	B8K	C5-C4-N9	4.33	111.97	106.35
2	2	4523	A2M	C5-C4-N3	-4.33	121.11	126.75
2	2	2363	A2M	C1'-N9-C8	-4.33	117.37	127.14
2	2	978	2MG	C2-N1-C6	-4.32	119.51	124.48
2	2	2522	7MG	C2-N3-C4	4.31	119.98	112.30
2	2	2050	OMG	C2-N3-C4	4.31	119.98	112.30
2	2	3867	A2M	C1'-N9-C8	-4.28	117.47	127.14
2	2	2380	B8W	N9-C8-N7	-4.28	108.06	113.91
2	2	729	2MG	N9-C4-N3	4.25	134.48	125.94
2	2	4472	B8W	N9-C8-N7	-4.25	108.10	113.91
2	2	4185	B8W	O6-C6-N1	4.24	124.86	119.01
2	2	1524	A2M	C5-C4-N3	-4.24	121.22	126.75
2	2	1574	B9B	N9-C8-N7	-4.23	108.13	113.91
2	2	4571	A2M	C1'-N9-C8	-4.23	117.59	127.14
2	2	3909	OMC	O2-C2-N1	4.14	127.43	118.89
2	2	3899	BGH	C4-C5-N7	4.13	108.58	104.91
2	2	4185	B8W	N9-C8-N7	-4.12	108.28	113.91
2	2	3899	BGH	N9-C8-N7	4.11	108.85	103.33
2	2	4083	5MU	O4-C4-C5	-4.06	120.19	124.90
2	2	1517	2MG	N9-C4-N3	4.05	134.07	125.94
2	2	2754	B9B	N9-C8-N7	-4.05	108.38	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	3899	BGH	C5-C4-N9	4.04	111.60	106.35
2	2	237	B9B	N9-C8-N7	-4.03	108.40	113.91
2	2	3723	A2M	C1'-N9-C8	-4.01	118.07	127.14
2	2	3867	A2M	N3-C4-N9	4.00	133.68	127.08
2	2	2363	A2M	N3-C4-N9	4.00	133.67	127.08
2	2	4571	A2M	N3-C4-N9	3.98	133.65	127.08
2	2	1326	A2M	C1'-N9-C8	-3.97	118.17	127.14
2	2	3718	A2M	C1'-N9-C8	-3.96	118.20	127.14
2	2	1326	A2M	N3-C4-N9	3.95	133.60	127.08
2	2	1524	A2M	C1'-N9-C8	-3.93	118.26	127.14
2	2	3723	A2M	N3-C4-N9	3.91	133.52	127.08
2	2	2401	A2M	C1'-N9-C8	-3.91	118.32	127.14
2	2	3825	A2M	C1'-N9-C8	-3.90	118.32	127.14
2	2	4523	A2M	C1'-N9-C8	-3.90	118.33	127.14
2	2	4690	B8K	C5-C4-N9	3.85	111.34	106.35
2	2	3825	A2M	N3-C4-N9	3.84	133.41	127.08
2	2	2401	A2M	N3-C4-N9	3.84	133.41	127.08
2	2	3718	A2M	N3-C4-N9	3.84	133.40	127.08
2	2	1659	I4U	C5-C4-N3	-3.81	119.11	124.91
2	2	1534	A2M	N3-C4-N9	3.81	133.36	127.08
2	2	3897	B8K	C4-C5-N7	3.79	108.28	104.91
2	2	4472	B8W	N3-C4-N9	3.78	132.24	126.99
2	2	1534	A2M	C1'-N9-C8	-3.78	118.60	127.14
2	2	3897	B8K	N9-C8-N7	3.78	108.40	103.33
2	2	4620	OMU	N3-C2-N1	3.77	119.90	114.89
2	2	4872	2MG	CM2-N2-C2	-3.77	115.54	123.86
2	2	398	A2M	N3-C4-N9	3.76	133.28	127.08
2	2	2380	B8W	C61-O6-C6	-3.75	113.50	117.21
2	2	4523	A2M	N3-C4-N9	3.75	133.25	127.08
2	2	2380	B8W	N3-C4-N9	3.74	132.18	126.99
2	2	1574	B9B	N3-C4-N9	3.74	132.18	126.99
2	2	1605	7MG	C5-C4-N3	-3.73	121.03	128.13
2	2	2297	E7G	C5-C4-N3	-3.73	121.03	128.13
2	2	1524	A2M	N3-C4-N9	3.71	133.19	127.08
2	2	4550	7MG	C5-C4-N3	-3.70	121.08	128.13
2	2	3825	A2M	C5-N7-C8	3.70	108.77	103.51
2	2	3899	BGH	C5-C4-N3	-3.70	121.08	128.13
2	2	1456	B8Q	C6-N1-C2	-3.69	118.48	121.79
2	2	398	A2M	C1'-N9-C8	-3.69	118.80	127.14
2	2	1534	A2M	C2-N3-C4	3.68	120.45	111.75
2	2	1605	7MG	C5-C4-N9	3.68	111.12	106.35
2	2	3825	A2M	C2-N3-C4	3.67	120.42	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4571	A2M	C2-N3-C4	3.67	120.42	111.75
2	2	3723	A2M	C2-N3-C4	3.67	120.41	111.75
2	2	2380	B8W	O6-C6-N1	3.66	124.06	119.01
2	2	2363	A2M	C2-N3-C4	3.66	120.39	111.75
2	2	1326	A2M	C2-N3-C4	3.66	120.39	111.75
2	2	4083	5MU	C5M-C5-C4	3.64	122.77	118.77
2	2	2401	A2M	C2-N3-C4	3.63	120.33	111.75
2	2	2401	A2M	C5-N7-C8	3.62	108.65	103.51
2	2	1871	A2M	C2-N3-C4	3.61	120.28	111.75
2	2	3723	A2M	C5-N7-C8	3.61	108.63	103.51
2	2	3867	A2M	C2-N3-C4	3.60	120.26	111.75
2	2	3718	A2M	C2-N3-C4	3.59	120.24	111.75
2	2	1871	A2M	N3-C4-N9	3.59	133.00	127.08
2	2	4523	A2M	C2-N3-C4	3.57	120.19	111.75
2	2	398	A2M	C2-N3-C4	3.57	120.19	111.75
2	2	1534	A2M	C5-N7-C8	3.56	108.57	103.51
2	2	4523	A2M	C5-N7-C8	3.55	108.55	103.51
5	8	14	OMU	N3-C2-N1	3.53	119.57	114.89
2	2	1326	A2M	C5-N7-C8	3.53	108.52	103.51
2	2	4550	7MG	C5-C4-N9	3.52	110.92	106.35
2	2	4564	M7A	C2-N3-C4	3.52	120.07	111.75
2	2	2363	A2M	C5-N7-C8	3.51	108.50	103.51
2	2	398	A2M	C5-N7-C8	3.51	108.50	103.51
2	2	1871	A2M	C5-N7-C8	3.51	108.50	103.51
2	2	2297	E7G	C5-C4-N9	3.50	110.89	106.35
2	2	1524	A2M	C2-N3-C4	3.50	120.02	111.75
2	2	1348	P4U	C5-C4-N3	-3.50	119.59	124.91
2	2	237	B9B	N3-C2-N1	-3.49	119.94	125.42
5	8	14	OMU	C5-C4-N3	3.48	120.05	114.84
2	2	3867	A2M	C5-N7-C8	3.48	108.45	103.51
2	2	4472	B8W	N1-C2-N3	-3.47	119.97	125.42
2	2	2754	B9B	N3-C2-N1	-3.46	119.99	125.42
2	2	3718	A2M	C5-N7-C8	3.46	108.42	103.51
2	2	2522	7MG	C5-C4-N3	-3.45	121.56	128.13
2	2	2522	7MG	C5-C4-N9	3.44	110.81	106.35
2	2	4185	B8W	N1-C2-N3	-3.41	120.08	125.42
2	2	2380	B8W	N1-C2-N3	-3.38	120.11	125.42
2	2	4620	OMU	C5-C4-N3	3.38	119.89	114.84
2	2	4529	B8W	N9-C8-N7	-3.38	109.30	113.91
2	2	978	2MG	N9-C4-N3	3.37	132.71	125.94
2	2	4472	B8W	C5-N7-C8	3.36	108.29	103.51
2	2	1524	A2M	C5-N7-C8	3.36	108.28	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4571	A2M	C5-N7-C8	3.35	108.27	103.51
2	2	1574	B9B	N3-C2-N1	-3.34	120.17	125.42
2	2	1871	A2M	C1'-N9-C8	-3.29	119.71	127.14
2	2	4690	B8K	C6-C5-C4	-3.25	115.93	122.62
2	2	4529	B8W	N1-C2-N3	-3.24	120.34	125.42
2	2	2050	OMG	C2-N1-C6	-3.20	119.27	125.10
2	2	2364	OMG	C2-N1-C6	-3.19	119.28	125.10
2	2	3897	B8K	C5-C4-N3	-3.19	122.05	128.13
2	2	1909	P7G	N9-C8-N7	3.17	107.92	103.38
2	2	3897	B8K	C6-C5-C4	-3.17	116.08	122.62
2	2	4637	OMG	C2-N1-C6	-3.16	119.33	125.10
2	2	1883	OMG	C2-N1-C6	-3.15	119.35	125.10
2	2	2424	OMG	C2-N1-C6	-3.14	119.37	125.10
2	2	4494	OMG	C2-N1-C6	-3.13	119.39	125.10
2	2	4529	B8W	O6-C6-C5	-3.13	113.05	116.97
2	2	2861	OMC	O2-C2-N3	-3.12	117.25	122.33
2	2	4536	OMC	O2-C2-N3	-3.11	117.27	122.33
2	2	1316	OMG	C2-N1-C6	-3.11	119.43	125.10
2	2	4690	B8K	C5-C4-N3	-3.10	122.22	128.13
2	2	1625	OMG	C2-N1-C6	-3.10	119.44	125.10
2	2	4623	OMG	C2-N1-C6	-3.09	119.47	125.10
2	2	4472	B8W	O6-C6-N1	3.08	123.27	119.01
2	2	2380	B8W	C5-N7-C8	3.07	107.87	103.51
2	2	373	OMG	C2-N1-C6	-3.06	119.51	125.10
2	2	2522	7MG	N9-C8-N7	3.04	107.72	103.38
2	2	1522	OMG	C2-N1-C6	-3.02	119.59	125.10
2	2	4083	5MU	C6-C5-C4	3.01	120.55	118.03
5	8	14	OMU	O4-C4-C5	-3.01	119.87	125.16
2	2	2380	B8W	C4-N9-C1'	-3.01	119.43	126.59
2	2	2773	OMG	C2-N1-C6	-3.00	119.62	125.10
2	2	4185	B8W	C5-N7-C8	3.00	107.77	103.51
2	2	4870	OMG	C2-N1-C6	-2.98	119.67	125.10
2	2	4872	2MG	N9-C8-N7	-2.94	107.85	113.39
2	2	1574	B9B	C5-N7-C8	2.93	107.67	103.51
2	2	4185	B8W	N2-C2-N1	-2.92	112.71	117.25
2	2	4597	UR3	C6-N1-C2	-2.92	119.17	121.79
2	2	4483	B8T	O2-C2-N3	-2.91	117.60	122.33
2	2	978	2MG	N9-C8-N7	-2.89	107.94	113.39
2	2	3899	BGH	C6-C5-C4	-2.89	116.66	122.62
2	2	2380	B8W	N2-C2-N1	-2.89	112.76	117.25
2	2	2522	7MG	C4-C5-N7	2.89	109.54	105.53
2	2	3887	OMC	O2-C2-N3	-2.87	117.66	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4185	B8W	C61-O6-C6	-2.87	114.37	117.21
2	2	4872	2MG	N9-C4-N3	2.86	131.68	125.94
2	2	1883	OMG	O6-C6-C5	-2.85	119.04	126.60
2	2	4620	OMU	O4-C4-C5	-2.84	120.17	125.16
2	2	1517	2MG	C5-C6-N1	2.83	120.36	113.19
2	2	4483	B8T	O3'-C3'-C2'	2.82	120.94	111.82
2	2	1524	A2M	C4'-O4'-C1'	-2.82	103.26	109.47
2	2	1605	7MG	N9-C8-N7	2.81	107.40	103.38
2	2	2401	A2M	C2'-C1'-N9	-2.81	108.80	113.53
2	2	1574	B9B	C61-O6-C6	-2.81	112.12	117.47
2	2	237	B9B	C5-N7-C8	2.81	107.50	103.51
2	2	4529	B8W	N2-C2-N1	-2.80	112.89	117.25
2	2	1883	OMG	C5-C6-N1	2.80	120.31	113.19
2	2	2754	B9B	C5-N7-C8	2.80	107.49	103.51
2	2	3909	OMC	C5-C4-N4	2.80	124.98	120.57
2	2	373	OMG	C5-C6-N1	2.80	120.29	113.19
2	2	3899	BGH	O6-C6-N1	-2.77	114.81	120.12
2	2	729	2MG	C5-C6-N1	2.75	120.19	113.19
2	2	4671	B8T	C6-C5-C4	2.75	120.32	116.96
2	2	2422	OMC	O2-C2-N3	-2.74	117.87	122.33
2	2	2424	OMG	C5-C6-N1	2.74	120.14	113.19
2	2	978	2MG	C5-C6-N1	2.73	120.12	113.19
2	2	4597	UR3	C3U-N3-C2	2.72	122.09	117.31
2	2	4870	OMG	C5-C6-N1	2.71	120.08	113.19
2	2	2364	OMG	C5-C6-N1	2.71	120.06	113.19
2	2	1909	P7G	C71-N7-C5	2.71	130.93	124.52
2	2	4623	OMG	C5-C6-N1	2.70	120.05	113.19
2	2	4872	2MG	C5-C6-N1	2.70	120.04	113.19
2	2	1316	OMG	C5-C6-N1	2.69	120.01	113.19
2	2	2364	OMG	C5-C4-N9	2.69	110.50	105.63
2	2	4472	B8W	C4-N9-C1'	-2.68	120.20	126.59
2	2	4623	OMG	C5-C4-N9	2.68	110.49	105.63
2	2	3897	B8K	O6-C6-N1	-2.68	114.98	120.12
2	2	2297	E7G	N9-C8-N7	2.68	107.20	103.38
2	2	4637	OMG	C5-C6-N1	2.67	119.97	113.19
2	2	4637	OMG	O4'-C1'-N9	2.67	114.47	108.36
2	2	4494	OMG	C5-C6-N1	2.67	119.97	113.19
2	2	2050	OMG	C5-C6-N1	2.67	119.96	113.19
2	2	1625	OMG	C5-C6-N1	2.66	119.95	113.19
2	2	2050	OMG	C5-C4-N9	2.66	110.45	105.63
2	2	1522	OMG	C5-C6-N1	2.65	119.93	113.19
2	2	1316	OMG	C5-C4-N9	2.65	110.44	105.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1517	2MG	O6-C6-C5	-2.65	119.56	126.60
2	2	2773	OMG	C5-C6-N1	2.65	119.92	113.19
2	2	4637	OMG	C5-C4-N9	2.65	110.43	105.63
2	2	4083	5MU	O2-C2-N1	-2.63	119.29	122.79
2	2	4690	B8K	C2-N1-C6	-2.61	120.34	125.10
2	2	4550	7MG	C4-C5-N7	2.59	109.12	105.53
2	2	1605	7MG	C4-C5-N7	2.59	109.12	105.53
2	2	3909	OMC	C4-N3-C2	2.58	124.42	120.25
2	2	4550	7MG	N9-C8-N7	2.58	107.07	103.38
2	2	3909	OMC	C1'-N1-C2	2.58	124.18	118.42
2	2	373	OMG	O6-C6-C5	-2.56	119.80	126.60
2	2	2773	OMG	C5-C4-N9	2.56	110.28	105.63
2	2	1625	OMG	C5-C4-N9	2.56	110.27	105.63
2	2	2364	OMG	O6-C6-C5	-2.55	119.85	126.60
2	2	4472	B8W	C2-N1-C6	2.53	119.95	115.93
2	2	2424	OMG	O6-C6-C5	-2.53	119.89	126.60
2	2	1522	OMG	O6-C6-C5	-2.53	119.89	126.60
2	2	1625	OMG	O6-C6-C5	-2.53	119.89	126.60
2	2	237	B9B	C2-N3-C4	2.52	120.86	113.89
2	2	4494	OMG	O6-C6-C5	-2.52	119.91	126.60
2	2	729	2MG	N9-C8-N7	-2.51	108.66	113.39
2	2	373	OMG	C5-C4-N9	2.51	110.19	105.63
2	2	4529	B8W	C5-N7-C8	2.51	107.08	103.51
2	2	4637	OMG	O6-C6-C5	-2.50	119.96	126.60
2	2	4494	OMG	C5-C4-N9	2.50	110.17	105.63
2	2	4872	2MG	O6-C6-C5	-2.50	119.97	126.60
2	2	729	2MG	O6-C6-C5	-2.50	119.97	126.60
2	2	1522	OMG	C5-C4-N9	2.50	110.16	105.63
2	2	1316	OMG	O6-C6-C5	-2.48	120.01	126.60
2	2	1605	7MG	C2-N1-C6	-2.48	120.57	125.10
2	2	978	2MG	O6-C6-C5	-2.48	120.03	126.60
2	2	237	B9B	C61-O6-C6	-2.48	112.76	117.47
2	2	2297	E7G	C2-N1-C6	-2.48	120.58	125.10
2	2	4472	B8W	C2-N3-C4	2.48	120.73	113.89
2	2	4623	OMG	O6-C6-C5	-2.47	120.04	126.60
2	2	1517	2MG	N9-C8-N7	-2.47	108.74	113.39
2	2	978	2MG	N1-C2-N3	-2.47	120.14	123.95
2	2	373	OMG	O4'-C1'-N9	2.46	113.99	108.36
2	2	2754	B9B	C2-N3-C4	2.46	120.69	113.89
2	2	2050	OMG	O6-C6-C5	-2.46	120.08	126.60
2	2	2380	B8W	C1'-N9-C8	2.45	132.68	127.14
2	2	2773	OMG	O6-C6-C5	-2.45	120.10	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4564	M7A	C5-C4-N3	-2.44	120.90	126.62
2	2	4494	OMG	O4'-C1'-N9	2.44	113.94	108.36
2	2	2786	B9H	O3'-C3'-C4'	2.43	118.09	111.05
2	2	4870	OMG	O6-C6-C5	-2.43	120.14	126.60
2	2	4472	B8W	C5-C6-N1	-2.43	120.08	123.46
2	2	4623	OMG	O4'-C1'-N9	2.43	113.92	108.36
2	2	3880	P7G	N9-C8-N7	2.43	106.85	103.38
2	2	2861	OMC	C1'-N1-C2	2.42	123.82	118.42
2	2	1316	OMG	O4'-C1'-N9	2.42	113.89	108.36
2	2	1517	2MG	N1-C2-N3	-2.41	120.23	123.95
2	2	3909	OMC	C5-C4-N3	-2.41	117.23	121.33
2	2	3869	OMC	O2-C2-N3	-2.40	118.43	122.33
2	2	4529	B8W	C6-C5-N7	-2.40	130.45	133.63
2	2	2754	B9B	C61-O6-C6	-2.39	112.91	117.47
2	2	1871	A2M	C2'-C1'-N9	-2.39	109.51	113.53
2	2	4472	B8W	C4-C5-N7	-2.38	107.72	110.62
2	2	2786	B9H	O2-C2-N1	-2.38	117.15	122.72
2	2	4185	B8W	C2-N3-C4	2.37	120.45	113.89
2	2	2364	OMG	O4'-C1'-N9	2.37	113.79	108.36
2	2	4483	B8T	O3'-C3'-C4'	2.37	117.90	111.05
2	2	1456	B8Q	C31-N3-C2	2.36	121.22	117.79
2	2	3897	B8K	C2-N1-C6	-2.36	120.80	125.10
2	2	1574	B9B	C2-N3-C4	2.36	120.40	113.89
2	2	3899	BGH	N1-C2-N3	-2.35	118.94	123.32
2	2	2380	B8W	C2-N1-C6	2.35	119.66	115.93
2	2	2424	OMG	N9-C4-N3	2.35	130.65	125.94
2	2	3899	BGH	C2-N1-C6	-2.34	120.83	125.10
2	2	4529	B8W	C5-C6-N1	-2.34	120.21	123.46
2	2	4550	7MG	C2-N1-C6	-2.32	120.86	125.10
2	2	2424	OMG	C5-C4-N9	2.32	109.84	105.63
2	2	237	B9B	C1'-N9-C8	-2.32	121.90	127.14
2	2	4623	OMG	C4-C5-N7	-2.32	107.06	110.72
2	2	1883	OMG	C2'-C1'-N9	-2.31	109.73	114.22
2	2	4185	B8W	C4-N9-C1'	-2.31	121.09	126.59
2	2	729	2MG	N1-C2-N3	-2.31	120.39	123.95
2	2	3897	B8K	N1-C2-N3	-2.30	119.03	123.32
2	2	1883	OMG	O4'-C1'-N9	2.30	113.61	108.36
2	2	4623	OMG	N9-C8-N7	-2.29	109.07	113.39
2	2	4623	OMG	N2-C2-N1	2.29	121.59	116.71
2	2	4083	5MU	O4-C4-N3	-2.28	115.74	120.12
2	2	1625	OMG	O4'-C1'-N9	2.28	113.58	108.36
2	2	4530	UR3	C6-N1-C2	-2.28	119.74	121.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	237	B9B	C4-N9-C8	2.28	108.20	105.73
2	2	373	OMG	N9-C8-N7	-2.27	109.11	113.39
5	8	14	OMU	C1'-N1-C2	2.27	121.68	117.57
2	2	4529	B8W	C2-N1-C6	2.27	119.53	115.93
2	2	2380	B8W	C2-N3-C4	2.26	120.14	113.89
2	2	1456	B8Q	C1'-N1-C2	2.26	120.80	116.99
2	2	4564	M7A	C4-N9-C1'	-2.25	121.25	126.60
2	2	4870	OMG	N9-C8-N7	-2.25	109.15	113.39
2	2	4637	OMG	N2-C2-N1	2.25	121.50	116.71
2	2	373	OMG	C2'-C1'-N9	-2.24	109.86	114.22
2	2	1883	OMG	C5-C4-N9	2.24	109.70	105.63
2	2	2050	OMG	O4'-C1'-N9	2.24	113.49	108.36
2	2	4690	B8K	N1-C2-N3	-2.24	119.14	123.32
2	2	4472	B8W	N2-C2-N1	-2.24	113.77	117.25
2	2	3909	OMC	C6-N1-C2	-2.23	116.62	120.49
2	2	4870	OMG	N9-C4-N3	2.23	130.41	125.94
2	2	1316	OMG	C4-C5-N7	-2.22	107.20	110.72
5	8	14	OMU	CM2-O2'-C2'	2.22	120.35	114.52
2	2	4185	B8W	C2-N1-C6	2.22	119.46	115.93
2	2	4690	B8K	O6-C6-C5	-2.22	122.10	127.54
2	2	4472	B8W	C1'-N9-C8	2.21	132.13	127.14
2	2	2522	7MG	C2-N1-C6	-2.21	121.07	125.10
2	2	4637	OMG	C4-C5-N7	-2.20	107.25	110.72
2	2	4494	OMG	N9-C4-N3	2.18	130.31	125.94
2	2	4529	B8W	C2-N3-C4	2.18	119.91	113.89
2	2	1883	OMG	N9-C4-N3	2.17	130.31	125.94
2	2	373	OMG	C4-C5-N7	-2.17	107.29	110.72
2	2	4536	OMC	C1'-N1-C2	2.17	123.26	118.42
2	2	2424	OMG	O4'-C1'-N9	2.16	113.29	108.36
2	2	1522	OMG	O4'-C1'-N9	2.15	113.28	108.36
2	2	1574	B9B	C4-N9-C8	2.15	108.06	105.73
2	2	1625	OMG	N9-C4-N3	2.14	130.23	125.94
2	2	4872	2MG	C1'-N9-C4	-2.14	120.15	126.50
2	2	2754	B9B	C4-N9-C8	2.13	108.03	105.73
2	2	4483	B8T	C6-C5-C4	2.12	119.56	116.96
2	2	978	2MG	C8-N7-C5	2.12	108.08	104.24
2	2	2522	7MG	C6-C5-C4	-2.12	118.25	122.62
2	2	2380	B8W	C5-C6-N1	-2.11	120.52	123.46
2	2	2050	OMG	C4-C5-N7	-2.10	107.39	110.72
2	2	4872	2MG	C8-N7-C5	2.10	108.04	104.24
2	2	4472	B8W	C5-C4-N9	2.10	108.22	105.78
2	2	1659	I4U	O2-C2-N3	-2.09	118.93	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4483	B8T	C5-C4-N3	-2.09	119.23	122.59
2	2	2786	B9H	C21-O2'-C2'	2.08	119.98	114.52
2	2	2522	7MG	O6-C6-C5	-2.08	122.44	127.54
2	2	4620	OMU	O2-C2-N1	-2.07	120.03	122.79
2	2	2861	OMC	O2-C2-N1	2.07	123.17	118.89
2	2	2422	OMC	C1'-N1-C2	2.07	123.04	118.42
2	2	4536	OMC	O2-C2-N1	2.07	123.16	118.89
2	2	2363	A2M	C4-N9-C1'	2.07	131.52	126.59
2	2	1605	7MG	O6-C6-C5	-2.06	122.49	127.54
2	2	2773	OMG	C4-C5-N7	-2.05	107.47	110.72
2	2	2297	E7G	C6-C5-C4	-2.05	118.39	122.62
2	2	4483	B8T	C6-N1-C2	-2.05	116.94	120.49
2	2	4185	B8W	C5-C6-N1	-2.03	120.63	123.46
2	2	1348	P4U	O2-C2-N3	-2.03	119.03	122.33
2	2	4870	OMG	C5-C4-N9	2.03	109.31	105.63
2	2	2364	OMG	C4-C5-N7	-2.03	107.51	110.72
2	2	2364	OMG	N2-C2-N1	2.02	121.01	116.71
2	2	2297	E7G	O6-C6-C5	-2.02	122.59	127.54
2	2	2522	7MG	N1-C2-N3	-2.02	119.56	123.32
2	2	4571	A2M	C4-N9-C1'	2.02	131.40	126.59
2	2	373	OMG	N2-C2-N1	2.02	121.00	116.71
2	2	1522	OMG	C4-C5-N7	-2.01	107.54	110.72
2	2	1316	OMG	N2-C2-N1	2.01	120.98	116.71
2	2	4872	2MG	N1-C2-N3	-2.00	120.85	123.95
2	2	2050	OMG	N2-C2-N1	2.00	120.98	116.71

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	8	14	OMU	C1'-C2'-O2'-CM2
2	2	237	B9B	C5-C6-O6-C61
2	2	237	B9B	N1-C6-O6-C61
2	2	237	B9B	C3'-C4'-C5'-O5'
2	2	237	B9B	O4'-C4'-C5'-O5'
2	2	398	A2M	O4'-C4'-C5'-O5'
2	2	1348	P4U	N3-C4-O4-C41
2	2	1574	B9B	C5-C6-O6-C61
2	2	1574	B9B	N1-C6-O6-C61
2	2	1574	B9B	C62-C61-O6-C6
2	2	1625	OMG	C3'-C4'-C5'-O5'
2	2	1871	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	1871	A2M	C3'-C4'-C5'-O5'
2	2	1883	OMG	C3'-C4'-C5'-O5'
2	2	2364	OMG	C1'-C2'-O2'-CM2
2	2	2380	B8W	C5-C6-O6-C61
2	2	2380	B8W	N1-C6-O6-C61
2	2	2424	OMG	O4'-C4'-C5'-O5'
2	2	2424	OMG	C3'-C4'-C5'-O5'
2	2	2754	B9B	C5-C6-O6-C61
2	2	2754	B9B	N1-C6-O6-C61
2	2	2754	B9B	C62-C61-O6-C6
2	2	2786	B9H	C1'-C2'-O2'-C21
2	2	4185	B8W	C5-C6-O6-C61
2	2	4472	B8W	C5-C6-O6-C61
2	2	4472	B8W	N1-C6-O6-C61
2	2	4550	7MG	O4'-C4'-C5'-O5'
2	2	4550	7MG	C3'-C4'-C5'-O5'
2	2	4637	OMG	O4'-C4'-C5'-O5'
2	2	4637	OMG	C1'-C2'-O2'-CM2
2	2	4870	OMG	O4'-C4'-C5'-O5'
2	2	4870	OMG	C3'-C4'-C5'-O5'
2	2	4872	2MG	O4'-C4'-C5'-O5'
2	2	398	A2M	C3'-C4'-C5'-O5'
2	2	1883	OMG	O4'-C4'-C5'-O5'
2	2	2364	OMG	O4'-C4'-C5'-O5'
2	2	3867	A2M	C3'-C4'-C5'-O5'
2	2	3897	B8K	O4'-C4'-C5'-O5'
2	2	4529	B8W	C3'-C4'-C5'-O5'
2	2	4529	B8W	O4'-C4'-C5'-O5'
2	2	4637	OMG	C3'-C4'-C5'-O5'
2	2	4872	2MG	C3'-C4'-C5'-O5'
2	2	237	B9B	O6-C61-C62-C63
2	2	1625	OMG	O4'-C4'-C5'-O5'
2	2	1909	P7G	O4'-C4'-C5'-O5'
2	2	2364	OMG	C3'-C4'-C5'-O5'
2	2	3867	A2M	O4'-C4'-C5'-O5'
2	2	3897	B8K	C3'-C4'-C5'-O5'
2	2	3880	P7G	O4'-C4'-C5'-O5'
2	2	1909	P7G	C3'-C4'-C5'-O5'
2	2	3701	OMC	C3'-C4'-C5'-O5'
2	2	3701	OMC	O4'-C4'-C5'-O5'
2	2	3880	P7G	C3'-C4'-C5'-O5'
2	2	1524	A2M	O4'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
2	2	2297	E7G	C72-C71-N7-C8
2	2	2754	B9B	O6-C61-C62-C63
2	2	1534	A2M	C4'-C5'-O5'-P
2	2	237	B9B	C62-C61-O6-C6
2	2	4185	B8W	N1-C6-O6-C61
2	2	3867	A2M	C4'-C5'-O5'-P
2	2	373	OMG	C4'-C5'-O5'-P
2	2	3887	OMC	C4'-C5'-O5'-P
2	2	4523	A2M	C4'-C5'-O5'-P
2	2	1524	A2M	O4'-C1'-N9-C8
2	2	1625	OMG	C4'-C5'-O5'-P
2	2	4637	OMG	C4'-C5'-O5'-P
2	2	3897	B8K	C4'-C5'-O5'-P
2	2	2422	OMC	O4'-C4'-C5'-O5'
2	2	4870	OMG	C4'-C5'-O5'-P
2	2	1909	P7G	C72-C71-N7-C8
2	2	1517	2MG	C4'-C5'-O5'-P
2	2	3909	OMC	O4'-C4'-C5'-O5'
2	2	729	2MG	O4'-C4'-C5'-O5'
2	2	1534	A2M	O4'-C4'-C5'-O5'
2	2	3909	OMC	C2'-C1'-N1-C2
2	2	1659	I4U	C43-C41-O4-C4
2	2	3899	BGH	O4'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	1574	B9B	1	0
2	2	4472	B8W	1	0
2	2	4083	5MU	1	0
2	2	2522	7MG	1	0
2	2	3723	A2M	1	0
2	2	4620	OMU	1	0
2	2	1517	2MG	1	0
2	2	2363	A2M	1	0
2	2	4494	OMG	1	0
2	2	729	2MG	1	0
5	8	14	OMU	1	0
2	2	4571	A2M	1	0
2	2	1871	A2M	1	0
2	2	4483	B8T	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	3718	A2M	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	30,34,34	0.83	1 (3%)	46,54,54	1.77	11 (23%)

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	-	5/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	w	801	GTP	C2-N3	2.13	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	w	801	GTP	C5-C4-N3	-5.20	120.02	128.46
60	w	801	GTP	C2-N3-C4	4.68	120.63	112.30
60	w	801	GTP	N9-C4-N3	3.39	132.76	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	w	801	GTP	PA-O3A-PB	-3.29	121.53	132.83
60	w	801	GTP	C2-N1-C6	-2.95	119.73	125.10
60	w	801	GTP	PB-O3B-PG	-2.70	123.56	132.83
60	w	801	GTP	C5-C6-N1	2.59	119.76	113.19
60	w	801	GTP	N9-C8-N7	-2.59	108.52	113.39
60	w	801	GTP	C8-N7-C5	2.54	108.83	104.24
60	w	801	GTP	O6-C6-C5	-2.40	120.24	126.60
60	w	801	GTP	C3'-C2'-C1'	2.00	105.23	101.43

There are no chirality outliers.

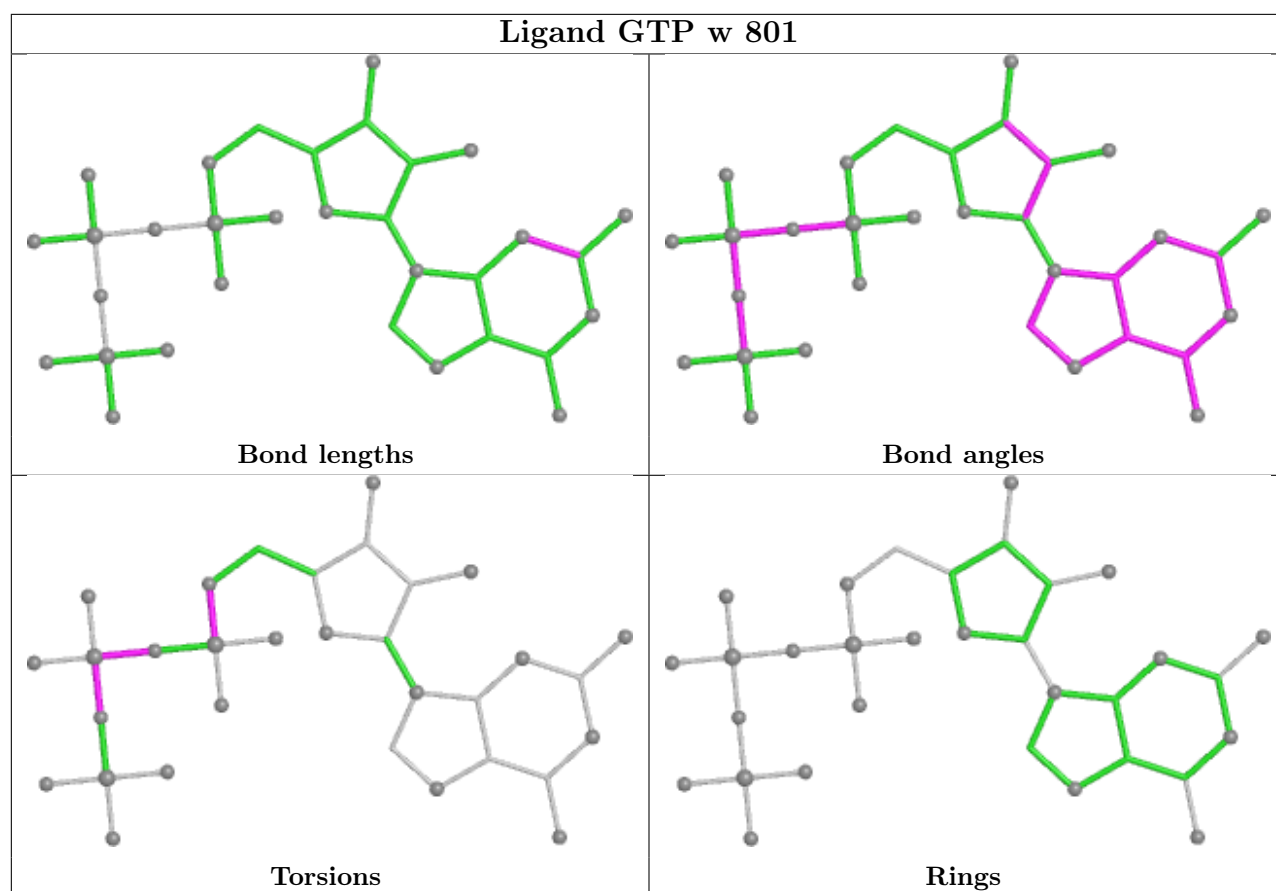
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	w	801	GTP	C5'-O5'-PA-O3A
60	w	801	GTP	PA-O3A-PB-O1B
60	w	801	GTP	C5'-O5'-PA-O2A
60	w	801	GTP	PG-O3B-PB-O3A
60	w	801	GTP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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.

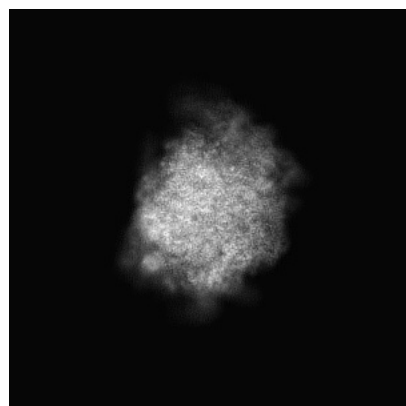
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35651. These allow visual inspection of the internal detail of the map and identification of artifacts.

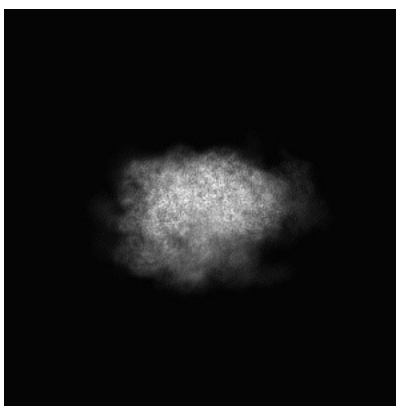
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

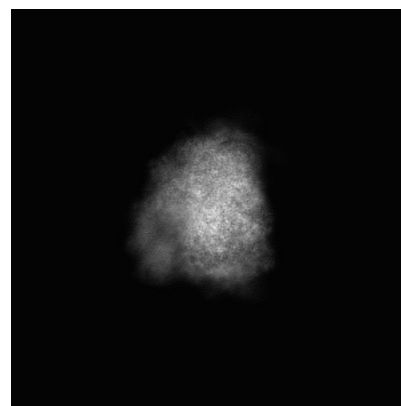
6.1.1 Primary map



X

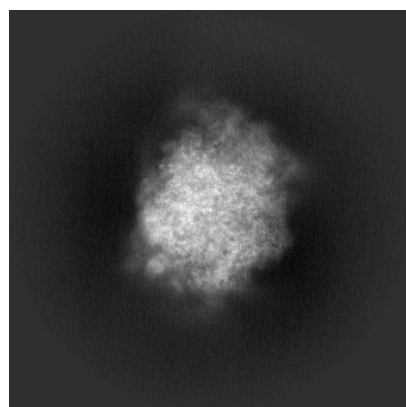


Y

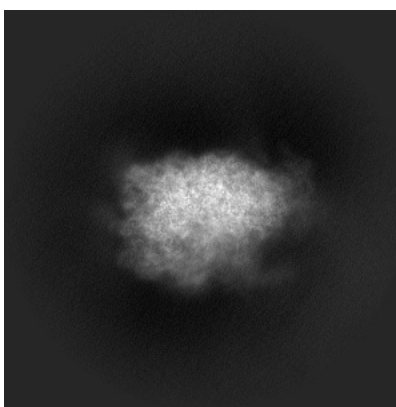


Z

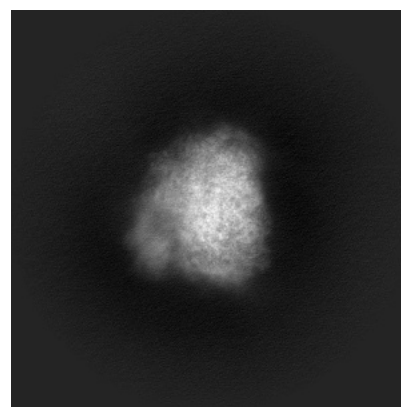
6.1.2 Raw map



X



Y

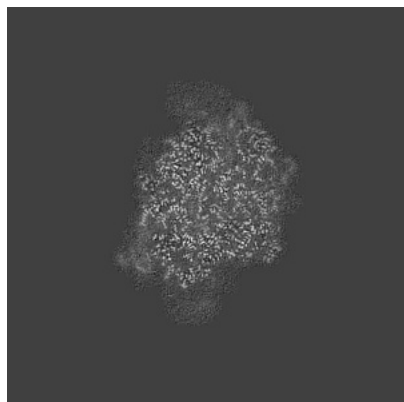


Z

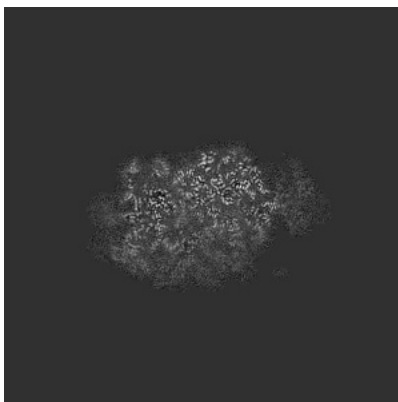
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

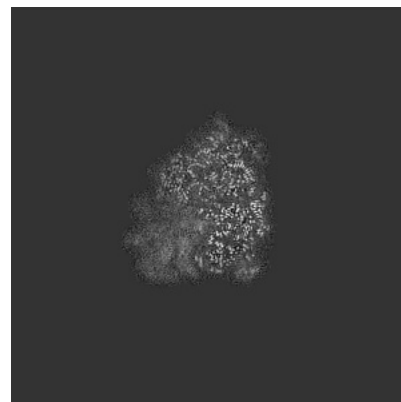
6.2.1 Primary map



X Index: 200

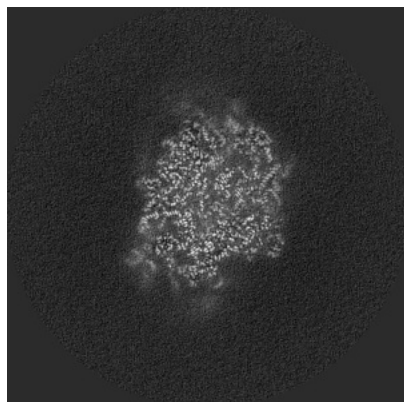


Y Index: 200

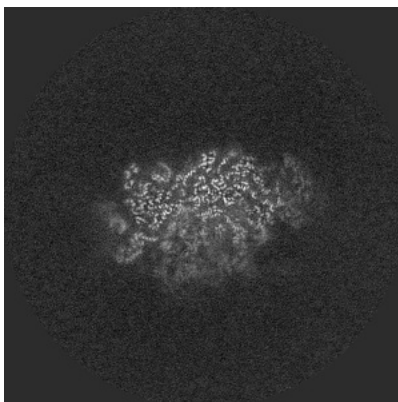


Z Index: 200

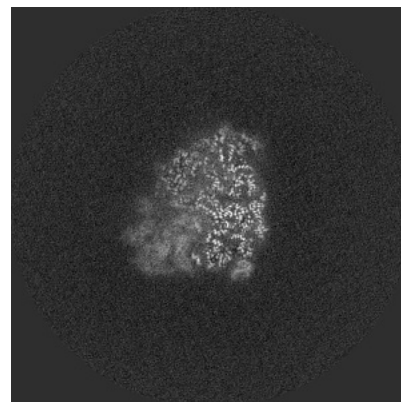
6.2.2 Raw map



X Index: 200



Y Index: 200

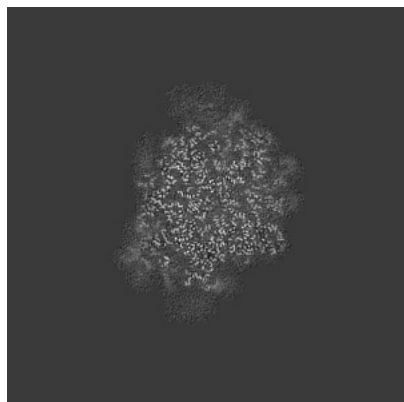


Z Index: 200

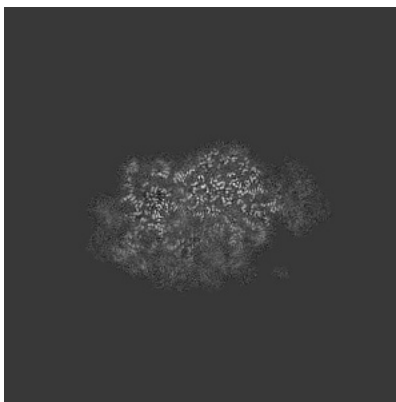
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

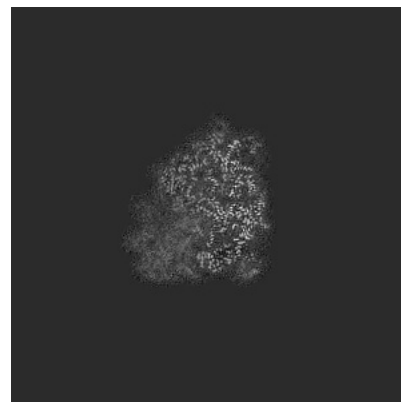
6.3.1 Primary map



X Index: 206

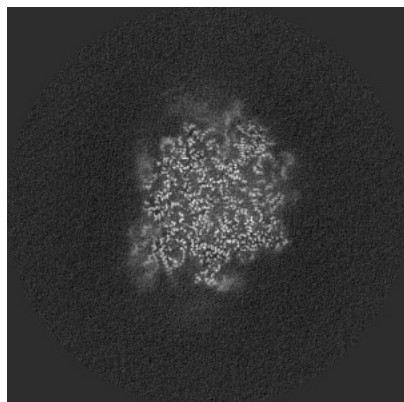


Y Index: 199

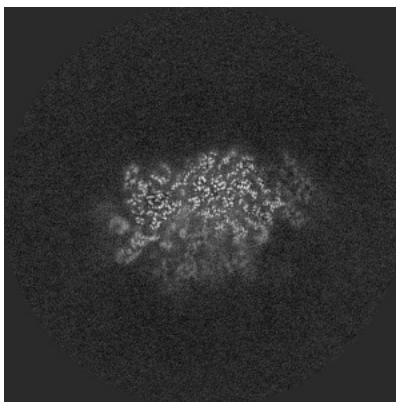


Z Index: 198

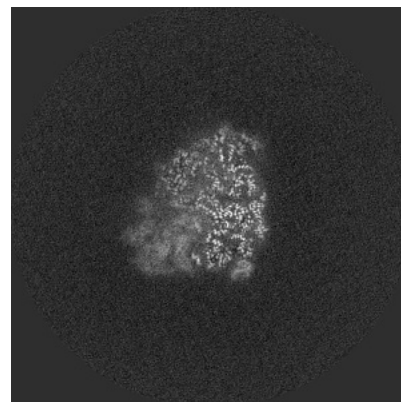
6.3.2 Raw map



X Index: 206



Y Index: 199

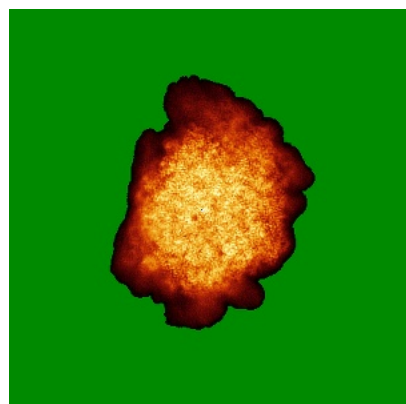


Z Index: 200

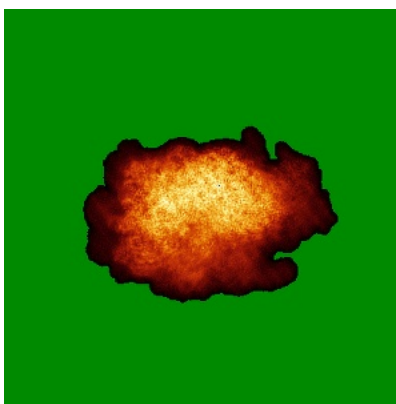
The images above show the largest variance slices of the map in three orthogonal directions.

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

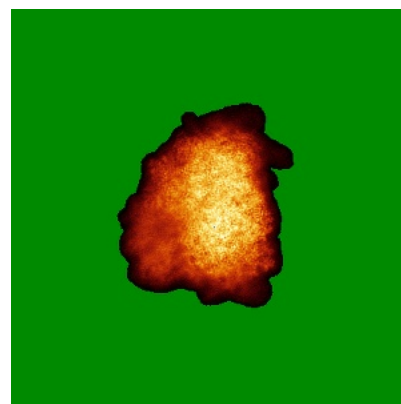
6.4.1 Primary map



X

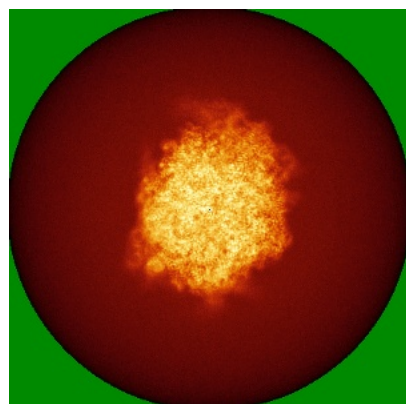


Y

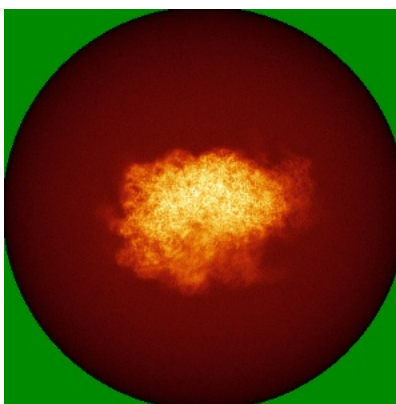


Z

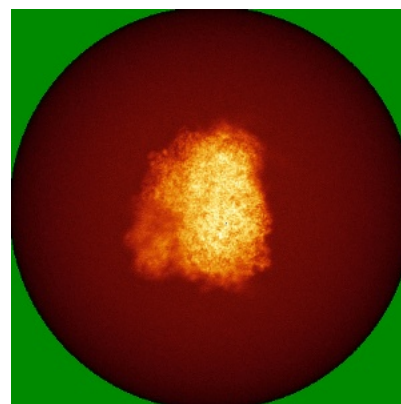
6.4.2 Raw map



X



Y

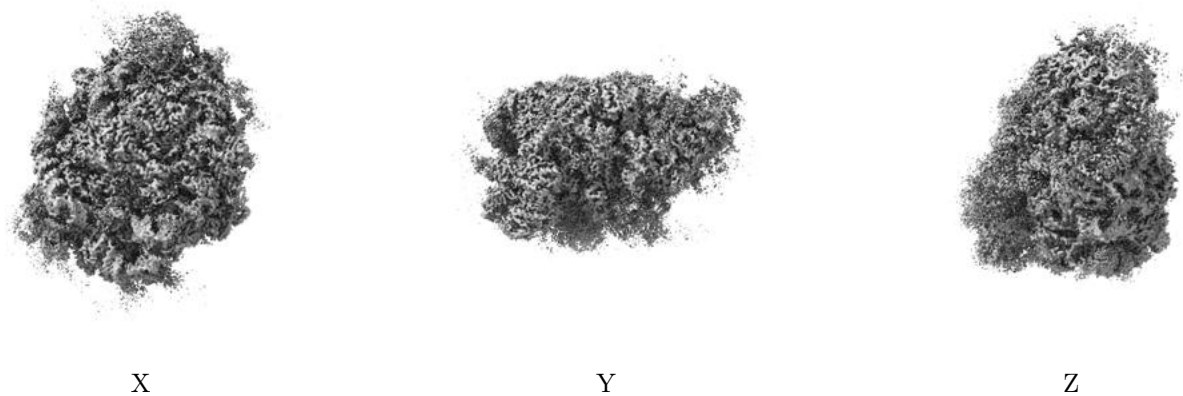


Z

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.

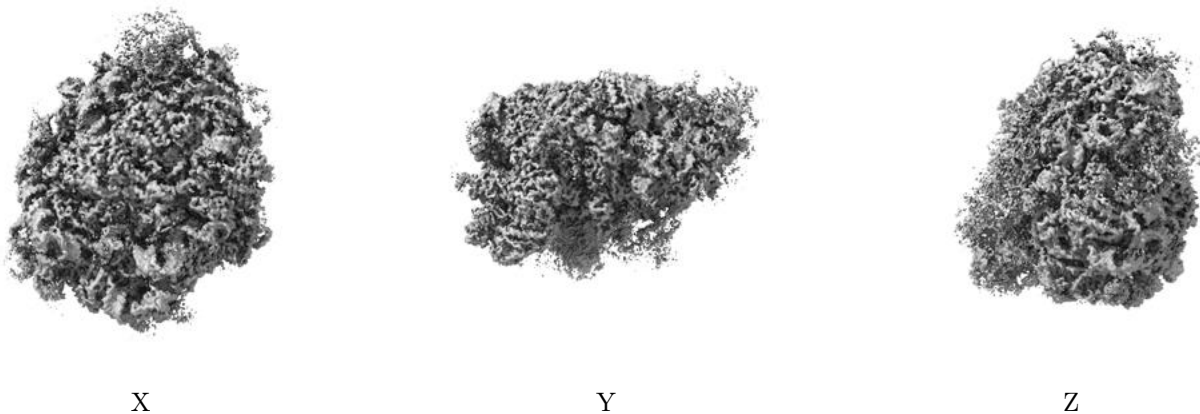
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. 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.

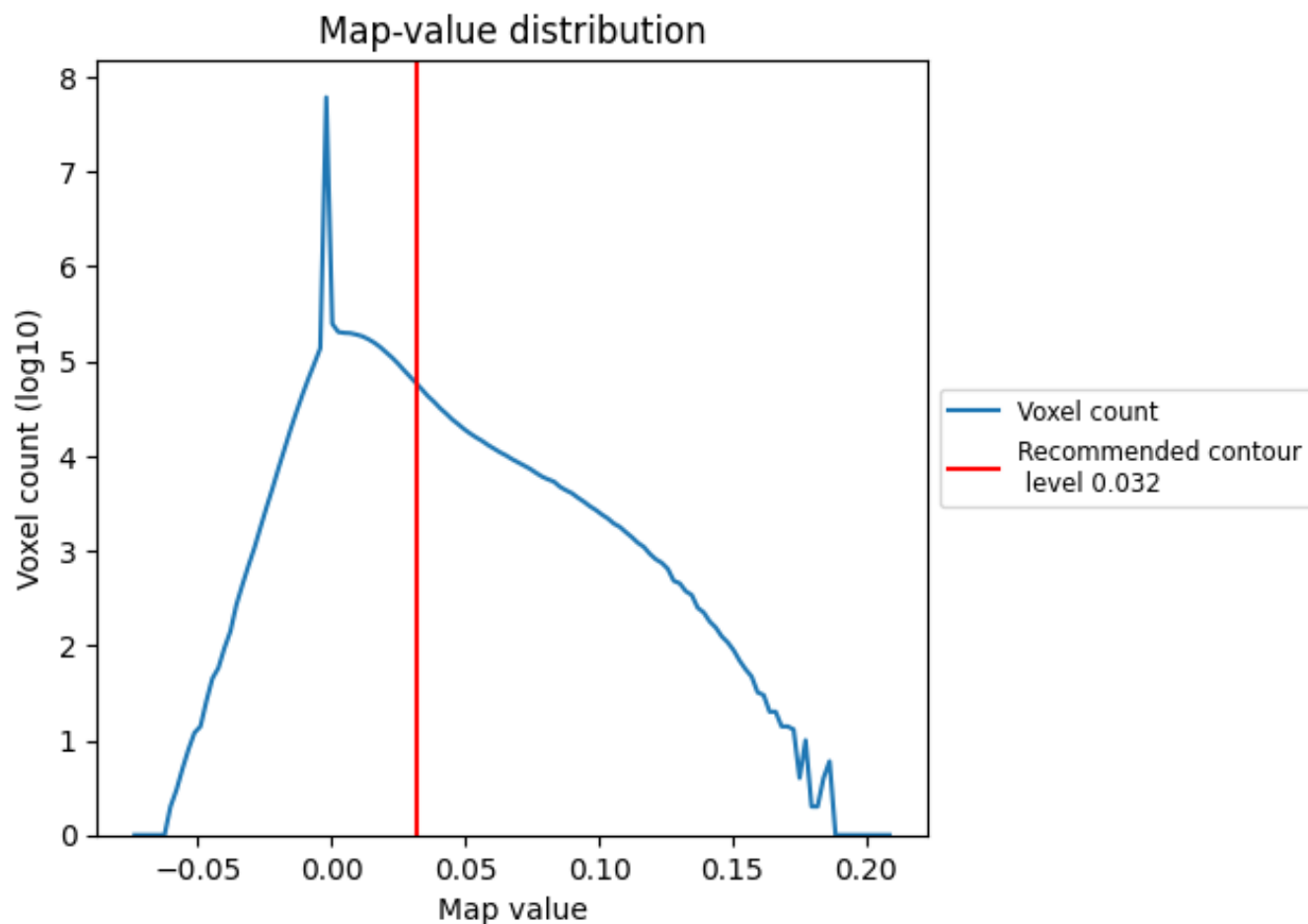
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

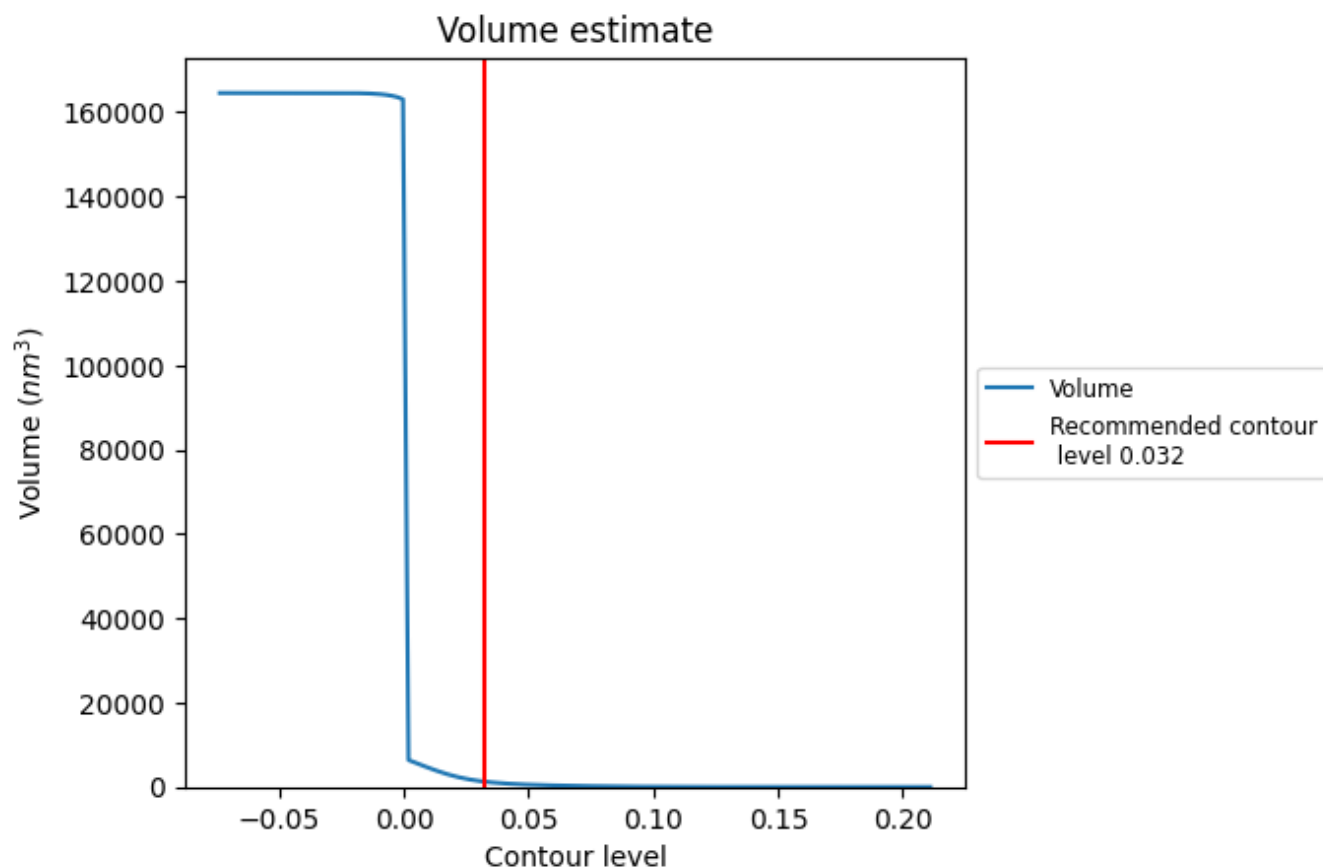
This section contains the results of statistical analysis of the map.

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.

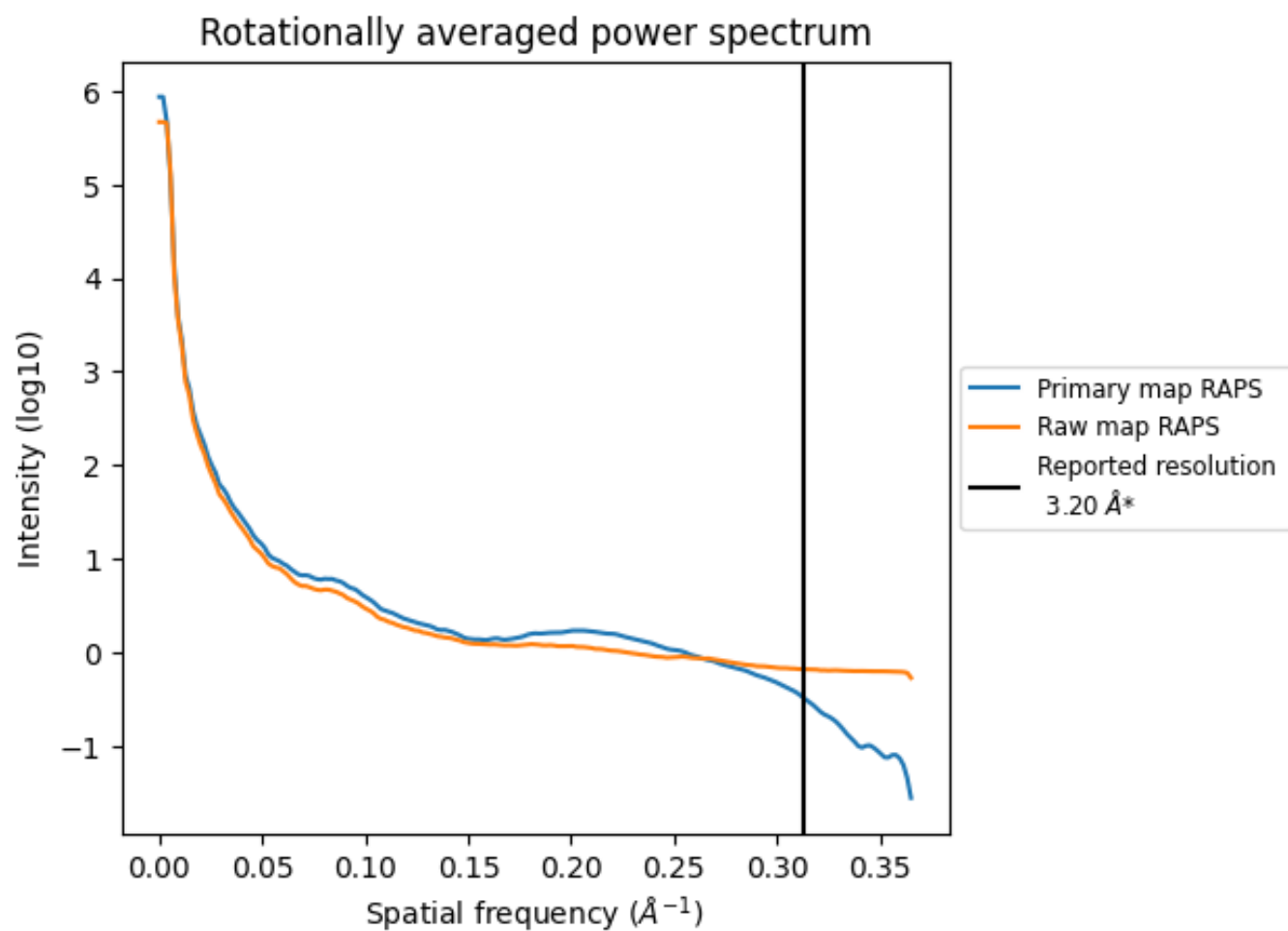
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1286 nm^3 ; this corresponds to an approximate mass of 1162 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 ⓘ

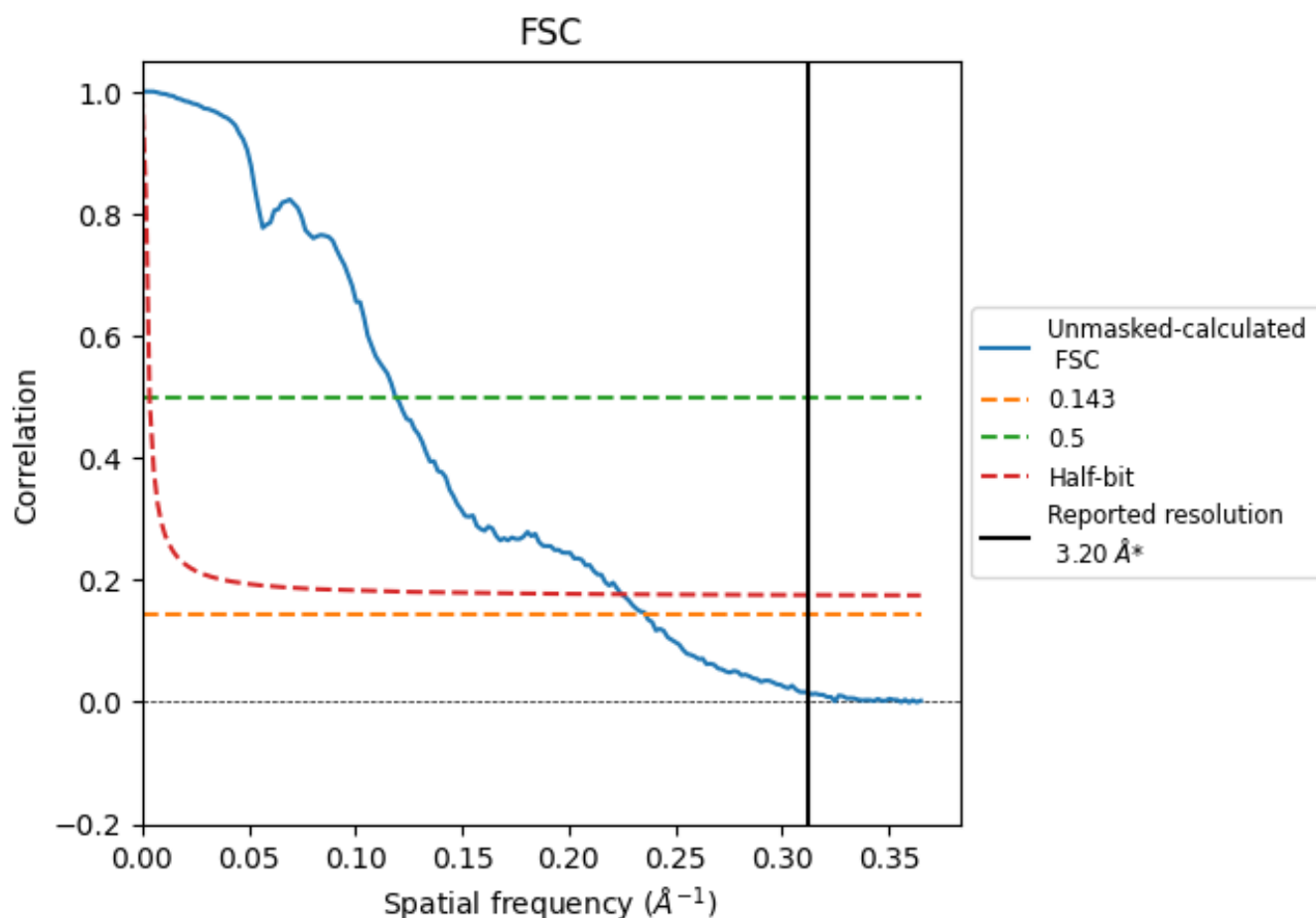


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

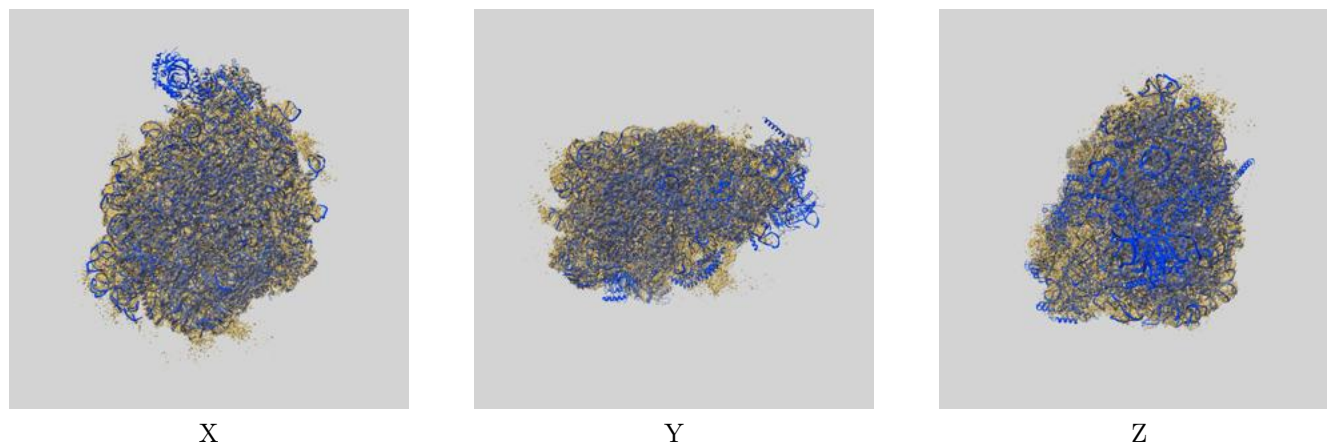
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	8.41	4.45

*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 4.24 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

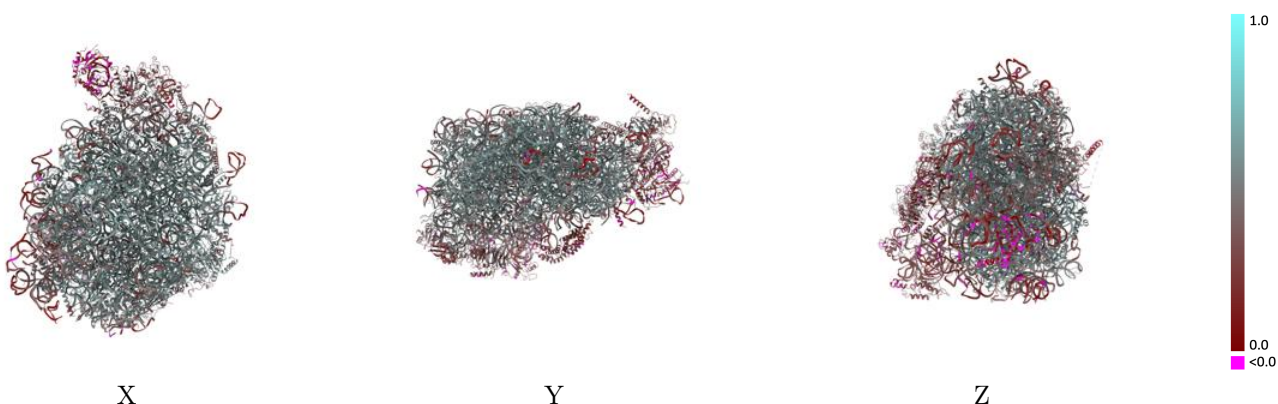
This section contains information regarding the fit between EMDB map EMD-35651 and PDB model 8IPY. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



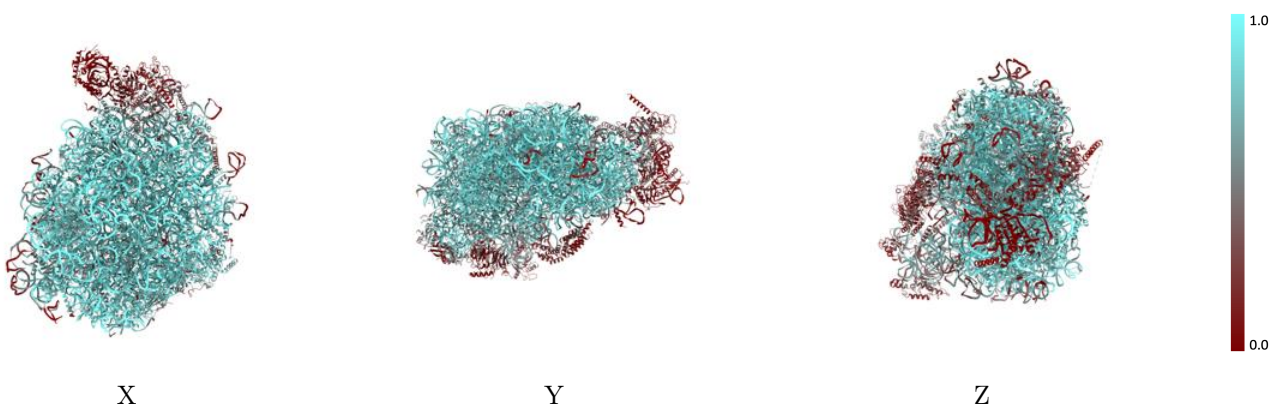
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



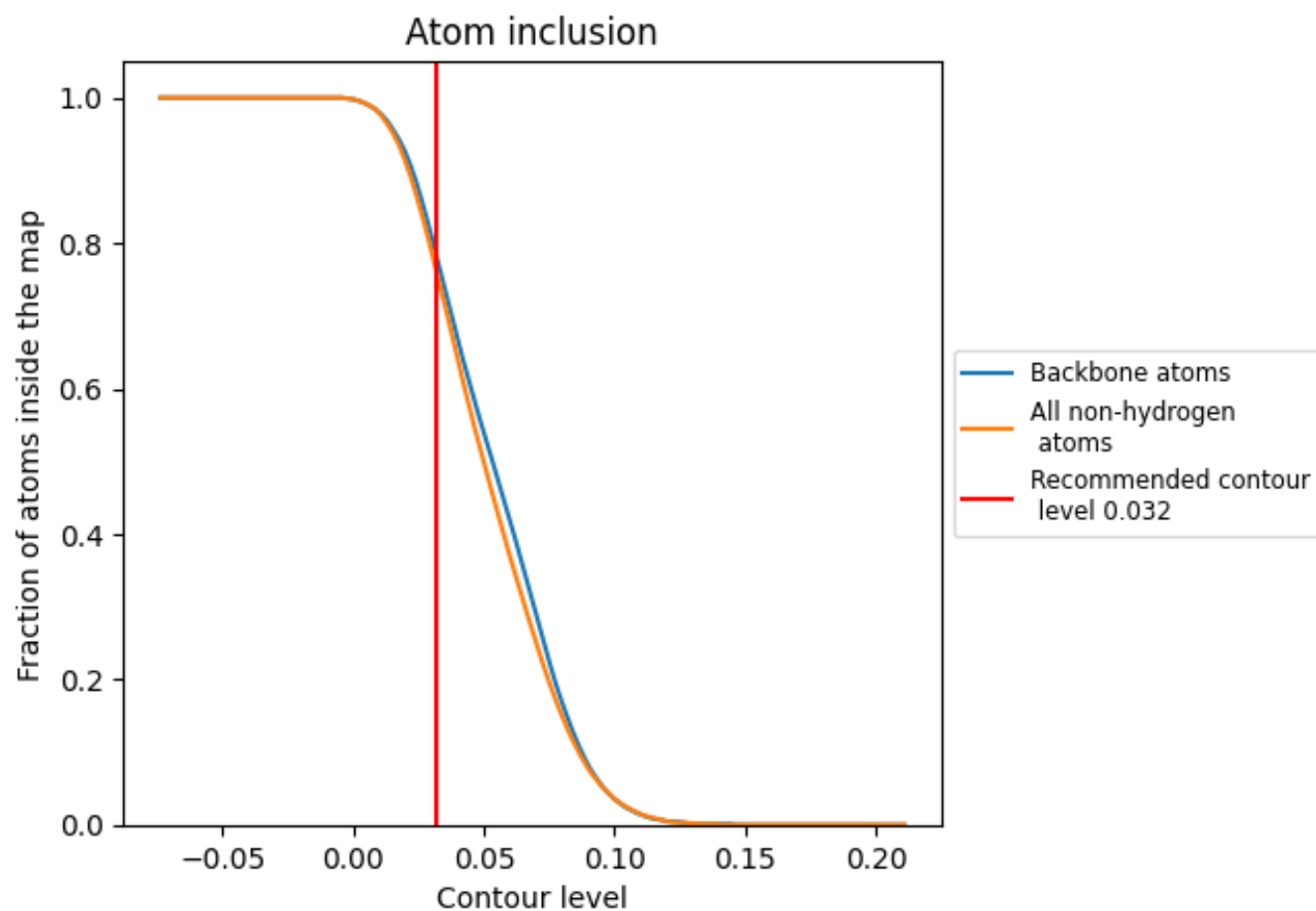
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 76% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.4550
1	 0.1910	 0.3760
2	 0.8690	 0.4650
3	 0.7220	 0.2860
4	 0.7210	 0.4550
6	 0.7640	 0.4940
7	 0.8360	 0.5340
8	 0.9400	 0.5330
9	 0.6160	 0.4430
A	 0.5310	 0.3820
B	 0.9000	 0.5510
C	 0.2390	 0.2200
D	 0.9190	 0.5520
E	 0.6830	 0.4780
F	 0.8660	 0.5320
G	 0.7080	 0.4640
H	 0.8610	 0.5290
I	 0.8250	 0.5220
J	 0.7560	 0.4930
K	 0.8250	 0.4970
L	 0.8970	 0.5490
M	 0.9570	 0.5650
N	 0.1680	 0.2300
O	 0.7180	 0.5040
P	 0.9720	 0.5700
Q	 0.8290	 0.5100
R	 0.2500	 0.2090
S	 0.8860	 0.5270
T	 0.5770	 0.3150
U	 0.8960	 0.5420
V	 0.8970	 0.5380
W	 0.1220	 0.3400
X	 0.7960	 0.5140
Y	 0.8650	 0.5350
Z	 0.9280	 0.5600



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Chain	Atom inclusion	Q-score
a	 0.8740	 0.5190
b	 0.9190	 0.5480
c	 0.0030	 0.1510
d	 0.7750	 0.5030
e	 0.9050	 0.5430
f	 0.3610	 0.3410
g	 0.7730	 0.4970
h	 0.8790	 0.5370
i	 0.7890	 0.4960
j	 0.8370	 0.5250
k	 0.9470	 0.5680
l	 0.9280	 0.5570
m	 0.8640	 0.5280
n	 0.9510	 0.5670
o	 0.7930	 0.4870
p	 0.9040	 0.5370
q	 0.3710	 0.4000
r	 0.3250	 0.3040
t	 0.0870	 0.2720
u	 0.4560	 0.3610
v	 0.5690	 0.4210
w	 0.7280	 0.4680
x	 0.0020	 0.1540
y	 0.3500	 0.3070
z	 0.6580	 0.4570