



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 03:37 PM JST

PDB ID : 8INK / pdb_00008ink
EMDB ID : EMD-35599
Title : human nuclear pre-60S ribosomal particle - State D
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-03-10
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

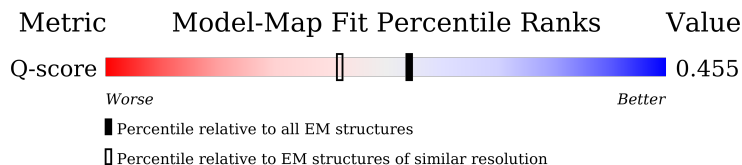
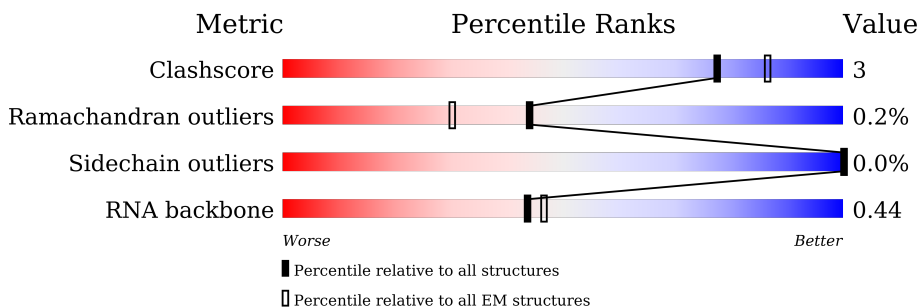
1 Overall quality at a glance

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	
2	6	245	
3	7	163	

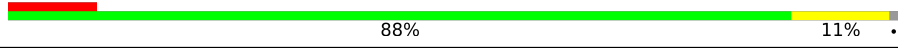
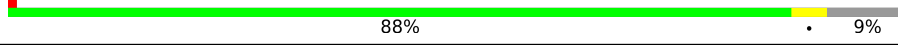
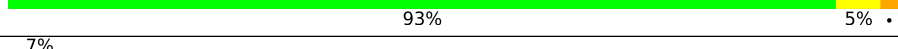
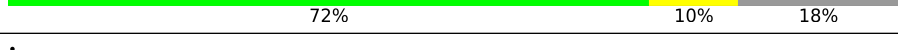
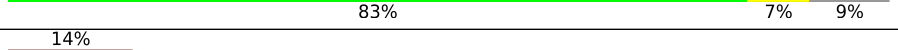
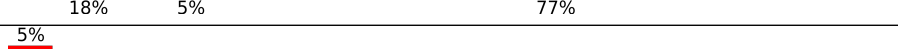
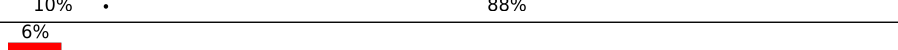
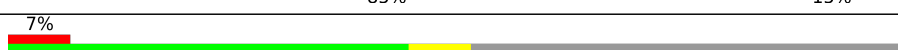
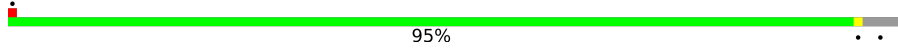
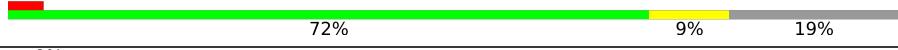
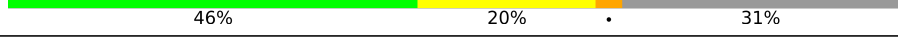
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Mol	Chain	Length	Quality of chain
4	8	156	
5	9	134	
6	A	159	
7	B	403	
8	D	427	
9	E	115	
10	F	117	
11	G	266	
12	H	123	
13	I	192	
14	J	260	
15	K	105	
16	L	148	
17	M	97	
18	O	70	
19	P	51	
20	Q	211	
21	S	215	
22	U	204	
23	V	203	
24	X	92	
25	Z	188	
26	a	196	
27	b	176	
28	e	140	

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Mol	Chain	Length	Quality of chain
29	g	156	
30	h	145	
31	i	136	
32	l	137	
33	m	257	
34	n	110	
35	o	288	
36	p	248	
37	r	360	
38	u	549	
39	w	731	
40	y	165	
41	z	129	
42	C	178	
43	R	297	
44	W	485	
45	T	160	
46	4	634	
47	Y	184	
48	k	135	
49	j	125	
50	d	128	
51	3	120	
52	v	239	
53	2	5054	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 152807 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 protein called Eukaryotic translation initiation factor 6.

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

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

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

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

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

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

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

- Molecule 6 is a protein called 60S ribosomal protein L29.

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

- Molecule 7 is a protein called 60S ribosomal protein L3.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	241	Total	C	N	O	S	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 L36.

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

- Molecule 16 is a protein called 60S ribosomal protein L27a.

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

- Molecule 17 is a protein called 60S ribosomal protein L37.

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

- Molecule 18 is a protein called 60S ribosomal protein L38.

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

- Molecule 19 is a protein called 60S ribosomal protein L39.

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

- Molecule 20 is a protein called 60S ribosomal protein L13.

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

- Molecule 21 is a protein called 60S ribosomal protein L14.

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

- Molecule 22 is a protein called 60S ribosomal protein L15.

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

- Molecule 23 is a protein called 60S ribosomal protein L13a.

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

- Molecule 24 is a protein called 60S ribosomal protein L37a.

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

- Molecule 25 is a protein called 60S ribosomal protein L18.

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

- Molecule 26 is a protein called 60S ribosomal protein L19.

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

- Molecule 27 is a protein called 60S ribosomal protein L18a.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	117	Total	C	N	O	S	0	0
			958	612	179	166	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 37 is a protein called Coiled-coil domain-containing protein 86.

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

- Molecule 38 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	u	68	Total	C	N	O	S	0	0
			578	362	121	92	3		

- Molecule 39 is a protein called G Protein Nucleolar 2.

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

- Molecule 40 is a protein called 60S ribosomal protein L12.

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

- Molecule 41 is a protein called Protein LLP homolog.

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

- Molecule 42 is a protein called 60S ribosomal protein L11.

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

- Molecule 43 is a protein called 60S ribosomal protein L5.

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

- Molecule 44 is a protein called Notchless protein homolog 1.

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

- Molecule 45 is a protein called 60S ribosomal protein L21.

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

- Molecule 46 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4	611	Total	C	N	O	S	0	0
			5016	3151	918	920	27		

- Molecule 47 is a protein called 60S ribosomal protein L17.

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

- Molecule 48 is a protein called 60S ribosomal protein L32.

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

- Molecule 49 is a protein called 60S ribosomal protein L31.

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

- Molecule 50 is a protein called 60S ribosomal protein L22.

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

- Molecule 51 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	115	Total	C	N	O	P	0	0
			2453	1093	437	808	115		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	92	C	G	conflict	GB NR_023363
3	93	G	C	conflict	GB NR_023363
3	95	C	U	conflict	GB NR_023363
3	96	U	G	conflict	GB NR_023363

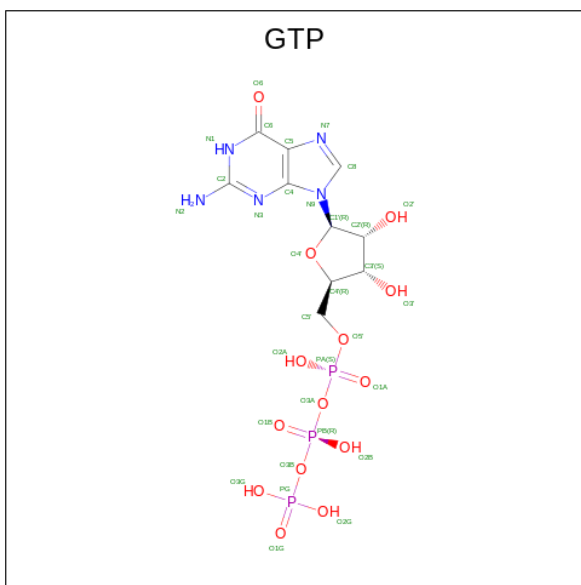
- Molecule 52 is a protein called mRNA turnover protein 4 homolog.

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

- Molecule 53 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	3495	Total	C	N	O	P	0	0
			75023	33449	13712	24368	3494		

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



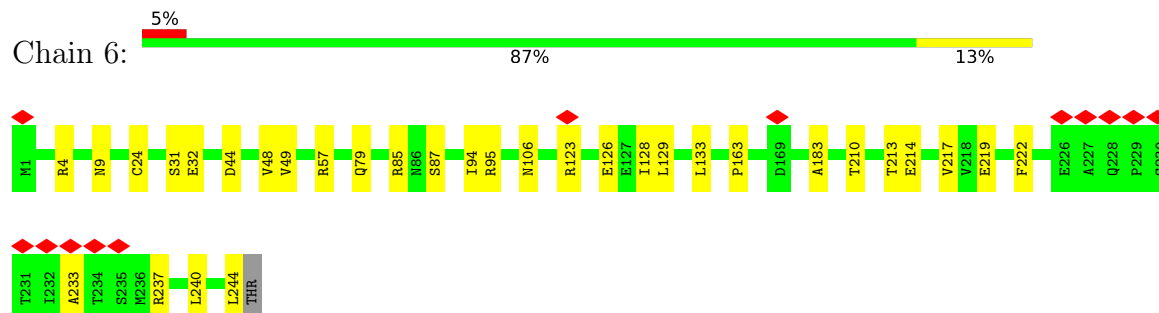
Mol	Chain	Residues	Atoms					AltConf
54	w	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

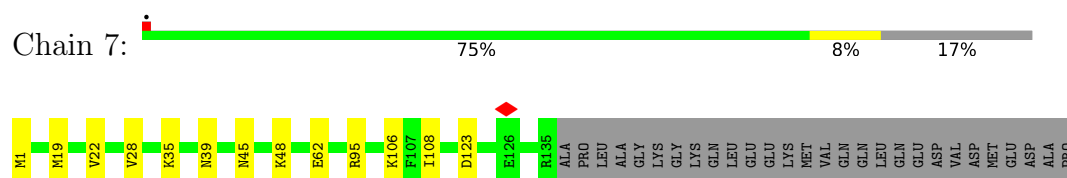
Mol	Chain	Residues	Atoms	AltConf
55	w	1	Total Mg 1 1	0

LEU	HIS	LYS	LYS	PRO	LYS	SER	ASP	GLU	THR	ARG	LEU	ALA	THR	ALA	MET	GLY	LYS	THR	ASN	PRO	PHE	SER	SER	THR	ASN	GLU	LYS	LYS	GLN	LYS	ASN	PHE	MET	MET	ARG	TYR	SER	GLN	ASN	VAL	ARG			
SER	LYS	ASN	LYS	ARG	ARG	PHE	ARG	GLU	LYS	GLN	LEU	ALA	LEU	ARG	ASP	ALA	LEU	LEU	LYS	ARG	LYS	ARG	GLY	MET	LYS																			

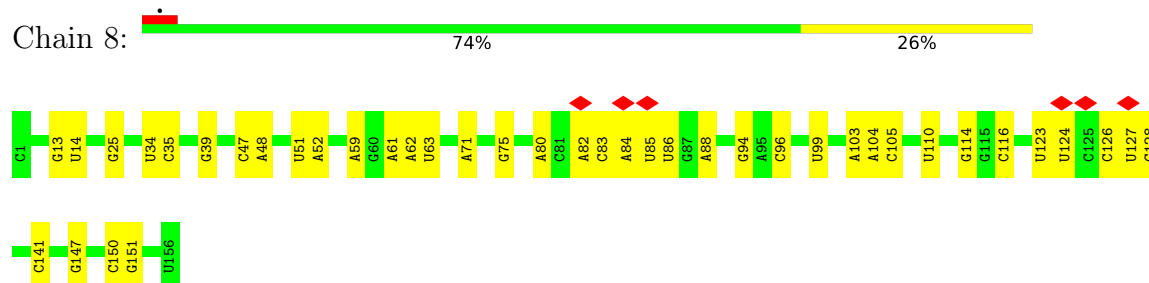
- Molecule 2: Eukaryotic translation initiation factor 6



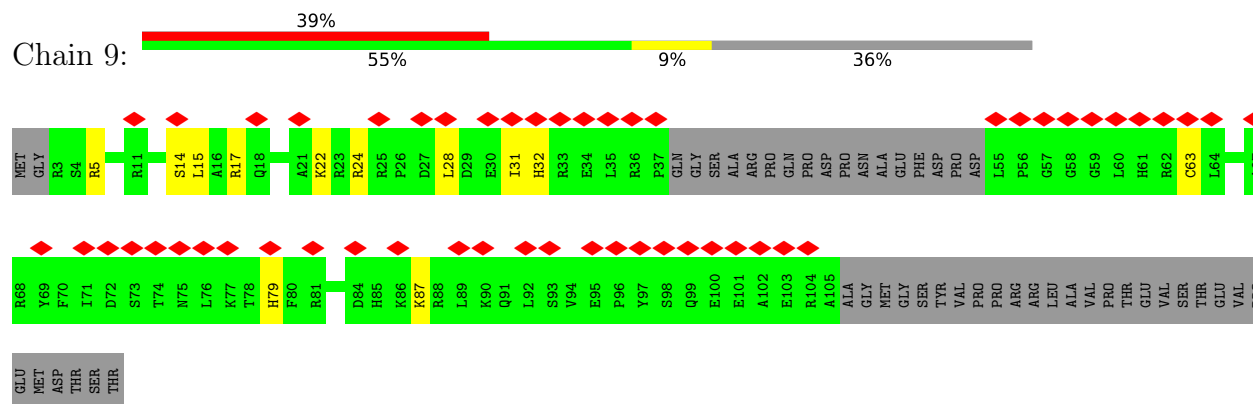
- Molecule 3: Probable ribosome biogenesis protein RLP24



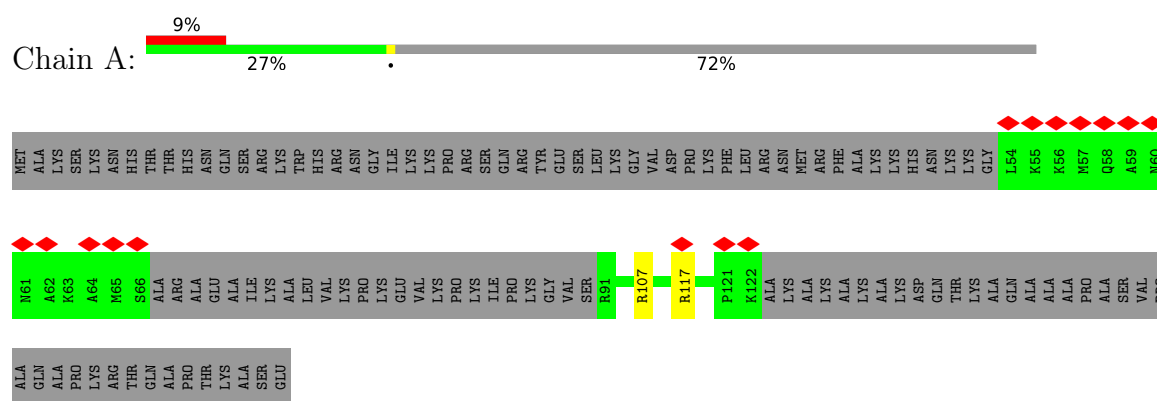
- Molecule 4: 5.8S rRNA



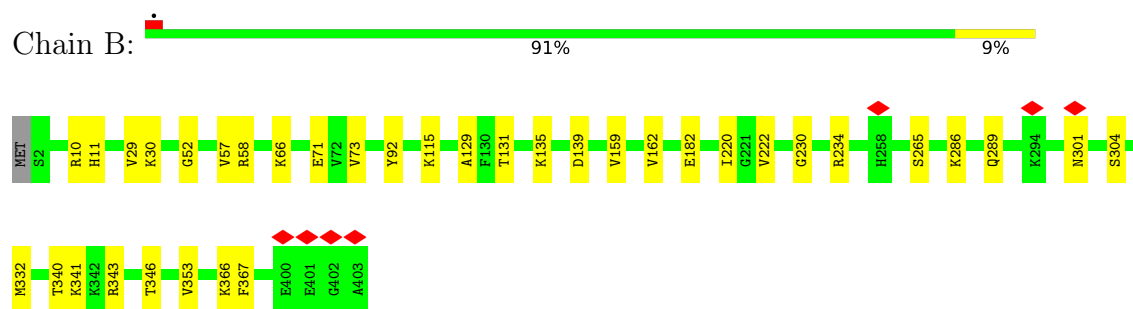
- Molecule 5: Zinc finger protein 593



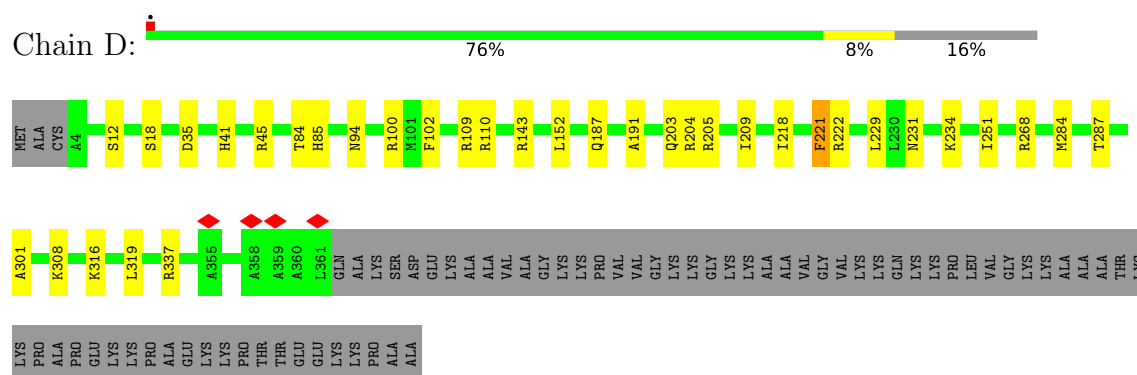
- Molecule 6: 60S ribosomal protein L29



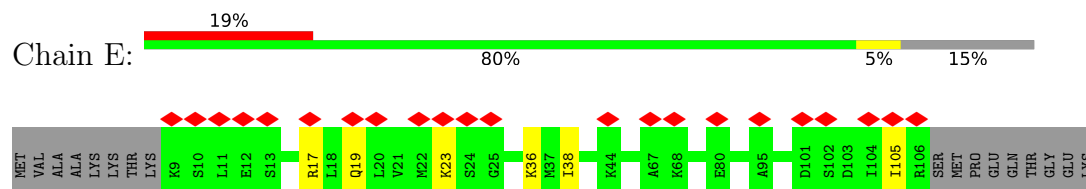
- Molecule 7: 60S ribosomal protein L3



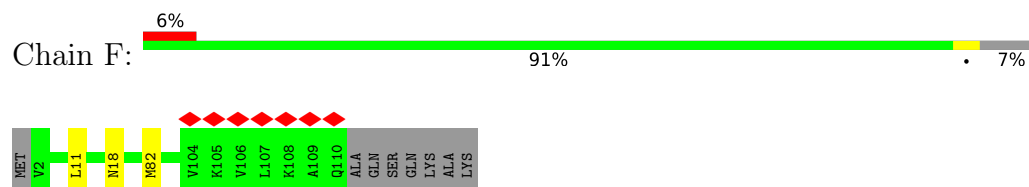
- Molecule 8: 60S ribosomal protein L4



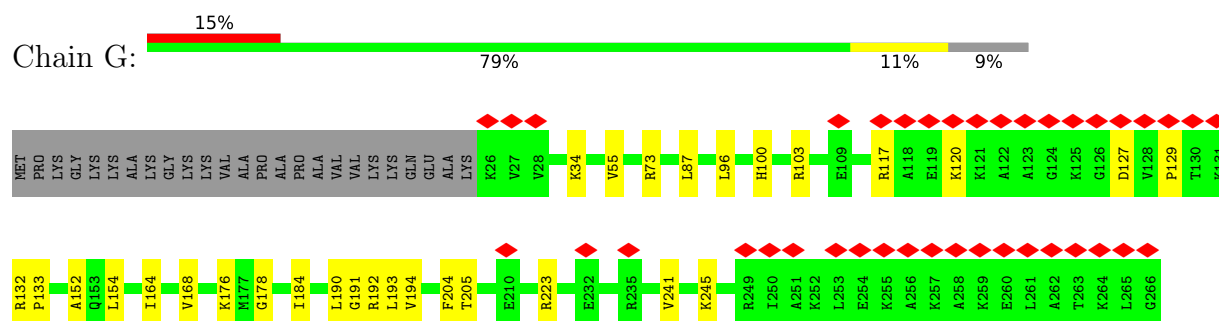
- Molecule 9: 60S ribosomal protein L30



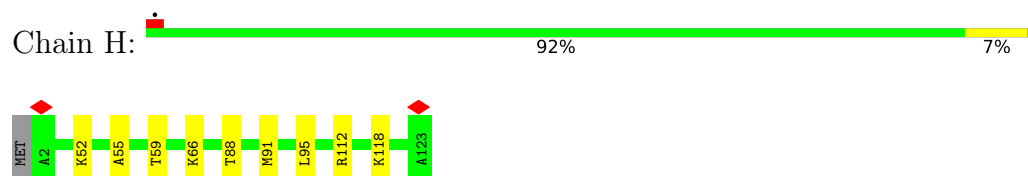
- Molecule 10: 60S ribosomal protein L34



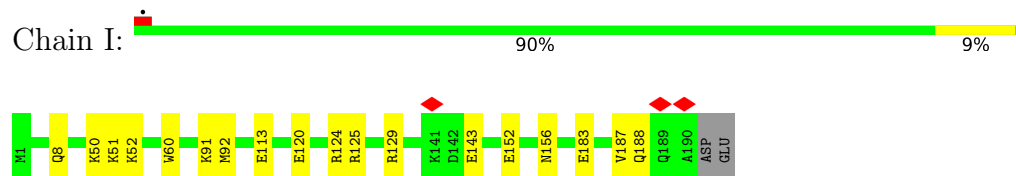
- Molecule 11: 60S ribosomal protein L7a



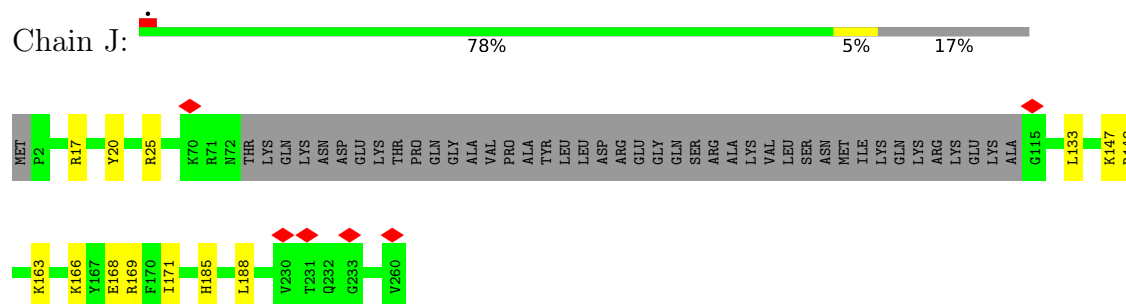
- Molecule 12: 60S ribosomal protein L35



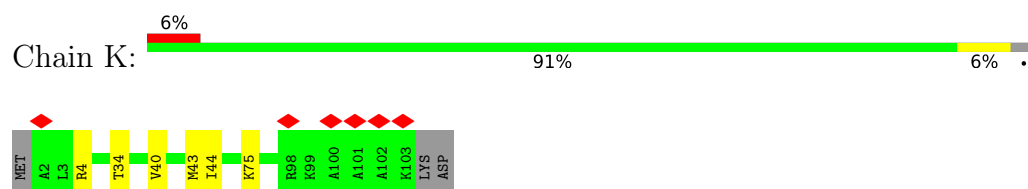
- Molecule 13: 60S ribosomal protein L9



- Molecule 14: Ribosome biogenesis protein NSA2 homolog

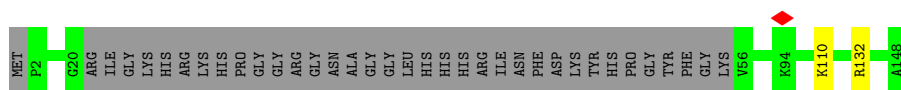


- Molecule 15: 60S ribosomal protein L36



- Molecule 16: 60S ribosomal protein L27a





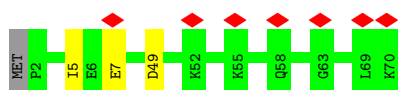
- Molecule 17: 60S ribosomal protein L37

Chain M: 80% 8% 11%



- Molecule 18: 60S ribosomal protein L38

Chain O: 10% 94% . .



- Molecule 19: 60S ribosomal protein L39

Chain P: 84% 14% .



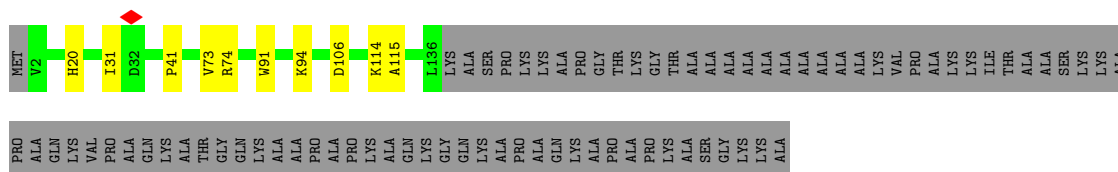
- Molecule 20: 60S ribosomal protein L13

Chain Q: 9% 93% 6%



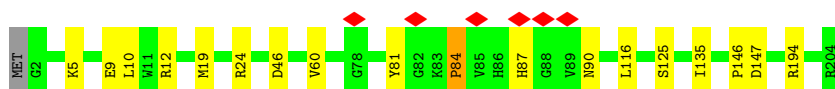
- Molecule 21: 60S ribosomal protein L14

Chain S: 58% 5% 37%



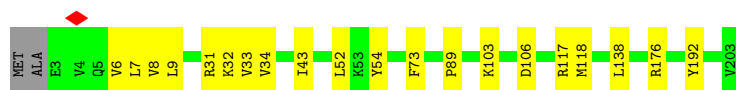
- Molecule 22: 60S ribosomal protein L15

Chain U: 91% 8% .



- Molecule 23: 60S ribosomal protein L13a

Chain V:  89% 10%



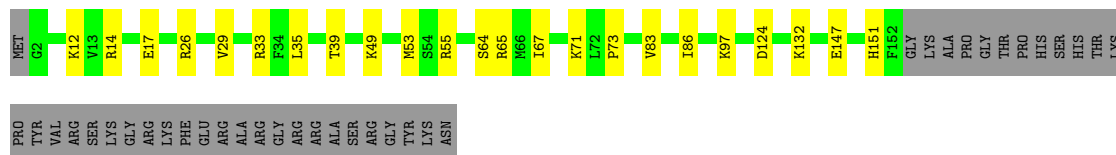
- Molecule 24: 60S ribosomal protein L37a

Chain X:  7% 86% 13%



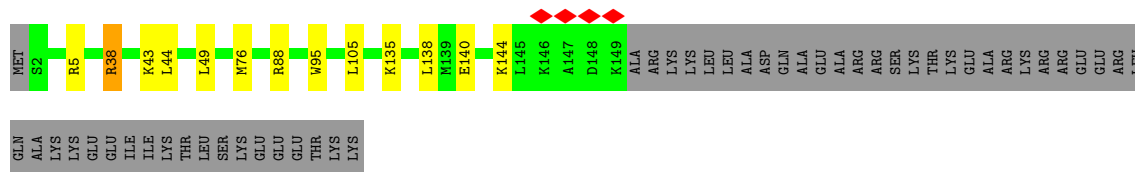
- Molecule 25: 60S ribosomal protein L18

Chain Z:  68% 12% 20%



- Molecule 26: 60S ribosomal protein L19

Chain a:  69% 6% 24%



- Molecule 27: 60S ribosomal protein L18a

Chain b:  88% 12%

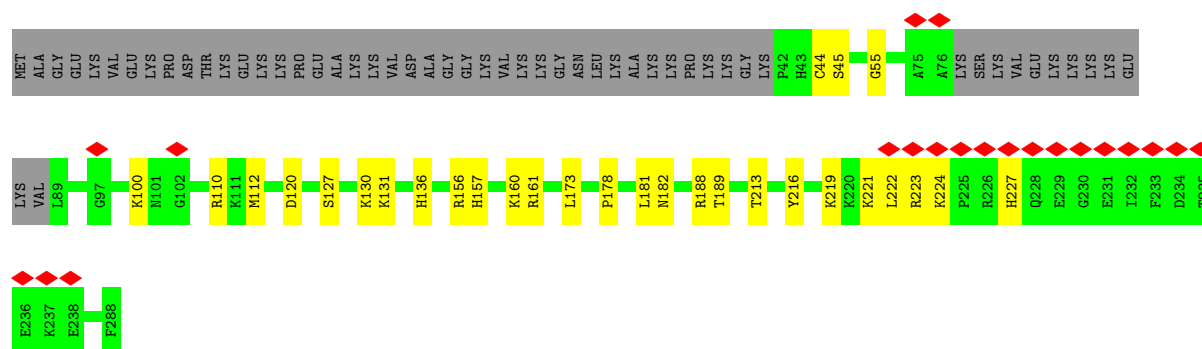


- Molecule 28: 60S ribosomal protein L23

Chain e:  80% 14% 6%

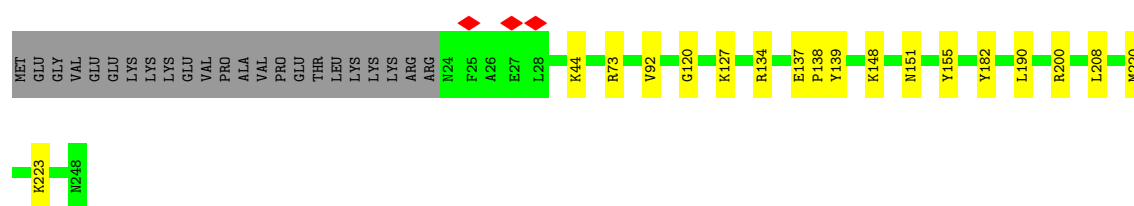


- Molecule 29: 60S ribosomal protein L23a



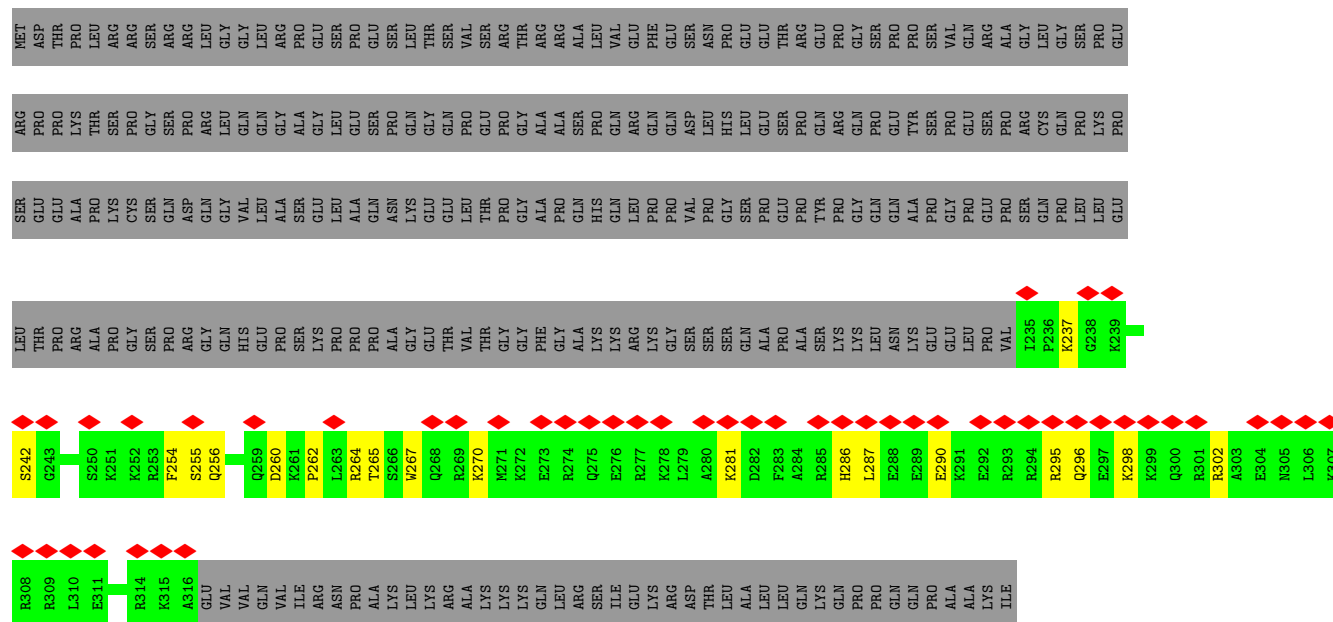
- Molecule 36: 60S ribosomal protein L7

Chain p: 83% 7% 9%



- Molecule 37: Coiled-coil domain-containing protein 86

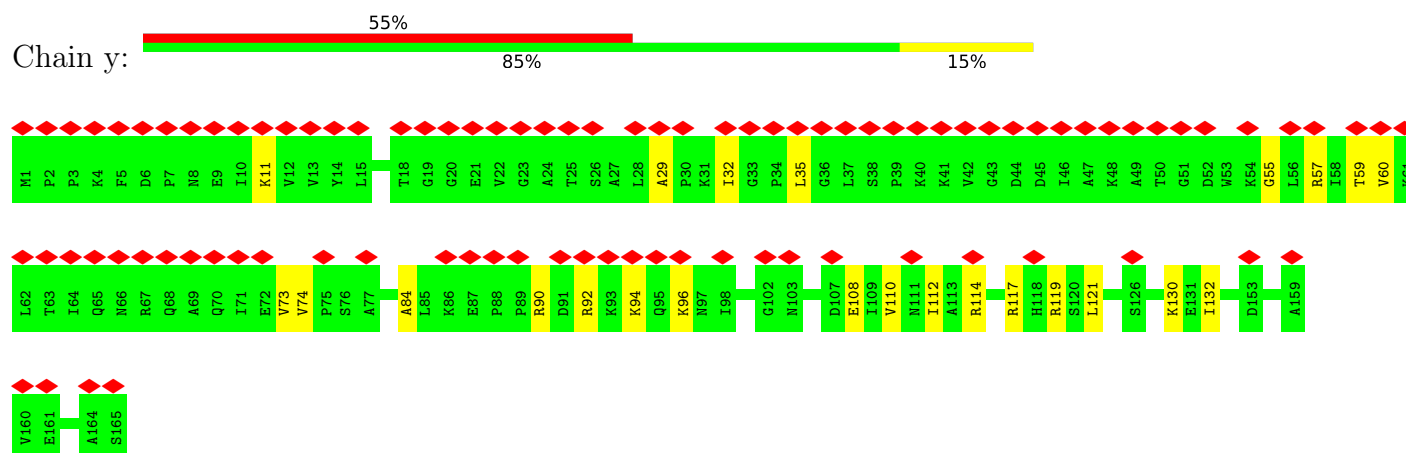
Chain r: 14% 18% 5% 77%



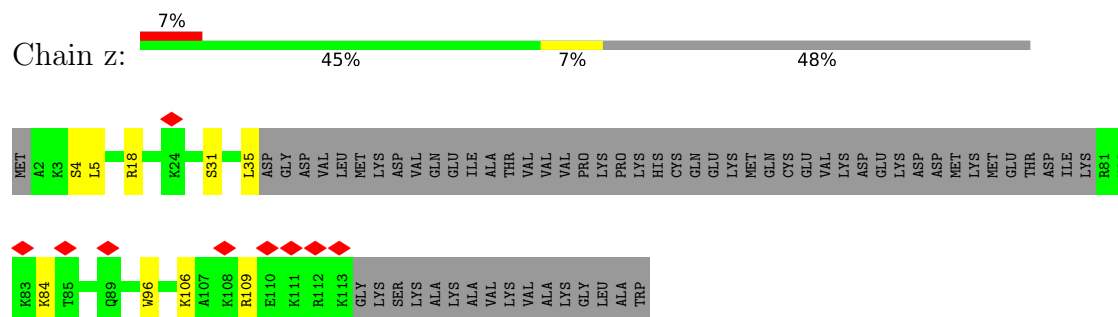
- Molecule 38: Guanine nucleotide-binding protein-like 3

Chain u: 5% 10% 88%

- Molecule 40: 60S ribosomal protein L12



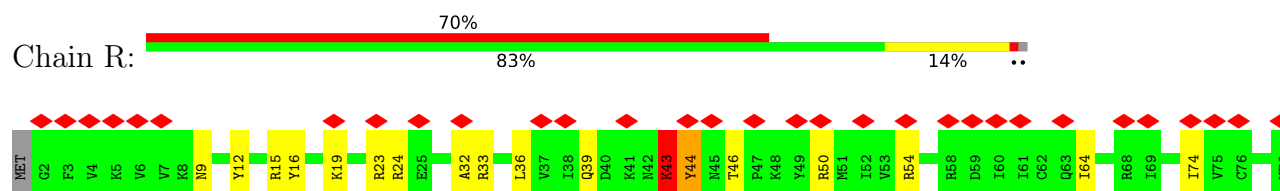
- Molecule 41: Protein LLP homolog

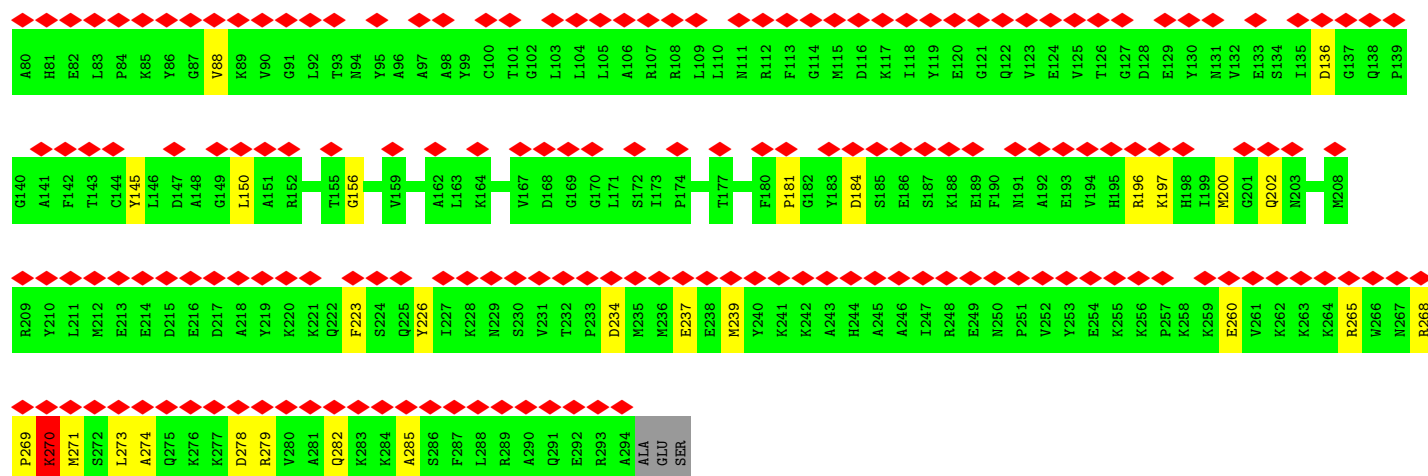


- Molecule 42: 60S ribosomal protein L11

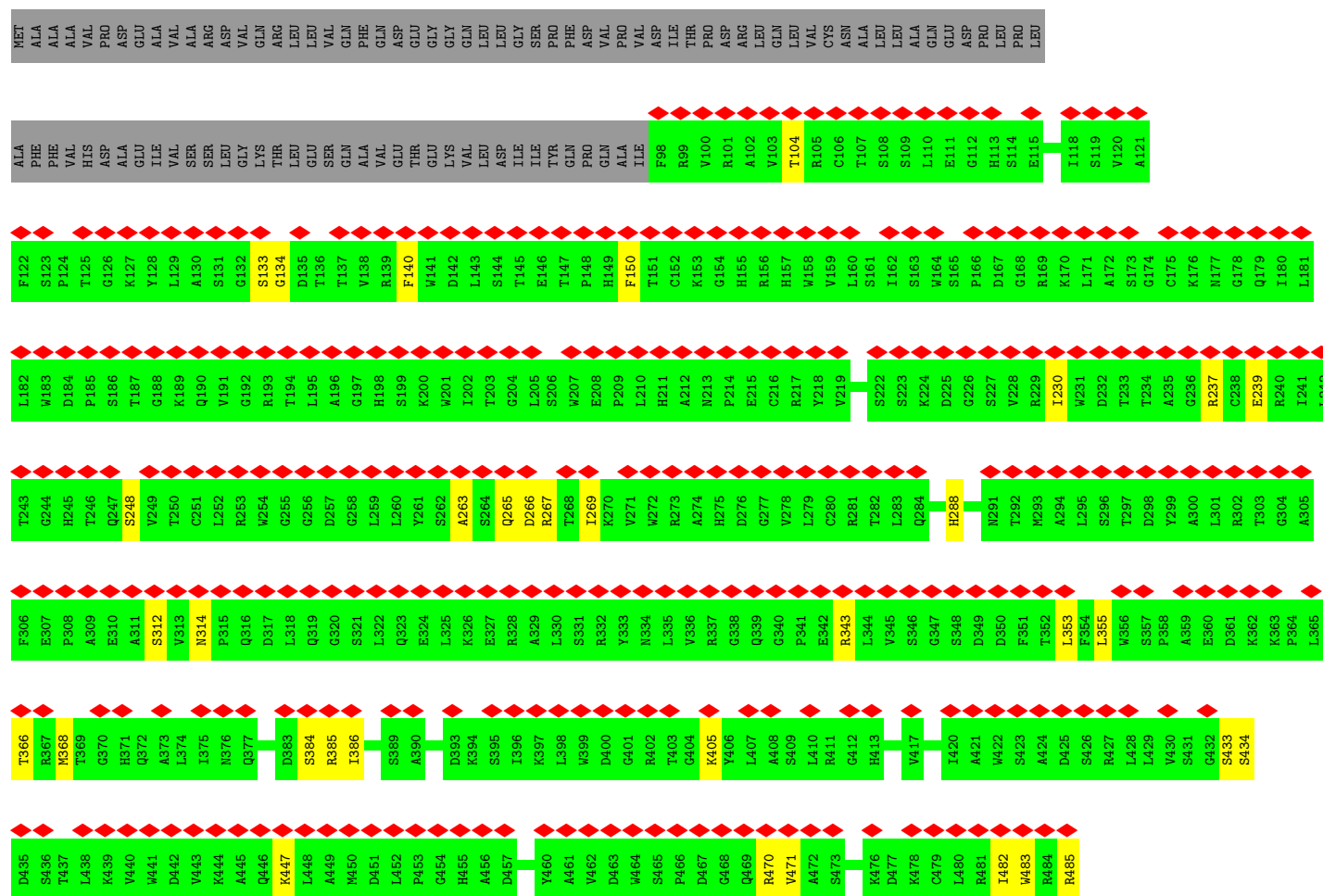
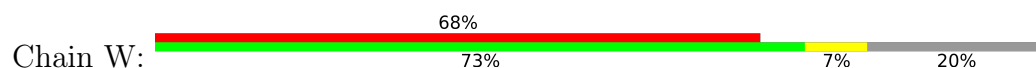


- Molecule 43: 60S ribosomal protein L5



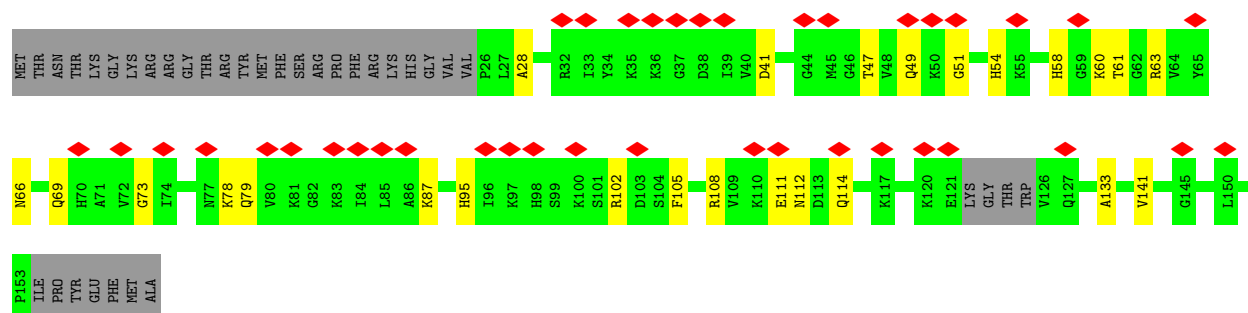


• Molecule 44: Notchless protein homolog 1

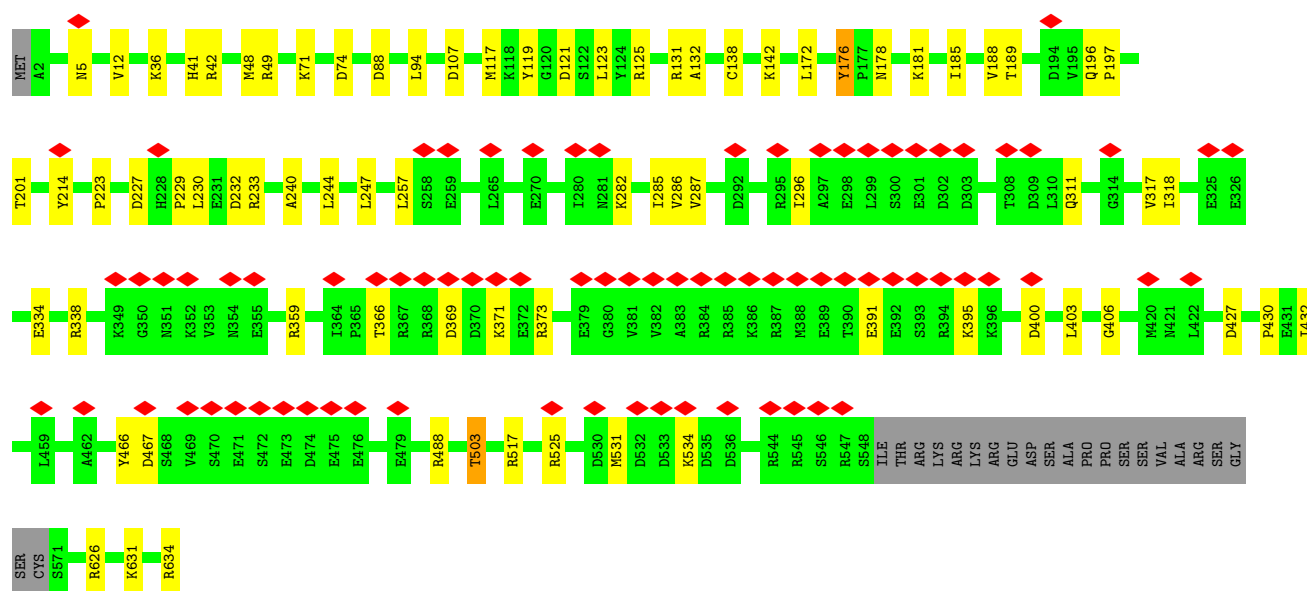
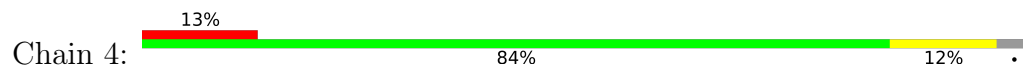


• Molecule 45: 60S ribosomal protein L21

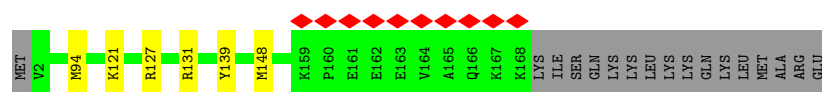
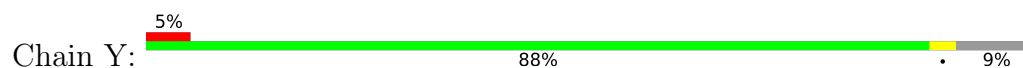




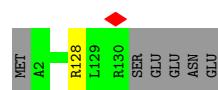
• Molecule 46: GTP-binding protein 4



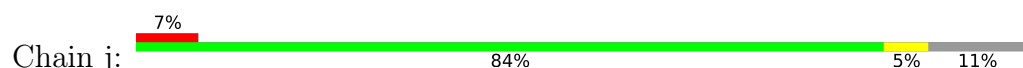
• Molecule 47: 60S ribosomal protein L17

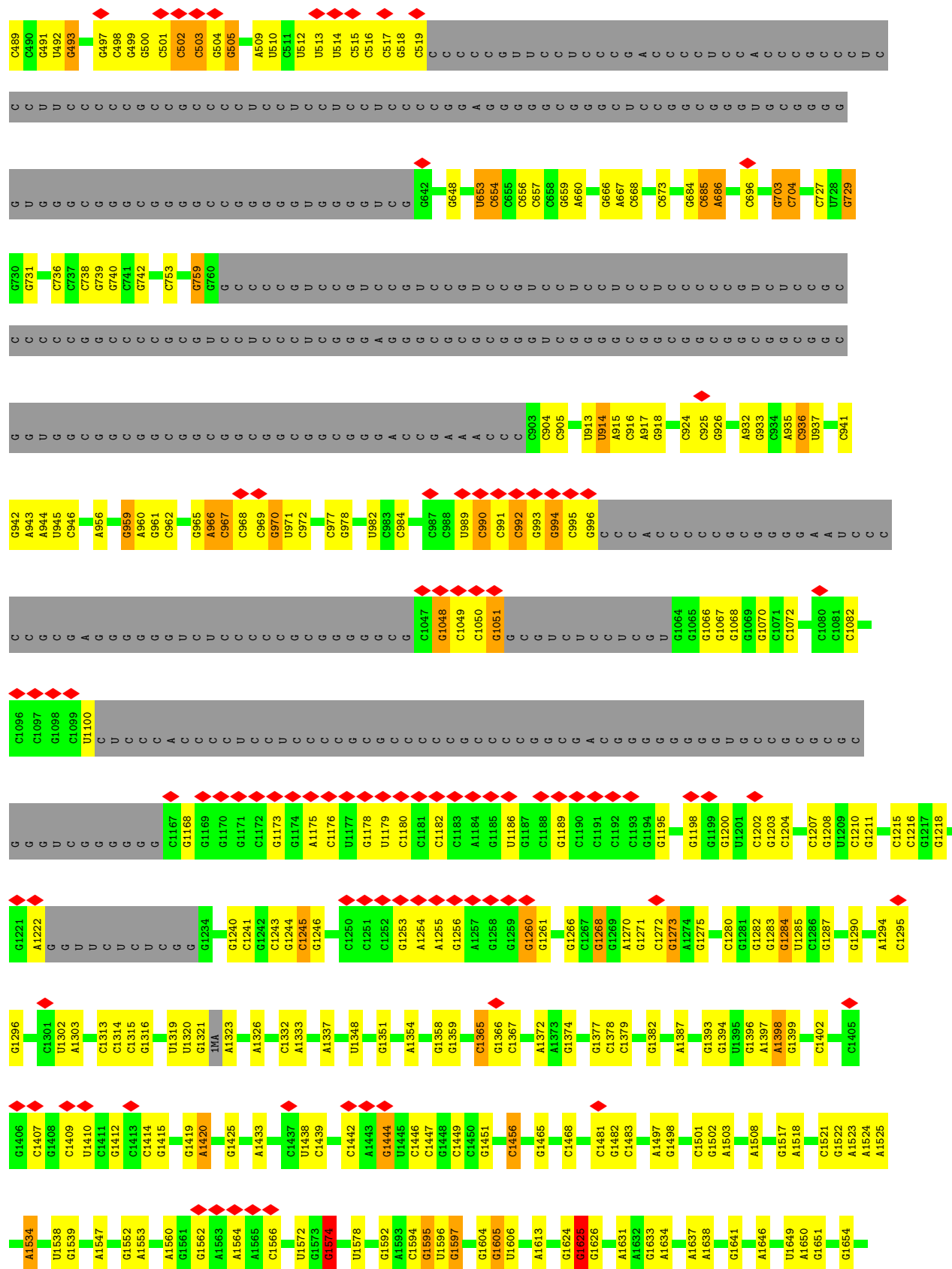


• Molecule 48: 60S ribosomal protein L32

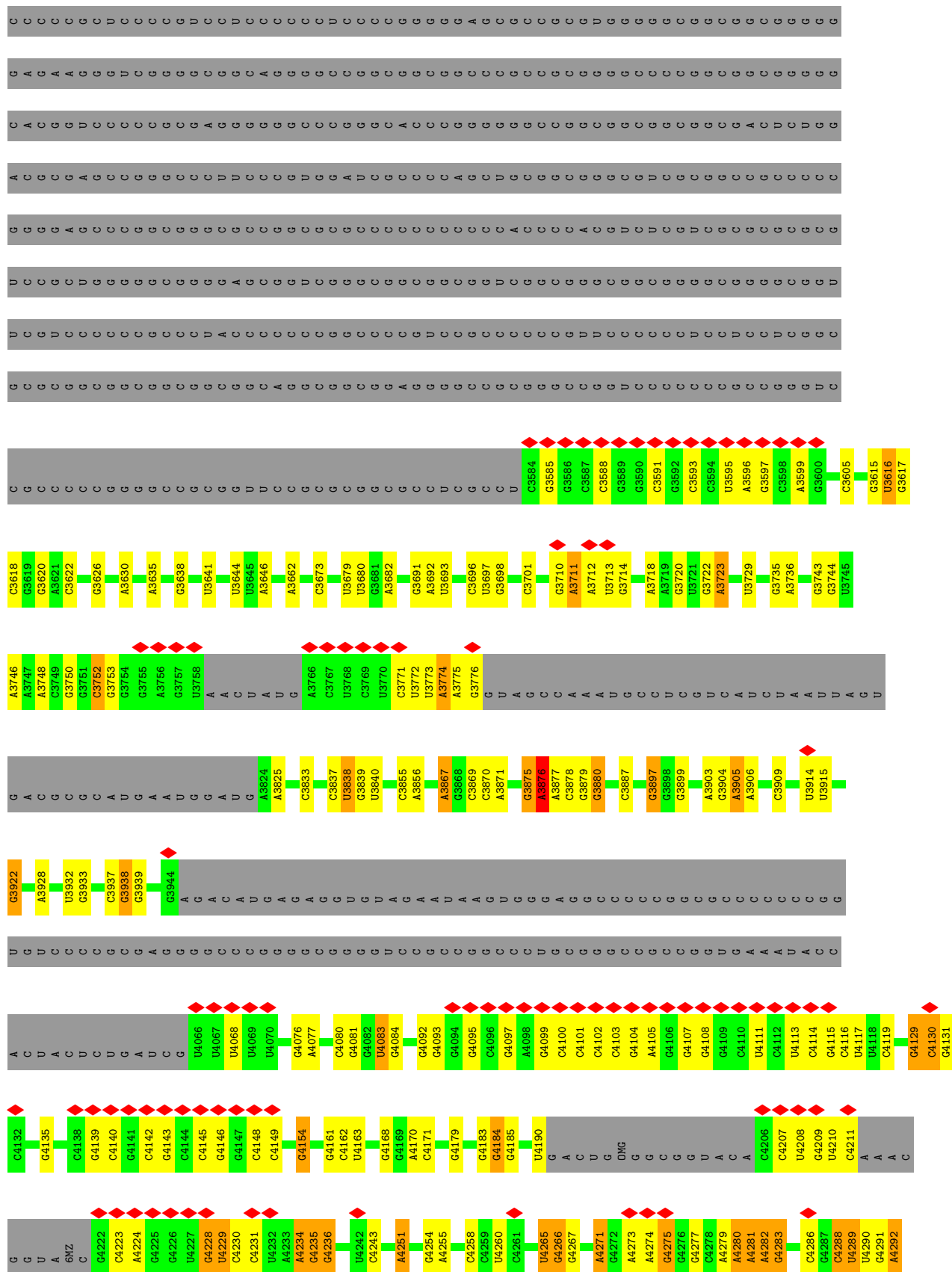


• Molecule 49: 60S ribosomal protein L31











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24229	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	0.205	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.031	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: A2M, E7G, 2MG, P7G, B8T, OMU, GTP, P4U, B8Q, OMC, MG, 7MG, 5MU, I4U, UR3, B8K, B9H, BGH, B8W, M7A, B9B, 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	0.37	1/2772 (0.0%)	0.72	0/3738
2	6	0.27	0/1877	0.66	0/2554
3	7	0.31	0/1181	0.64	0/1563
4	8	0.21	0/3679	0.38	0/5732
5	9	0.30	0/723	0.70	0/961
6	A	0.28	0/354	0.69	0/465
7	B	0.27	0/3315	0.66	4/4435 (0.1%)
8	D	0.27	0/2907	0.61	3/3905 (0.1%)
9	E	0.32	0/774	0.72	0/1038
10	F	0.26	0/878	0.56	0/1170
11	G	0.34	0/1960	0.70	2/2637 (0.1%)
12	H	0.31	0/1023	0.60	0/1351
13	I	0.29	0/1537	0.68	0/2066
14	J	0.24	0/1808	0.52	0/2414
15	K	0.29	0/843	0.68	0/1115
16	L	0.25	0/893	0.57	0/1193
17	M	0.27	0/720	0.61	0/952
18	O	0.28	0/575	0.65	0/761
19	P	0.26	0/454	0.54	0/599
20	Q	0.29	0/1732	0.62	0/2315
21	S	0.34	0/1133	0.72	2/1516 (0.1%)
22	U	0.42	1/1746 (0.1%)	0.79	6/2338 (0.3%)
23	V	0.29	0/1682	0.59	1/2250 (0.0%)
24	X	0.28	0/718	0.61	0/953
25	Z	0.24	0/1239	0.59	1/1658 (0.1%)
26	a	0.30	0/1255	0.74	4/1662 (0.2%)
27	b	0.26	0/1501	0.55	0/2013
28	e	0.26	0/993	0.63	0/1332
29	g	0.27	0/975	0.60	2/1312 (0.2%)
30	h	0.26	0/1132	0.59	0/1504
31	i	0.28	0/1130	0.66	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	l	0.26	0/1017	0.57	0/1364
33	m	0.29	0/1936	0.70	4/2596 (0.2%)
34	n	0.25	0/895	0.64	2/1198 (0.2%)
35	o	0.28	0/1935	0.71	2/2596 (0.1%)
36	p	0.34	0/1916	0.64	1/2553 (0.0%)
37	r	0.38	0/732	0.79	0/960
38	u	0.37	0/585	0.85	4/767 (0.5%)
39	w	0.28	0/3541	0.65	0/4775
40	y	0.37	0/1269	0.81	2/1712 (0.1%)
41	z	0.32	0/587	0.76	0/767
42	C	0.34	0/1341	0.84	3/1793 (0.2%)
43	R	0.34	0/2428	0.82	6/3252 (0.2%)
44	W	0.27	0/3093	0.66	2/4196 (0.0%)
45	T	0.31	0/1018	0.80	4/1357 (0.3%)
46	4	0.34	0/5099	0.82	13/6840 (0.2%)
47	Y	0.24	0/1383	0.56	0/1856
48	k	0.25	0/1082	0.59	0/1443
49	j	0.28	0/933	0.63	0/1256
50	d	0.35	0/864	0.88	4/1160 (0.3%)
51	3	0.24	0/2739	0.49	2/4266 (0.0%)
52	v	0.29	0/1806	0.68	0/2420
53	2	0.26	2/82131 (0.0%)	0.46	21/128040 (0.0%)
All	All	0.28	4/161839 (0.0%)	0.56	95/236176 (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
1	N	0	1
8	D	0	1
34	n	0	1
38	u	0	1
40	y	0	1
43	R	0	2
45	T	0	1
46	4	0	1
53	2	0	1
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	84	PRO	CG-CD	-12.94	1.06	1.50
53	2	3876	A	N9-C4	7.22	1.52	1.37
1	N	190	ARG	CA-C	6.92	1.62	1.52
53	2	3876	A	C1'-N9	5.56	1.55	1.47

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	U	84	PRO	N-CD-CG	-18.54	75.38	103.20
53	2	1871	A2M	OP2-P-O3'	-15.77	70.50	105.20
53	2	1871	A2M	OP1-P-O3'	14.46	137.01	105.20
53	2	1872	G	OP1-P-OP2	-13.41	79.36	119.60
22	U	84	PRO	CA-CB-CG	-11.79	82.11	104.50
22	U	84	PRO	CB-CG-CD	10.20	138.72	106.10
53	2	1872	G	O5'-P-OP1	-9.52	79.44	108.00
53	2	3876	A	N9-C1'-C2'	7.97	125.95	114.00
46	4	230	LEU	CA-CB-CG	7.67	143.16	116.30
46	4	503	THR	CA-C-N	7.66	135.49	121.70
46	4	503	THR	C-N-CA	7.66	135.49	121.70
53	2	3876	A	C8-N9-C1'	7.42	149.95	127.70
53	2	1872	G	O5'-P-OP2	7.23	129.68	108.00
46	4	406	GLY	CA-C-N	7.22	135.34	121.54
46	4	406	GLY	C-N-CA	7.22	135.34	121.54
26	a	38	ARG	CA-C-N	7.22	135.33	121.54
26	a	38	ARG	C-N-CA	7.22	135.33	121.54
44	W	266	ASP	CA-C-N	7.22	135.32	121.54
44	W	266	ASP	C-N-CA	7.22	135.32	121.54
42	C	18	ARG	CA-C-N	7.18	131.02	120.90
42	C	18	ARG	C-N-CA	7.18	131.02	120.90
22	U	84	PRO	CA-N-CD	-7.09	102.08	112.00
46	4	41	HIS	CA-C-N	7.07	135.04	121.54
46	4	41	HIS	C-N-CA	7.07	135.04	121.54
53	2	3876	A	C8-N9-C4	-6.95	84.96	105.80
50	d	54	GLY	CA-C-N	6.69	134.32	121.54
50	d	54	GLY	C-N-CA	6.69	134.32	121.54
46	4	391	GLU	CA-C-N	6.66	134.25	121.54
46	4	391	GLU	C-N-CA	6.66	134.25	121.54
34	n	105	LEU	CA-C-N	6.62	137.96	121.80
34	n	105	LEU	C-N-CA	6.62	137.96	121.80
29	g	117	TYR	CA-C-N	6.52	131.65	122.46
29	g	117	TYR	C-N-CA	6.52	131.65	122.46
46	4	430	PRO	CA-C-N	6.49	133.93	121.54
46	4	430	PRO	C-N-CA	6.49	133.93	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	4	176	TYR	CB-CA-C	6.43	118.87	109.48
35	o	127	SER	CA-C-N	6.34	131.40	122.08
35	o	127	SER	C-N-CA	6.34	131.40	122.08
43	R	270	LYS	CA-C-N	-6.33	111.89	122.64
43	R	270	LYS	C-N-CA	-6.33	111.89	122.64
53	2	2760	G	P-O3'-C3'	6.11	129.37	120.20
7	B	304	SER	CA-C-N	6.09	133.18	121.54
7	B	304	SER	C-N-CA	6.09	133.18	121.54
36	p	220	MET	CA-CB-CG	6.09	126.28	114.10
11	G	129	PRO	CA-C-N	5.98	131.31	122.82
11	G	129	PRO	C-N-CA	5.98	131.31	122.82
22	U	146	PRO	CA-C-N	5.94	132.89	121.54
22	U	146	PRO	C-N-CA	5.94	132.89	121.54
43	R	43	LYS	CA-C-N	5.92	132.84	121.54
43	R	43	LYS	C-N-CA	5.92	132.84	121.54
43	R	234	ASP	CA-C-N	5.89	130.73	122.08
43	R	234	ASP	C-N-CA	5.89	130.73	122.08
25	Z	83	VAL	N-CA-C	5.88	112.51	106.21
53	2	1678	C	P-O3'-C3'	5.85	128.97	120.20
53	2	3774	A	P-O3'-C3'	5.83	128.95	120.20
40	y	94	LYS	CA-C-N	5.81	131.07	122.82
40	y	94	LYS	C-N-CA	5.81	131.07	122.82
23	V	31	ARG	N-CA-C	5.79	117.69	110.91
53	2	914	U	P-O3'-C3'	5.79	128.88	120.20
26	a	76	MET	CA-C-N	5.79	132.75	121.41
26	a	76	MET	C-N-CA	5.79	132.75	121.41
33	m	179	ILE	CA-C-N	5.78	132.58	121.54
33	m	179	ILE	C-N-CA	5.78	132.58	121.54
8	D	221	PHE	CA-C-N	5.76	132.54	121.54
8	D	221	PHE	C-N-CA	5.76	132.54	121.54
50	d	66	SER	CA-C-N	5.71	132.44	121.54
50	d	66	SER	C-N-CA	5.71	132.44	121.54
38	u	4	PRO	CA-C-N	5.70	132.42	121.54
38	u	4	PRO	C-N-CA	5.70	132.42	121.54
42	C	41	GLU	N-CA-CB	5.66	119.05	110.28
53	2	3876	A	N7-C8-N9	5.65	130.74	113.80
45	T	69	GLN	CA-C-N	5.50	132.05	121.54
45	T	69	GLN	C-N-CA	5.50	132.05	121.54
53	2	2033	A	P-O3'-C3'	5.48	128.42	120.20
53	2	3905	A	P-O3'-C3'	5.38	128.27	120.20
53	2	1980	U	P-O3'-C3'	5.36	128.24	120.20
51	3	51	G	C2'-C3'-O3'	5.34	121.70	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	S	31	ILE	CA-C-N	5.32	131.71	121.54
21	S	31	ILE	C-N-CA	5.32	131.71	121.54
53	2	1931	C	C2'-C3'-O3'	5.32	117.47	109.50
46	4	12	VAL	CA-CB-CG1	5.24	119.31	110.40
53	2	1931	C	P-O3'-C3'	5.21	128.01	120.20
45	T	54	HIS	CA-C-N	5.19	131.46	121.54
45	T	54	HIS	C-N-CA	5.19	131.46	121.54
51	3	51	G	P-O3'-C3'	5.18	127.98	120.20
53	2	4913	G	P-O3'-C3'	5.16	127.94	120.20
7	B	29	VAL	CA-C-N	5.12	131.33	121.54
7	B	29	VAL	C-N-CA	5.12	131.33	121.54
33	m	13	GLY	CA-C-N	5.09	131.26	121.54
33	m	13	GLY	C-N-CA	5.09	131.26	121.54
53	2	4636	U	C2'-C3'-O3'	5.08	117.12	109.50
53	2	1808	C	C2'-C3'-O3'	5.08	121.31	113.70
38	u	13	MET	CA-C-N	5.03	131.14	121.54
38	u	13	MET	C-N-CA	5.03	131.14	121.54
8	D	319	LEU	CA-CB-CG	5.01	133.85	116.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	2	3876	A	Sidechain
46	4	503	THR	Peptide
8	D	231	ASN	Peptide
1	N	380	ASN	Peptide
43	R	196	ARG	Sidechain
43	R	43	LYS	Peptide
45	T	63	ARG	Sidechain
34	n	106	TYR	Peptide
38	u	54	ALA	Peptide
40	y	55	GLY	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	22	0
2	6	1852	0	1828	20	0
3	7	1159	0	1224	10	0
4	8	3315	0	1685	11	0
5	9	711	0	724	12	0
6	A	352	0	398	3	0
7	B	3244	0	3389	21	0
8	D	2853	0	3028	25	0
9	E	764	0	804	4	0
10	F	868	0	963	2	0
11	G	1927	0	2074	21	0
12	H	1015	0	1148	7	0
13	I	1518	0	1601	11	0
14	J	1772	0	1892	10	0
15	K	832	0	917	6	0
16	L	877	0	938	2	0
17	M	705	0	741	7	0
18	O	569	0	637	2	0
19	P	444	0	483	5	0
20	Q	1701	0	1818	9	0
21	S	1111	0	1174	8	0
22	U	1701	0	1749	13	0
23	V	1650	0	1794	13	0
24	X	708	0	760	8	0
25	Z	1223	0	1330	15	0
26	a	1239	0	1363	10	0
27	b	1461	0	1502	16	0
28	e	979	0	1039	11	0
29	g	958	0	1027	5	0
30	h	1115	0	1205	11	0
31	i	1107	0	1182	10	0
32	l	1002	0	1068	3	0
33	m	1898	0	1993	15	0
34	n	876	0	912	5	0
35	o	1897	0	2046	23	0
36	p	1878	0	2009	12	0
37	r	723	0	770	16	0
38	u	578	0	643	10	0
39	w	3472	0	3529	33	0
40	y	1250	0	1305	17	0
41	z	581	0	656	7	0
42	C	1319	0	1358	12	0
43	R	2382	0	2410	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	W	3018	0	2959	19	0
45	T	1001	0	1064	17	0
46	4	5016	0	5153	46	0
47	Y	1355	0	1389	5	0
48	k	1064	0	1160	1	0
49	j	918	0	964	3	0
50	d	850	0	868	6	0
51	3	2453	0	1243	19	0
52	v	1771	0	1810	20	0
53	2	75023	0	37751	304	0
54	w	32	0	12	0	0
55	w	1	0	0	0	0
All	All	152807	0	116286	731	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 (731) 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)
53:2:4083:5MU:C5	53:2:4083:5MU:C4	1.79	1.64
40:y:121:LEU:HD22	52:v:58:ASN:ND2	1.46	1.29
43:R:19:LYS:NZ	53:2:4265:U:O4	1.78	1.17
45:T:49:GLN:NE2	53:2:4282:A:N3	2.06	1.02
53:2:4297:G:H1	53:2:4313:A:H2	0.98	0.96
40:y:121:LEU:HD22	52:v:58:ASN:HD21	1.20	0.95
53:2:4297:G:N1	53:2:4313:A:C2	2.41	0.88
43:R:268:ARG:NH2	53:2:1175:A:N3	2.22	0.88
53:2:1976:G:H1	53:2:1991:A:H62	1.23	0.85
15:K:34:THR:HG21	53:2:276:C:OP2	1.78	0.84
15:K:4:ARG:HD3	53:2:1481:C:H41	1.42	0.83
26:a:95:TRP:CZ2	53:2:1572:U:H4'	2.15	0.81
39:w:32:MET:SD	53:2:3922:G:C6	2.74	0.81
40:y:121:LEU:CD2	52:v:58:ASN:HD21	1.95	0.80
1:N:85:LEU:O	1:N:89:HIS:HB3	1.83	0.79
53:2:4297:G:N1	53:2:4313:A:H2	1.75	0.79
39:w:23:ARG:NH2	53:2:3922:G:N7	2.30	0.79
43:R:43:LYS:HG3	53:2:1820:C:N4	1.97	0.78
2:6:129:LEU:O	2:6:133:LEU:HB2	1.84	0.77
45:T:79:GLN:NE2	53:2:1800:U:OP1	2.18	0.76
53:2:2452:G:H21	53:2:2507:A:H62	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:C:75:ARG:HD2	51:3:40:U:O2	1.87	0.75
43:R:268:ARG:O	43:R:270:LYS:N	2.19	0.75
25:Z:64:SER:HG	53:2:1501:C:HO2'	1.34	0.73
6:A:107:ARG:HH21	53:2:1268:G:P	2.11	0.73
20:Q:44:ARG:NH1	53:2:186:G:OP2	2.22	0.73
35:o:173:LEU:HB2	35:o:189:THR:O	1.88	0.72
43:R:279:ARG:NH1	53:2:1176:C:O2'	2.19	0.72
22:U:90:ASN:ND2	53:2:3928:A:OP1	2.23	0.72
22:U:12:ARG:NH1	53:2:279:A:N7	2.39	0.71
45:T:58:HIS:O	53:2:1732:C:O2'	2.07	0.71
37:r:302:ARG:HH21	51:3:104:C:H4'	1.56	0.70
36:p:73:ARG:NH2	53:2:727:C:OP1	2.25	0.69
41:z:106:LYS:NZ	53:2:4740:G:OP1	2.26	0.68
53:2:1858:A:H2'	53:2:1859:C:H6	1.59	0.66
5:9:22:LYS:NZ	53:2:2845:A:O3'	2.29	0.66
40:y:121:LEU:CD2	52:v:58:ASN:ND2	2.41	0.66
43:R:50:ARG:NH2	51:3:6:C:O2'	2.22	0.65
26:a:95:TRP:CE2	53:2:1572:U:H4'	2.31	0.65
43:R:150:LEU:HD21	53:2:4280:A:N1	2.12	0.64
39:w:32:MET:SD	53:2:3922:G:C5	2.90	0.64
1:N:102:LYS:NZ	53:2:3744:G:OP1	2.31	0.64
45:T:102:ARG:NH1	53:2:1801:A:O2'	2.31	0.64
2:6:9:ASN:ND2	53:2:4596:C:OP1	2.31	0.64
53:2:1732:C:H42	53:2:1797:G:H21	1.44	0.64
46:4:119:TYR:OH	53:2:4448:G:OP2	2.15	0.63
53:2:4288:C:O3'	53:2:4289:U:H3'	1.98	0.63
1:N:102:LYS:HD3	53:2:3743:G:H4'	1.80	0.63
41:z:109:ARG:NH1	53:2:4740:G:OP1	2.31	0.63
43:R:150:LEU:HD21	53:2:4280:A:C6	2.34	0.63
53:2:4740:G:H1'	53:2:4742:G:H5''	1.80	0.62
17:M:80:GLU:OE1	53:2:134:G:N2	2.33	0.62
25:Z:35:LEU:O	25:Z:39:THR:HB	2.00	0.62
43:R:271:MET:HE3	53:2:1175:A:C2	2.35	0.61
43:R:268:ARG:C	43:R:270:LYS:H	2.07	0.61
24:X:23:ARG:NH2	53:2:2875:C:OP1	2.33	0.61
36:p:138:PRO:HB3	51:3:84:U:OP2	1.99	0.61
32:l:16:PHE:HB3	32:l:27:THR:H	1.66	0.61
43:R:88:VAL:HG22	43:R:239:MET:HG2	1.83	0.60
25:Z:73:PRO:O	53:2:1456:B8Q:O2'	2.18	0.60
53:2:1797:G:H2'	53:2:1798:G:C8	2.37	0.60
43:R:44:TYR:OH	53:2:1822:U:H2'	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:94:ASN:HD22	8:D:102:PHE:HB2	1.66	0.60
31:i:69:LYS:NZ	53:2:2576:G:OP1	2.35	0.60
53:2:4322:G:H21	53:2:4325:A:H62	1.50	0.60
39:w:348:TRP:HA	39:w:361:ASP:O	2.02	0.59
53:2:1858:A:H2'	53:2:1859:C:C6	2.36	0.59
11:G:245:LYS:NZ	53:2:4161:G:H21	2.00	0.59
50:d:22:THR:O	50:d:109:SER:HA	2.03	0.59
41:z:31:SER:O	41:z:35:LEU:HB2	2.03	0.59
53:2:4271:A:H62	53:2:4331:G:H22	1.50	0.58
28:e:28:CYS:SG	28:e:29:ALA:N	2.75	0.58
47:Y:94:MET:HG2	47:Y:148:MET:HE2	1.84	0.58
33:m:233:ARG:NH1	53:2:4184:G:OP1	2.37	0.58
12:H:112:ARG:NH1	53:2:264:C:O2	2.36	0.58
40:y:90:ARG:HH21	40:y:92:ARG:HA	1.68	0.58
14:J:17:ARG:HB3	14:J:20:TYR:HB2	1.86	0.58
23:V:89:PRO:HD3	53:2:1914:C:H4'	1.86	0.58
33:m:45:VAL:HG12	33:m:61:VAL:HG22	1.86	0.58
39:w:267:ARG:HH21	39:w:464:ASN:HB3	1.69	0.58
17:M:52:LYS:NZ	53:2:375:G:OP2	2.34	0.57
44:W:140:PHE:HB2	44:W:150:PHE:HB2	1.86	0.57
53:2:2362:U:H2'	53:2:2363:A2M:H8	1.86	0.57
43:R:12:TYR:O	43:R:16:TYR:HB2	2.03	0.57
2:6:244:LEU:HD21	46:4:359:ARG:HE	1.70	0.57
23:V:34:VAL:HG12	23:V:103:LYS:HB2	1.85	0.57
15:K:40:VAL:HG11	22:U:5:LYS:HG2	1.85	0.57
27:b:170:LYS:HE3	53:2:4875:G:H5''	1.87	0.57
39:w:352:THR:HG23	53:2:4539:U:H5''	1.86	0.56
15:K:75:LYS:NZ	53:2:3720:G:OP1	2.35	0.56
52:v:208:TRP:HA	52:v:214:ARG:O	2.05	0.56
43:R:24:ARG:NH2	51:3:13:A:O2'	2.39	0.56
13:I:92:MET:O	13:I:143:GLU:HA	2.05	0.56
23:V:7:LEU:HB3	23:V:33:VAL:HG12	1.88	0.56
53:2:1976:G:H1	53:2:1991:A:N6	1.97	0.56
7:B:289:GLN:OE1	7:B:301:ASN:ND2	2.39	0.56
26:a:105:LEU:HD23	26:a:138:LEU:HD23	1.88	0.56
53:2:1797:G:H2'	53:2:1798:G:H8	1.70	0.56
4:8:83:C:H42	30:h:50:ARG:HH12	1.52	0.56
8:D:234:LYS:NZ	53:2:1365:C:H41	2.04	0.56
35:o:110:ARG:NH2	53:2:967:C:H2'	2.20	0.56
27:b:87:ARG:HH22	53:2:2034:G:H5''	1.70	0.56
35:o:173:LEU:O	35:o:188:ARG:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:T:41:ASP:HB3	45:T:61:THR:HG22	1.87	0.56
43:R:156:GLY:HA2	43:R:181:PRO:HG3	1.87	0.56
2:6:24:CYS:HB3	2:6:48:VAL:HG12	1.89	0.55
1:N:303:GLN:O	1:N:307:CYS:HB2	2.07	0.55
18:O:5:ILE:HG22	18:O:7:GLU:H	1.70	0.55
41:z:84:LYS:NZ	53:2:4904:G:N7	2.54	0.55
47:Y:131:ARG:NH1	53:2:1597:G:OP2	2.35	0.55
35:o:222:LEU:HD12	35:o:223:ARG:HG2	1.88	0.55
53:2:4297:G:O6	53:2:4313:A:N1	2.40	0.55
53:2:1732:C:N4	53:2:1797:G:H21	2.04	0.55
22:U:81:TYR:OH	53:2:1625:OMG:HM22	2.07	0.55
46:4:287:VAL:HA	46:4:318:ILE:O	2.07	0.55
53:2:493:G:N1	53:2:660:A:C2	2.73	0.55
35:o:44:CYS:SG	35:o:45:SER:N	2.79	0.54
36:p:182:TYR:HB3	36:p:200:ARG:HG3	1.88	0.54
1:N:190:ARG:HH21	1:N:193:TRP:HE1	1.54	0.54
16:L:110:LYS:NZ	53:2:1396:G:N7	2.55	0.54
26:a:5:ARG:NH2	53:2:2385:U:OP1	2.40	0.54
39:w:91:SER:O	39:w:95:PHE:HB2	2.06	0.54
44:W:133:SER:OG	44:W:134:GLY:N	2.40	0.54
46:4:285:ILE:HG12	46:4:334:GLU:HG3	1.88	0.54
52:v:42:ILE:HD11	52:v:92:VAL:HG13	1.89	0.54
53:2:4209:G:N1	53:2:4224:A:N7	2.56	0.54
5:9:24:ARG:NH2	53:2:3837:C:OP1	2.41	0.54
46:4:286:VAL:O	46:4:317:VAL:HA	2.07	0.54
53:2:39:A:H61	53:2:1681:G:H5''	1.72	0.54
28:e:87:SER:HA	28:e:96:LEU:O	2.07	0.54
33:m:244:GLY:HA3	53:2:3746:A:H5''	1.90	0.54
43:R:223:PHE:HB3	43:R:226:TYR:HB2	1.89	0.54
8:D:109:ARG:NH2	53:2:2343:G:OP2	2.40	0.54
11:G:245:LYS:HZ1	53:2:4161:G:N2	2.06	0.54
13:I:187:VAL:HG12	13:I:188:GLN:HG3	1.90	0.54
51:3:28:C:H1'	51:3:54:A:H61	1.74	0.53
51:3:41:G:N3	51:3:44:C:N4	2.56	0.53
53:2:1870:C:H2'	53:2:1871:A2M:H8	1.89	0.53
2:6:49:VAL:HG11	2:6:87:SER:HB3	1.91	0.53
8:D:234:LYS:HZ1	53:2:1365:C:H41	1.55	0.53
8:D:143:ARG:NH1	53:2:2300:A:N7	2.56	0.53
53:2:4429:C:H2'	53:2:4430:G:O4'	2.08	0.53
1:N:146:LYS:O	1:N:150:ALA:HB2	2.07	0.53
8:D:218:ILE:O	8:D:222:ARG:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:r:254:PHE:CE2	53:2:4693:C:H5''	2.43	0.53
1:N:97:ARG:HE	1:N:133:LEU:HD22	1.74	0.53
2:6:57:ARG:HH12	7:B:66:LYS:HE3	1.74	0.53
19:P:37:TYR:O	53:2:362:A:N6	2.41	0.53
39:w:354:MET:HE2	53:2:3752:C:H3'	1.90	0.53
53:2:1319:U:O2	53:2:1323:A:N6	2.42	0.53
26:a:88:ARG:O	53:2:2725:A:N6	2.42	0.53
28:e:90:ARG:HD3	28:e:123:LYS:HD2	1.90	0.53
53:2:4748:U:H3	53:2:4952:G:H1	1.56	0.53
2:6:233:ALA:O	2:6:237:ARG:HB3	2.09	0.53
46:4:178:ASN:ND2	46:4:197:PRO:O	2.42	0.53
44:W:471:VAL:HB	44:W:483:TRP:HB2	1.91	0.53
53:2:4275:G:P	53:2:4275:G:H3'	2.48	0.53
37:r:281:LYS:HE3	38:u:55:PRO:HD3	1.90	0.52
2:6:163:PRO:HA	2:6:183:ALA:HB1	1.91	0.52
43:R:50:ARG:O	43:R:64:ILE:HA	2.08	0.52
53:2:990:C:N4	53:2:992:C:O2'	2.42	0.52
1:N:385:LYS:HG3	42:C:58:ARG:HE	1.74	0.52
5:9:14:SER:HB2	53:2:2843:U:H5''	1.91	0.52
5:9:22:LYS:HD2	53:2:2846:G:H5''	1.90	0.52
53:2:3641:U:OP2	53:2:3646:A:N6	2.43	0.52
53:2:1992:U:H5'	53:2:1993:C:H5'	1.90	0.52
27:b:1:MET:SD	27:b:43:ARG:NH1	2.82	0.52
53:2:1868:A:H2'	53:2:1869:G:O4'	2.09	0.52
42:C:48:PRO:HB3	42:C:72:CYS:HB2	1.91	0.52
46:4:172:LEU:HD21	46:4:247:LEU:HD23	1.90	0.52
42:C:131:TYR:CE2	53:2:4260:U:H1'	2.45	0.52
53:2:2396:A:N7	53:2:2814:C:O2'	2.42	0.52
53:2:3616:U:OP2	53:2:3617:G:N2	2.43	0.52
1:N:191:ASN:OD1	1:N:194:ASN:ND2	2.42	0.51
14:J:188:LEU:HD21	44:W:288:HIS:HA	1.92	0.51
45:T:78:LYS:HD2	45:T:87:LYS:HD2	1.92	0.51
53:2:3697:U:H5''	53:2:3698:G:H5'	1.92	0.51
2:6:31:SER:OG	2:6:32:GLU:N	2.43	0.51
38:u:1:MET:SD	53:2:2041:A:C2	3.02	0.51
52:v:49:ARG:HD3	52:v:126:ARG:HH22	1.74	0.51
7:B:57:VAL:HG12	7:B:73:VAL:HG12	1.93	0.51
19:P:34:LYS:HE3	53:2:361:C:H4'	1.90	0.51
45:T:105:PHE:CE2	53:2:1802:A:H4'	2.44	0.51
1:N:349:GLU:HB3	1:N:352:LYS:HB2	1.91	0.51
33:m:136:VAL:HG12	33:m:148:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:o:156:ARG:NH1	53:2:4940:C:OP1	2.43	0.51
37:r:254:PHE:HE2	53:2:4693:C:H5''	1.76	0.51
17:M:14:LYS:HE2	53:2:2405:G:H5''	1.92	0.51
53:2:505:G:H1	53:2:653:U:H3	1.58	0.51
11:G:245:LYS:CE	53:2:4161:G:H21	2.24	0.51
35:o:110:ARG:HH22	53:2:967:C:H2'	1.75	0.51
53:2:1433:A:N6	53:2:1451:G:O2'	2.44	0.51
53:2:2395:A:HO2'	53:2:2806:A:HO2'	1.58	0.51
53:2:4289:U:H1'	53:2:4320:G:O2'	2.11	0.51
11:G:164:ILE:O	11:G:168:VAL:HB	2.11	0.51
28:e:66:LYS:O	28:e:73:ARG:NH2	2.44	0.51
27:b:15:ARG:HD2	27:b:25:PRO:HG2	1.92	0.51
5:9:5:ARG:HB3	53:2:1604:G:H21	1.74	0.51
25:Z:49:LYS:HG2	25:Z:53:MET:HE3	1.93	0.51
40:y:119:ARG:NH2	53:2:1973:G:OP1	2.44	0.51
43:R:273:LEU:HD22	51:3:108:G:OP1	2.11	0.51
44:W:237:ARG:NH1	53:2:1991:A:H4'	2.26	0.51
53:2:3722:G:H2'	53:2:3723:A2M:H8	1.92	0.51
3:7:1:MET:HE3	46:4:432:ILE:HD12	1.93	0.51
21:S:41:PRO:HG3	21:S:73:VAL:HG13	1.92	0.51
27:b:15:ARG:HB3	27:b:27:LEU:HD23	1.93	0.51
31:i:57:MET:HE3	31:i:61:LYS:HE2	1.92	0.51
39:w:450:ASP:OD1	39:w:455:ARG:NH1	2.44	0.50
49:j:22:THR:HG23	49:j:122:VAL:HB	1.94	0.50
5:9:28:LEU:O	5:9:32:HIS:ND1	2.41	0.50
13:I:113:GLU:HG2	13:I:125:ARG:HG2	1.92	0.50
53:2:1552:G:O2'	53:2:1574:B9B:N2	2.44	0.50
53:2:4277:G:N2	53:2:4332:C:O2	2.45	0.50
8:D:152:LEU:HD23	8:D:251:ILE:HG12	1.94	0.50
27:b:87:ARG:NH1	53:2:2034:G:OP2	2.44	0.50
30:h:87:ARG:NH2	53:2:404:U:O3'	2.44	0.50
33:m:29:LEU:O	33:m:123:ARG:NH1	2.42	0.50
1:N:146:LYS:HA	1:N:190:ARG:HH12	1.76	0.50
1:N:383:THR:HA	42:C:63:ARG:HH12	1.76	0.50
40:y:29:ALA:HA	40:y:32:ILE:HG22	1.91	0.50
40:y:110:VAL:HG12	40:y:114:ARG:HE	1.76	0.50
43:R:260:GLU:OE2	51:3:1:G:C8	2.64	0.50
46:4:138:CYS:O	46:4:142:LYS:HB2	2.12	0.50
40:y:60:VAL:HG22	40:y:73:VAL:HG12	1.94	0.50
53:2:382:G:N1	53:2:385:A:OP2	2.42	0.50
53:2:2335:C:H2'	53:2:2336:G:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:2759:G:O2'	53:2:2762:G:N2	2.44	0.50
6:A:117:ARG:HD2	53:2:1273:G:H8	1.77	0.50
53:2:1972:G:H1	53:2:1994:C:H5	1.58	0.50
53:2:2452:G:N2	53:2:2507:A:H62	2.05	0.50
16:L:132:ARG:NH2	53:2:1468:C:OP1	2.45	0.50
35:o:100:LYS:HB3	53:2:684:G:H4'	1.93	0.50
46:4:132:ALA:HA	53:2:4407:G:H1'	1.92	0.50
53:2:184:U:O2	53:2:255:C:N4	2.44	0.50
53:2:4277:G:N1	53:2:4332:C:N3	2.59	0.50
53:2:966:A:OP2	53:2:2256:C:N4	2.45	0.49
53:2:996:G:O2'	53:2:1048:G:N2	2.44	0.49
53:2:1864:G:H2'	53:2:1865:G:O4'	2.11	0.49
53:2:4573:G:N2	53:2:4722:G:OP2	2.45	0.49
35:o:224:LYS:HB3	35:o:227:HIS:HB2	1.94	0.49
39:w:214:ILE:O	39:w:248:LYS:NZ	2.45	0.49
46:4:467:ASP:OD1	46:4:467:ASP:N	2.45	0.49
20:Q:63:THR:HG22	20:Q:65:ARG:H	1.77	0.49
2:6:79:GLN:OE1	3:7:1:MET:N	2.45	0.49
13:I:91:LYS:HB2	13:I:183:GLU:HB3	1.93	0.49
46:4:517:ARG:NH2	46:4:534:LYS:O	2.45	0.49
53:2:4234:A:OP2	53:2:4292:A:N6	2.45	0.49
14:J:25:ARG:HH22	37:r:242:SER:HB3	1.78	0.49
53:2:4321:U:H3	53:2:4326:G:H1	1.61	0.49
40:y:96:LYS:HB2	53:2:1979:A:OP1	2.11	0.49
53:2:2601:A:N6	53:2:2744:A:OP2	2.46	0.49
1:N:74:LEU:HD12	1:N:77:PHE:HB2	1.94	0.49
3:7:19:MET:SD	3:7:19:MET:N	2.85	0.49
8:D:284:MET:HE2	8:D:287:THR:HA	1.94	0.49
39:w:210:LEU:HD12	39:w:365:VAL:HG11	1.95	0.49
40:y:130:LYS:HB3	53:2:1994:C:H4'	1.95	0.49
53:2:1245:C:H2'	53:2:1246:G:H8	1.78	0.49
25:Z:67:ILE:O	25:Z:71:LYS:HB2	2.11	0.49
39:w:32:MET:HG2	53:2:3922:G:O6	2.12	0.49
39:w:175:ASP:HB3	39:w:178:LYS:HB2	1.94	0.49
43:R:39:GLN:NE2	43:R:46:THR:O	2.45	0.49
46:4:400:ASP:HA	46:4:403:LEU:HG	1.95	0.49
27:b:66:GLN:O	53:2:729:2MG:N2	2.40	0.49
45:T:108:ARG:O	45:T:112:ASN:HB2	2.13	0.49
46:4:188:VAL:HG13	46:4:189:THR:HG23	1.94	0.49
53:2:3938:G:N2	53:2:4171:C:OP2	2.46	0.49
21:S:91:TRP:CZ2	53:2:4870:OMG:H2'	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:106:ASP:OD2	35:o:161:ARG:NH2	2.46	0.49
39:w:32:MET:HG2	53:2:3922:G:C6	2.48	0.49
11:G:117:ARG:NH1	11:G:127:ASP:O	2.45	0.48
12:H:88:THR:HB	12:H:91:MET:HB2	1.94	0.48
38:u:7:LYS:NZ	53:2:1933:G:OP2	2.45	0.48
5:9:28:LEU:H	5:9:31:ILE:HD12	1.78	0.48
9:E:19:GLN:O	9:E:23:LYS:NZ	2.46	0.48
23:V:176:ARG:HD3	53:2:4769:G:H5''	1.95	0.48
39:w:402:LYS:HB3	39:w:405:TYR:HD2	1.77	0.48
26:a:44:LEU:HD22	26:a:49:LEU:HD22	1.94	0.48
33:m:117:GLU:O	33:m:162:ASN:ND2	2.47	0.48
42:C:108:GLY:HA3	53:2:4251:A:H5''	1.95	0.48
44:W:470:ARG:HB3	44:W:482:ILE:HD11	1.95	0.48
53:2:4130:C:H42	53:2:4154:G:H22	1.59	0.48
53:2:4338:G:OP1	53:2:4339:A:N6	2.46	0.48
4:8:94:G:OP2	17:M:72:ARG:NH2	2.46	0.48
5:9:17:ARG:HD2	53:2:3838:U:H5'	1.93	0.48
35:o:130:LYS:HG3	53:2:1284:G:H21	1.79	0.48
53:2:1270:A:H8	53:2:2106:G:H21	1.59	0.48
3:7:22:VAL:HG22	3:7:28:VAL:HG22	1.94	0.48
19:P:33:ASN:ND2	19:P:35:ILE:O	2.45	0.48
43:R:54:ARG:NH2	51:3:6:C:H5''	2.29	0.48
53:2:2459:G:N2	53:2:2462:C:OP2	2.47	0.48
2:6:4:ARG:NH1	2:6:210:THR:O	2.47	0.48
11:G:245:LYS:NZ	53:2:4161:G:N2	2.61	0.48
26:a:38:ARG:NH2	53:2:2527:A:OP1	2.44	0.48
5:9:87:LYS:HE2	53:2:3617:G:H1	1.76	0.48
43:R:9:ASN:H	43:R:12:TYR:HB3	1.78	0.48
8:D:218:ILE:O	8:D:221:PHE:C	2.56	0.48
33:m:70:LYS:NZ	53:2:2503:G:N7	2.61	0.48
39:w:32:MET:CG	53:2:3922:G:O6	2.61	0.48
43:R:274:ALA:O	43:R:278:ASP:HB2	2.13	0.48
47:Y:127:ARG:HB2	47:Y:139:TYR:HB3	1.96	0.48
8:D:100:ARG:NH2	53:2:1521:C:OP1	2.47	0.48
36:p:92:VAL:O	36:p:120:GLY:HA2	2.14	0.48
1:N:108:ARG:NH1	1:N:111:ASN:OD1	2.47	0.48
13:I:8:GLN:OE1	37:r:256:GLN:NE2	2.47	0.48
53:2:1797:G:O2'	53:2:1798:G:H5'	2.14	0.48
7:B:115:LYS:HD2	7:B:129:ALA:HB3	1.96	0.47
7:B:353:VAL:O	41:z:18:ARG:NH1	2.44	0.47
20:Q:62:PRO:HG3	53:2:74:G:H1'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:115:ALA:HB1	23:V:192:TYR:HB3	1.96	0.47
39:w:314:GLY:HA2	39:w:360:ILE:HB	1.95	0.47
46:4:285:ILE:HD11	46:4:338:ARG:HD2	1.95	0.47
53:2:170:C:O2'	53:2:172:C:N4	2.46	0.47
53:2:184:U:O2'	53:2:253:G:N2	2.45	0.47
5:9:15:LEU:HD22	53:2:4660:G:H4'	1.97	0.47
8:D:187:GLN:NE2	8:D:203:GLN:OE1	2.47	0.47
24:X:59:SER:O	53:2:2652:G:N2	2.47	0.47
44:W:343:ARG:NH2	44:W:384:SER:O	2.45	0.47
7:B:57:VAL:HG23	7:B:366:LYS:HB3	1.96	0.47
22:U:194:ARG:NH1	53:2:79:C:OP1	2.47	0.47
30:h:1:MET:N	53:2:226:G:OP2	2.43	0.47
31:i:59:LYS:HG2	53:2:4148:C:H5'	1.96	0.47
44:W:433:SER:OG	44:W:434:SER:N	2.48	0.47
53:2:158:A:N1	53:2:276:C:O2'	2.43	0.47
1:N:158:ASN:O	1:N:162:GLN:HB2	2.15	0.47
12:H:95:LEU:O	53:2:135:G:N2	2.47	0.47
53:2:253:G:N2	53:2:254:G:O6	2.46	0.47
53:2:3620:G:OP1	53:2:3622:C:N4	2.46	0.47
25:Z:29:VAL:O	25:Z:33:ARG:HB2	2.14	0.47
27:b:95:ARG:NH1	27:b:112:ASP:OD2	2.48	0.47
7:B:131:THR:O	7:B:135:LYS:NZ	2.48	0.47
11:G:152:ALA:HA	11:G:205:THR:HA	1.97	0.47
11:G:154:LEU:HB3	11:G:204:PHE:HB2	1.96	0.47
13:I:152:GLU:O	13:I:156:ASN:HB2	2.14	0.47
18:O:49:ASP:OD1	18:O:49:ASP:N	2.48	0.47
33:m:138:SER:HB2	33:m:147:ARG:HB3	1.95	0.47
35:o:157:HIS:HB3	35:o:160:LYS:HD2	1.96	0.47
36:p:223:LYS:NZ	53:2:1896:A:OP1	2.48	0.47
40:y:59:THR:HG23	40:y:74:VAL:HG23	1.96	0.47
43:R:184:ASP:OD1	43:R:184:ASP:N	2.48	0.47
53:2:4281:A:O2'	53:2:4283:G:OP2	2.33	0.47
53:2:4776:G:O2'	53:2:4858:C:N4	2.47	0.47
7:B:10:ARG:NH1	7:B:11:HIS:O	2.48	0.47
28:e:37:LEU:HD21	28:e:105:ILE:HD11	1.96	0.47
39:w:37:THR:HG23	39:w:40:ARG:HH21	1.80	0.47
53:2:4297:G:C6	53:2:4313:A:N1	2.83	0.47
30:h:14:ASN:ND2	53:2:228:C:O2'	2.48	0.47
38:u:26:ARG:HD2	53:2:1859:C:OP1	2.14	0.47
43:R:32:ALA:O	43:R:36:LEU:HB2	2.14	0.47
46:4:257:LEU:HD21	46:4:296:ILE:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:4:525:ARG:NH2	46:4:531:MET:O	2.48	0.47
49:j:18:ASN:O	49:j:90:ARG:NH2	2.48	0.47
53:2:2020:U:H2'	53:2:2021:G:H8	1.80	0.47
4:8:83:C:N3	30:h:50:ARG:NH2	2.52	0.47
5:9:17:ARG:NH2	53:2:2860:C:OP1	2.48	0.47
12:H:118:LYS:HE3	20:Q:48:PRO:HG3	1.97	0.47
30:h:54:GLU:HG2	30:h:108:ARG:HB2	1.96	0.47
32:l:112:ARG:NH1	53:2:2264:C:OP1	2.47	0.47
44:W:230:ILE:O	44:W:239:GLU:N	2.48	0.47
51:3:2:U:H3	51:3:117:G:H22	1.63	0.47
37:r:255:SER:HA	37:r:264:ARG:HH22	1.79	0.46
42:C:114:ASP:OD1	42:C:114:ASP:N	2.47	0.46
43:R:74:ILE:O	51:3:114:U:O2'	2.32	0.46
52:v:28:GLU:HA	52:v:31:ARG:HG2	1.97	0.46
53:2:968:C:O2'	53:2:970:G:OP2	2.33	0.46
53:2:994:G:N7	53:2:1050:C:N4	2.63	0.46
4:8:99:U:OP1	29:g:67:ARG:NH2	2.47	0.46
39:w:32:MET:CG	53:2:3922:G:C6	2.98	0.46
46:4:371:LYS:HB2	46:4:373:ARG:HH21	1.80	0.46
14:J:148:ARG:NH1	39:w:61:GLN:O	2.47	0.46
20:Q:140:SER:HA	20:Q:143:GLU:HG2	1.97	0.46
25:Z:55:ARG:NH2	53:2:1351:G:O6	2.48	0.46
53:2:4228:G:N2	53:2:4229:U:O4	2.47	0.46
3:7:62:GLU:HG3	3:7:108:ILE:HD11	1.98	0.46
4:8:116:C:O2'	29:g:55:ARG:NH2	2.47	0.46
35:o:131:LYS:O	35:o:136:HIS:NE2	2.48	0.46
46:4:71:LYS:NZ	46:4:74:ASP:OD2	2.43	0.46
53:2:1595:G:H1'	53:2:1597:G:H21	1.81	0.46
7:B:162:VAL:O	7:B:182:GLU:HA	2.15	0.46
11:G:96:LEU:O	11:G:100:HIS:HB2	2.16	0.46
31:i:36:ARG:NH2	53:2:2580:U:OP1	2.46	0.46
46:4:626:ARG:HH21	46:4:631:LYS:HE2	1.80	0.46
53:2:1414:C:H2'	53:2:1415:G:H8	1.81	0.46
34:n:100:ARG:NH1	53:2:4753:U:OP1	2.48	0.46
39:w:183:VAL:HB	46:4:5:ASN:HD21	1.81	0.46
46:4:227:ASP:OD1	46:4:227:ASP:N	2.46	0.46
31:i:88:ASP:OD1	31:i:88:ASP:N	2.47	0.46
1:N:153:LYS:HE2	1:N:192:ILE:HB	1.98	0.46
7:B:220:ILE:HB	7:B:346:THR:HB	1.97	0.46
11:G:73:ARG:NH1	11:G:241:VAL:O	2.47	0.46
22:U:46:ASP:OD1	22:U:46:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:38:THR:HA	24:X:45:THR:HA	1.98	0.46
27:b:92:ASN:ND2	38:u:51:PRO:O	2.49	0.46
40:y:114:ARG:HA	40:y:117:ARG:HG2	1.96	0.46
45:T:41:ASP:HA	45:T:60:LYS:O	2.16	0.46
53:2:1398:A:OP2	53:2:1420:A:N6	2.49	0.46
5:9:63:CYS:SG	5:9:79:HIS:NE2	2.80	0.46
22:U:10:LEU:HG	22:U:19:MET:HE2	1.97	0.46
52:v:153:LEU:HB3	52:v:158:LEU:HD12	1.96	0.46
23:V:6:VAL:HG12	23:V:32:LYS:HG3	1.97	0.46
27:b:80:ILE:HG12	27:b:129:VAL:HG23	1.98	0.46
48:k:128:ARG:NH1	53:2:2306:G:OP1	2.49	0.46
53:2:35:U:H4'	53:2:1525:A:H2	1.81	0.46
4:8:75:G:OP2	30:h:74:TYR:OH	2.33	0.45
7:B:222:VAL:O	7:B:343:ARG:NH1	2.49	0.45
11:G:176:LYS:HD2	15:K:43:MET:HE1	1.98	0.45
47:Y:127:ARG:NH1	53:2:2420:A:OP2	2.48	0.45
52:v:23:LYS:HD3	53:2:1960:A:H2'	1.98	0.45
53:2:1859:C:H42	53:2:1875:C:H42	1.62	0.45
53:2:2874:U:N3	53:2:3693:U:O2	2.49	0.45
11:G:178:GLY:O	11:G:223:ARG:NH2	2.49	0.45
46:4:36:LYS:HG2	46:4:123:LEU:HD13	1.98	0.45
46:4:223:PRO:HD2	46:4:240:ALA:HB2	1.97	0.45
46:4:369:ASP:N	46:4:369:ASP:OD1	2.44	0.45
7:B:139:ASP:OD2	41:z:96:TRP:NE1	2.48	0.45
46:4:71:LYS:HD2	53:2:4441:A:H5'	1.98	0.45
52:v:177:LYS:NZ	52:v:178:GLU:O	2.48	0.45
7:B:230:GLY:O	7:B:234:ARG:HB2	2.15	0.45
11:G:103:ARG:NH2	11:G:192:ARG:O	2.49	0.45
26:a:43:LYS:HE3	53:2:2708:U:H1'	1.99	0.45
30:h:10:ASP:HB3	30:h:13:LYS:HB2	1.97	0.45
32:l:7:TRP:O	32:l:11:ARG:HB2	2.16	0.45
39:w:307:ASP:OD1	39:w:307:ASP:N	2.46	0.45
1:N:293:PRO:HB2	1:N:330:LEU:HD21	1.99	0.45
28:e:51:ARG:NH1	53:2:4620:OMU:OP1	2.50	0.45
33:m:144:LYS:HB3	33:m:160:SER:HB2	1.97	0.45
53:2:2521:G:H2'	53:2:2522:7MG:H82	1.97	0.45
8:D:204:ARG:NH1	8:D:205:ARG:O	2.50	0.45
14:J:147:LYS:HD3	14:J:171:ILE:HD11	1.98	0.45
26:a:105:LEU:HD22	26:a:135:LYS:HG3	1.98	0.45
33:m:126:LEU:HD21	33:m:156:LYS:HE3	1.98	0.45
36:p:139:TYR:OH	51:3:83:A:H2'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:w:84:THR:OG1	39:w:85:ARG:N	2.50	0.45
53:2:1207:C:H2'	53:2:1208:G:H8	1.81	0.45
35:o:223:ARG:HD2	35:o:224:LYS:HG2	1.99	0.45
46:4:176:TYR:O	46:4:181:LYS:NZ	2.45	0.45
44:W:248:SER:HB3	44:W:265:GLN:HG3	1.98	0.45
46:4:172:LEU:HD13	46:4:244:LEU:HD23	1.98	0.45
1:N:113:ILE:HG21	1:N:118:LEU:HD13	1.98	0.45
8:D:84:THR:OG1	8:D:85:HIS:N	2.49	0.45
33:m:104:VAL:O	33:m:139:HIS:NE2	2.45	0.45
42:C:143:ASP:OD1	42:C:143:ASP:N	2.49	0.45
43:R:23:ARG:O	43:R:23:ARG:NH1	2.45	0.45
53:2:2486:G:O6	53:2:2492:C:N4	2.50	0.45
53:2:2663:G:H21	53:2:2676:A:HO2'	1.63	0.45
2:6:240:LEU:O	2:6:244:LEU:HB2	2.17	0.45
37:r:260:ASP:HA	37:r:264:ARG:HE	1.81	0.45
43:R:202:GLN:NE2	43:R:237:GLU:OE2	2.49	0.45
45:T:66:ASN:HB2	45:T:73:GLY:HA3	1.98	0.45
2:6:214:GLU:HA	2:6:217:VAL:HG12	1.99	0.44
31:i:88:ASP:OD1	31:i:121:ARG:NH2	2.44	0.44
34:n:104:MET:HE2	34:n:104:MET:HB3	1.79	0.44
36:p:190:LEU:HD21	36:p:208:LEU:HD21	1.99	0.44
45:T:51:GLY:O	45:T:95:HIS:NE2	2.50	0.44
46:4:395:LYS:HG3	46:4:400:ASP:HB2	1.99	0.44
52:v:25:ASN:HA	52:v:28:GLU:HG2	2.00	0.44
31:i:47:ASP:HB3	31:i:69:LYS:HB3	1.99	0.44
35:o:161:ARG:O	35:o:182:ASN:ND2	2.51	0.44
37:r:287:LEU:HD11	38:u:63:GLU:HG3	1.98	0.44
46:4:311:GLN:HB3	46:4:317:VAL:HG12	1.98	0.44
53:2:224:U:HO2'	53:2:243:A:HO2'	1.64	0.44
53:2:703:G:H2'	53:2:704:C:H4'	1.99	0.44
27:b:27:LEU:HD21	45:T:141:VAL:HG11	2.00	0.44
27:b:95:ARG:NH2	53:2:1951:G:O2'	2.50	0.44
33:m:20:VAL:HA	33:m:23:ARG:HG3	1.99	0.44
13:I:120:GLU:OE1	13:I:124:ARG:NH1	2.47	0.44
31:i:25:ILE:HA	31:i:43:VAL:HG12	1.97	0.44
42:C:21:CYS:HA	42:C:72:CYS:O	2.17	0.44
36:p:127:LYS:HB2	45:T:133:ALA:HB3	1.98	0.44
38:u:6:LEU:HB3	38:u:7:LYS:H	1.74	0.44
39:w:51:ASN:OD1	39:w:55:LYS:N	2.50	0.44
39:w:327:ILE:HG12	39:w:359:LEU:HD23	2.00	0.44
43:R:268:ARG:C	43:R:270:LYS:N	2.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:d:96:LEU:HD12	50:d:100:LEU:HD23	1.98	0.44
52:v:48:MET:O	52:v:126:ARG:NH1	2.50	0.44
13:I:51:LYS:HB2	13:I:52:LYS:HE2	1.99	0.44
22:U:24:ARG:NE	53:2:3938:G:OP1	2.50	0.44
52:v:60:TRP:HH2	52:v:112:VAL:HG23	1.82	0.44
17:M:20:ARG:NH2	17:M:39:TYR:OH	2.44	0.44
43:R:33:ARG:NH2	51:3:7:G:O3'	2.51	0.44
44:W:355:LEU:HB2	44:W:366:THR:HG22	2.00	0.44
50:d:35:ASP:OD2	50:d:35:ASP:N	2.48	0.44
53:2:2101:C:H2'	53:2:2102:G:H2'	2.00	0.44
8:D:268:ARG:HB3	53:2:654:C:H5'	1.99	0.44
13:I:60:TRP:HB2	53:2:4764:A:N1	2.33	0.44
41:z:4:SER:OG	41:z:5:LEU:N	2.51	0.44
43:R:282:GLN:HA	43:R:285:ALA:HB3	2.00	0.44
53:2:1868:A:N3	53:2:1869:G:H1'	2.32	0.44
2:6:106:ASN:ND2	28:e:136:ALA:O	2.51	0.44
4:8:141:C:H5''	22:U:60:VAL:HG21	1.99	0.44
22:U:125:SER:HB2	53:2:3937:C:H1'	2.00	0.44
25:Z:12:LYS:HD2	25:Z:14:ARG:HH21	1.82	0.44
31:i:5:MET:HG2	31:i:77:TYR:HE2	1.82	0.44
43:R:260:GLU:OE1	51:3:1:G:N7	2.50	0.44
53:2:1868:A:C2	53:2:1869:G:H1'	2.53	0.44
53:2:2706:G:N2	53:2:2708:U:O4'	2.51	0.44
4:8:13:G:O2'	47:Y:121:LYS:O	2.34	0.43
8:D:12:SER:HB3	8:D:18:SER:HB3	2.00	0.43
44:W:104:THR:OG1	44:W:485:ARG:O	2.35	0.43
44:W:405:LYS:HD2	44:W:405:LYS:HA	1.80	0.43
53:2:2418:A:N1	53:2:2429:A:O2'	2.48	0.43
7:B:92:TYR:HB2	7:B:159:VAL:HB	1.98	0.43
9:E:17:ARG:HH22	9:E:105:ILE:HG22	1.83	0.43
53:2:62:A:N3	53:2:77:U:O2'	2.47	0.43
53:2:1604:G:H2'	53:2:1605:7MG:H82	2.00	0.43
53:2:3932:U:H2'	53:2:3933:G:H8	1.84	0.43
6:A:117:ARG:HD2	53:2:1273:G:C8	2.52	0.43
8:D:316:LYS:NZ	53:2:1282:G:OP2	2.49	0.43
24:X:30:GLU:HA	24:X:33:GLN:HG2	2.00	0.43
45:T:47:THR:HA	53:2:4282:A:N6	2.34	0.43
50:d:72:VAL:HG11	50:d:83:LEU:HD21	2.00	0.43
53:2:989:U:H3	53:2:1051:G:H8	1.66	0.43
53:2:4301:U:O4	53:2:4309:G:O6	2.37	0.43
22:U:84:PRO:O	22:U:87:HIS:ND1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:o:223:ARG:HA	35:o:224:LYS:HA	1.81	0.43
46:4:229:PRO:HB2	46:4:233:ARG:HG3	2.00	0.43
14:J:169:ARG:NH2	39:w:61:GLN:OE1	2.51	0.43
23:V:43:ILE:HD11	23:V:138:LEU:HD13	1.99	0.43
28:e:32:THR:HG23	28:e:34:ALA:H	1.82	0.43
34:n:105:LEU:HB3	34:n:106:TYR:H	1.67	0.43
43:R:50:ARG:HA	43:R:145:TYR:O	2.17	0.43
43:R:150:LEU:HD11	53:2:4280:A:N6	2.33	0.43
45:T:111:GLU:HA	45:T:114:GLN:HG3	2.00	0.43
2:6:85:ARG:HD2	2:6:94:ILE:HD13	2.01	0.43
21:S:20:HIS:NE2	53:2:936:C:H5'	2.33	0.43
30:h:55:VAL:HG12	30:h:106:ILE:HA	2.00	0.43
35:o:221:LYS:NZ	35:o:223:ARG:O	2.45	0.43
42:C:31:ASP:N	42:C:31:ASP:OD1	2.52	0.43
46:4:196:GLN:HG2	46:4:201:THR:HB	2.00	0.43
53:2:1538:U:H2'	53:2:1539:G:H8	1.84	0.43
7:B:10:ARG:NH2	7:B:265:SER:O	2.51	0.43
8:D:191:ALA:HB2	53:2:2334:C:C5	2.54	0.43
25:Z:17:GLU:OE1	25:Z:26:ARG:NH2	2.49	0.43
53:2:4620:OMU:OP2	53:2:4670:C:N4	2.47	0.43
11:G:245:LYS:HE3	53:2:4161:G:H21	1.83	0.43
24:X:80:LYS:HD2	33:m:98:ILE:HD12	2.01	0.43
27:b:69:GLU:HG2	27:b:101:THR:HG22	2.01	0.43
40:y:84:ALA:HB1	40:y:108:GLU:HG3	2.01	0.43
44:W:263:ALA:HA	44:W:269:ILE:HG22	2.01	0.43
44:W:312:SER:OG	44:W:314:ASN:O	2.36	0.43
53:2:456:C:H2'	53:2:457:G:H8	1.84	0.43
53:2:2378:G:N2	53:2:2381:A:OP2	2.44	0.43
53:2:3855:C:H2'	53:2:3856:A:H8	1.83	0.43
7:B:52:GLY:HA2	7:B:341[A]:LYS:HE3	2.01	0.43
8:D:209:ILE:HB	8:D:229:LEU:HD13	2.01	0.43
25:Z:124:ASP:OD1	25:Z:124:ASP:N	2.52	0.43
46:4:131:ARG:HH21	53:2:4407:G:H5''	1.84	0.43
50:d:23:LEU:HG	50:d:70:ILE:HB	2.00	0.43
51:3:38:U:N3	51:3:41:G:OP2	2.51	0.43
53:2:502:C:H3'	53:2:503:C:H3'	2.01	0.43
53:2:4092:G:H3'	53:2:4093:G:H21	1.84	0.43
37:r:295:ARG:HA	37:r:298:LYS:HG2	2.01	0.42
39:w:462:PRO:HG2	39:w:465:ALA:HB3	2.00	0.42
43:R:43:LYS:HD3	53:2:1819:G:N7	2.33	0.42
44:W:385:ARG:HB3	44:W:386:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:2364:OMG:HM23	53:2:2364:OMG:H1'	1.80	0.42
7:B:30:LYS:NZ	53:2:4717:A:OP2	2.52	0.42
8:D:337:ARG:NH1	35:o:55:GLY:O	2.50	0.42
14:J:133:LEU:HD22	14:J:148:ARG:HB3	2.01	0.42
24:X:57:CYS:O	24:X:61:MET:HA	2.19	0.42
36:p:134:ARG:HA	36:p:137:GLU:HG3	2.01	0.42
39:w:312:SER:HB2	39:w:360:ILE:HD11	2.01	0.42
2:6:44:ASP:OD1	2:6:44:ASP:N	2.51	0.42
37:r:237:LYS:HA	37:r:237:LYS:HD3	1.93	0.42
46:4:121:ASP:H	46:4:125:ARG:HD3	1.85	0.42
53:2:4432:C:H2'	53:2:4433:G:H8	1.84	0.42
1:N:109:ASN:HB3	53:2:3711:A:H1'	2.01	0.42
2:6:123:ARG:HA	2:6:126:GLU:HG2	2.01	0.42
2:6:213:THR:OG1	46:4:214:TYR:O	2.37	0.42
2:6:219:GLU:O	2:6:222:PHE:O	2.37	0.42
13:I:129:ARG:HH22	53:2:4704:C:H4'	1.83	0.42
46:4:107:ASP:N	46:4:107:ASP:OD1	2.50	0.42
52:v:69:LYS:HA	52:v:69:LYS:HD3	1.76	0.42
53:2:35:U:O2'	53:2:1651:G:N3	2.45	0.42
20:Q:201:GLU:HA	20:Q:204:GLU:HB3	2.00	0.42
23:V:106:ASP:O	53:2:4910:G:N2	2.53	0.42
31:i:105:ALA:HA	31:i:108:ARG:HE	1.84	0.42
33:m:116:LEU:HD13	33:m:164:ALA:HB2	2.02	0.42
34:n:33:VAL:HG23	34:n:38:GLU:HB2	2.02	0.42
36:p:148:LYS:HD2	53:2:942:G:H3'	2.02	0.42
43:R:265:ARG:HA	43:R:265:ARG:HD3	1.95	0.42
52:v:96:LEU:HD21	52:v:102:LEU:HD21	2.02	0.42
1:N:131:LYS:HB3	1:N:131:LYS:HE3	1.87	0.42
8:D:234:LYS:HG2	53:2:1374:G:H1'	2.00	0.42
8:D:301:ALA:HB1	25:Z:132:LYS:HD3	2.01	0.42
11:G:117:ARG:HA	11:G:120:LYS:HG2	2.02	0.42
23:V:52:LEU:HD13	38:u:5:LYS:HB3	2.01	0.42
23:V:54:TYR:OH	23:V:73:PHE:O	2.36	0.42
37:r:286:HIS:NE2	37:r:290:GLU:OE2	2.53	0.42
53:2:2295:C:H2'	53:2:2296:G:H8	1.85	0.42
53:2:4918:C:H2'	53:2:4919:G:H8	1.84	0.42
19:P:10:LYS:NZ	53:2:2782:U:OP2	2.44	0.42
27:b:147:ASP:HB3	27:b:150:ILE:HB	2.01	0.42
29:g:100:VAL:HG21	29:g:109:ILE:HD11	2.02	0.42
40:y:11:LYS:HZ3	40:y:35:LEU:HD13	1.83	0.42
46:4:634:ARG:NH2	53:2:1594:C:N3	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:42:ILE:HB	52:v:206:TYR:HB2	2.02	0.42
53:2:1868:A:H8	53:2:1868:A:O5'	2.02	0.42
7:B:58:ARG:O	7:B:71:GLU:HA	2.20	0.42
10:F:82:MET:HE2	10:F:82:MET:HB2	1.98	0.42
14:J:166:LYS:O	39:w:44:TYR:OH	2.35	0.42
42:C:109:ILE:HG22	42:C:111:GLU:H	1.85	0.42
42:C:110:GLN:HG3	53:2:4251:A:H1'	2.01	0.42
44:W:353:LEU:HB2	44:W:368:MET:HB2	2.01	0.42
46:4:94:LEU:HD11	53:2:4438:U:C2	2.55	0.42
11:G:132:ARG:HA	11:G:133:PRO:HD3	1.88	0.42
35:o:112:MET:HE3	35:o:112:MET:HB3	1.93	0.42
43:R:197:LYS:HA	43:R:200:MET:HE3	2.01	0.42
44:W:447:LYS:HD2	44:W:447:LYS:HA	1.88	0.42
4:8:96:C:H5''	12:H:66:LYS:HG2	2.01	0.42
33:m:104:VAL:HA	33:m:107:MET:HG3	2.01	0.42
46:4:42:ARG:HD3	53:2:4519:C:C2	2.54	0.42
52:v:135:VAL:HG21	52:v:190:LEU:HD21	2.02	0.42
53:2:959:G:O2'	53:2:2263:A:N6	2.51	0.42
53:2:1732:C:H42	53:2:1797:G:N2	2.15	0.42
8:D:110:ARG:NH2	53:2:1508:A:OP1	2.53	0.41
10:F:11:LEU:HG	10:F:18:ASN:HD21	1.84	0.41
23:V:8:VAL:HG12	23:V:117:ARG:HG3	2.02	0.41
40:y:112:ILE:HG22	40:y:132:ILE:HD13	2.02	0.41
53:2:4080:C:H2'	53:2:4081:G:H8	1.85	0.41
53:2:4620:OMU:H1'	53:2:4620:OMU:HM23	1.82	0.41
19:P:9:ILE:HD12	19:P:51:LEU:HD21	2.01	0.41
23:V:32:LYS:H	23:V:32:LYS:HG2	1.67	0.41
25:Z:86:ILE:HD13	25:Z:86:ILE:HA	1.95	0.41
28:e:85:ARG:HE	28:e:100:ASP:HA	1.85	0.41
43:R:15:ARG:NH2	53:2:4266:G:OP2	2.54	0.41
53:2:1332:C:H2'	53:2:1333:A:H8	1.85	0.41
7:B:286:LYS:HB3	7:B:332:MET:HE3	2.01	0.41
11:G:34:LYS:NZ	53:2:4129:B8W:O2'	2.42	0.41
38:u:3:ARG:HA	38:u:4:PRO:HD3	1.93	0.41
50:d:107:LYS:NZ	53:2:2717:G:OP1	2.50	0.41
3:7:123:ASP:OD1	46:4:488:ARG:NH2	2.51	0.41
28:e:24:ALA:HB3	28:e:39:ILE:HD12	2.02	0.41
35:o:219:LYS:HD2	53:2:1290:G:H5''	2.02	0.41
51:3:72:U:O2'	51:3:74:A:OP2	2.30	0.41
53:2:1734:G:N2	53:2:1796:U:H3	2.19	0.41
53:2:4522:G:OP1	53:2:4525:C:N4	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:169:LEU:HD12	1:N:184:MET:HE1	2.03	0.41
20:Q:197:LYS:HD2	53:2:4358:U:H4'	2.02	0.41
30:h:131:GLU:HA	30:h:134:LYS:HE3	2.03	0.41
53:2:990:C:N4	53:2:1051:G:O2'	2.53	0.41
53:2:3870:C:H2'	53:2:3871:A:H8	1.86	0.41
8:D:41:HIS:O	8:D:45:ARG:HB2	2.20	0.41
30:h:31:SER:HA	30:h:48:PRO:HA	2.01	0.41
36:p:44:LYS:HB3	36:p:44:LYS:HE3	1.86	0.41
38:u:16:HIS:ND1	53:2:3875:G:O2'	2.51	0.41
39:w:87:ILE:HG21	39:w:92:LEU:HD13	2.02	0.41
43:R:200:MET:HG3	43:R:202:GLN:HG3	2.03	0.41
49:j:24:GLU:OE1	49:j:87:ARG:NH2	2.48	0.41
52:v:29:GLU:HG2	52:v:32:LYS:HZ1	1.85	0.41
53:2:422:C:H2'	53:2:423:G:H8	1.85	0.41
53:2:1260:G:H2'	53:2:1261:G:H8	1.85	0.41
53:2:2773:OMG:HM22	53:2:2774:C:H5'	2.01	0.41
3:7:35:LYS:O	3:7:39:ASN:ND2	2.44	0.41
3:7:45:ASN:HB3	3:7:48:LYS:HB2	2.02	0.41
3:7:95:ARG:HA	3:7:95:ARG:HD2	1.90	0.41
8:D:35:ASP:OD1	8:D:35:ASP:N	2.54	0.41
25:Z:65:ARG:NH1	53:2:1502:G:OP1	2.53	0.41
39:w:23:ARG:NH2	53:2:3922:G:C8	2.87	0.41
53:2:1444:G:H22	53:2:2104:G:H22	1.68	0.41
53:2:2843:U:O2'	53:2:4632:U:OP1	2.39	0.41
4:8:47:C:H1'	4:8:61:A:H2'	2.02	0.41
23:V:9:LEU:HD23	23:V:118:MET:HB2	2.01	0.41
37:r:265:THR:OG1	37:r:270:LYS:NZ	2.45	0.41
37:r:267:TRP:HH2	53:2:2025:A:C2	2.39	0.41
45:T:49:GLN:CG	53:2:4282:A:N3	2.84	0.41
46:4:232:ASP:OD1	46:4:232:ASP:N	2.51	0.41
53:2:419:A:N3	53:2:1332:C:O2'	2.51	0.41
53:2:685:C:O2'	53:2:686:A:N7	2.53	0.41
53:2:1605:7MG:H2'	53:2:1606:U:O4'	2.20	0.41
53:2:4492:U:H5''	53:2:4493:U:H5'	2.01	0.41
53:2:4638:U:OP1	53:2:5044:A:O2'	2.38	0.41
1:N:140:HIS:O	1:N:144:ASP:HB2	2.21	0.41
11:G:191:GLY:HA2	11:G:194:VAL:HG12	2.02	0.41
13:I:50:LYS:HE2	53:2:759:G:OP1	2.20	0.41
15:K:44:ILE:HG13	22:U:9:GLU:HB2	2.03	0.41
17:M:49:TRP:O	53:2:1646:A:O2'	2.38	0.41
21:S:114:LYS:HD2	53:2:4929:C:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:g:48:ARG:NH2	53:2:2475:G:O6	2.52	0.41
34:n:83:MET:HE3	34:n:83:MET:HB3	1.86	0.41
35:o:178:PRO:HB2	35:o:181:LEU:HD23	2.02	0.41
36:p:151:ASN:O	36:p:155:TYR:HB2	2.20	0.41
37:r:295:ARG:HG3	37:r:296:GLN:HE21	1.85	0.41
45:T:28:ALA:N	51:3:9:C:OP1	2.50	0.41
46:4:48:MET:HG3	46:4:117:MET:HE2	2.03	0.41
46:4:185:ILE:O	46:4:189:THR:OG1	2.34	0.41
12:H:55:ALA:O	12:H:59:THR:OG1	2.36	0.41
17:M:25:LYS:HE2	17:M:25:LYS:HB3	1.97	0.41
21:S:94:LYS:NZ	53:2:4872:2MG:OP2	2.52	0.41
24:X:21:SER:HA	24:X:24:LYS:HE2	2.03	0.41
27:b:144:GLN:HA	37:r:262:PRO:HD3	2.03	0.41
39:w:258:ASP:OD1	39:w:258:ASP:N	2.53	0.41
7:B:57:VAL:HG22	7:B:367:PHE:HB3	2.03	0.40
14:J:185:HIS:HB3	14:J:188:LEU:HB2	2.03	0.40
43:R:136:ASP:OD1	43:R:136:ASP:N	2.54	0.40
51:3:13:A:OP2	51:3:66:G:N2	2.52	0.40
3:7:106:LYS:HE2	46:4:466:TYR:HA	2.02	0.40
20:Q:190:ARG:NH2	53:2:1393:G:O2'	2.54	0.40
25:Z:97:LYS:HE3	25:Z:97:LYS:HB2	1.93	0.40
25:Z:147:GLU:OE2	25:Z:151:HIS:NE2	2.47	0.40
26:a:140:GLU:O	26:a:144:LYS:HB2	2.21	0.40
53:2:1976:G:C6	53:2:1991:A:N6	2.90	0.40
53:2:2447:U:H2'	53:2:2448:G:H8	1.85	0.40
2:6:95:ARG:HH11	2:6:128:ILE:HD11	1.86	0.40
11:G:87:LEU:HD12	11:G:184:ILE:HG22	2.02	0.40
21:S:74:ARG:NH1	53:2:736:C:OP1	2.26	0.40
22:U:116:LEU:HD22	22:U:135:ILE:HD11	2.04	0.40
35:o:120:ASP:OD1	53:2:2263:A:O2'	2.39	0.40
35:o:213:THR:H	35:o:216:TYR:HB3	1.86	0.40
44:W:237:ARG:HH12	53:2:1991:A:H4'	1.86	0.40
46:4:244:LEU:O	46:4:282:LYS:NZ	2.53	0.40
53:2:1699:A:OP1	53:2:2085:G:O2'	2.39	0.40
53:2:4235:G:C5	53:2:4292:A:N7	2.90	0.40
4:8:61:A:OP1	12:H:52:LYS:NZ	2.48	0.40
9:E:36:LYS:HB2	9:E:36:LYS:HE3	1.89	0.40
9:E:38:ILE:HD13	9:E:38:ILE:HA	1.95	0.40
27:b:48:VAL:HG11	27:b:54:MET:HE2	2.02	0.40
28:e:67:LYS:HA	28:e:73:ARG:HH22	1.85	0.40
46:4:49:ARG:NH1	53:2:4515:G:OP1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:1865:G:C2'	53:2:1866:U:H5'	2.51	0.40
53:2:4236:G:O2'	53:2:4328:G:H1'	2.21	0.40
8:D:308:LYS:HD3	53:2:1702:C:H4'	2.02	0.40
11:G:55:VAL:HG21	29:g:41:ARG:HD2	2.03	0.40
11:G:190:LEU:HD23	11:G:193:LEU:HD12	2.03	0.40
14:J:163:LYS:HB2	14:J:168:GLU:HB2	2.04	0.40
20:Q:96:ILE:HD12	20:Q:117:LEU:HD11	2.04	0.40
24:X:9:GLY:O	53:2:1553:A:O2'	2.39	0.40
39:w:15:SER:OG	39:w:16:LYS:N	2.54	0.40
40:y:57:ARG:HH12	40:y:92:ARG:HE	1.69	0.40
52:v:190:LEU:HD23	52:v:190:LEU:HA	1.97	0.40
53:2:188:G:N2	53:2:191:G:O6	2.43	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%)	313 (97%)	11 (3%)	0	100	100
2	6	242/245 (99%)	227 (94%)	15 (6%)	0	100	100
3	7	133/163 (82%)	130 (98%)	3 (2%)	0	100	100
5	9	82/134 (61%)	75 (92%)	7 (8%)	0	100	100
6	A	41/159 (26%)	41 (100%)	0	0	100	100
7	B	401/403 (100%)	384 (96%)	17 (4%)	0	100	100
8	D	356/427 (83%)	335 (94%)	21 (6%)	0	100	100
9	E	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
10	F	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
11	G	239/266 (90%)	231 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	H	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
13	I	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
14	J	213/260 (82%)	208 (98%)	5 (2%)	0	100	100
15	K	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
16	L	108/148 (73%)	101 (94%)	7 (6%)	0	100	100
17	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
18	O	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
19	P	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
20	Q	208/211 (99%)	198 (95%)	10 (5%)	0	100	100
21	S	133/215 (62%)	126 (95%)	7 (5%)	0	100	100
22	U	201/204 (98%)	190 (94%)	10 (5%)	1 (0%)	24	59
23	V	199/203 (98%)	191 (96%)	8 (4%)	0	100	100
24	X	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
25	Z	149/188 (79%)	147 (99%)	2 (1%)	0	100	100
26	a	146/196 (74%)	143 (98%)	3 (2%)	0	100	100
27	b	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
28	e	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
29	g	115/156 (74%)	111 (96%)	4 (4%)	0	100	100
30	h	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
31	i	133/136 (98%)	128 (96%)	4 (3%)	1 (1%)	16	50
32	l	123/137 (90%)	117 (95%)	6 (5%)	0	100	100
33	m	246/257 (96%)	224 (91%)	22 (9%)	0	100	100
34	n	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
35	o	231/288 (80%)	217 (94%)	14 (6%)	0	100	100
36	p	224/248 (90%)	217 (97%)	7 (3%)	0	100	100
37	r	80/360 (22%)	76 (95%)	4 (5%)	0	100	100
38	u	64/549 (12%)	57 (89%)	5 (8%)	2 (3%)	3	22
39	w	427/731 (58%)	411 (96%)	13 (3%)	3 (1%)	18	52
40	y	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
41	z	63/129 (49%)	63 (100%)	0	0	100	100
42	C	163/178 (92%)	152 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	R	291/297 (98%)	271 (93%)	17 (6%)	3 (1%)	12	45
44	W	386/485 (80%)	369 (96%)	16 (4%)	1 (0%)	36	68
45	T	120/160 (75%)	109 (91%)	11 (9%)	0	100	100
46	4	607/634 (96%)	558 (92%)	46 (8%)	3 (0%)	24	59
47	Y	165/184 (90%)	156 (94%)	9 (6%)	0	100	100
48	k	127/135 (94%)	121 (95%)	6 (5%)	0	100	100
49	j	109/125 (87%)	104 (95%)	5 (5%)	0	100	100
50	d	102/128 (80%)	92 (90%)	10 (10%)	0	100	100
52	v	215/239 (90%)	204 (95%)	11 (5%)	0	100	100
All	All	8770/11363 (77%)	8341 (95%)	415 (5%)	14 (0%)	44	73

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	u	55	PRO
44	W	267	ARG
38	u	14	THR
39	w	27	ALA
46	4	88	ASP
43	R	44	TYR
22	U	147	ASP
31	i	31	ASP
39	w	323	LYS
43	R	269	PRO
39	w	132	VAL
43	R	270	LYS
46	4	366	THR
46	4	427	ASP

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
2	6	212/213 (100%)	212 (100%)	0	100	100
3	7	126/149 (85%)	126 (100%)	0	100	100
5	9	74/114 (65%)	74 (100%)	0	100	100
6	A	34/126 (27%)	34 (100%)	0	100	100
7	B	349/349 (100%)	349 (100%)	0	100	100
8	D	298/348 (86%)	298 (100%)	0	100	100
9	E	83/97 (86%)	83 (100%)	0	100	100
10	F	94/100 (94%)	94 (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	K	86/89 (97%)	86 (100%)	0	100	100
16	L	94/121 (78%)	94 (100%)	0	100	100
17	M	73/80 (91%)	73 (100%)	0	100	100
18	O	64/65 (98%)	64 (100%)	0	100	100
19	P	47/48 (98%)	47 (100%)	0	100	100
20	Q	176/177 (99%)	176 (100%)	0	100	100
21	S	115/161 (71%)	115 (100%)	0	100	100
22	U	171/172 (99%)	171 (100%)	0	100	100
23	V	173/174 (99%)	173 (100%)	0	100	100
24	X	74/75 (99%)	74 (100%)	0	100	100
25	Z	136/165 (82%)	136 (100%)	0	100	100
26	a	133/175 (76%)	133 (100%)	0	100	100
27	b	157/157 (100%)	156 (99%)	1 (1%)	78	84
28	e	101/107 (94%)	101 (100%)	0	100	100
29	g	105/133 (79%)	105 (100%)	0	100	100
30	h	124/135 (92%)	124 (100%)	0	100	100
31	i	117/118 (99%)	117 (100%)	0	100	100
32	l	109/121 (90%)	109 (100%)	0	100	100
33	m	190/199 (96%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	n	88/89 (99%)	88 (100%)	0	100	100
35	o	208/252 (82%)	208 (100%)	0	100	100
36	p	195/215 (91%)	195 (100%)	0	100	100
37	r	76/312 (24%)	76 (100%)	0	100	100
38	u	62/485 (13%)	62 (100%)	0	100	100
39	w	385/654 (59%)	385 (100%)	0	100	100
40	y	137/137 (100%)	137 (100%)	0	100	100
41	z	61/115 (53%)	61 (100%)	0	100	100
42	C	138/149 (93%)	138 (100%)	0	100	100
43	R	246/250 (98%)	245 (100%)	1 (0%)	84	86
44	W	322/404 (80%)	322 (100%)	0	100	100
45	T	109/140 (78%)	109 (100%)	0	100	100
46	4	554/574 (96%)	554 (100%)	0	100	100
47	Y	147/163 (90%)	147 (100%)	0	100	100
48	k	115/121 (95%)	115 (100%)	0	100	100
49	j	101/110 (92%)	101 (100%)	0	100	100
50	d	94/115 (82%)	94 (100%)	0	100	100
52	v	194/214 (91%)	193 (100%)	1 (0%)	81	85
All	All	7727/9828 (79%)	7724 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	b	77	ASN
43	R	270	LYS
52	v	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	34	GLN
1	N	37	HIS
1	N	48	GLN
1	N	89	HIS
1	N	288	HIS

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Mol	Chain	Res	Type
1	N	319	ASN
1	N	427	ASN
2	6	33	ASN
2	6	50	HIS
2	6	82	GLN
2	6	156	ASN
3	7	17	HIS
3	7	24	ASN
3	7	122	GLN
3	7	130	ASN
3	7	132	HIS
5	9	85	HIS
7	B	109	HIS
7	B	121	ASN
7	B	167	GLN
7	B	208	ASN
8	D	94	ASN
8	D	317	ASN
8	D	329	ASN
10	F	110	GLN
11	G	225	ASN
13	I	116	ASN
13	I	138	GLN
13	I	162	GLN
14	J	4	ASN
14	J	21	HIS
14	J	55	HIS
14	J	202	ASN
14	J	232	GLN
14	J	255	ASN
17	M	13	ASN
20	Q	104	ASN
20	Q	149	GLN
21	S	125	ASN
22	U	57	GLN
22	U	109	HIS
23	V	184	ASN
25	Z	7	HIS
26	a	39	GLN
27	b	117	HIS
28	e	50	ASN
29	g	125	ASN

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Mol	Chain	Res	Type
30	h	20	ASN
33	m	86	GLN
33	m	162	ASN
33	m	187	HIS
33	m	215	ASN
33	m	217	GLN
34	n	99	HIS
37	r	256	GLN
39	w	63	GLN
39	w	236	HIS
39	w	255	ASN
39	w	393	HIS
40	y	66	ASN
41	z	89	GLN
42	C	46	GLN
42	C	97	ASN
43	R	131	ASN
43	R	225	GLN
44	W	177	ASN
44	W	245	HIS
46	4	5	ASN
46	4	84	ASN
46	4	218	GLN
46	4	246	HIS
46	4	436	HIS
46	4	538	HIS
47	Y	28	ASN
47	Y	97	ASN
47	Y	133	HIS
48	k	24	GLN
48	k	57	ASN
48	k	63	ASN
48	k	101	HIS
49	j	69	ASN
49	j	79	ASN
49	j	121	ASN
50	d	17	GLN
50	d	41	GLN
52	v	58	ASN
52	v	91	GLN
52	v	147	HIS
52	v	152	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	8	155/156 (99%)	30 (19%)	0
51	3	113/120 (94%)	25 (22%)	2 (1%)
53	2	3472/5054 (68%)	869 (25%)	19 (0%)
All	All	3740/5330 (70%)	924 (24%)	21 (0%)

All (924) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	8	25	G
4	8	34	U
4	8	35	C
4	8	39	G
4	8	48	A
4	8	51	U
4	8	52	A
4	8	59	A
4	8	62	A
4	8	63	U
4	8	71	A
4	8	80	A
4	8	82	A
4	8	84	A
4	8	85	U
4	8	86	U
4	8	88	A
4	8	103	A
4	8	104	A
4	8	105	C
4	8	110	U
4	8	114	G
4	8	123	U
4	8	124	U
4	8	126	C
4	8	127	U
4	8	128	C
4	8	147	G
4	8	150	C
4	8	151	G
51	3	7	G
51	3	10	C
51	3	11	A

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Mol	Chain	Res	Type
51	3	22	A
51	3	41	G
51	3	48	G
51	3	49	A
51	3	51	G
51	3	52	C
51	3	53	U
51	3	54	A
51	3	56	G
51	3	60	G
51	3	62	U
51	3	63	C
51	3	64	G
51	3	72	U
51	3	73	U
51	3	74	A
51	3	75	G
51	3	83	A
51	3	84	U
51	3	85	G
51	3	100	A
51	3	110	G
53	2	39	A
53	2	42	A
53	2	44	A
53	2	48	G
53	2	56	A
53	2	59	A
53	2	64	A
53	2	65	A
53	2	69	A
53	2	72	C
53	2	73	A
53	2	84	A
53	2	91	G
53	2	98	A
53	2	108	A
53	2	109	G
53	2	110	C
53	2	112	C
53	2	119	G
53	2	120	A

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Mol	Chain	Res	Type
53	2	131	C
53	2	132	G
53	2	134	G
53	2	135	G
53	2	136	C
53	2	144	G
53	2	145	G
53	2	152	U
53	2	158	A
53	2	159	C
53	2	183	C
53	2	185	C
53	2	186	G
53	2	188	G
53	2	197	A
53	2	200	U
53	2	209	U
53	2	216	C
53	2	217	C
53	2	218	A
53	2	220	C
53	2	234	G
53	2	237	B9B
53	2	254	G
53	2	255	C
53	2	256	G
53	2	265	C
53	2	266	C
53	2	267	G
53	2	279	A
53	2	280	G
53	2	297	U
53	2	306	A
53	2	315	G
53	2	316	U
53	2	340	C
53	2	347	A
53	2	363	A
53	2	387	G
53	2	398	A2M
53	2	407	A
53	2	408	A

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Mol	Chain	Res	Type
53	2	409	G
53	2	410	A
53	2	412	G
53	2	432	U
53	2	433	A
53	2	440	U
53	2	449	C
53	2	450	G
53	2	452	A
53	2	453	G
53	2	454	U
53	2	461	G
53	2	464	G
53	2	465	G
53	2	467	U
53	2	484	U
53	2	485	C
53	2	486	C
53	2	489	C
53	2	491	G
53	2	492	U
53	2	493	G
53	2	497	G
53	2	498	C
53	2	499	G
53	2	500	G
53	2	501	C
53	2	502	C
53	2	503	C
53	2	504	G
53	2	505	G
53	2	509	A
53	2	510	U
53	2	512	U
53	2	513	U
53	2	514	U
53	2	515	C
53	2	516	C
53	2	517	C
53	2	518	G
53	2	519	C
53	2	648	G

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Mol	Chain	Res	Type
53	2	653	U
53	2	654	C
53	2	656	C
53	2	657	C
53	2	659	G
53	2	666	G
53	2	667	A
53	2	668	C
53	2	673	C
53	2	685	C
53	2	686	A
53	2	696	C
53	2	703	G
53	2	704	C
53	2	731	G
53	2	738	C
53	2	739	G
53	2	740	G
53	2	742	G
53	2	753	C
53	2	759	G
53	2	904	C
53	2	905	C
53	2	913	U
53	2	914	U
53	2	915	A
53	2	916	C
53	2	917	A
53	2	918	G
53	2	924	C
53	2	925	C
53	2	926	G
53	2	932	A
53	2	933	G
53	2	935	A
53	2	936	C
53	2	937	U
53	2	941	C
53	2	943	A
53	2	944	A
53	2	945	U
53	2	946	C

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Mol	Chain	Res	Type
53	2	956	A
53	2	959	G
53	2	960	A
53	2	961	G
53	2	962	C
53	2	965	G
53	2	966	A
53	2	967	C
53	2	969	C
53	2	970	G
53	2	971	U
53	2	972	C
53	2	977	C
53	2	982	U
53	2	984	C
53	2	990	C
53	2	991	C
53	2	992	C
53	2	993	G
53	2	994	G
53	2	995	C
53	2	1048	G
53	2	1049	C
53	2	1051	G
53	2	1066	G
53	2	1067	G
53	2	1068	G
53	2	1070	G
53	2	1072	C
53	2	1082	C
53	2	1100	U
53	2	1168	G
53	2	1173	G
53	2	1178	G
53	2	1179	U
53	2	1180	C
53	2	1182	C
53	2	1186	U
53	2	1189	G
53	2	1195	G
53	2	1198	G
53	2	1200	G

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Mol	Chain	Res	Type
53	2	1202	C
53	2	1203	G
53	2	1204	C
53	2	1210	C
53	2	1211	G
53	2	1215	C
53	2	1216	C
53	2	1218	G
53	2	1222	A
53	2	1240	G
53	2	1241	C
53	2	1243	C
53	2	1244	G
53	2	1245	C
53	2	1253	G
53	2	1254	A
53	2	1255	A
53	2	1256	G
53	2	1260	G
53	2	1266	G
53	2	1268	G
53	2	1271	G
53	2	1272	C
53	2	1273	G
53	2	1275	G
53	2	1280	C
53	2	1283	G
53	2	1284	G
53	2	1285	U
53	2	1287	G
53	2	1294	A
53	2	1295	C
53	2	1296	G
53	2	1302	U
53	2	1303	A
53	2	1313	C
53	2	1314	C
53	2	1315	C
53	2	1320	U
53	2	1321	G
53	2	1337	A
53	2	1354	A

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Mol	Chain	Res	Type
53	2	1358	G
53	2	1359	G
53	2	1365	C
53	2	1366	G
53	2	1367	C
53	2	1372	A
53	2	1377	G
53	2	1378	C
53	2	1379	C
53	2	1382	G
53	2	1387	A
53	2	1394	G
53	2	1397	A
53	2	1398	A
53	2	1399	G
53	2	1402	C
53	2	1407	C
53	2	1409	C
53	2	1410	U
53	2	1412	G
53	2	1419	G
53	2	1420	A
53	2	1425	G
53	2	1438	U
53	2	1439	C
53	2	1442	C
53	2	1444	G
53	2	1446	C
53	2	1447	C
53	2	1449	C
53	2	1465	G
53	2	1482	G
53	2	1483	C
53	2	1497	A
53	2	1498	G
53	2	1503	A
53	2	1518	A
53	2	1523	A
53	2	1534	A2M
53	2	1547	A
53	2	1560	A
53	2	1562	G

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Mol	Chain	Res	Type
53	2	1564	A
53	2	1566	C
53	2	1574	B9B
53	2	1578	U
53	2	1592	G
53	2	1595	G
53	2	1596	U
53	2	1597	G
53	2	1613	A
53	2	1624	G
53	2	1625	OMG
53	2	1626	G
53	2	1631	A
53	2	1633	G
53	2	1634	A
53	2	1637	A
53	2	1638	A
53	2	1641	G
53	2	1649	U
53	2	1650	A
53	2	1654	G
53	2	1661	C
53	2	1670	G
53	2	1672	U
53	2	1673	U
53	2	1674	C
53	2	1675	C
53	2	1676	C
53	2	1677	U
53	2	1678	C
53	2	1679	A
53	2	1680	G
53	2	1691	G
53	2	1697	G
53	2	1699	A
53	2	1700	G
53	2	1701	A
53	2	1703	C
53	2	1704	C
53	2	1705	G
53	2	1707	C
53	2	1708	G

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Mol	Chain	Res	Type
53	2	1709	C
53	2	1715	C
53	2	1716	G
53	2	1718	C
53	2	1719	A
53	2	1721	G
53	2	1724	G
53	2	1726	U
53	2	1729	A
53	2	1796	U
53	2	1798	G
53	2	1803	G
53	2	1804	A
53	2	1806	G
53	2	1809	C
53	2	1810	G
53	2	1813	U
53	2	1815	G
53	2	1816	C
53	2	1817	U
53	2	1820	C
53	2	1823	G
53	2	1824	G
53	2	1829	G
53	2	1832	C
53	2	1833	G
53	2	1834	U
53	2	1836	G
53	2	1837	A
53	2	1842	G
53	2	1854	G
53	2	1855	G
53	2	1856	C
53	2	1861	U
53	2	1865	G
53	2	1866	U
53	2	1870	C
53	2	1871	A2M
53	2	1882	U
53	2	1883	OMG
53	2	1891	A
53	2	1897	A

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Mol	Chain	Res	Type
53	2	1900	C
53	2	1918	U
53	2	1919	G
53	2	1920	C
53	2	1921	C
53	2	1922	G
53	2	1925	G
53	2	1931	C
53	2	1932	A
53	2	1935	C
53	2	1939	A
53	2	1940	G
53	2	1942	A
53	2	1943	A
53	2	1944	A
53	2	1948	G
53	2	1952	G
53	2	1956	A
53	2	1959	U
53	2	1966	C
53	2	1972	G
53	2	1974	U
53	2	1975	G
53	2	1980	U
53	2	1981	G
53	2	1984	A
53	2	1985	G
53	2	1990	A
53	2	1997	U
53	2	2001	G
53	2	2002	A
53	2	2003	G
53	2	2004	U
53	2	2007	G
53	2	2008	U
53	2	2011	C
53	2	2017	A
53	2	2018	C
53	2	2025	A
53	2	2026	A
53	2	2033	A
53	2	2034	G

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Mol	Chain	Res	Type
53	2	2040	A
53	2	2044	U
53	2	2046	G
53	2	2048	U
53	2	2055	G
53	2	2056	G
53	2	2069	A
53	2	2084	C
53	2	2085	G
53	2	2090	U
53	2	2091	C
53	2	2092	G
53	2	2093	A
53	2	2094	G
53	2	2095	A
53	2	2096	G
53	2	2097	U
53	2	2098	G
53	2	2101	C
53	2	2102	G
53	2	2104	G
53	2	2105	A
53	2	2106	G
53	2	2110	C
53	2	2111	G
53	2	2112	G
53	2	2250	C
53	2	2251	G
53	2	2253	A
53	2	2254	G
53	2	2255	C
53	2	2256	C
53	2	2258	C
53	2	2259	G
53	2	2260	C
53	2	2269	C
53	2	2289	C
53	2	2300	A
53	2	2301	G
53	2	2306	G
53	2	2313	A
53	2	2314	G

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Mol	Chain	Res	Type
53	2	2316	G
53	2	2333	G
53	2	2346	C
53	2	2348	G
53	2	2351	C
53	2	2360	A
53	2	2395	A
53	2	2410	C
53	2	2416	G
53	2	2417	A
53	2	2422	OMC
53	2	2425	U
53	2	2441	C
53	2	2450	G
53	2	2463	G
53	2	2464	C
53	2	2465	C
53	2	2471	G
53	2	2474	G
53	2	2475	G
53	2	2478	C
53	2	2484	A
53	2	2486	G
53	2	2487	G
53	2	2488	C
53	2	2489	C
53	2	2490	U
53	2	2491	C
53	2	2493	G
53	2	2494	U
53	2	2495	U
53	2	2496	G
53	2	2497	C
53	2	2498	C
53	2	2502	G
53	2	2503	G
53	2	2504	C
53	2	2505	C
53	2	2506	G
53	2	2507	A
53	2	2511	A
53	2	2512	A

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Mol	Chain	Res	Type
53	2	2513	A
53	2	2519	U
53	2	2529	A
53	2	2537	A
53	2	2543	A
53	2	2544	G
53	2	2545	U
53	2	2546	G
53	2	2547	G
53	2	2554	U
53	2	2555	G
53	2	2559	G
53	2	2560	C
53	2	2563	C
53	2	2566	G
53	2	2567	G
53	2	2573	A
53	2	2583	C
53	2	2587	A
53	2	2589	C
53	2	2600	A
53	2	2601	A
53	2	2618	G
53	2	2627	C
53	2	2643	G
53	2	2653	C
53	2	2661	U
53	2	2662	G
53	2	2669	C
53	2	2670	C
53	2	2674	A
53	2	2675	G
53	2	2687	U
53	2	2694	G
53	2	2695	A
53	2	2696	A
53	2	2707	U
53	2	2708	U
53	2	2710	C
53	2	2711	G
53	2	2719	C
53	2	2721	G

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Mol	Chain	Res	Type
53	2	2723	U
53	2	2724	G
53	2	2726	G
53	2	2739	C
53	2	2742	G
53	2	2743	A
53	2	2746	A
53	2	2753	G
53	2	2756	G
53	2	2759	G
53	2	2761	U
53	2	2762	G
53	2	2763	U
53	2	2769	U
53	2	2770	C
53	2	2787	A
53	2	2788	U
53	2	2790	U
53	2	2815	A
53	2	2826	U
53	2	2827	G
53	2	2828	U
53	2	2842	G
53	2	2846	G
53	2	2882	A
53	2	2897	G
53	2	2901	G
53	2	2902	G
53	2	2904	U
53	2	2905	C
53	2	2906	G
53	2	2908	U
53	2	2910	G
53	2	3585	G
53	2	3588	C
53	2	3591	C
53	2	3593	C
53	2	3595	U
53	2	3596	A
53	2	3597	G
53	2	3599	A
53	2	3605	C

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Mol	Chain	Res	Type
53	2	3615	G
53	2	3616	U
53	2	3618	C
53	2	3626	G
53	2	3630	A
53	2	3635	A
53	2	3638	G
53	2	3644	U
53	2	3662	A
53	2	3673	C
53	2	3679	U
53	2	3680	U
53	2	3682	A
53	2	3691	G
53	2	3692	A
53	2	3696	C
53	2	3710	G
53	2	3711	A
53	2	3712	A
53	2	3713	U
53	2	3714	G
53	2	3729	U
53	2	3735	G
53	2	3736	A
53	2	3748	A
53	2	3750	G
53	2	3753	G
53	2	3771	C
53	2	3772	U
53	2	3773	U
53	2	3774	A
53	2	3775	A
53	2	3776	G
53	2	3833	C
53	2	3838	U
53	2	3839	G
53	2	3840	U
53	2	3867	A2M
53	2	3875	G
53	2	3876	A
53	2	3877	A
53	2	3878	C

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Mol	Chain	Res	Type
53	2	3879	G
53	2	3880	P7G
53	2	3897	B8K
53	2	3903	A
53	2	3904	G
53	2	3905	A
53	2	3906	A
53	2	3914	U
53	2	3915	U
53	2	3922	G
53	2	3938	G
53	2	3939	G
53	2	4068	U
53	2	4076	G
53	2	4077	A
53	2	4084	G
53	2	4095	G
53	2	4097	G
53	2	4099	G
53	2	4100	C
53	2	4101	C
53	2	4102	C
53	2	4103	C
53	2	4104	G
53	2	4105	A
53	2	4107	G
53	2	4108	G
53	2	4111	U
53	2	4113	U
53	2	4114	C
53	2	4115	G
53	2	4116	C
53	2	4117	U
53	2	4119	C
53	2	4130	C
53	2	4131	G
53	2	4135	G
53	2	4139	G
53	2	4140	C
53	2	4142	C
53	2	4143	G
53	2	4145	C

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Mol	Chain	Res	Type
53	2	4146	G
53	2	4149	C
53	2	4154	G
53	2	4162	C
53	2	4163	U
53	2	4168	G
53	2	4170	A
53	2	4179	G
53	2	4183	G
53	2	4184	G
53	2	4190	U
53	2	4207	C
53	2	4208	U
53	2	4210	U
53	2	4211	C
53	2	4223	C
53	2	4228	G
53	2	4229	U
53	2	4230	C
53	2	4231	C
53	2	4234	A
53	2	4235	G
53	2	4236	G
53	2	4243	C
53	2	4251	A
53	2	4254	G
53	2	4255	A
53	2	4258	C
53	2	4265	U
53	2	4266	G
53	2	4267	G
53	2	4271	A
53	2	4273	A
53	2	4274	A
53	2	4275	G
53	2	4279	A
53	2	4280	A
53	2	4281	A
53	2	4282	A
53	2	4283	G
53	2	4286	C
53	2	4288	C

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Mol	Chain	Res	Type
53	2	4289	U
53	2	4290	U
53	2	4291	G
53	2	4292	A
53	2	4297	G
53	2	4302	U
53	2	4313	A
53	2	4315	A
53	2	4319	C
53	2	4326	G
53	2	4329	G
53	2	4330	G
53	2	4332	C
53	2	4341	C
53	2	4342	C
53	2	4343	U
53	2	4347	G
53	2	4348	A
53	2	4349	C
53	2	4350	C
53	2	4354	U
53	2	4355	G
53	2	4368	G
53	2	4371	G
53	2	4372	U
53	2	4381	A
53	2	4387	C
53	2	4395	U
53	2	4396	A
53	2	4401	G
53	2	4413	C
53	2	4414	A
53	2	4415	A
53	2	4416	G
53	2	4417	C
53	2	4418	G
53	2	4419	U
53	2	4420	U
53	2	4421	C
53	2	4422	A
53	2	4423	U
53	2	4424	A

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Mol	Chain	Res	Type
53	2	4425	G
53	2	4427	G
53	2	4428	A
53	2	4429	C
53	2	4433	G
53	2	4437	U
53	2	4440	G
53	2	4446	U
53	2	4447	C
53	2	4448	G
53	2	4449	A
53	2	4450	U
53	2	4451	G
53	2	4452	U
53	2	4453	C
53	2	4455	G
53	2	4464	A
53	2	4465	U
53	2	4466	C
53	2	4475	G
53	2	4476	C
53	2	4484	A
53	2	4498	U
53	2	4499	G
53	2	4500	U
53	2	4503	A
53	2	4510	A
53	2	4512	U
53	2	4513	A
53	2	4518	A
53	2	4519	C
53	2	4524	G
53	2	4529	B8W
53	2	4531	U
53	2	4538	G
53	2	4545	G
53	2	4548	A
53	2	4550	7MG
53	2	4555	U
53	2	4556	U
53	2	4557	U
53	2	4558	U

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Mol	Chain	Res	Type
53	2	4560	C
53	2	4584	A
53	2	4589	A
53	2	4590	A
53	2	4600	G
53	2	4601	U
53	2	4606	G
53	2	4607	A
53	2	4608	G
53	2	4627	U
53	2	4635	A
53	2	4636	U
53	2	4637	OMG
53	2	4656	A
53	2	4670	C
53	2	4672	A
53	2	4677	U
53	2	4678	G
53	2	4684	A
53	2	4694	G
53	2	4695	C
53	2	4703	U
53	2	4707	A
53	2	4708	A
53	2	4709	U
53	2	4720	C
53	2	4730	C
53	2	4731	G
53	2	4733	C
53	2	4734	A
53	2	4740	G
53	2	4741	C
53	2	4742	G
53	2	4745	G
53	2	4751	G
53	2	4754	G
53	2	4757	C
53	2	4759	C
53	2	4761	G
53	2	4764	A
53	2	4765	G
53	2	4771	C

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Mol	Chain	Res	Type
53	2	4773	C
53	2	4775	C
53	2	4776	G
53	2	4859	C
53	2	4870	OMG
53	2	4871	C
53	2	4872	2MG
53	2	4874	A
53	2	4875	G
53	2	4877	G
53	2	4882	U
53	2	4883	C
53	2	4887	C
53	2	4889	G
53	2	4895	C
53	2	4900	C
53	2	4901	G
53	2	4910	G
53	2	4912	G
53	2	4914	C
53	2	4915	G
53	2	4916	G
53	2	4927	G
53	2	4928	C
53	2	4934	A
53	2	4940	C
53	2	4941	G
53	2	4943	A
53	2	4949	G
53	2	4975	G
53	2	4976	U
53	2	4988	U
53	2	4989	U
53	2	4991	U
53	2	5014	A
53	2	5017	G
53	2	5022	U
53	2	5024	C
53	2	5026	U
53	2	5027	C
53	2	5028	G
53	2	5030	U

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Mol	Chain	Res	Type
53	2	5031	G
53	2	5034	A
53	2	5041	G
53	2	5047	C
53	2	5050	C
53	2	5054	C
53	2	5055	G
53	2	5061	A
53	2	5069	U

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	3	51	G
51	3	72	U
53	2	914	U
53	2	1633	G
53	2	1678	C
53	2	1808	C
53	2	1931	C
53	2	1980	U
53	2	2017	A
53	2	2033	A
53	2	2760	G
53	2	3596	A
53	2	3752	C
53	2	3774	A
53	2	3905	A
53	2	4235	G
53	2	4415	A
53	2	4555	U
53	2	4636	U
53	2	4707	A
53	2	4913	G

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

68 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$
53	OMU	2	4620	53	19,22,23	2.92	8 (42%)	26,31,34	1.70	5 (19%)
53	B8K	2	3897	53	24,28,29	3.44	11 (45%)	30,42,45	2.55	11 (36%)
53	OMC	2	2861	53	19,22,23	3.04	8 (42%)	26,31,34	1.18	3 (11%)
53	A2M	2	2363	53	22,25,26	3.20	9 (40%)	31,36,39	2.98	11 (35%)
53	BGH	2	3899	53	25,29,30	4.52	17 (68%)	31,43,46	2.59	11 (35%)
53	OMC	2	2804	53	19,22,23	2.96	8 (42%)	26,31,34	0.76	0
53	OMC	2	3887	53	19,22,23	3.04	8 (42%)	26,31,34	1.06	2 (7%)
53	A2M	2	4523	53	22,25,26	3.18	9 (40%)	31,36,39	3.04	11 (35%)
53	5MU	2	4083	53	19,22,23	7.24	8 (42%)	28,32,35	3.38	10 (35%)
53	A2M	2	1524	53	22,25,26	3.18	9 (40%)	31,36,39	3.00	11 (35%)
53	A2M	2	2401	53	22,25,26	3.20	10 (45%)	31,36,39	2.97	11 (35%)
53	I4U	2	1659	53	21,24,25	3.51	9 (42%)	27,34,37	1.15	2 (7%)
53	A2M	2	1871	53	22,25,26	3.20	10 (45%)	31,36,39	3.13	12 (38%)
53	B8W	2	4472	53	23,26,27	2.80	5 (21%)	33,38,41	2.50	14 (42%)
53	OMG	2	2364	53	23,26,27	2.63	8 (34%)	33,38,41	2.76	10 (30%)
53	B8W	2	4185	53	23,26,27	2.73	6 (26%)	33,38,41	2.65	12 (36%)
53	A2M	2	3718	53	22,25,26	3.23	9 (40%)	31,36,39	2.84	10 (32%)
53	7MG	2	2522	53	22,26,27	3.73	10 (45%)	29,39,42	1.99	8 (27%)
53	B8T	2	4483	53	19,22,23	3.61	8 (42%)	26,31,34	1.45	5 (19%)
53	OMC	2	3701	53	19,22,23	3.02	8 (42%)	26,31,34	0.75	0
53	A2M	2	1534	53	22,25,26	3.20	9 (40%)	31,36,39	3.10	12 (38%)
53	B9B	2	1574	53	25,28,29	1.71	6 (24%)	35,40,43	5.16	11 (31%)
53	2MG	2	978	53	23,26,27	3.01	9 (39%)	32,38,41	2.23	9 (28%)
53	OMG	2	1883	53	23,26,27	2.68	8 (34%)	33,38,41	2.68	11 (33%)
53	UR3	2	4597	53	19,22,23	2.75	7 (36%)	26,32,35	1.91	4 (15%)
53	B8T	2	4671	53	19,22,23	3.57	8 (42%)	26,31,34	0.94	1 (3%)
53	B8W	2	4129	53	23,26,27	2.75	6 (26%)	33,38,41	2.75	12 (36%)
53	OMC	2	2365	53	19,22,23	2.90	8 (42%)	26,31,34	0.81	0
53	OMC	2	2422	53	19,22,23	2.99	8 (42%)	26,31,34	1.18	3 (11%)
53	OMC	2	4536	53	19,22,23	3.00	8 (42%)	26,31,34	1.08	2 (7%)
53	B8Q	2	1456	53	17,22,23	2.91	5 (29%)	22,32,35	2.24	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	E7G	2	2297	53	24,27,28	3.89	11 (45%)	30,40,43	2.10	7 (23%)
53	OMG	2	4623	53	23,26,27	2.59	9 (39%)	33,38,41	2.72	13 (39%)
53	B8W	2	2380	53	23,26,27	2.70	5 (21%)	33,38,41	2.50	14 (42%)
53	OMG	2	2424	53	23,26,27	2.65	8 (34%)	33,38,41	2.72	9 (27%)
4	OMU	8	14	4,53	19,22,23	3.04	8 (42%)	26,31,34	1.74	5 (19%)
53	7MG	2	4550	53	22,26,27	3.85	10 (45%)	29,39,42	1.99	9 (31%)
53	OMG	2	373	53	23,26,27	2.66	9 (39%)	33,38,41	2.66	13 (39%)
53	B9B	2	237	53	25,28,29	1.72	6 (24%)	35,40,43	5.19	11 (31%)
53	B9H	2	2786	53	20,25,26	3.27	3 (15%)	22,35,38	2.36	6 (27%)
53	UR3	2	4530	53	19,22,23	2.83	7 (36%)	26,32,35	1.33	3 (11%)
53	A2M	2	4571	53	22,25,26	3.21	9 (40%)	31,36,39	3.00	10 (32%)
53	2MG	2	729	53	23,26,27	2.92	8 (34%)	32,38,41	2.41	9 (28%)
53	OMG	2	1316	53	23,26,27	2.66	8 (34%)	33,38,41	2.75	12 (36%)
53	P4U	2	1348	53	21,24,25	3.48	8 (38%)	27,33,36	1.14	2 (7%)
53	7MG	2	1605	53	22,26,27	3.73	10 (45%)	29,39,42	2.01	10 (34%)
53	OMG	2	4494	53	23,26,27	2.73	8 (34%)	33,38,41	2.86	10 (30%)
53	OMG	2	4637	53	23,26,27	2.67	8 (34%)	33,38,41	2.80	10 (30%)
53	M7A	2	4564	53	20,25,26	1.99	3 (15%)	28,37,40	3.91	7 (25%)
53	B8K	2	4690	53	24,28,29	3.27	11 (45%)	30,42,45	2.57	11 (36%)
53	OMG	2	2773	53	23,26,27	2.70	8 (34%)	33,38,41	2.76	10 (30%)
53	A2M	2	1326	53	22,25,26	3.20	9 (40%)	31,36,39	2.98	10 (32%)
53	OMG	2	1522	53	23,26,27	2.63	8 (34%)	33,38,41	2.74	11 (33%)
53	P7G	2	1909	53	24,28,29	4.05	11 (45%)	27,41,44	1.50	3 (11%)
53	A2M	2	3723	53	22,25,26	3.15	9 (40%)	31,36,39	2.98	10 (32%)
53	OMG	2	1625	53	23,26,27	2.71	8 (34%)	33,38,41	2.76	10 (30%)
53	A2M	2	3825	53	22,25,26	3.18	9 (40%)	31,36,39	3.01	10 (32%)
53	OMC	2	3869	53	19,22,23	2.96	8 (42%)	26,31,34	0.93	1 (3%)
53	P7G	2	3880	53	24,28,29	4.01	11 (45%)	27,41,44	1.45	3 (11%)
53	OMG	2	4870	53	23,26,27	2.70	8 (34%)	33,38,41	2.94	10 (30%)
53	2MG	2	4872	53	23,26,27	2.85	9 (39%)	32,38,41	2.30	10 (31%)
53	B8W	2	4529	53	23,26,27	2.77	5 (21%)	33,38,41	2.57	13 (39%)
53	B9B	2	2754	53	25,28,29	1.75	5 (20%)	35,40,43	5.24	11 (31%)
53	A2M	2	398	53	22,25,26	3.22	9 (40%)	31,36,39	2.97	10 (32%)
53	A2M	2	3867	53	22,25,26	3.16	9 (40%)	31,36,39	3.07	10 (32%)
53	OMG	2	2050	53	23,26,27	2.64	8 (34%)	33,38,41	2.71	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	2MG	2	1517	53	23,26,27	2.95	9 (39%)	32,38,41	2.26	9 (28%)
53	OMC	2	3909	53	19,22,23	3.13	8 (42%)	26,31,34	1.95	7 (26%)

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
53	OMU	2	4620	53	-	0/9/27/28	0/2/2/2
53	B8K	2	3897	53	-	3/11/41/42	0/3/3/3
53	OMC	2	2861	53	-	0/9/27/28	0/2/2/2
53	A2M	2	2363	53	-	0/9/27/28	0/3/3/3
53	BGH	2	3899	53	-	1/13/43/44	0/3/3/3
53	OMC	2	2804	53	-	0/9/27/28	0/2/2/2
53	OMC	2	3887	53	-	1/9/27/28	0/2/2/2
53	A2M	2	4523	53	-	1/9/27/28	0/3/3/3
53	5MU	2	4083	53	-	0/7/25/26	0/2/2/2
53	A2M	2	1524	53	-	1/9/27/28	0/3/3/3
53	A2M	2	2401	53	-	0/9/27/28	0/3/3/3
53	I4U	2	1659	53	-	2/9/29/30	0/2/2/2
53	A2M	2	1871	53	-	2/9/27/28	0/3/3/3
53	B8W	2	4472	53	-	2/9/27/28	0/3/3/3
53	OMG	2	2364	53	-	2/9/27/28	0/3/3/3
53	B8W	2	4185	53	-	0/9/27/28	0/3/3/3
53	A2M	2	3718	53	-	0/9/27/28	0/3/3/3
53	7MG	2	2522	53	-	0/7/37/38	0/3/3/3
53	B8T	2	4483	53	-	0/7/27/28	0/2/2/2
53	OMC	2	3701	53	-	2/9/27/28	0/2/2/2
53	A2M	2	1534	53	-	2/9/27/28	0/3/3/3
53	B9B	2	1574	53	-	4/11/29/30	0/3/3/3
53	2MG	2	978	53	-	0/9/27/28	0/3/3/3
53	OMG	2	1883	53	-	2/9/27/28	0/3/3/3
53	UR3	2	4597	53	-	0/7/25/26	0/2/2/2
53	B8T	2	4671	53	-	0/7/27/28	0/2/2/2
53	B8W	2	4129	53	-	4/9/27/28	0/3/3/3
53	OMC	2	2365	53	-	1/9/27/28	0/2/2/2
53	OMC	2	2422	53	-	1/9/27/28	0/2/2/2
53	OMC	2	4536	53	-	0/9/27/28	0/2/2/2
53	B8Q	2	1456	53	-	0/7/42/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	E7G	2	2297	53	-	1/9/39/40	0/3/3/3
53	OMG	2	4623	53	-	0/9/27/28	0/3/3/3
53	B8W	2	2380	53	-	3/9/27/28	0/3/3/3
53	OMG	2	2424	53	-	2/9/27/28	0/3/3/3
4	OMU	8	14	4,53	-	1/9/27/28	0/2/2/2
53	7MG	2	4550	53	-	2/7/37/38	0/3/3/3
53	OMG	2	373	53	-	1/9/27/28	0/3/3/3
53	B9B	2	237	53	-	4/11/29/30	0/3/3/3
53	B9H	2	2786	53	-	2/12/47/48	0/2/2/2
53	UR3	2	4530	53	-	0/7/25/26	0/2/2/2
53	A2M	2	4571	53	-	0/9/27/28	0/3/3/3
53	2MG	2	729	53	-	2/9/27/28	0/3/3/3
53	OMG	2	1316	53	-	0/9/27/28	0/3/3/3
53	P4U	2	1348	53	-	1/10/29/30	0/2/2/2
53	7MG	2	1605	53	-	0/7/37/38	0/3/3/3
53	OMG	2	4494	53	-	0/9/27/28	0/3/3/3
53	OMG	2	4637	53	-	4/9/27/28	0/3/3/3
53	M7A	2	4564	53	-	0/7/37/38	0/3/3/3
53	B8K	2	4690	53	-	0/11/41/42	0/3/3/3
53	OMG	2	2773	53	-	1/9/27/28	0/3/3/3
53	A2M	2	1326	53	-	0/9/27/28	0/3/3/3
53	OMG	2	1522	53	-	0/9/27/28	0/3/3/3
53	P7G	2	1909	53	-	2/10/40/41	0/3/3/3
53	A2M	2	3723	53	-	1/9/27/28	0/3/3/3
53	OMG	2	1625	53	-	2/9/27/28	0/3/3/3
53	A2M	2	3825	53	-	0/9/27/28	0/3/3/3
53	OMC	2	3869	53	-	2/9/27/28	0/2/2/2
53	P7G	2	3880	53	-	4/10/40/41	0/3/3/3
53	OMG	2	4870	53	-	2/9/27/28	0/3/3/3
53	2MG	2	4872	53	-	2/9/27/28	0/3/3/3
53	B8W	2	4529	53	-	4/9/27/28	0/3/3/3
53	B9B	2	2754	53	-	3/11/29/30	0/3/3/3
53	A2M	2	398	53	-	2/9/27/28	0/3/3/3
53	A2M	2	3867	53	-	3/9/27/28	0/3/3/3
53	OMG	2	2050	53	-	0/9/27/28	0/3/3/3
53	2MG	2	1517	53	-	3/9/27/28	0/3/3/3
53	OMC	2	3909	53	-	3/9/27/28	0/2/2/2

All (560) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	4083	5MU	C4-C5	20.77	1.79	1.44
53	2	4083	5MU	C6-N1	16.04	1.65	1.38
53	2	4083	5MU	C6-C5	-11.52	1.15	1.34
53	2	4083	5MU	C4-N3	-11.04	1.18	1.38
53	2	1659	I4U	C4-N3	10.62	1.45	1.31
53	2	2786	B9H	C2-N3	10.24	1.50	1.37
53	2	1348	P4U	C4-N3	10.13	1.44	1.31
53	2	3880	P7G	C5-N7	9.48	1.46	1.35
53	2	1909	P7G	C8-N9	9.38	1.51	1.46
53	2	2297	E7G	C5-N7	9.26	1.46	1.35
53	2	1909	P7G	C5-N7	9.24	1.45	1.35
53	2	4550	7MG	C8-N9	9.20	1.51	1.46
53	2	4472	B8W	O6-C6	9.10	1.49	1.35
53	2	3897	B8K	C8-N9	9.07	1.51	1.46
53	2	1871	A2M	C3'-C4'	-9.01	1.30	1.53
53	2	3899	BGH	C2'-C1'	-9.00	1.29	1.53
53	2	1326	A2M	C3'-C4'	-8.97	1.30	1.53
53	2	398	A2M	C3'-C4'	-8.96	1.30	1.53
53	2	3899	BGH	O4'-C1'	8.94	1.63	1.42
53	2	4523	A2M	C3'-C4'	-8.92	1.30	1.53
53	2	4571	A2M	C3'-C4'	-8.90	1.30	1.53
53	2	3718	A2M	C3'-C4'	-8.86	1.30	1.53
53	2	2401	A2M	C3'-C4'	-8.85	1.30	1.53
53	2	1524	A2M	C3'-C4'	-8.83	1.30	1.53
53	2	4550	7MG	C5-N7	8.83	1.45	1.35
53	2	2363	A2M	C3'-C4'	-8.81	1.30	1.53
53	2	3825	A2M	C3'-C4'	-8.72	1.30	1.53
53	2	4129	B8W	O6-C6	8.71	1.48	1.35
53	2	1534	A2M	C3'-C4'	-8.71	1.30	1.53
53	2	3723	A2M	C3'-C4'	-8.69	1.30	1.53
53	2	3880	P7G	C8-N9	8.68	1.50	1.46
53	2	3867	A2M	C3'-C4'	-8.66	1.30	1.53
53	2	4529	B8W	O6-C6	8.62	1.48	1.35
53	2	2297	E7G	C8-N9	8.57	1.50	1.46
53	2	1605	7MG	C5-N7	8.56	1.45	1.35
53	2	2522	7MG	C5-N7	8.56	1.45	1.35
53	2	4690	B8K	C8-N9	8.54	1.50	1.46
53	2	4185	B8W	O6-C6	8.53	1.48	1.35
53	2	1605	7MG	C8-N9	8.50	1.50	1.46
53	2	2522	7MG	C8-N9	8.46	1.50	1.46
53	2	2380	B8W	O6-C6	8.43	1.48	1.35
53	2	1456	B8Q	C6-C5	8.30	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	978	2MG	C2-N3	8.03	1.47	1.31
53	2	4529	B8W	C2-N2	8.01	1.49	1.33
53	2	4185	B8W	C2-N2	7.97	1.49	1.33
53	2	4129	B8W	C2-N2	7.96	1.49	1.33
53	2	4472	B8W	C2-N2	7.93	1.49	1.33
53	2	3718	A2M	O4'-C4'	7.77	1.62	1.45
53	2	1517	2MG	C2-N3	7.76	1.46	1.31
53	2	2380	B8W	C2-N2	7.74	1.49	1.33
53	2	4872	2MG	C2-N3	7.72	1.46	1.31
53	2	729	2MG	C2-N3	7.72	1.46	1.31
53	2	3899	BGH	C8-N9	7.67	1.50	1.46
53	2	1871	A2M	O4'-C4'	7.61	1.62	1.45
53	2	3825	A2M	O4'-C4'	7.61	1.62	1.45
53	2	1534	A2M	O4'-C4'	7.58	1.61	1.45
53	2	2401	A2M	O4'-C4'	7.57	1.61	1.45
53	2	398	A2M	O4'-C4'	7.56	1.61	1.45
53	2	3899	BGH	O4'-C4'	-7.56	1.28	1.45
53	2	3723	A2M	O4'-C4'	7.53	1.61	1.45
53	2	4571	A2M	O4'-C4'	7.52	1.61	1.45
53	2	1326	A2M	O4'-C4'	7.50	1.61	1.45
53	2	2363	A2M	O4'-C4'	7.45	1.61	1.45
53	2	4523	A2M	O4'-C4'	7.42	1.61	1.45
53	2	3867	A2M	O4'-C4'	7.40	1.61	1.45
53	2	4483	B8T	C2-N3	7.38	1.51	1.36
53	2	1524	A2M	O4'-C4'	7.33	1.61	1.45
53	2	4671	B8T	C2-N3	7.26	1.51	1.36
4	8	14	OMU	C2-N1	7.24	1.50	1.38
53	2	2786	B9H	C2-N1	7.09	1.48	1.38
53	2	4671	B8T	C4-N3	6.97	1.44	1.32
53	2	4671	B8T	C6-C5	6.91	1.51	1.35
53	2	4483	B8T	C4-N3	6.88	1.44	1.32
53	2	4620	OMU	C2-N1	6.86	1.49	1.38
53	2	978	2MG	C2-N2	6.81	1.48	1.33
53	2	729	2MG	C4-N3	6.77	1.50	1.34
4	8	14	OMU	C2-N3	6.77	1.50	1.38
53	2	2786	B9H	C6-C5	6.73	1.48	1.33
53	2	3909	OMC	C6-C5	6.70	1.50	1.35
53	2	4483	B8T	C6-C5	6.70	1.50	1.35
53	2	3897	B8K	C2-N3	6.68	1.49	1.33
53	2	4597	UR3	C6-C5	6.66	1.50	1.35
53	2	4530	UR3	C6-C5	6.66	1.50	1.35
53	2	1517	2MG	C2-N2	6.63	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	729	2MG	C2-N2	6.61	1.48	1.33
53	2	4690	B8K	C2-N3	6.59	1.49	1.33
53	2	4530	UR3	C2-N1	6.57	1.48	1.38
53	2	978	2MG	C4-N3	6.47	1.49	1.34
53	2	1517	2MG	C4-N3	6.46	1.49	1.34
53	2	3887	OMC	C2-N3	6.45	1.49	1.36
53	2	1456	B8Q	C2-N3	6.44	1.46	1.35
53	2	4620	OMU	C2-N3	6.42	1.49	1.38
53	2	4494	OMG	C2-N3	6.39	1.48	1.33
53	2	3701	OMC	C2-N3	6.39	1.49	1.36
53	2	4494	OMG	C4-N3	6.36	1.49	1.34
53	2	2861	OMC	C2-N3	6.34	1.49	1.36
53	2	4671	B8T	C4-N4	6.33	1.48	1.35
53	2	2422	OMC	C2-N3	6.33	1.49	1.36
53	2	4483	B8T	C4-N4	6.32	1.48	1.35
53	2	2297	E7G	C8-N7	6.31	1.51	1.45
53	2	1625	OMG	C2-N3	6.30	1.48	1.33
53	2	4870	OMG	C2-N3	6.27	1.48	1.33
53	2	3869	OMC	C2-N3	6.27	1.49	1.36
53	2	4536	OMC	C2-N3	6.26	1.49	1.36
53	2	1625	OMG	C4-N3	6.25	1.49	1.34
53	2	2773	OMG	C2-N3	6.25	1.48	1.33
53	2	4872	2MG	C2-N2	6.21	1.47	1.33
53	2	1909	P7G	C4-N9	6.18	1.44	1.35
53	2	4870	OMG	C4-N3	6.18	1.48	1.34
53	2	2804	OMC	C2-N3	6.17	1.48	1.36
53	2	1909	P7G	C4-N3	6.17	1.48	1.37
53	2	3880	P7G	C4-N9	6.15	1.44	1.35
53	2	4597	UR3	C2-N3	6.14	1.50	1.39
53	2	1659	I4U	C2-N3	6.14	1.48	1.36
53	2	3880	P7G	C4-N3	6.13	1.48	1.37
53	2	3899	BGH	C4-N9	6.11	1.44	1.37
53	2	1625	OMG	C2-N2	6.11	1.48	1.34
53	2	1883	OMG	C2-N3	6.10	1.47	1.33
53	2	2773	OMG	C4-N3	6.10	1.48	1.34
53	2	4637	OMG	C2-N3	6.10	1.47	1.33
53	2	4637	OMG	C4-N3	6.07	1.48	1.34
53	2	4872	2MG	C4-N3	6.06	1.48	1.34
53	2	3701	OMC	C6-C5	6.06	1.49	1.35
53	2	2773	OMG	C2-N2	6.05	1.48	1.34
53	2	1316	OMG	C2-N3	6.04	1.47	1.33
53	2	4870	OMG	C2-N2	6.02	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	1316	OMG	C4-N3	6.02	1.48	1.34
53	2	1348	P4U	C2-N3	6.01	1.48	1.36
53	2	2424	OMG	C2-N3	6.01	1.47	1.33
53	2	1348	P4U	C6-C5	6.01	1.49	1.35
53	2	3897	B8K	C4-N9	6.01	1.44	1.37
53	2	1883	OMG	C4-N3	6.00	1.48	1.34
53	2	2365	OMC	C2-N3	6.00	1.48	1.36
53	2	373	OMG	C2-N2	5.99	1.48	1.34
53	2	1883	OMG	C2-N2	5.97	1.48	1.34
53	2	4494	OMG	C2-N2	5.96	1.48	1.34
53	2	2424	OMG	C2-N2	5.96	1.48	1.34
53	2	2861	OMC	C6-C5	5.96	1.48	1.35
53	2	2424	OMG	C4-N3	5.96	1.48	1.34
53	2	2364	OMG	C2-N3	5.94	1.47	1.33
53	2	2050	OMG	C4-N3	5.94	1.48	1.34
53	2	373	OMG	C2-N3	5.94	1.47	1.33
53	2	4536	OMC	C6-C5	5.93	1.48	1.35
53	2	373	OMG	C4-N3	5.92	1.48	1.34
53	2	1659	I4U	C6-C5	5.92	1.48	1.35
53	2	1316	OMG	C2-N2	5.92	1.48	1.34
53	2	2365	OMC	C6-C5	5.89	1.48	1.35
53	2	4637	OMG	C2-N2	5.88	1.48	1.34
53	2	4564	M7A	C4-N9	5.87	1.49	1.38
53	2	2050	OMG	C2-N3	5.87	1.47	1.33
53	2	1522	OMG	C4-N3	5.87	1.48	1.34
53	2	2804	OMC	C6-C5	5.87	1.48	1.35
53	2	1522	OMG	C2-N3	5.86	1.47	1.33
53	2	1909	P7G	C2-N2	5.86	1.48	1.34
53	2	2364	OMG	C4-N3	5.86	1.48	1.34
53	2	2050	OMG	C2-N2	5.85	1.48	1.34
53	2	1522	OMG	C2-N2	5.84	1.48	1.34
53	2	4597	UR3	C2-N1	5.83	1.46	1.38
53	2	3880	P7G	C2-N2	5.83	1.48	1.34
53	2	3880	P7G	C8-N7	5.80	1.51	1.45
53	2	2754	B9B	C2-N2	5.79	1.45	1.33
53	2	3887	OMC	C6-C5	5.79	1.48	1.35
53	2	3869	OMC	C6-C5	5.78	1.48	1.35
53	2	4550	7MG	C2-N3	5.77	1.47	1.33
53	2	2364	OMG	C2-N2	5.74	1.47	1.34
53	2	2422	OMC	C6-C5	5.74	1.48	1.35
53	2	4623	OMG	C2-N2	5.71	1.47	1.34
53	2	3909	OMC	C4-N4	5.71	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	4530	UR3	C2-N3	5.68	1.50	1.39
53	2	4623	OMG	C4-N3	5.67	1.47	1.34
53	2	2522	7MG	C2-N3	5.64	1.46	1.33
53	2	2297	E7G	C4-N9	5.62	1.44	1.37
53	2	1605	7MG	C2-N3	5.62	1.46	1.33
53	2	3899	BGH	C4-N3	5.60	1.47	1.34
53	2	237	B9B	C2-N2	5.60	1.45	1.33
53	2	2297	E7G	C2-N3	5.60	1.46	1.33
53	2	4623	OMG	C2-N3	5.59	1.46	1.33
53	2	3899	BGH	C2-N3	5.59	1.46	1.33
53	2	1574	B9B	C2-N2	5.57	1.45	1.33
4	8	14	OMU	C6-C5	5.55	1.47	1.35
53	2	4550	7MG	C4-N3	5.54	1.47	1.34
53	2	2297	E7G	C4-N3	5.52	1.47	1.34
53	2	2522	7MG	C4-N3	5.52	1.47	1.34
53	2	4620	OMU	C6-C5	5.50	1.47	1.35
53	2	1909	P7G	C8-N7	5.48	1.51	1.45
53	2	1605	7MG	C4-N3	5.46	1.47	1.34
53	2	3909	OMC	C2-N1	5.46	1.51	1.40
53	2	3909	OMC	C2-N3	5.43	1.47	1.36
53	2	2522	7MG	C4-N9	5.34	1.43	1.37
53	2	3880	P7G	C2-N1	5.28	1.45	1.33
53	2	3701	OMC	C4-N3	5.27	1.45	1.34
53	2	1909	P7G	C2-N1	5.21	1.45	1.33
53	2	4550	7MG	C4-N9	5.20	1.43	1.37
53	2	4483	B8T	C2-N1	5.16	1.51	1.40
53	2	1605	7MG	C4-N9	5.16	1.43	1.37
53	2	2422	OMC	C2-N1	5.14	1.51	1.40
53	2	2861	OMC	C2-N1	5.13	1.51	1.40
53	2	3887	OMC	C4-N3	5.10	1.44	1.34
53	2	2861	OMC	C4-N3	5.06	1.44	1.34
53	2	2804	OMC	C4-N3	5.05	1.44	1.34
53	2	2297	E7G	C2-N2	5.04	1.46	1.34
53	2	3887	OMC	C2-N1	5.03	1.50	1.40
53	2	3869	OMC	C4-N3	5.01	1.44	1.34
53	2	4690	B8K	C4-N9	5.00	1.43	1.37
53	2	4536	OMC	C2-N1	4.98	1.50	1.40
53	2	4536	OMC	C4-N3	4.96	1.44	1.34
53	2	2422	OMC	C4-N3	4.95	1.44	1.34
53	2	3899	BGH	C2-N2	4.88	1.45	1.34
53	2	3867	A2M	O4'-C1'	-4.88	1.30	1.42
53	2	3701	OMC	C4-N4	4.87	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	3887	OMC	C4-N4	4.86	1.45	1.33
53	2	2861	OMC	C4-N4	4.86	1.45	1.33
53	2	2365	OMC	C4-N4	4.83	1.45	1.33
53	2	4550	7MG	C2-N2	4.81	1.45	1.34
53	2	2804	OMC	C4-N4	4.80	1.45	1.33
53	2	4536	OMC	C4-N4	4.79	1.45	1.33
53	2	1605	7MG	C2-N2	4.79	1.45	1.34
53	2	2422	OMC	C4-N4	4.77	1.45	1.33
53	2	3869	OMC	C4-N4	4.76	1.45	1.33
53	2	2365	OMC	C4-N3	4.74	1.44	1.34
53	2	2522	7MG	C2-N2	4.74	1.45	1.34
53	2	1326	A2M	O4'-C1'	-4.67	1.30	1.42
53	2	1524	A2M	O4'-C1'	-4.67	1.30	1.42
53	2	1456	B8Q	C2-N1	4.66	1.45	1.38
53	2	1534	A2M	O4'-C1'	-4.64	1.31	1.42
53	2	2363	A2M	O4'-C1'	-4.64	1.31	1.42
53	2	398	A2M	O4'-C1'	-4.60	1.31	1.42
53	2	4523	A2M	O4'-C1'	-4.59	1.31	1.42
53	2	3869	OMC	C2-N1	4.59	1.49	1.40
53	2	3825	A2M	O4'-C1'	-4.57	1.31	1.42
53	2	1534	A2M	C6-N6	4.56	1.45	1.34
53	2	3825	A2M	C6-N6	4.56	1.45	1.34
53	2	2401	A2M	O4'-C1'	-4.56	1.31	1.42
53	2	3718	A2M	C6-N6	4.56	1.45	1.34
53	2	1524	A2M	C6-N6	4.55	1.45	1.34
53	2	3897	B8K	C4-N3	4.55	1.45	1.34
53	2	4571	A2M	O4'-C1'	-4.54	1.31	1.42
53	2	1871	A2M	C6-N6	4.53	1.45	1.34
53	2	4523	A2M	C6-N6	4.52	1.45	1.34
53	2	3718	A2M	O4'-C1'	-4.52	1.31	1.42
53	2	3723	A2M	C6-N6	4.51	1.45	1.34
53	2	2401	A2M	C6-N6	4.50	1.45	1.34
53	2	3909	OMC	C4-N3	4.49	1.43	1.34
53	2	1348	P4U	C2-N1	4.49	1.49	1.40
53	2	4083	5MU	C2-N3	4.49	1.46	1.38
53	2	3723	A2M	O4'-C1'	-4.49	1.31	1.42
53	2	1326	A2M	C6-N6	4.48	1.45	1.34
53	2	3701	OMC	C2-N1	4.48	1.49	1.40
53	2	398	A2M	C6-N6	4.48	1.45	1.34
53	2	4571	A2M	C6-N6	4.47	1.45	1.34
53	2	4671	B8T	C2-N1	4.47	1.49	1.40
53	2	3899	BGH	C5-N7	4.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	3867	A2M	C6-N6	4.44	1.45	1.34
53	2	2804	OMC	C2-N1	4.43	1.49	1.40
53	2	1659	I4U	C5-C4	4.39	1.48	1.43
53	2	4690	B8K	C4-N3	4.38	1.44	1.34
53	2	2363	A2M	C6-N6	4.37	1.45	1.34
53	2	1348	P4U	O4-C4	4.37	1.40	1.35
53	2	4564	M7A	C6-N6	4.29	1.44	1.34
53	2	3897	B8K	C5-N7	4.29	1.47	1.39
53	2	1871	A2M	O4'-C1'	-4.28	1.31	1.42
53	2	3897	B8K	C5-C6	4.25	1.54	1.43
53	2	978	2MG	C2-N1	4.24	1.43	1.36
4	8	14	OMU	C4-N3	4.24	1.46	1.38
53	2	1659	I4U	C2-N1	4.20	1.49	1.40
53	2	1517	2MG	C2-N1	4.20	1.43	1.36
53	2	4690	B8K	C5-N7	4.18	1.46	1.39
53	2	3899	BGH	C5-C6	4.17	1.54	1.43
53	2	2365	OMC	C2-N1	4.15	1.49	1.40
53	2	1348	P4U	C5-C4	4.13	1.48	1.43
53	2	4690	B8K	C5-C6	4.05	1.54	1.43
53	2	2364	OMG	C5-N7	-4.03	1.31	1.39
53	2	4872	2MG	C2-N1	4.03	1.43	1.36
53	2	1625	OMG	C5-N7	-3.99	1.31	1.39
53	2	1316	OMG	C5-N7	-3.99	1.31	1.39
53	2	4494	OMG	C5-N7	-3.97	1.31	1.39
53	2	2050	OMG	C5-N7	-3.92	1.31	1.39
53	2	2424	OMG	C5-N7	-3.91	1.31	1.39
53	2	1883	OMG	C5-N7	-3.85	1.31	1.39
53	2	729	2MG	C2-N1	3.84	1.42	1.36
53	2	4620	OMU	C4-N3	3.83	1.45	1.38
53	2	4550	7MG	C5-C6	3.82	1.53	1.43
53	2	1522	OMG	C5-N7	-3.80	1.31	1.39
53	2	4637	OMG	C5-N7	-3.80	1.31	1.39
53	2	373	OMG	C5-N7	-3.75	1.31	1.39
53	2	1909	P7G	C2-N3	3.73	1.46	1.37
53	2	4870	OMG	C5-N7	-3.70	1.31	1.39
53	2	4671	B8T	C5-C4	3.68	1.48	1.40
53	2	2773	OMG	C5-N7	-3.68	1.31	1.39
53	2	1605	7MG	C2-N1	3.68	1.46	1.37
53	2	2522	7MG	C5-C6	3.65	1.53	1.43
53	2	3897	B8K	C71-N7	3.64	1.47	1.39
53	2	1605	7MG	C5-C6	3.63	1.52	1.43
53	2	2297	E7G	C5-C6	3.63	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	4623	OMG	C5-N7	-3.62	1.32	1.39
53	2	3880	P7G	C2-N3	3.62	1.46	1.37
53	2	3909	OMC	C6-N1	3.61	1.46	1.38
53	2	1909	P7G	C6-N1	3.60	1.44	1.38
53	2	4564	M7A	C5-N7	3.59	1.48	1.39
53	2	3880	P7G	C6-N1	3.57	1.44	1.38
53	2	3899	BGH	C71-N7	3.55	1.47	1.39
53	2	4483	B8T	C6-N1	3.55	1.46	1.38
53	2	4550	7MG	C2-N1	3.54	1.46	1.37
53	2	3899	BGH	O2'-C2'	3.54	1.51	1.42
53	2	4690	B8K	C6-N1	3.54	1.45	1.38
53	2	2522	7MG	C2-N1	3.52	1.46	1.37
53	2	2754	B9B	O6-C6	3.50	1.40	1.35
53	2	4483	B8T	C5-C4	3.50	1.48	1.40
53	2	3897	B8K	C2-N2	3.50	1.42	1.34
53	2	4690	B8K	C2-N2	3.50	1.42	1.34
53	2	4690	B8K	C71-N7	3.49	1.47	1.39
53	2	4083	5MU	C2-N1	3.47	1.44	1.38
53	2	3897	B8K	C6-N1	3.47	1.45	1.38
53	2	4530	UR3	C6-N1	3.39	1.46	1.38
53	2	1605	7MG	C6-N1	3.39	1.45	1.38
53	2	237	B9B	O6-C6	3.36	1.40	1.35
53	2	3887	OMC	C6-N1	3.35	1.46	1.38
53	2	1909	P7G	C5-C4	3.31	1.43	1.37
53	2	2297	E7G	C2-N1	3.31	1.45	1.37
53	2	1883	OMG	O6-C6	-3.30	1.17	1.23
53	2	1574	B9B	O6-C6	3.28	1.40	1.35
53	2	3880	P7G	O6-C6	-3.28	1.18	1.23
53	2	4550	7MG	C6-N1	3.27	1.44	1.38
53	2	2050	OMG	O6-C6	-3.26	1.17	1.23
53	2	1348	P4U	C6-N1	3.26	1.45	1.38
53	2	2522	7MG	C6-N1	3.25	1.44	1.38
53	2	2861	OMC	C6-N1	3.23	1.45	1.38
53	2	3899	BGH	C2-N1	3.22	1.45	1.37
53	2	2422	OMC	C6-N1	3.22	1.45	1.38
53	2	2365	OMC	C6-N1	3.21	1.45	1.38
53	2	3869	OMC	C6-N1	3.21	1.45	1.38
53	2	1659	I4U	C6-N1	3.21	1.45	1.38
53	2	4637	OMG	O6-C6	-3.21	1.17	1.23
53	2	1522	OMG	O6-C6	-3.20	1.17	1.23
53	2	729	2MG	C5-N7	-3.20	1.32	1.39
53	2	2773	OMG	C6-N1	3.20	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	3899	BGH	C6-N1	3.18	1.44	1.38
53	2	1909	P7G	O6-C6	-3.18	1.18	1.23
53	2	373	OMG	C6-N1	3.18	1.44	1.38
53	2	1517	2MG	C5-N7	-3.16	1.32	1.39
53	2	4690	B8K	C2-N1	3.16	1.45	1.37
53	2	3897	B8K	C2-N1	3.16	1.45	1.37
53	2	2364	OMG	O6-C6	-3.15	1.17	1.23
53	2	1316	OMG	O6-C6	-3.15	1.17	1.23
53	2	4623	OMG	O6-C6	-3.14	1.17	1.23
53	2	4623	OMG	C6-N1	3.14	1.44	1.38
53	2	2804	OMC	C6-N1	3.13	1.45	1.38
53	2	3880	P7G	C5-C4	3.12	1.43	1.37
53	2	4671	B8T	C6-N1	3.12	1.45	1.38
53	2	4536	OMC	C6-N1	3.11	1.45	1.38
53	2	4870	OMG	O6-C6	-3.11	1.17	1.23
53	2	4494	OMG	O6-C6	-3.10	1.17	1.23
53	2	2424	OMG	O6-C6	-3.09	1.17	1.23
53	2	4620	OMU	O4-C4	-3.08	1.18	1.24
53	2	373	OMG	O6-C6	-3.07	1.17	1.23
53	2	4529	B8W	C5-N7	-3.06	1.33	1.39
53	2	3701	OMC	C6-N1	3.06	1.45	1.38
53	2	2773	OMG	O6-C6	-3.05	1.17	1.23
53	2	4870	OMG	C6-N1	3.05	1.44	1.38
53	2	2380	B8W	C5-C4	-3.05	1.33	1.39
53	2	2297	E7G	C6-N1	3.05	1.44	1.38
53	2	2424	OMG	C6-N1	3.01	1.44	1.38
53	2	2380	B8W	C5-N7	-3.01	1.33	1.39
53	2	1316	OMG	C6-N1	3.01	1.44	1.38
53	2	4185	B8W	C5-C4	-3.01	1.33	1.39
53	2	1625	OMG	O6-C6	-3.00	1.17	1.23
53	2	1522	OMG	C6-N1	3.00	1.44	1.38
53	2	4597	UR3	C6-N1	3.00	1.45	1.38
53	2	1883	OMG	C6-N1	2.99	1.44	1.38
53	2	4494	OMG	C6-N1	2.99	1.44	1.38
53	2	3899	BGH	O3'-C3'	-2.99	1.35	1.43
53	2	3897	B8K	C5-C4	2.97	1.47	1.38
53	2	1534	A2M	O3'-C3'	2.97	1.50	1.43
53	2	1625	OMG	C6-N1	2.96	1.44	1.38
53	2	4637	OMG	C6-N1	2.95	1.44	1.38
53	2	2050	OMG	C6-N1	2.94	1.44	1.38
53	2	2754	B9B	C5-C4	-2.94	1.33	1.39
53	2	4083	5MU	O4-C4	-2.93	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	978	2MG	C5-N7	-2.92	1.33	1.39
53	2	3825	A2M	O3'-C3'	2.92	1.49	1.43
53	2	2364	OMG	C6-N1	2.92	1.44	1.38
53	2	4129	B8W	C5-N7	-2.92	1.33	1.39
53	2	1524	A2M	O3'-C3'	2.90	1.49	1.43
53	2	3718	A2M	O3'-C3'	2.89	1.49	1.43
53	2	4185	B8W	C5-N7	-2.88	1.33	1.39
53	2	3867	A2M	O3'-C3'	2.88	1.49	1.43
53	2	4571	A2M	C5-C4	-2.88	1.33	1.39
53	2	2363	A2M	O3'-C3'	2.87	1.49	1.43
53	2	4872	2MG	C5-N7	-2.87	1.33	1.39
53	2	237	B9B	C5-C4	-2.87	1.33	1.39
53	2	4472	B8W	C5-C4	-2.87	1.33	1.39
53	2	2363	A2M	C5-C4	-2.86	1.33	1.39
53	2	2401	A2M	O3'-C3'	2.85	1.49	1.43
53	2	1574	B9B	C5-C4	-2.85	1.33	1.39
4	8	14	OMU	O4-C4	-2.84	1.19	1.24
53	2	398	A2M	O3'-C3'	2.84	1.49	1.43
53	2	4083	5MU	O2-C2	-2.84	1.17	1.23
53	2	2365	OMC	O2-C2	-2.84	1.18	1.23
53	2	2363	A2M	O2'-C2'	-2.83	1.35	1.42
53	2	398	A2M	C5-C4	-2.81	1.33	1.39
53	2	1326	A2M	O3'-C3'	2.80	1.49	1.43
4	8	14	OMU	C6-N1	2.80	1.44	1.38
53	2	4671	B8T	O2-C2	-2.79	1.18	1.23
53	2	2804	OMC	O2-C2	-2.79	1.18	1.23
53	2	3867	A2M	C5-C4	-2.79	1.33	1.39
53	2	1659	I4U	O2-C2	-2.78	1.18	1.23
53	2	1659	I4U	O4-C4	2.78	1.40	1.35
53	2	1348	P4U	O2-C2	-2.78	1.18	1.23
53	2	1326	A2M	C5-C4	-2.76	1.33	1.39
53	2	3869	OMC	O2-C2	-2.76	1.18	1.23
53	2	1524	A2M	O2'-C2'	-2.76	1.35	1.42
53	2	3899	BGH	O6-C6	-2.75	1.18	1.23
53	2	1534	A2M	C5-C4	-2.75	1.33	1.39
53	2	1871	A2M	O3'-C3'	2.74	1.49	1.43
53	2	2401	A2M	C5-C4	-2.74	1.33	1.39
53	2	4571	A2M	O3'-C3'	2.74	1.49	1.43
53	2	4571	A2M	O2'-C2'	-2.74	1.35	1.42
53	2	3723	A2M	O3'-C3'	2.73	1.49	1.43
53	2	4483	B8T	O2-C2	-2.73	1.18	1.23
53	2	4129	B8W	C4-N3	2.71	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	3909	OMC	C5-C4	2.70	1.49	1.42
53	2	729	2MG	C5-C6	2.70	1.54	1.44
53	2	3825	A2M	C5-C4	-2.69	1.34	1.39
53	2	978	2MG	C5-C6	2.69	1.54	1.44
53	2	2401	A2M	O2'-C2'	-2.69	1.35	1.42
53	2	1574	B9B	C5-N7	-2.68	1.34	1.39
53	2	4523	A2M	C5-C4	-2.68	1.34	1.39
53	2	1659	I4U	O4-C41	-2.68	1.40	1.47
53	2	4523	A2M	O3'-C3'	2.68	1.49	1.43
53	2	4872	2MG	C5-C6	2.68	1.54	1.44
53	2	4623	OMG	C5-C6	2.68	1.54	1.44
53	2	1534	A2M	O2'-C2'	-2.67	1.35	1.42
53	2	4536	OMC	O2-C2	-2.67	1.18	1.23
53	2	4529	B8W	C5-C4	-2.66	1.34	1.39
53	2	3718	A2M	O2'-C2'	-2.66	1.35	1.42
53	2	3723	A2M	C5-C4	-2.65	1.34	1.39
53	2	2363	A2M	C5-N7	-2.65	1.34	1.39
53	2	4690	B8K	C5-C4	2.65	1.46	1.38
53	2	4472	B8W	C8-N9	-2.65	1.32	1.37
53	2	4529	B8W	C8-N9	-2.65	1.32	1.37
53	2	1534	A2M	C8-N9	-2.64	1.32	1.37
53	2	3718	A2M	C5-C4	-2.64	1.34	1.39
53	2	237	B9B	C5-N7	-2.64	1.34	1.39
53	2	1871	A2M	C5-C4	-2.62	1.34	1.39
53	2	1517	2MG	C5-C6	2.61	1.54	1.44
53	2	1605	7MG	O6-C6	-2.61	1.18	1.23
53	2	3825	A2M	O2'-C2'	-2.60	1.35	1.42
53	2	2754	B9B	C5-N7	-2.60	1.34	1.39
53	2	2363	A2M	C8-N9	-2.60	1.32	1.37
53	2	2773	OMG	C5-C6	2.59	1.54	1.44
53	2	3718	A2M	C8-N9	-2.59	1.32	1.37
53	2	4523	A2M	O2'-C2'	-2.59	1.36	1.42
53	2	2773	OMG	C2-N1	2.59	1.44	1.37
53	2	4870	OMG	C5-C6	2.58	1.54	1.44
53	2	2522	7MG	O6-C6	-2.58	1.18	1.23
53	2	398	A2M	C8-N9	-2.56	1.32	1.37
53	2	3701	OMC	O2-C2	-2.56	1.19	1.23
53	2	4872	2MG	C4-N9	-2.56	1.31	1.38
53	2	4494	OMG	C5-C6	2.56	1.53	1.44
53	2	398	A2M	O2'-C2'	-2.56	1.36	1.42
53	2	4571	A2M	C8-N9	-2.56	1.32	1.37
53	2	3701	OMC	C5-C4	2.55	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	3887	OMC	O2-C2	-2.55	1.19	1.23
53	2	4472	B8W	C5-N7	-2.55	1.34	1.39
53	2	373	OMG	C2-N1	2.55	1.44	1.37
53	2	2422	OMC	O2-C2	-2.55	1.19	1.23
53	2	1524	A2M	C5-C4	-2.54	1.34	1.39
53	2	1871	A2M	O2'-C2'	-2.54	1.36	1.42
53	2	1522	OMG	C5-C6	2.54	1.53	1.44
53	2	4637	OMG	C5-C6	2.54	1.53	1.44
53	2	2861	OMC	O2-C2	-2.54	1.19	1.23
53	2	4620	OMU	C6-N1	2.53	1.44	1.38
53	2	3718	A2M	C5-N7	-2.53	1.34	1.39
53	2	1871	A2M	C8-N9	-2.53	1.33	1.37
53	2	2297	E7G	O6-C6	-2.52	1.18	1.23
53	2	978	2MG	C6-N1	2.52	1.43	1.38
53	2	4530	UR3	C4-N3	2.52	1.46	1.40
53	2	4620	OMU	O2-C2	-2.51	1.18	1.23
53	2	1326	A2M	O2'-C2'	-2.50	1.36	1.42
53	2	4129	B8W	C5-C4	-2.49	1.34	1.39
53	2	2401	A2M	C8-N9	-2.49	1.33	1.37
53	2	3867	A2M	C8-N9	-2.48	1.33	1.37
53	2	4550	7MG	O6-C6	-2.48	1.18	1.23
53	2	3723	A2M	O2'-C2'	-2.48	1.36	1.42
53	2	373	OMG	C5-C6	2.47	1.53	1.44
53	2	2364	OMG	C5-C6	2.47	1.53	1.44
53	2	1517	2MG	C6-N1	2.47	1.43	1.38
53	2	1316	OMG	C5-C6	2.47	1.53	1.44
53	2	2050	OMG	C5-C6	2.47	1.53	1.44
53	2	3723	A2M	C8-N9	-2.46	1.33	1.37
53	2	1625	OMG	C5-C6	2.46	1.53	1.44
53	2	4571	A2M	C5-N7	-2.46	1.34	1.39
53	2	1522	OMG	C2-N1	2.46	1.43	1.37
53	2	4870	OMG	C2-N1	2.45	1.43	1.37
53	2	3825	A2M	C8-N9	-2.42	1.33	1.37
53	2	2804	OMC	C5-C4	2.41	1.48	1.42
53	2	2861	OMC	C5-C4	2.41	1.48	1.42
53	2	398	A2M	C5-N7	-2.41	1.34	1.39
53	2	3867	A2M	O2'-C2'	-2.41	1.36	1.42
53	2	1625	OMG	C2-N1	2.40	1.43	1.37
53	2	1883	OMG	C2-N1	2.40	1.43	1.37
4	8	14	OMU	C5-C4	2.40	1.48	1.43
53	2	4637	OMG	C2-N1	2.40	1.43	1.37
53	2	1326	A2M	C8-N9	-2.39	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	2050	OMG	C2-N1	2.39	1.43	1.37
53	2	2364	OMG	C2-N1	2.39	1.43	1.37
53	2	2380	B8W	C8-N9	-2.38	1.33	1.37
53	2	1316	OMG	C2-N1	2.38	1.43	1.37
53	2	1883	OMG	C5-C6	2.37	1.53	1.44
53	2	4623	OMG	C2-N1	2.37	1.43	1.37
53	2	2424	OMG	C2-N1	2.36	1.43	1.37
53	2	1534	A2M	C5-N7	-2.36	1.34	1.39
53	2	3867	A2M	C5-N7	-2.35	1.34	1.39
53	2	4494	OMG	C2-N1	2.35	1.43	1.37
53	2	4523	A2M	C8-N9	-2.35	1.33	1.37
53	2	2424	OMG	C5-C6	2.35	1.53	1.44
53	2	2401	A2M	C5-N7	-2.35	1.34	1.39
53	2	1524	A2M	C8-N9	-2.32	1.33	1.37
4	8	14	OMU	O2-C2	-2.30	1.18	1.23
53	2	3909	OMC	O2-C2	-2.30	1.19	1.23
53	2	1456	B8Q	C6-N1	2.30	1.43	1.38
53	2	3887	OMC	C5-C4	2.28	1.48	1.42
53	2	1871	A2M	C5-N7	-2.26	1.34	1.39
53	2	1524	A2M	C5-N7	-2.25	1.34	1.39
53	2	4536	OMC	C5-C4	2.24	1.48	1.42
53	2	2365	OMC	C5-C4	2.24	1.48	1.42
53	2	978	2MG	C4-N9	-2.23	1.32	1.38
53	2	1326	A2M	C5-N7	-2.23	1.34	1.39
53	2	4185	B8W	C8-N9	-2.23	1.33	1.37
53	2	4623	OMG	C4-N9	-2.21	1.32	1.38
53	2	237	B9B	C8-N9	-2.21	1.33	1.37
53	2	3825	A2M	C5-N7	-2.20	1.34	1.39
53	2	1517	2MG	O6-C6	-2.20	1.19	1.23
53	2	729	2MG	C6-N1	2.19	1.42	1.38
53	2	4597	UR3	C5-C4	2.19	1.49	1.43
53	2	4872	2MG	C6-N1	2.19	1.42	1.38
53	2	3723	A2M	C5-N7	-2.18	1.34	1.39
53	2	1574	B9B	C8-N9	-2.16	1.33	1.37
53	2	4872	2MG	O6-C6	-2.15	1.19	1.23
53	2	1517	2MG	C4-N9	-2.15	1.32	1.38
53	2	4620	OMU	C5-C4	2.14	1.48	1.43
53	2	4523	A2M	C5-N7	-2.12	1.35	1.39
53	2	1871	A2M	O5'-C5'	-2.12	1.39	1.44
53	2	4530	UR3	C5-C4	2.11	1.49	1.43
53	2	4597	UR3	C4-N3	2.11	1.45	1.40
53	2	4597	UR3	O2-C2	-2.10	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	3869	OMC	C5-C4	2.10	1.47	1.42
53	2	4129	B8W	C8-N9	-2.09	1.33	1.37
53	2	373	OMG	C4-N9	-2.09	1.32	1.38
53	2	1574	B9B	C5-C6	-2.08	1.37	1.41
53	2	2422	OMC	C5-C4	2.07	1.47	1.42
53	2	978	2MG	O6-C6	-2.07	1.19	1.23
53	2	2754	B9B	C8-N9	-2.06	1.33	1.37
53	2	237	B9B	C5-C6	-2.06	1.37	1.41
53	2	3899	BGH	C5-C4	2.05	1.44	1.38
53	2	2401	A2M	C4-N9	-2.04	1.33	1.37
53	2	729	2MG	O6-C6	-2.01	1.19	1.23
53	2	1456	B8Q	O2-C2	-2.01	1.18	1.22
53	2	4185	B8W	C4-N3	2.01	1.36	1.34
53	2	4530	UR3	O2-C2	-2.00	1.18	1.22

All (558) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	2754	B9B	O6-C6-C5	21.49	143.78	116.57
53	2	1574	B9B	O6-C6-C5	21.23	143.45	116.57
53	2	237	B9B	O6-C6-C5	21.10	143.28	116.57
53	2	2754	B9B	O6-C6-N1	-18.48	94.26	120.00
53	2	237	B9B	O6-C6-N1	-18.11	94.78	120.00
53	2	1574	B9B	O6-C6-N1	-18.09	94.80	120.00
53	2	4564	M7A	C5-C6-N6	13.75	147.23	123.74
53	2	4564	M7A	N6-C6-N1	-11.72	92.67	118.35
53	2	4083	5MU	C5-C4-N3	10.06	123.89	115.31
53	2	4870	OMG	C1'-N9-C8	-9.57	99.44	126.70
53	2	4870	OMG	C1'-N9-C4	9.35	154.26	126.50
53	2	4129	B8W	C5-C4-N3	-9.05	117.01	127.19
53	2	4494	OMG	C1'-N9-C4	8.91	152.96	126.50
53	2	1625	OMG	C1'-N9-C4	8.67	152.26	126.50
53	2	2364	OMG	C1'-N9-C4	8.65	152.18	126.50
53	2	1522	OMG	C1'-N9-C4	8.52	151.81	126.50
53	2	2424	OMG	C1'-N9-C4	8.51	151.77	126.50
53	2	2773	OMG	C1'-N9-C4	8.45	151.60	126.50
53	2	2050	OMG	C1'-N9-C4	8.44	151.59	126.50
53	2	4637	OMG	C1'-N9-C4	8.43	151.55	126.50
53	2	1522	OMG	C1'-N9-C8	-8.43	102.70	126.70
53	2	4494	OMG	C1'-N9-C8	-8.41	102.75	126.70
53	2	2773	OMG	C1'-N9-C8	-8.27	103.15	126.70
53	2	2424	OMG	C1'-N9-C8	-8.27	103.17	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	1625	OMG	C1'-N9-C8	-8.21	103.32	126.70
53	2	4637	OMG	C1'-N9-C8	-8.21	103.33	126.70
53	2	2050	OMG	C1'-N9-C8	-8.20	103.37	126.70
53	2	2364	OMG	C1'-N9-C8	-8.18	103.40	126.70
53	2	4623	OMG	C1'-N9-C4	8.18	150.79	126.50
53	2	1316	OMG	C1'-N9-C4	8.15	150.70	126.50
53	2	4623	OMG	C1'-N9-C8	-8.14	103.52	126.70
53	2	1316	OMG	C1'-N9-C8	-8.03	103.84	126.70
53	2	1883	OMG	C1'-N9-C4	8.00	150.26	126.50
53	2	1883	OMG	C1'-N9-C8	-7.96	104.03	126.70
53	2	4083	5MU	C5-C6-N1	-7.88	115.23	123.34
53	2	373	OMG	C1'-N9-C8	-7.76	104.60	126.70
53	2	373	OMG	C1'-N9-C4	7.75	149.52	126.50
53	2	4597	UR3	C4-N3-C2	-7.64	117.37	124.56
53	2	729	2MG	C2-N3-C4	7.50	121.34	112.04
53	2	4185	B8W	C5-C4-N3	-7.37	118.90	127.19
53	2	4529	B8W	C5-C4-N3	-7.23	119.06	127.19
53	2	1534	A2M	N6-C6-N1	-7.04	102.93	118.35
53	2	4083	5MU	C4-N3-C2	-7.02	118.26	127.35
53	2	1326	A2M	N6-C6-N1	-7.02	102.98	118.35
53	2	3825	A2M	N6-C6-N1	-6.96	103.10	118.35
53	2	4523	A2M	N6-C6-N1	-6.96	103.10	118.35
53	2	398	A2M	N6-C6-N1	-6.95	103.13	118.35
53	2	237	B9B	C5-C4-N3	-6.90	119.42	127.19
53	2	1517	2MG	C2-N3-C4	6.89	120.58	112.04
53	2	1871	A2M	N6-C6-N1	-6.83	103.39	118.35
53	2	2786	B9H	C31-N3-C2	6.81	125.72	117.21
53	2	978	2MG	C2-N3-C4	6.81	120.48	112.04
53	2	3867	A2M	N6-C6-N1	-6.75	103.56	118.35
53	2	3723	A2M	N6-C6-N1	-6.74	103.58	118.35
53	2	4571	A2M	N6-C6-N1	-6.69	103.70	118.35
53	2	2363	A2M	N6-C6-N1	-6.68	103.73	118.35
53	2	1524	A2M	N6-C6-N1	-6.63	103.84	118.35
53	2	2401	A2M	N6-C6-N1	-6.61	103.88	118.35
53	2	729	2MG	C5-C4-N3	-6.53	117.86	128.46
53	2	2754	B9B	C5-C4-N3	-6.50	119.88	127.19
53	2	1574	B9B	C5-C4-N3	-6.50	119.88	127.19
53	2	3718	A2M	N6-C6-N1	-6.48	104.15	118.35
53	2	4571	A2M	N3-C2-N1	-6.43	118.54	128.60
53	2	4472	B8W	C5-C4-N3	-6.43	119.96	127.19
53	2	2380	B8W	C5-C4-N3	-6.37	120.02	127.19
53	2	3897	B8K	C72-C71-N7	6.37	128.44	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	4690	B8K	C72-C71-N7	6.35	128.41	118.86
53	2	4185	B8W	N2-C2-N3	6.31	127.07	117.25
53	2	2380	B8W	N2-C2-N3	6.29	127.04	117.25
53	2	1871	A2M	N3-C2-N1	-6.29	118.76	128.60
53	2	3867	A2M	N3-C2-N1	-6.28	118.77	128.60
53	2	3825	A2M	N3-C2-N1	-6.28	118.78	128.60
53	2	398	A2M	N3-C2-N1	-6.27	118.80	128.60
53	2	4129	B8W	N2-C2-N3	6.25	126.98	117.25
53	2	4529	B8W	N2-C2-N3	6.24	126.96	117.25
53	2	2363	A2M	N3-C2-N1	-6.23	118.85	128.60
53	2	1326	A2M	N3-C2-N1	-6.23	118.86	128.60
53	2	2401	A2M	N3-C2-N1	-6.22	118.86	128.60
53	2	4872	2MG	C2-N3-C4	6.20	119.72	112.04
53	2	1524	A2M	N3-C2-N1	-6.20	118.91	128.60
53	2	4523	A2M	N3-C2-N1	-6.20	118.91	128.60
53	2	4523	A2M	N9-C8-N7	-6.20	105.44	113.91
53	2	3899	BGH	C72-C71-N7	6.18	128.16	118.86
53	2	1534	A2M	N3-C2-N1	-6.18	118.94	128.60
53	2	3723	A2M	N3-C2-N1	-6.12	119.02	128.60
53	2	2401	A2M	N9-C8-N7	-6.11	105.55	113.91
53	2	4564	M7A	N3-C2-N1	-6.06	119.11	128.60
53	2	3867	A2M	N9-C8-N7	-6.06	105.63	113.91
53	2	4690	B8K	C5-C6-N1	6.05	121.65	110.99
53	2	4129	B8W	N3-C4-N9	6.04	135.37	126.99
53	2	1871	A2M	N9-C8-N7	-6.03	105.66	113.91
53	2	4571	A2M	N9-C8-N7	-6.03	105.67	113.91
53	2	1326	A2M	C5-C6-N6	6.02	136.52	123.43
53	2	4472	B8W	N2-C2-N3	6.01	126.60	117.25
53	2	3718	A2M	N3-C2-N1	-6.00	119.22	128.60
53	2	398	A2M	C5-C6-N6	6.00	136.48	123.43
53	2	3723	A2M	N9-C8-N7	-5.98	105.73	113.91
53	2	1534	A2M	C5-C6-N6	5.97	136.41	123.43
53	2	398	A2M	N9-C8-N7	-5.97	105.75	113.91
53	2	1326	A2M	N9-C8-N7	-5.95	105.77	113.91
53	2	3825	A2M	C5-C6-N6	5.94	136.36	123.43
53	2	4523	A2M	C5-C6-N6	5.94	136.35	123.43
53	2	1871	A2M	C5-C6-N6	5.92	136.31	123.43
53	2	3825	A2M	N9-C8-N7	-5.87	105.88	113.91
53	2	1534	A2M	N9-C8-N7	-5.86	105.90	113.91
53	2	4494	OMG	C5-C4-N3	-5.82	119.02	128.46
53	2	2401	A2M	C5-C6-N6	5.79	136.04	123.43
53	2	3723	A2M	C5-C6-N6	5.77	135.98	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	3899	BGH	C5-C6-N1	5.77	121.16	110.99
53	2	3718	A2M	C5-C6-N6	5.75	135.94	123.43
53	2	3867	A2M	C5-C6-N6	5.75	135.94	123.43
53	2	4571	A2M	C5-C6-N6	5.74	135.93	123.43
53	2	1524	A2M	C5-C6-N6	5.70	135.84	123.43
53	2	2363	A2M	N9-C8-N7	-5.69	106.13	113.91
53	2	1524	A2M	N9-C8-N7	-5.66	106.17	113.91
53	2	3897	B8K	C5-C6-N1	5.65	120.96	110.99
53	2	2363	A2M	C5-C6-N6	5.65	135.72	123.43
53	2	3909	OMC	O2-C2-N3	-5.63	113.18	122.33
53	2	1517	2MG	C5-C4-N3	-5.61	119.36	128.46
53	2	1625	OMG	C5-C4-N3	-5.57	119.42	128.46
53	2	1456	B8Q	N3-C2-N1	5.51	123.60	117.13
53	2	2401	A2M	C4-N9-C8	5.47	111.66	105.73
53	2	3718	A2M	N9-C8-N7	-5.41	106.51	113.91
53	2	4523	A2M	C4-N9-C8	5.41	111.59	105.73
53	2	3867	A2M	C4-N9-C8	5.38	111.55	105.73
53	2	4637	OMG	C5-C4-N3	-5.36	119.76	128.46
53	2	978	2MG	C5-C4-N3	-5.35	119.78	128.46
53	2	2786	B9H	C6-N1-C2	-5.33	117.01	121.79
53	2	4872	2MG	C5-C4-N3	-5.30	119.86	128.46
53	2	1871	A2M	C4-N9-C8	5.30	111.47	105.73
53	2	4872	2MG	C2-N1-C6	-5.29	118.39	124.48
53	2	2364	OMG	C5-C4-N3	-5.25	119.94	128.46
53	2	3723	A2M	C4-N9-C8	5.25	111.42	105.73
53	2	4571	A2M	C4-N9-C8	5.22	111.39	105.73
53	2	1316	OMG	C5-C4-N3	-5.21	120.01	128.46
53	2	1534	A2M	C4-N9-C8	5.19	111.36	105.73
53	2	3899	BGH	C2-N3-C4	5.19	121.55	112.30
53	2	398	A2M	C4-N9-C8	5.17	111.33	105.73
4	8	14	OMU	C4-N3-C2	-5.11	119.84	126.58
53	2	4620	OMU	C4-N3-C2	-5.09	119.86	126.58
53	2	2773	OMG	C5-C4-N3	-5.09	120.21	128.46
53	2	1524	A2M	C4-N9-C8	5.06	111.22	105.73
53	2	4870	OMG	C5-C4-N3	-5.06	120.25	128.46
53	2	1326	A2M	C4-N9-C8	5.05	111.20	105.73
53	2	1909	P7G	C4-C5-N7	5.04	109.33	106.67
53	2	3825	A2M	C4-N9-C8	5.03	111.18	105.73
53	2	3880	P7G	C4-C5-N7	5.02	109.32	106.67
53	2	2522	7MG	C5-C6-N1	5.01	119.82	110.99
53	2	4083	5MU	N3-C2-N1	5.00	121.53	114.89
53	2	2754	B9B	N2-C2-N3	5.00	125.03	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	2297	E7G	C5-C6-N1	5.00	119.80	110.99
53	2	1456	B8Q	C31-N3-C4	5.00	121.78	114.25
53	2	4564	M7A	N3-C4-N9	4.98	133.16	126.87
53	2	4550	7MG	C5-C6-N1	4.97	119.75	110.99
53	2	1605	7MG	C5-C6-N1	4.97	119.74	110.99
53	2	4529	B8W	O6-C6-N1	4.95	125.85	119.01
53	2	2424	OMG	C5-C4-N3	-4.94	120.45	128.46
53	2	237	B9B	N2-C2-N3	4.92	124.91	117.25
53	2	2050	OMG	C5-C4-N3	-4.91	120.49	128.46
53	2	4083	5MU	C5M-C5-C6	-4.90	116.31	122.85
53	2	1883	OMG	C5-C4-N3	-4.89	120.53	128.46
53	2	2297	E7G	C4-C5-N7	4.89	109.26	104.91
53	2	2363	A2M	C4-N9-C8	4.87	111.01	105.73
53	2	1456	B8Q	O2-C2-N3	-4.83	115.86	122.95
53	2	4185	B8W	N3-C4-N9	4.83	133.69	126.99
53	2	3897	B8K	C2-N3-C4	4.82	120.88	112.30
53	2	729	2MG	C2-N1-C6	-4.80	118.96	124.48
53	2	1574	B9B	N2-C2-N3	4.79	124.70	117.25
53	2	4690	B8K	C2-N3-C4	4.78	120.81	112.30
53	2	3718	A2M	C4-N9-C8	4.75	110.88	105.73
53	2	2363	A2M	C5-C4-N3	-4.75	120.55	126.75
53	2	1517	2MG	C2-N1-C6	-4.74	119.02	124.48
53	2	4472	B8W	N9-C8-N7	-4.74	107.43	113.91
53	2	3825	A2M	C5-C4-N3	-4.70	120.62	126.75
53	2	4494	OMG	C2-N3-C4	4.69	120.66	112.30
53	2	4530	UR3	C4-N3-C2	-4.67	120.17	124.56
53	2	1522	OMG	C5-C4-N3	-4.66	120.90	128.46
53	2	4529	B8W	N3-C4-N9	4.65	133.44	126.99
53	2	3867	A2M	C5-C4-N3	-4.63	120.70	126.75
53	2	1534	A2M	C5-C4-N3	-4.61	120.73	126.75
53	2	1871	A2M	C5-C4-N3	-4.61	120.74	126.75
53	2	3723	A2M	C5-C4-N3	-4.58	120.77	126.75
53	2	2363	A2M	C1'-N9-C8	-4.57	116.82	127.14
53	2	237	B9B	N3-C4-N9	4.55	133.30	126.99
53	2	4637	OMG	C2-N3-C4	4.53	120.37	112.30
53	2	2773	OMG	C2-N3-C4	4.51	120.34	112.30
53	2	373	OMG	C5-C4-N3	-4.51	121.14	128.46
53	2	3867	A2M	C1'-N9-C8	-4.48	117.03	127.14
53	2	1316	OMG	C2-N3-C4	4.47	120.27	112.30
53	2	1524	A2M	C5-C4-N3	-4.46	120.93	126.75
53	2	978	2MG	C2-N1-C6	-4.46	119.34	124.48
53	2	1625	OMG	C2-N3-C4	4.46	120.24	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	729	2MG	N9-C4-N3	4.45	134.87	125.94
53	2	4550	7MG	C2-N3-C4	4.44	120.22	112.30
53	2	1326	A2M	C5-C4-N3	-4.44	120.95	126.75
53	2	1605	7MG	C2-N3-C4	4.43	120.20	112.30
53	2	2424	OMG	C2-N3-C4	4.42	120.17	112.30
53	2	4870	OMG	C2-N3-C4	4.41	120.15	112.30
53	2	2297	E7G	C2-N3-C4	4.40	120.15	112.30
53	2	4571	A2M	C5-C4-N3	-4.39	121.03	126.75
53	2	4623	OMG	C5-C4-N3	-4.36	121.38	128.46
53	2	4523	A2M	C5-C4-N3	-4.35	121.08	126.75
53	2	2364	OMG	C2-N3-C4	4.35	120.04	112.30
53	2	4185	B8W	O6-C6-N1	4.34	124.99	119.01
53	2	1883	OMG	C2-N3-C4	4.34	120.03	112.30
53	2	4690	B8K	C4-C5-N7	4.33	108.76	104.91
53	2	2522	7MG	C2-N3-C4	4.33	120.01	112.30
53	2	2786	B9H	C21-O2'-C2'	4.31	125.83	114.52
53	2	4872	2MG	CM2-N2-C2	-4.30	114.36	123.86
53	2	1534	A2M	C1'-N9-C8	-4.30	117.43	127.14
53	2	2754	B9B	N9-C8-N7	-4.28	108.05	113.91
53	2	1522	OMG	C2-N3-C4	4.28	119.92	112.30
53	2	398	A2M	C5-C4-N3	-4.27	121.18	126.75
53	2	3718	A2M	C5-C4-N3	-4.27	121.18	126.75
53	2	3897	B8K	C4-C5-N7	4.26	108.70	104.91
53	2	4623	OMG	C2-N3-C4	4.25	119.88	112.30
53	2	1524	A2M	C1'-N9-C8	-4.25	117.55	127.14
53	2	3909	OMC	O2-C2-N1	4.24	127.64	118.89
53	2	2363	A2M	N3-C4-N9	4.23	134.05	127.08
53	2	2050	OMG	C2-N3-C4	4.22	119.82	112.30
53	2	237	B9B	N9-C8-N7	-4.22	108.15	113.91
53	2	2380	B8W	N9-C8-N7	-4.19	108.18	113.91
53	2	373	OMG	C2-N3-C4	4.19	119.76	112.30
53	2	1871	A2M	C1'-N9-C8	-4.18	117.69	127.14
53	2	3825	A2M	C1'-N9-C8	-4.18	117.70	127.14
53	2	4185	B8W	N9-C8-N7	-4.16	108.22	113.91
53	2	2401	A2M	C5-C4-N3	-4.16	121.33	126.75
53	2	3867	A2M	N3-C4-N9	4.15	133.92	127.08
53	2	1574	B9B	N9-C8-N7	-4.14	108.26	113.91
53	2	4571	A2M	C1'-N9-C8	-4.13	117.82	127.14
53	2	3899	BGH	C5-C4-N9	4.10	111.67	106.35
53	2	3723	A2M	C1'-N9-C8	-4.09	117.91	127.14
53	2	1659	I4U	C5-C4-N3	-4.08	118.71	124.91
53	2	1534	A2M	N3-C4-N9	4.04	133.74	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	1574	B9B	N3-C4-N9	4.03	132.59	126.99
53	2	1871	A2M	N3-C4-N9	4.03	133.73	127.08
53	2	3718	A2M	C1'-N9-C8	-3.99	118.14	127.14
53	2	3899	BGH	C4-C5-N7	3.98	108.45	104.91
53	2	3899	BGH	N9-C8-N7	3.96	108.65	103.33
53	2	2754	B9B	N3-C4-N9	3.95	132.47	126.99
53	2	3825	A2M	N3-C4-N9	3.95	133.58	127.08
53	2	1326	A2M	C1'-N9-C8	-3.94	118.23	127.14
53	2	3723	A2M	N3-C4-N9	3.94	133.58	127.08
53	2	1524	A2M	N3-C4-N9	3.94	133.57	127.08
53	2	4083	5MU	O4-C4-C5	-3.93	120.35	124.90
53	2	2401	A2M	C1'-N9-C8	-3.90	118.34	127.14
53	2	3897	B8K	N9-C8-N7	3.88	108.54	103.33
53	2	4690	B8K	C5-C4-N9	3.87	111.36	106.35
53	2	3897	B8K	C5-C4-N9	3.86	111.36	106.35
53	2	4571	A2M	N3-C4-N9	3.86	133.44	127.08
53	2	4523	A2M	C1'-N9-C8	-3.84	118.46	127.14
53	2	4472	B8W	N3-C4-N9	3.81	132.28	126.99
53	2	2297	E7G	C5-C4-N3	-3.79	120.91	128.13
53	2	4083	5MU	C5M-C5-C4	3.78	122.93	118.77
53	2	1456	B8Q	C6-N1-C2	-3.75	118.43	121.79
53	2	3825	A2M	C2-N3-C4	3.75	120.60	111.75
53	2	4472	B8W	C5-N7-C8	3.73	108.81	103.51
53	2	3718	A2M	N3-C4-N9	3.73	133.22	127.08
53	2	4523	A2M	N3-C4-N9	3.72	133.22	127.08
53	2	1871	A2M	C5-N7-C8	3.72	108.79	103.51
53	2	4523	A2M	C5-N7-C8	3.72	108.79	103.51
53	2	2401	A2M	N3-C4-N9	3.71	133.19	127.08
53	2	4620	OMU	N3-C2-N1	3.71	119.81	114.89
53	2	4472	B8W	N1-C2-N3	-3.70	119.61	125.42
53	2	1534	A2M	C2-N3-C4	3.69	120.47	111.75
53	2	398	A2M	C1'-N9-C8	-3.69	118.81	127.14
53	2	2363	A2M	C2-N3-C4	3.69	120.46	111.75
53	2	3899	BGH	C5-C4-N3	-3.68	121.12	128.13
53	2	4571	A2M	C2-N3-C4	3.67	120.42	111.75
53	2	1871	A2M	C2-N3-C4	3.67	120.42	111.75
53	2	1326	A2M	N3-C4-N9	3.66	133.11	127.08
53	2	1326	A2M	C2-N3-C4	3.66	120.39	111.75
53	2	398	A2M	N3-C4-N9	3.66	133.10	127.08
53	2	3867	A2M	C2-N3-C4	3.64	120.36	111.75
53	2	4550	7MG	C5-C4-N3	-3.62	121.24	128.13
53	2	1605	7MG	C5-C4-N9	3.62	111.04	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	2522	7MG	C5-C4-N3	-3.61	121.25	128.13
53	2	2380	B8W	N3-C4-N9	3.61	131.99	126.99
53	2	4571	A2M	C5-N7-C8	3.61	108.63	103.51
53	2	3723	A2M	C5-N7-C8	3.60	108.63	103.51
53	2	3723	A2M	C2-N3-C4	3.60	120.26	111.75
53	2	1524	A2M	C2-N3-C4	3.59	120.24	111.75
53	2	2754	B9B	N3-C2-N1	-3.59	119.79	125.42
53	2	2401	A2M	C5-N7-C8	3.59	108.61	103.51
53	2	4523	A2M	C2-N3-C4	3.59	120.23	111.75
53	2	4129	B8W	N1-C2-N3	-3.59	119.79	125.42
53	2	1326	A2M	C5-N7-C8	3.58	108.59	103.51
53	2	398	A2M	C2-N3-C4	3.57	120.19	111.75
53	2	4550	7MG	C5-C4-N9	3.57	110.98	106.35
53	2	3825	A2M	C5-N7-C8	3.57	108.58	103.51
53	2	3867	A2M	C5-N7-C8	3.56	108.57	103.51
53	2	398	A2M	C5-N7-C8	3.56	108.57	103.51
53	2	4564	M7A	C2-N3-C4	3.55	120.14	111.75
4	8	14	OMU	N3-C2-N1	3.53	119.58	114.89
53	2	1605	7MG	C5-C4-N3	-3.53	121.41	128.13
53	2	2297	E7G	C5-C4-N9	3.51	110.90	106.35
53	2	2522	7MG	C5-C4-N9	3.50	110.89	106.35
53	2	1534	A2M	C5-N7-C8	3.50	108.48	103.51
53	2	1517	2MG	N9-C4-N3	3.49	132.95	125.94
53	2	2401	A2M	C2-N3-C4	3.47	119.95	111.75
53	2	2380	B8W	O6-C6-N1	3.46	123.79	119.01
53	2	2363	A2M	C5-N7-C8	3.46	108.43	103.51
53	2	1348	P4U	C5-C4-N3	-3.46	119.65	124.91
53	2	4185	B8W	N1-C2-N3	-3.45	120.01	125.42
4	8	14	OMU	C5-C4-N3	3.40	119.93	114.84
53	2	4620	OMU	C5-C4-N3	3.40	119.92	114.84
53	2	2380	B8W	C61-O6-C6	-3.39	113.85	117.21
53	2	4690	B8K	C6-C5-C4	-3.39	115.63	122.62
53	2	3897	B8K	C5-C4-N3	-3.37	121.71	128.13
53	2	4690	B8K	N9-C8-N7	3.37	107.85	103.33
53	2	3718	A2M	C2-N3-C4	3.37	119.71	111.75
53	2	2364	OMG	C2-N1-C6	-3.34	119.00	125.10
53	2	4529	B8W	N9-C8-N7	-3.34	109.35	113.91
53	2	2380	B8W	N1-C2-N3	-3.33	120.19	125.42
53	2	1574	B9B	N3-C2-N1	-3.32	120.21	125.42
53	2	237	B9B	N3-C2-N1	-3.32	120.22	125.42
53	2	2422	OMC	O2-C2-N3	-3.31	116.94	122.33
53	2	4637	OMG	C2-N1-C6	-3.31	119.07	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	1909	P7G	N9-C8-N7	3.30	108.10	103.38
53	2	4494	OMG	C2-N1-C6	-3.27	119.14	125.10
53	2	4083	5MU	C6-C5-C4	3.27	120.76	118.03
53	2	1524	A2M	C5-N7-C8	3.24	108.11	103.51
53	2	2861	OMC	O2-C2-N3	-3.23	117.07	122.33
53	2	4483	B8T	O2-C2-N3	-3.23	117.08	122.33
53	2	978	2MG	N9-C4-N3	3.21	132.39	125.94
53	2	1316	OMG	C2-N1-C6	-3.21	119.25	125.10
53	2	4529	B8W	N1-C2-N3	-3.21	120.39	125.42
53	2	4129	B8W	N9-C8-N7	-3.20	109.54	113.91
53	2	3718	A2M	C5-N7-C8	3.17	108.01	103.51
53	2	2050	OMG	C2-N1-C6	-3.16	119.34	125.10
53	2	3909	OMC	C5-C4-N4	3.16	125.54	120.57
53	2	1883	OMG	C2-N1-C6	-3.11	119.43	125.10
53	2	3909	OMC	C4-N3-C2	3.10	125.27	120.25
53	2	4870	OMG	C2-N1-C6	-3.08	119.48	125.10
53	2	2773	OMG	C2-N1-C6	-3.07	119.50	125.10
53	2	1625	OMG	C2-N1-C6	-3.06	119.51	125.10
53	2	4129	B8W	C2-N3-C4	3.06	122.35	113.89
53	2	3897	B8K	C6-C5-C4	-3.05	116.34	122.62
53	2	2424	OMG	C2-N1-C6	-3.04	119.56	125.10
53	2	4185	B8W	C5-N7-C8	3.03	107.82	103.51
53	2	4623	OMG	C2-N1-C6	-3.03	119.57	125.10
53	2	4129	B8W	O6-C6-N1	3.02	123.18	119.01
53	2	4129	B8W	C5-N7-C8	3.01	107.79	103.51
53	2	4185	B8W	C61-O6-C6	-3.01	114.23	117.21
53	2	4536	OMC	O2-C2-N3	-3.01	117.44	122.33
53	2	373	OMG	C2-N1-C6	-3.00	119.63	125.10
53	2	2754	B9B	C5-N7-C8	2.99	107.75	103.51
53	2	1605	7MG	N9-C8-N7	2.98	107.65	103.38
53	2	4129	B8W	C61-O6-C6	-2.98	114.26	117.21
53	2	4690	B8K	C5-C4-N3	-2.98	122.46	128.13
53	2	3887	OMC	O2-C2-N3	-2.97	117.50	122.33
53	2	2380	B8W	C5-N7-C8	2.97	107.72	103.51
53	2	1522	OMG	C2-N1-C6	-2.96	119.69	125.10
53	2	4529	B8W	N2-C2-N1	-2.96	112.65	117.25
53	2	4623	OMG	C5-C4-N9	2.96	111.00	105.63
53	2	2786	B9H	O2'-C2'-C1'	2.95	114.83	109.08
53	2	4564	M7A	C4-N9-C1'	-2.94	119.61	126.60
53	2	4483	B8T	O3'-C3'-C2'	2.94	121.32	111.82
53	2	3899	BGH	C6-C5-C4	-2.92	116.60	122.62
53	2	237	B9B	C5-N7-C8	2.92	107.66	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	8	14	OMU	O4-C4-C5	-2.92	120.03	125.16
53	2	4872	2MG	N9-C4-N3	2.91	131.79	125.94
53	2	4620	OMU	O4-C4-C5	-2.91	120.04	125.16
53	2	2522	7MG	N9-C8-N7	2.89	107.51	103.38
53	2	2380	B8W	N2-C2-N1	-2.88	112.77	117.25
53	2	3899	BGH	O6-C6-N1	-2.88	114.60	120.12
53	2	729	2MG	C5-C6-N1	2.84	120.40	113.19
53	2	2861	OMC	C1'-N1-C2	2.84	124.75	118.42
53	2	4872	2MG	C5-C6-N1	2.83	120.39	113.19
53	2	1574	B9B	C5-N7-C8	2.83	107.52	103.51
53	2	3909	OMC	C5-C4-N3	-2.82	116.53	121.33
53	2	4872	2MG	N9-C8-N7	-2.82	108.08	113.39
53	2	4472	B8W	C2-N1-C6	2.82	120.41	115.93
53	2	1517	2MG	C5-C6-N1	2.82	120.34	113.19
53	2	978	2MG	C5-C6-N1	2.81	120.33	113.19
53	2	2522	7MG	C4-C5-N7	2.80	109.42	105.53
53	2	4494	OMG	C5-C6-N1	2.80	120.30	113.19
53	2	4637	OMG	C5-C6-N1	2.79	120.28	113.19
53	2	4185	B8W	N2-C2-N1	-2.79	112.92	117.25
53	2	978	2MG	N9-C8-N7	-2.78	108.15	113.39
53	2	237	B9B	C61-O6-C6	-2.78	112.17	117.47
53	2	4597	UR3	C3U-N3-C2	2.78	122.18	117.31
53	2	1574	B9B	C61-O6-C6	-2.77	112.19	117.47
53	2	1883	OMG	C5-C6-N1	2.77	120.21	113.19
53	2	4637	OMG	O4'-C1'-N9	2.75	114.65	108.36
53	2	2424	OMG	C5-C6-N1	2.75	120.16	113.19
53	2	4870	OMG	C5-C6-N1	2.74	120.16	113.19
53	2	1605	7MG	C4-C5-N7	2.74	109.34	105.53
53	2	4623	OMG	N2-C2-N1	2.73	122.53	116.71
53	2	2364	OMG	C5-C4-N9	2.73	110.58	105.63
53	2	3897	B8K	O6-C6-N1	-2.73	114.89	120.12
53	2	1883	OMG	O6-C6-C5	-2.72	119.38	126.60
53	2	1316	OMG	C5-C6-N1	2.71	120.08	113.19
53	2	2773	OMG	C5-C6-N1	2.71	120.07	113.19
53	2	2380	B8W	C4-N9-C1'	-2.70	120.15	126.59
53	2	4597	UR3	C6-N1-C2	-2.70	119.37	121.79
53	2	1348	P4U	O2-C2-N3	-2.70	117.95	122.33
53	2	2364	OMG	C5-C6-N1	2.66	119.94	113.19
53	2	4472	B8W	C4-C5-N7	-2.65	107.39	110.62
53	2	4472	B8W	C4-N9-C8	2.65	108.60	105.73
53	2	2050	OMG	C5-C6-N1	2.65	119.92	113.19
53	2	4671	B8T	C6-C5-C4	2.65	120.20	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	2786	B9H	O2-C2-N1	-2.64	116.53	122.72
53	2	4550	7MG	C4-C5-N7	2.64	109.20	105.53
53	2	4472	B8W	O6-C6-N1	2.64	122.66	119.01
53	2	2050	OMG	C5-C4-N9	2.62	110.38	105.63
53	2	1625	OMG	C5-C6-N1	2.62	119.84	113.19
53	2	373	OMG	C5-C6-N1	2.62	119.83	113.19
53	2	1517	2MG	O6-C6-C5	-2.62	119.66	126.60
53	2	1522	OMG	C5-C6-N1	2.62	119.83	113.19
53	2	4529	B8W	C5-N7-C8	2.61	107.21	103.51
53	2	4690	B8K	C2-N1-C6	-2.60	120.35	125.10
53	2	4550	7MG	N9-C8-N7	2.60	107.09	103.38
53	2	4530	UR3	C6-N1-C2	-2.59	119.47	121.79
53	2	2050	OMG	O6-C6-C5	-2.59	119.72	126.60
53	2	1522	OMG	C5-C4-N9	2.59	110.33	105.63
53	2	4129	B8W	N2-C2-N1	-2.59	113.23	117.25
53	2	1456	B8Q	C1'-N1-C2	2.59	121.36	116.99
53	2	4083	5MU	O2-C2-N1	-2.58	119.36	122.79
53	2	2297	E7G	N9-C8-N7	2.58	107.07	103.38
53	2	4472	B8W	C5-C6-N1	-2.58	119.87	123.46
53	2	4623	OMG	C5-C6-N1	2.57	119.71	113.19
53	2	4637	OMG	C5-C4-N9	2.57	110.29	105.63
53	2	978	2MG	N1-C2-N3	-2.57	119.98	123.95
53	2	2424	OMG	O6-C6-C5	-2.57	119.79	126.60
53	2	1909	P7G	C71-N7-C5	2.57	130.60	124.52
53	2	1517	2MG	N9-C8-N7	-2.56	108.56	113.39
53	2	4564	M7A	C5-C4-N3	-2.56	120.61	126.62
53	2	4483	B8T	O3'-C3'-C4'	2.56	118.46	111.05
53	2	978	2MG	O6-C6-C5	-2.56	119.80	126.60
53	2	373	OMG	C5-C4-N9	2.55	110.26	105.63
53	2	2364	OMG	O6-C6-C5	-2.55	119.83	126.60
53	2	373	OMG	O6-C6-C5	-2.55	119.84	126.60
53	2	4529	B8W	O6-C6-C5	-2.54	113.78	116.97
53	2	978	2MG	CM2-N2-C2	-2.54	118.25	123.86
53	2	1316	OMG	C5-C4-N9	2.54	110.24	105.63
4	8	14	OMU	C1'-N1-C2	2.54	122.16	117.57
53	2	2773	OMG	O6-C6-C5	-2.53	119.88	126.60
53	2	4690	B8K	O6-C6-N1	-2.53	115.26	120.12
53	2	2773	OMG	C5-C4-N9	2.53	110.22	105.63
53	2	4494	OMG	C5-C4-N9	2.53	110.22	105.63
53	2	1625	OMG	O6-C6-C5	-2.53	119.90	126.60
53	2	4623	OMG	C4-C5-N7	-2.52	106.73	110.72
53	2	3880	P7G	N9-C8-N7	2.51	106.97	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	2754	B9B	C2-N3-C4	2.50	120.80	113.89
53	2	4494	OMG	O6-C6-C5	-2.50	119.97	126.60
53	2	2422	OMC	C1'-N1-C2	2.49	123.99	118.42
53	2	1316	OMG	O6-C6-C5	-2.49	119.98	126.60
53	2	1625	OMG	C5-C4-N9	2.49	110.14	105.63
53	2	4185	B8W	C2-N3-C4	2.48	120.76	113.89
53	2	1883	OMG	C2'-C1'-N9	-2.48	109.41	114.22
53	2	2522	7MG	C2-N1-C6	-2.48	120.58	125.10
53	2	4870	OMG	O6-C6-C5	-2.47	120.06	126.60
53	2	2297	E7G	C2-N1-C6	-2.46	120.62	125.10
53	2	237	B9B	C2-N3-C4	2.45	120.67	113.89
53	2	2380	B8W	C2-N1-C6	2.45	119.83	115.93
53	2	729	2MG	O6-C6-C5	-2.45	120.09	126.60
53	2	1316	OMG	O4'-C1'-N9	2.45	113.97	108.36
53	2	3909	OMC	C6-N1-C2	-2.45	116.25	120.49
53	2	4637	OMG	O6-C6-C5	-2.44	120.13	126.60
53	2	4494	OMG	O4'-C1'-N9	2.43	113.92	108.36
53	2	373	OMG	O4'-C1'-N9	2.43	113.92	108.36
53	2	4472	B8W	C4-N9-C1'	-2.42	120.82	126.59
53	2	237	B9B	C4-N9-C8	2.42	108.35	105.73
53	2	729	2MG	N9-C8-N7	-2.42	108.84	113.39
53	2	3899	BGH	N1-C2-N3	-2.41	118.83	123.32
53	2	4872	2MG	O6-C6-C5	-2.41	120.21	126.60
53	2	4472	B8W	C2-N3-C4	2.41	120.54	113.89
53	2	2364	OMG	O4'-C1'-N9	2.41	113.86	108.36
53	2	4494	OMG	N9-C4-N3	2.40	130.76	125.94
53	2	1517	2MG	CM2-N2-C2	-2.40	118.57	123.86
53	2	2424	OMG	C5-C4-N9	2.40	109.98	105.63
53	2	2401	A2M	C2'-C1'-N9	-2.39	109.50	113.53
53	2	373	OMG	C2'-C1'-N9	-2.39	109.58	114.22
53	2	3899	BGH	C2-N1-C6	-2.39	120.75	125.10
53	2	1456	B8Q	C31-N3-C2	2.38	121.25	117.79
53	2	1605	7MG	C2-N1-C6	-2.38	120.77	125.10
53	2	1871	A2M	O4'-C4'-C3'	-2.37	100.42	105.11
53	2	1524	A2M	C4'-O4'-C1'	-2.37	104.25	109.47
53	2	2754	B9B	C61-O6-C6	-2.36	112.97	117.47
53	2	1517	2MG	N1-C2-N3	-2.36	120.30	123.95
53	2	3897	B8K	C2-N1-C6	-2.35	120.81	125.10
53	2	1883	OMG	O4'-C1'-N9	2.35	113.73	108.36
53	2	1534	A2M	O4'-C1'-C2'	-2.34	102.46	106.57
53	2	1522	OMG	O6-C6-C5	-2.34	120.39	126.60
53	2	4550	7MG	C2-N1-C6	-2.34	120.83	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	2363	A2M	C4-N9-C1'	2.33	132.15	126.59
53	2	4185	B8W	O6-C6-C5	-2.33	114.05	116.97
53	2	729	2MG	N1-C2-N3	-2.33	120.35	123.95
53	2	1574	B9B	C2-N3-C4	2.33	120.32	113.89
53	2	3869	OMC	O2-C2-N3	-2.32	118.56	122.33
53	2	4870	OMG	N9-C8-N7	-2.31	109.04	113.39
53	2	1871	A2M	C2'-C1'-N9	-2.31	109.64	113.53
53	2	4623	OMG	N9-C8-N7	-2.30	109.05	113.39
53	2	1883	OMG	C5-C4-N9	2.29	109.78	105.63
53	2	373	OMG	N9-C8-N7	-2.28	109.10	113.39
53	2	4083	5MU	O4-C4-N3	-2.28	115.75	120.12
53	2	4529	B8W	C2-N3-C4	2.27	120.17	113.89
53	2	4690	B8K	N1-C2-N3	-2.27	119.09	123.32
53	2	2050	OMG	O4'-C1'-N9	2.27	113.54	108.36
53	2	3880	P7G	C71-N7-C5	2.26	129.88	124.52
53	2	4529	B8W	C6-C5-N7	-2.26	130.63	133.63
53	2	3909	OMC	C1'-N1-C2	2.26	123.46	118.42
53	2	2380	B8W	C5-C6-N1	-2.25	120.33	123.46
53	2	1574	B9B	C4-N9-C8	2.25	108.16	105.73
53	2	1316	OMG	C4-C5-N7	-2.24	107.17	110.72
53	2	1625	OMG	N9-C4-N3	2.24	130.43	125.94
53	2	2754	B9B	C4-N9-C8	2.24	108.15	105.73
53	2	4472	B8W	N2-C2-N1	-2.23	113.78	117.25
53	2	2424	OMG	O4'-C1'-N9	2.23	113.46	108.36
53	2	4623	OMG	O4'-C1'-N9	2.22	113.44	108.36
53	2	4529	B8W	C5-C6-N1	-2.22	120.37	123.46
53	2	1316	OMG	N9-C8-N7	-2.21	109.22	113.39
53	2	373	OMG	N2-C2-N1	2.20	121.39	116.71
53	2	4637	OMG	C4-C5-N7	-2.18	107.27	110.72
53	2	2380	B8W	C2-N3-C4	2.17	119.90	113.89
53	2	4536	OMC	C1'-N1-C2	2.17	123.27	118.42
53	2	4870	OMG	N9-C4-N3	2.17	130.30	125.94
53	2	4129	B8W	C6-C5-N7	-2.17	130.75	133.63
53	2	4623	OMG	O6-C6-C5	-2.17	120.85	126.60
53	2	4530	UR3	C3U-N3-C4	2.16	120.98	117.89
53	2	1522	OMG	O4'-C1'-N9	2.16	113.31	108.36
53	2	2380	B8W	C1'-N9-C8	2.16	132.01	127.14
53	2	3897	B8K	N1-C2-N3	-2.16	119.30	123.32
53	2	1605	7MG	O6-C6-C5	-2.15	122.27	127.54
53	2	373	OMG	C4-C5-N7	-2.15	107.32	110.72
53	2	2861	OMC	O2-C2-N1	2.14	123.31	118.89
53	2	1522	OMG	N2-C2-N1	2.14	121.26	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	4529	B8W	C2-N1-C6	2.13	119.32	115.93
53	2	4550	7MG	O6-C6-C5	-2.13	122.32	127.54
53	2	1534	A2M	C2'-C1'-N9	2.12	117.11	113.53
53	2	4483	B8T	C6-N1-C2	-2.11	116.83	120.49
53	2	1883	OMG	N9-C8-N7	-2.11	109.42	113.39
53	2	2773	OMG	C4-C5-N7	-2.11	107.39	110.72
53	2	4870	OMG	C5-C4-N9	2.10	109.44	105.63
53	2	1605	7MG	C6-C5-C4	-2.10	118.30	122.62
53	2	1625	OMG	O4'-C1'-N9	2.09	113.14	108.36
53	2	4597	UR3	O2-C2-N3	-2.08	118.40	121.34
53	2	4550	7MG	C6-C5-C4	-2.08	118.33	122.62
53	2	2422	OMC	O2-C2-N1	2.08	123.19	118.89
53	2	4623	OMG	C6-C5-N7	2.08	134.11	130.25
53	2	2773	OMG	C2'-C1'-N9	-2.06	110.22	114.22
53	2	4483	B8T	C6-C5-C4	2.06	119.49	116.96
53	2	1522	OMG	C4-C5-N7	-2.06	107.46	110.72
53	2	4185	B8W	C2-N1-C6	2.05	119.19	115.93
53	2	2786	B9H	C32-C31-N3	2.05	116.75	112.47
53	2	2522	7MG	C6-C5-C4	-2.04	118.41	122.62
53	2	4129	B8W	C2-N1-C6	2.04	119.17	115.93
53	2	4523	A2M	C4'-O4'-C1'	-2.03	104.99	109.47
53	2	2364	OMG	C4-C5-N7	-2.03	107.51	110.72
53	2	729	2MG	C8-N7-C5	2.03	107.91	104.24
53	2	1316	OMG	C8-N7-C5	2.03	107.91	104.24
53	2	4872	2MG	C8-N7-C5	2.02	107.90	104.24
53	2	4872	2MG	C1'-N9-C4	-2.01	120.53	126.50
53	2	4620	OMU	O2-C2-N1	-2.01	120.12	122.79
53	2	3887	OMC	C1'-N1-C2	2.01	122.90	118.42
53	2	1605	7MG	N1-C2-N3	-2.00	119.58	123.32
53	2	1659	I4U	O2-C2-N3	-2.00	119.07	122.33

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	8	14	OMU	C1'-C2'-O2'-CM2
53	2	237	B9B	C5-C6-O6-C61
53	2	237	B9B	N1-C6-O6-C61
53	2	237	B9B	C3'-C4'-C5'-O5'
53	2	237	B9B	O4'-C4'-C5'-O5'
53	2	398	A2M	O4'-C4'-C5'-O5'
53	2	1348	P4U	N3-C4-O4-C41

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Mol	Chain	Res	Type	Atoms
53	2	1574	B9B	C5-C6-O6-C61
53	2	1574	B9B	N1-C6-O6-C61
53	2	1625	OMG	C3'-C4'-C5'-O5'
53	2	1871	A2M	O4'-C4'-C5'-O5'
53	2	1871	A2M	C3'-C4'-C5'-O5'
53	2	1883	OMG	O4'-C4'-C5'-O5'
53	2	1883	OMG	C3'-C4'-C5'-O5'
53	2	2380	B8W	C5-C6-O6-C61
53	2	2380	B8W	N1-C6-O6-C61
53	2	2424	OMG	C3'-C4'-C5'-O5'
53	2	2754	B9B	C5-C6-O6-C61
53	2	2754	B9B	N1-C6-O6-C61
53	2	2786	B9H	C1'-C2'-O2'-C21
53	2	4129	B8W	C5-C6-O6-C61
53	2	4129	B8W	N1-C6-O6-C61
53	2	4129	B8W	C3'-C4'-C5'-O5'
53	2	4472	B8W	C5-C6-O6-C61
53	2	4472	B8W	N1-C6-O6-C61
53	2	4529	B8W	C5-C6-O6-C61
53	2	4529	B8W	C3'-C4'-C5'-O5'
53	2	4529	B8W	O4'-C4'-C5'-O5'
53	2	4550	7MG	O4'-C4'-C5'-O5'
53	2	4550	7MG	C3'-C4'-C5'-O5'
53	2	4637	OMG	O4'-C4'-C5'-O5'
53	2	4637	OMG	C3'-C4'-C5'-O5'
53	2	4637	OMG	C1'-C2'-O2'-CM2
53	2	4870	OMG	O4'-C4'-C5'-O5'
53	2	4870	OMG	C3'-C4'-C5'-O5'
53	2	398	A2M	C3'-C4'-C5'-O5'
53	2	1625	OMG	O4'-C4'-C5'-O5'
53	2	2424	OMG	O4'-C4'-C5'-O5'
53	2	3897	B8K	O4'-C4'-C5'-O5'
53	2	4129	B8W	O4'-C4'-C5'-O5'
53	2	4872	2MG	O4'-C4'-C5'-O5'
53	2	729	2MG	O4'-C4'-C5'-O5'
53	2	2364	OMG	O4'-C4'-C5'-O5'
53	2	3880	P7G	C3'-C4'-C5'-O5'
53	2	3880	P7G	O4'-C4'-C5'-O5'
53	2	3897	B8K	C3'-C4'-C5'-O5'
53	2	4872	2MG	C3'-C4'-C5'-O5'
53	2	1517	2MG	O4'-C4'-C5'-O5'
53	2	1909	P7G	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
53	2	3909	OMC	O4'-C4'-C5'-O5'
53	2	1574	B9B	C62-C61-O6-C6
53	2	729	2MG	C3'-C4'-C5'-O5'
53	2	3701	OMC	O4'-C4'-C5'-O5'
53	2	1517	2MG	C3'-C4'-C5'-O5'
53	2	2364	OMG	C3'-C4'-C5'-O5'
53	2	3867	A2M	C3'-C4'-C5'-O5'
53	2	3880	P7G	N7-C71-C72-C73
53	2	3701	OMC	C3'-C4'-C5'-O5'
53	2	3867	A2M	C4'-C5'-O5'-P
53	2	1534	A2M	O4'-C4'-C5'-O5'
53	2	2786	B9H	C3'-C2'-O2'-C21
53	2	3723	A2M	O4'-C4'-C5'-O5'
53	2	3867	A2M	O4'-C4'-C5'-O5'
53	2	3899	BGH	O4'-C4'-C5'-O5'
53	2	3887	OMC	C4'-C5'-O5'-P
53	2	4529	B8W	N1-C6-O6-C61
53	2	2365	OMC	C3'-C2'-O2'-CM2
53	2	1574	B9B	O6-C61-C62-C63
53	2	1517	2MG	C4'-C5'-O5'-P
53	2	3897	B8K	C4'-C5'-O5'-P
53	2	2297	E7G	C72-C71-N7-C8
53	2	373	OMG	C4'-C5'-O5'-P
53	2	4637	OMG	C4'-C5'-O5'-P
53	2	3909	OMC	C3'-C4'-C5'-O5'
53	2	1524	A2M	C3'-C2'-O2'-CM'
53	2	3869	OMC	C3'-C2'-O2'-CM2
53	2	4523	A2M	C3'-C2'-O2'-CM'
53	2	2422	OMC	O4'-C4'-C5'-O5'
53	2	1909	P7G	C3'-C4'-C5'-O5'
53	2	2773	OMG	C3'-C4'-C5'-O5'
53	2	3869	OMC	C1'-C2'-O2'-CM2
53	2	3909	OMC	C2'-C1'-N1-C2
53	2	1534	A2M	C3'-C4'-C5'-O5'
53	2	2380	B8W	O4'-C4'-C5'-O5'
53	2	1659	I4U	C42-C41-O4-C4
53	2	1659	I4U	C43-C41-O4-C4
53	2	2754	B9B	C62-C61-O6-C6
53	2	3880	P7G	C4'-C5'-O5'-P

There are no ring outliers.

16 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	2	4620	OMU	3	0
53	2	2363	A2M	1	0
53	2	4083	5MU	1	0
53	2	1871	A2M	1	0
53	2	2364	OMG	1	0
53	2	2522	7MG	1	0
53	2	1574	B9B	1	0
53	2	4129	B8W	1	0
53	2	1456	B8Q	1	0
53	2	729	2MG	1	0
53	2	1605	7MG	2	0
53	2	2773	OMG	1	0
53	2	3723	A2M	1	0
53	2	1625	OMG	1	0
53	2	4870	OMG	1	0
53	2	4872	2MG	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	$\# Z > 2$
54	GTP	w	801	55	30,34,34	0.55	0	46,54,54	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	GTP	w	801	55	-	1/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

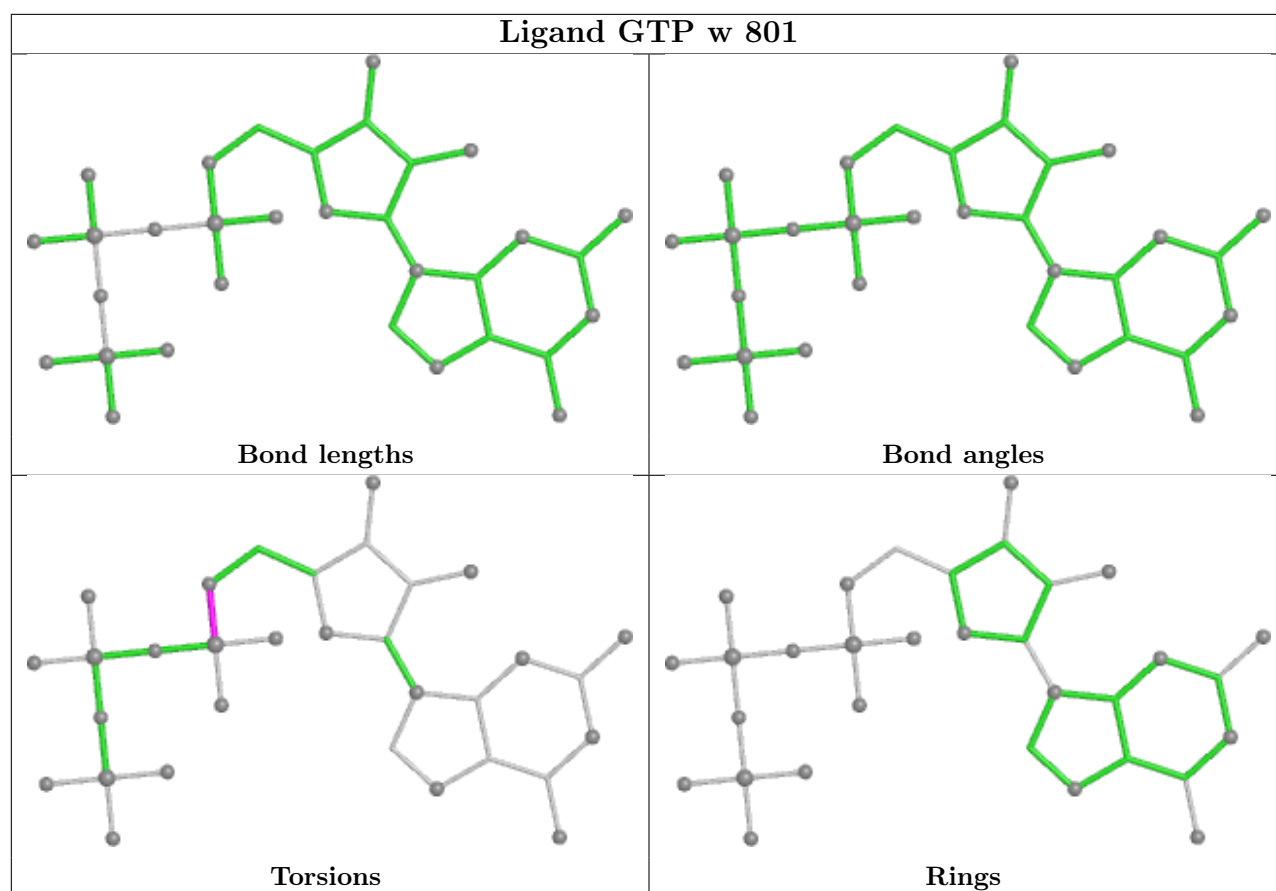
All (1) torsion outliers are listed below:

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

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.

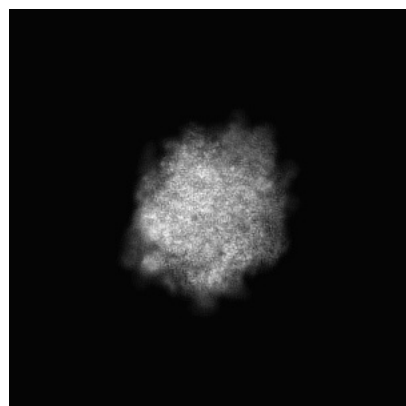
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35599. These allow visual inspection of the internal detail of the map and identification of artifacts.

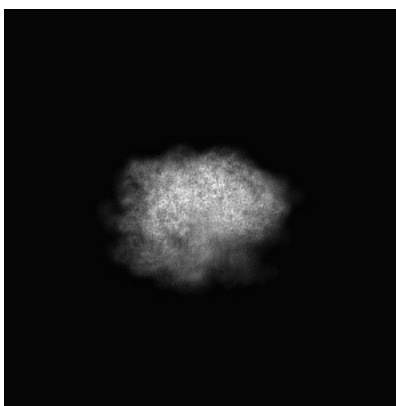
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

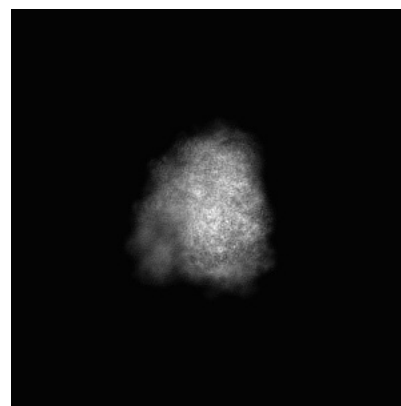
6.1.1 Primary map



X

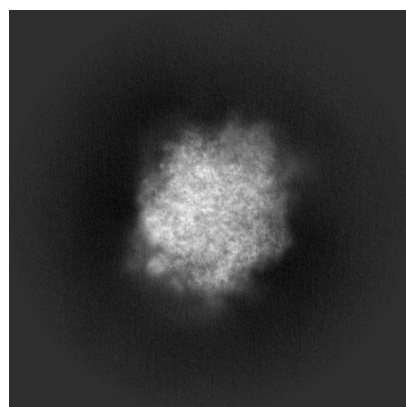


Y

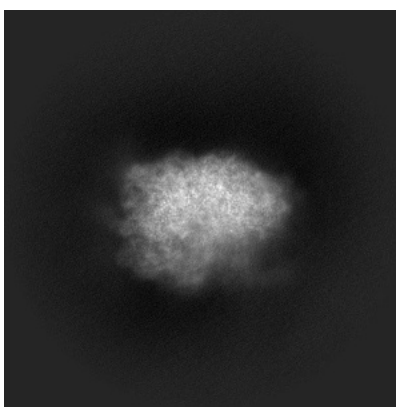


Z

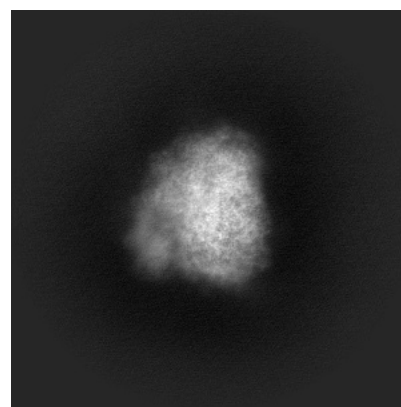
6.1.2 Raw map



X



Y

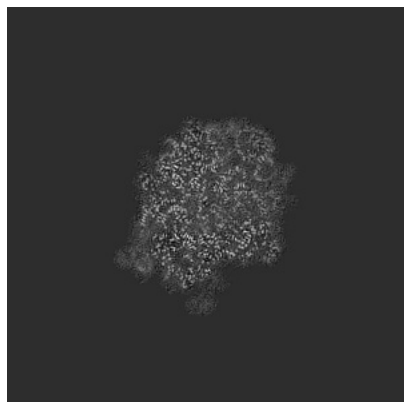


Z

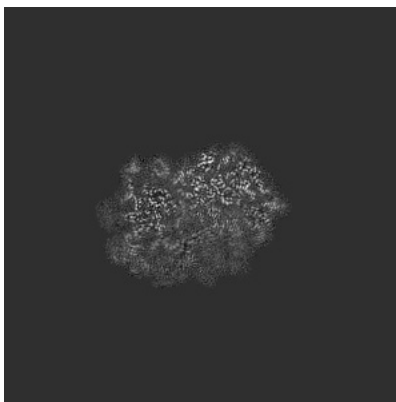
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

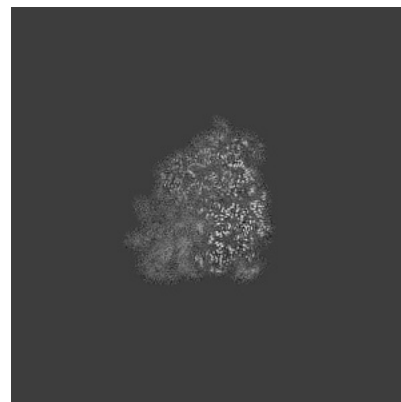
6.2.1 Primary map



X Index: 200

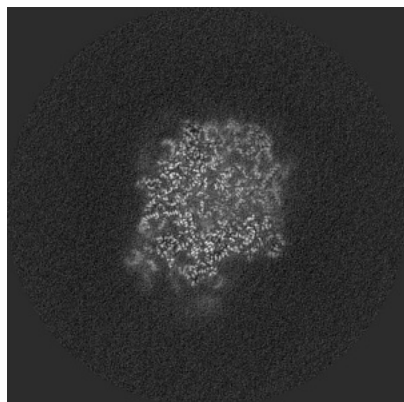


Y Index: 200

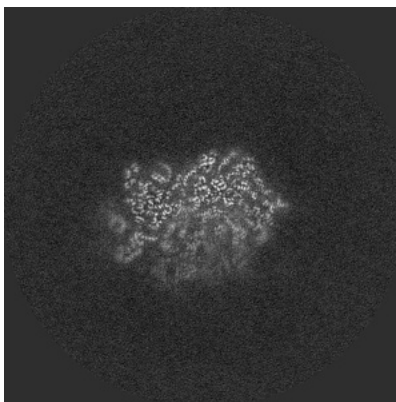


Z Index: 200

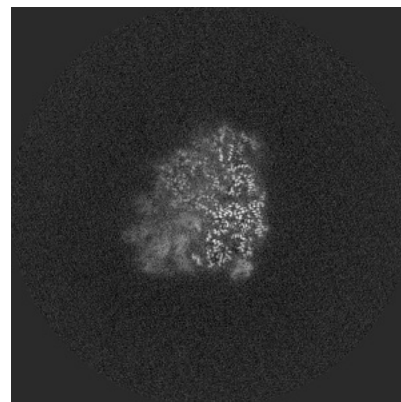
6.2.2 Raw map



X Index: 200



Y Index: 200

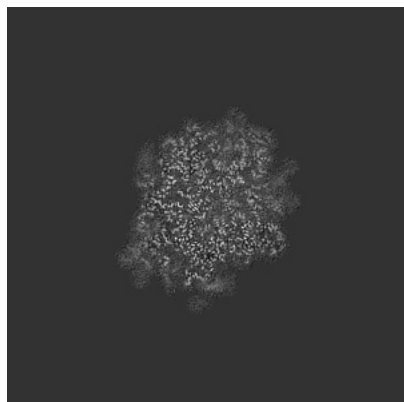


Z Index: 200

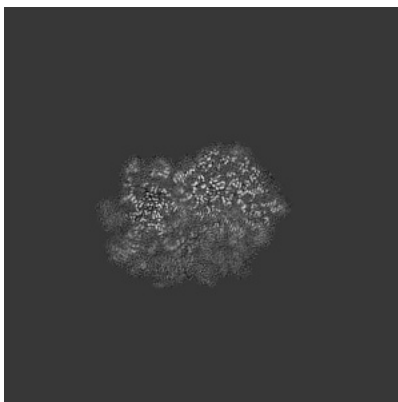
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

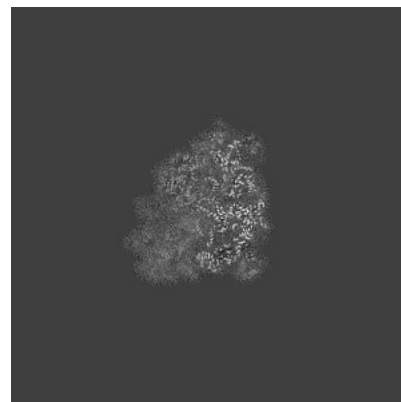
6.3.1 Primary map



X Index: 206

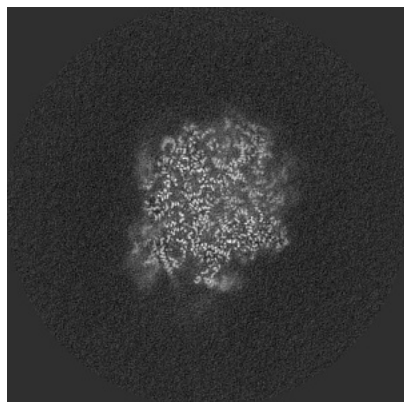


Y Index: 199

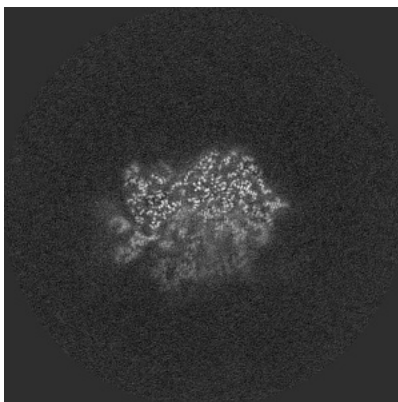


Z Index: 198

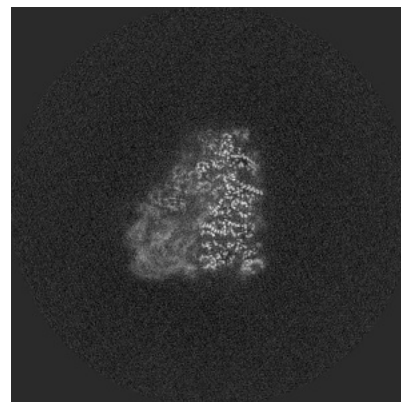
6.3.2 Raw map



X Index: 206



Y Index: 199

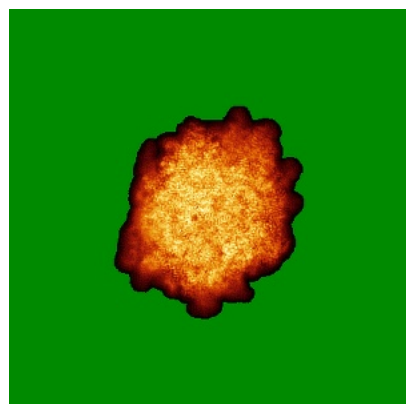


Z Index: 190

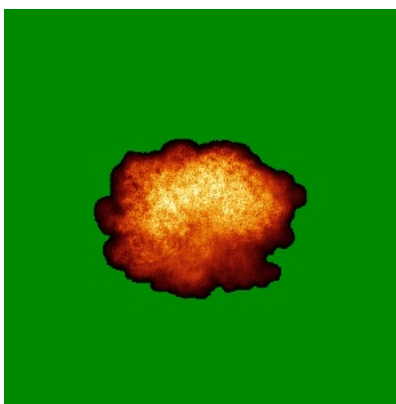
The images above show the largest variance slices of the map in three orthogonal directions.

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

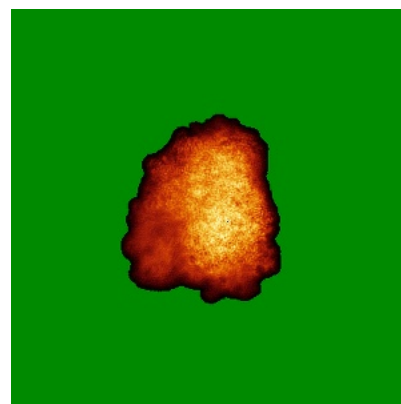
6.4.1 Primary map



X

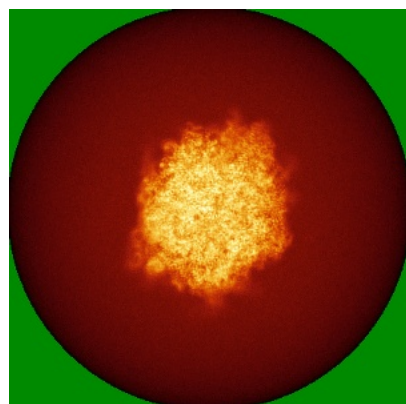


Y

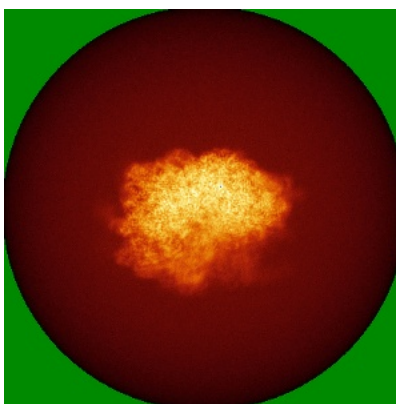


Z

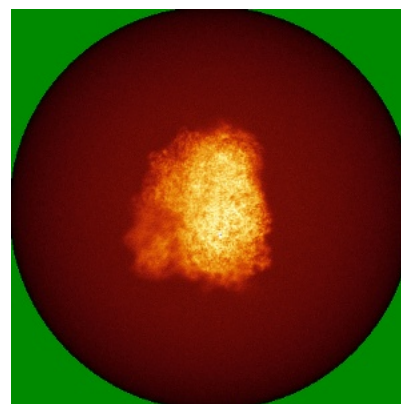
6.4.2 Raw map



X



Y

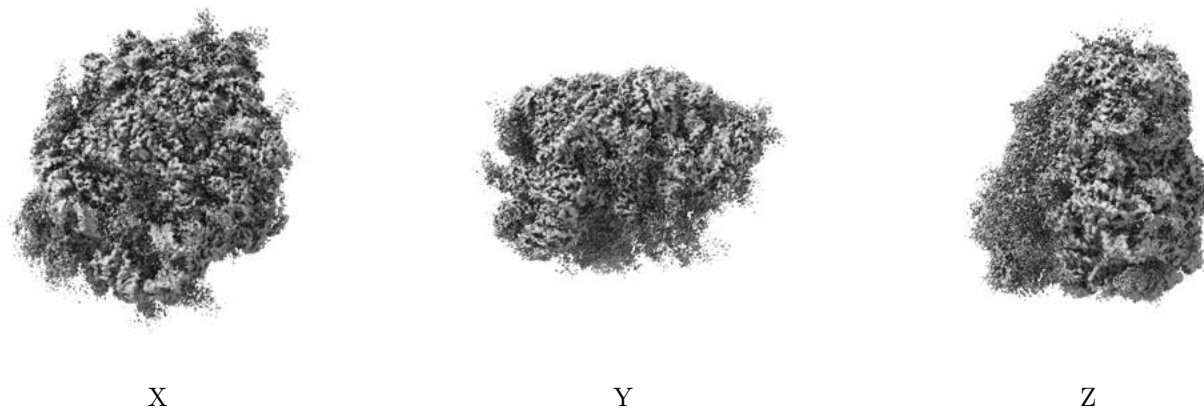


Z

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 0.031. 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.

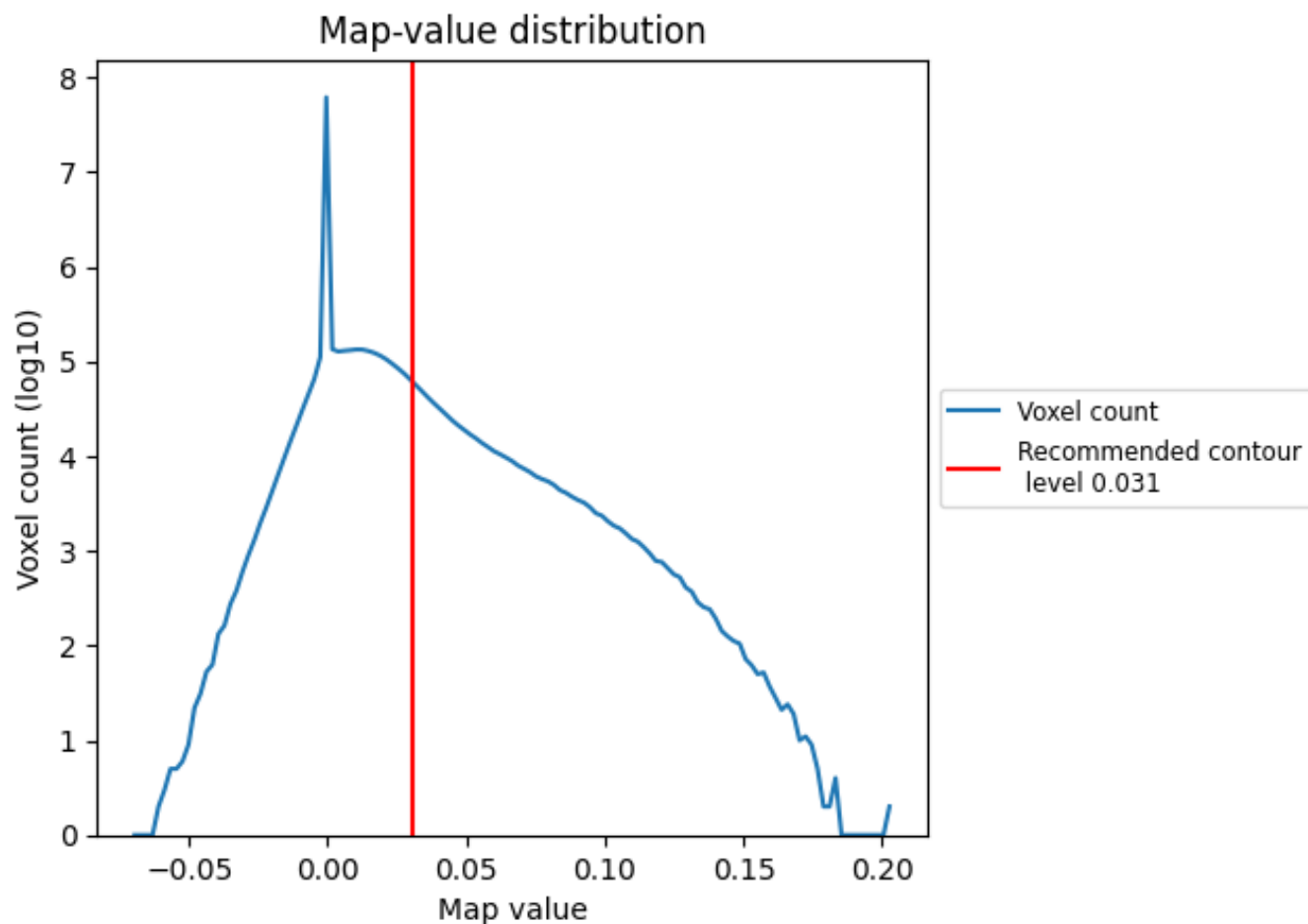
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

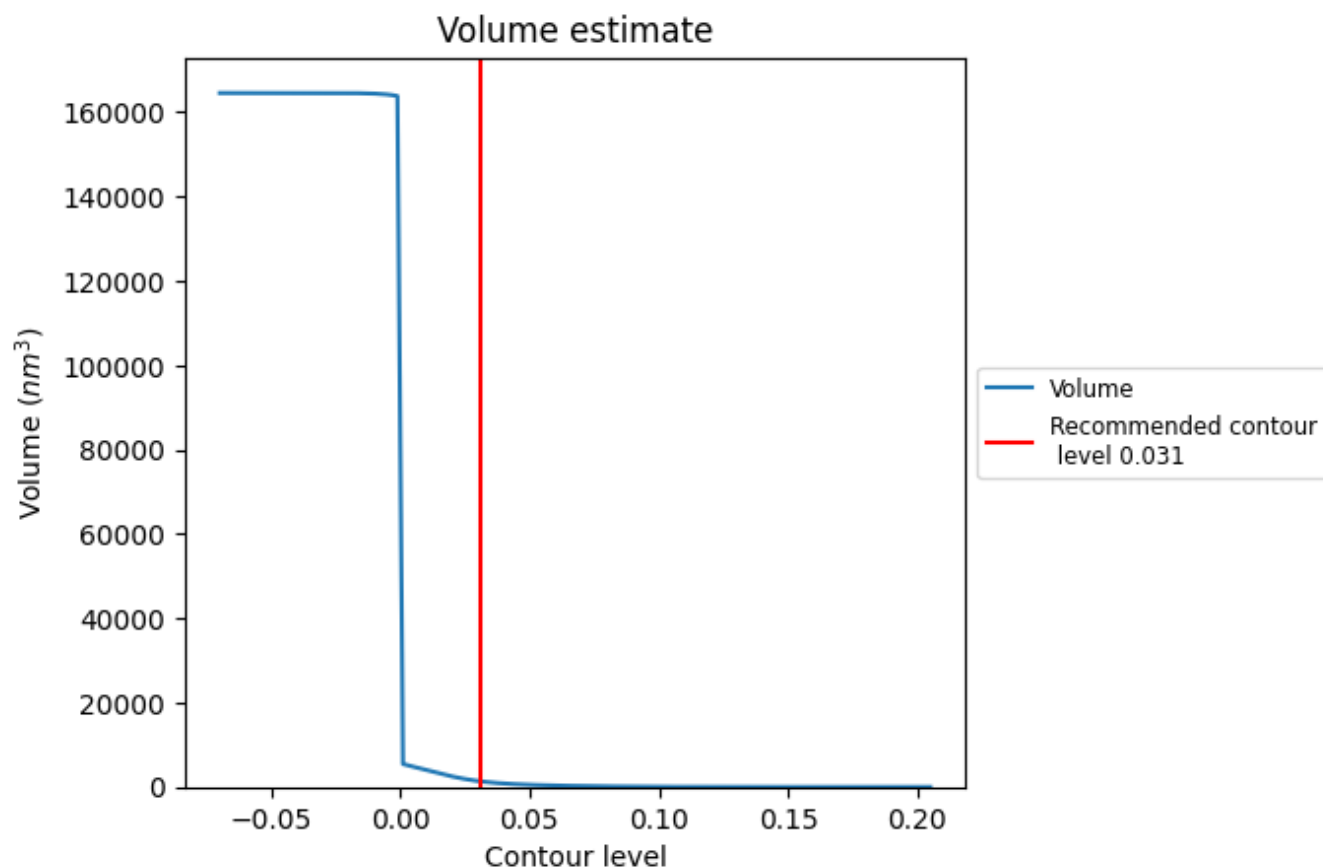
This section contains the results of statistical analysis of the map.

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.

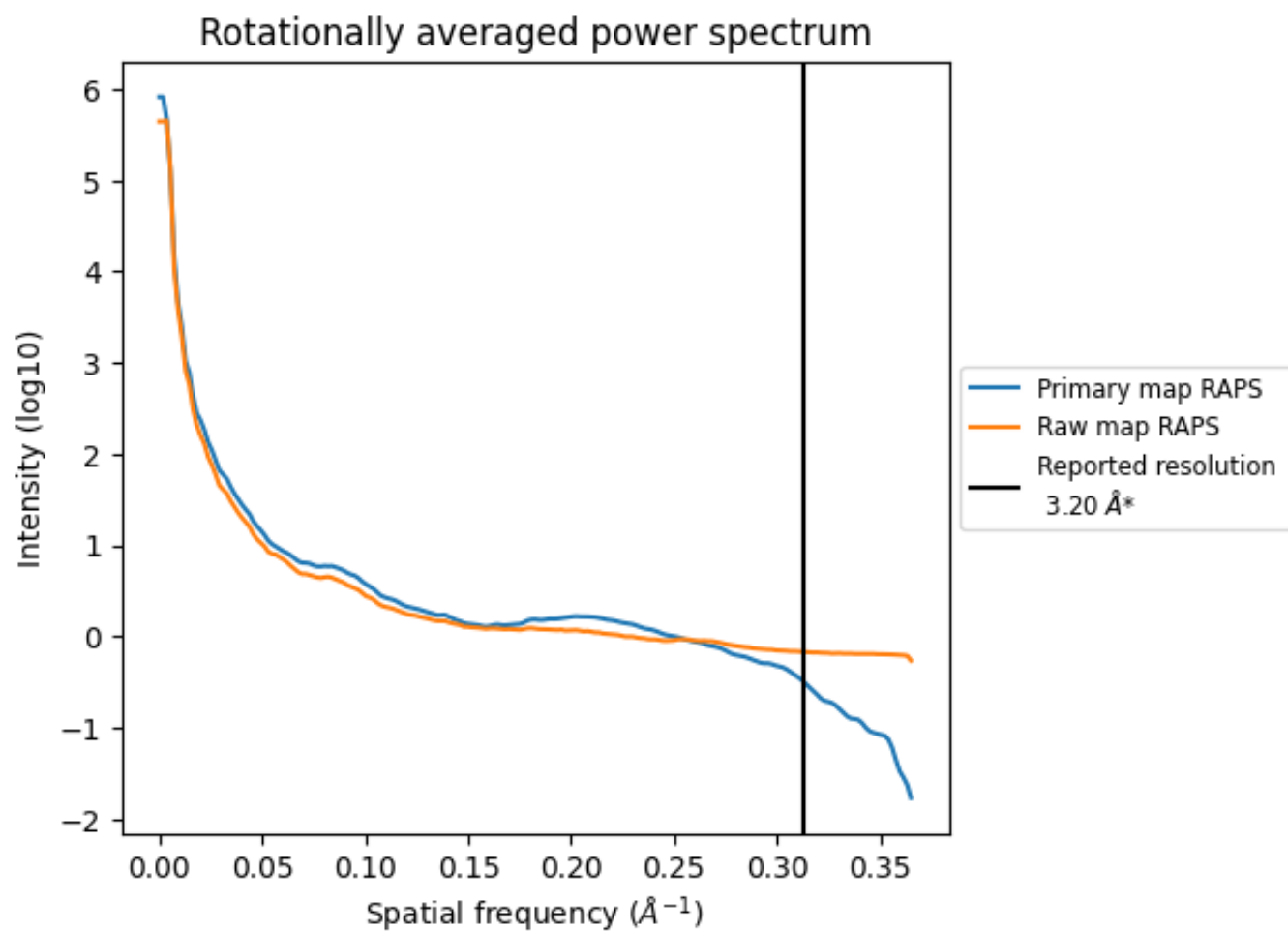
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1338 nm^3 ; this corresponds to an approximate mass of 1209 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 ⓘ

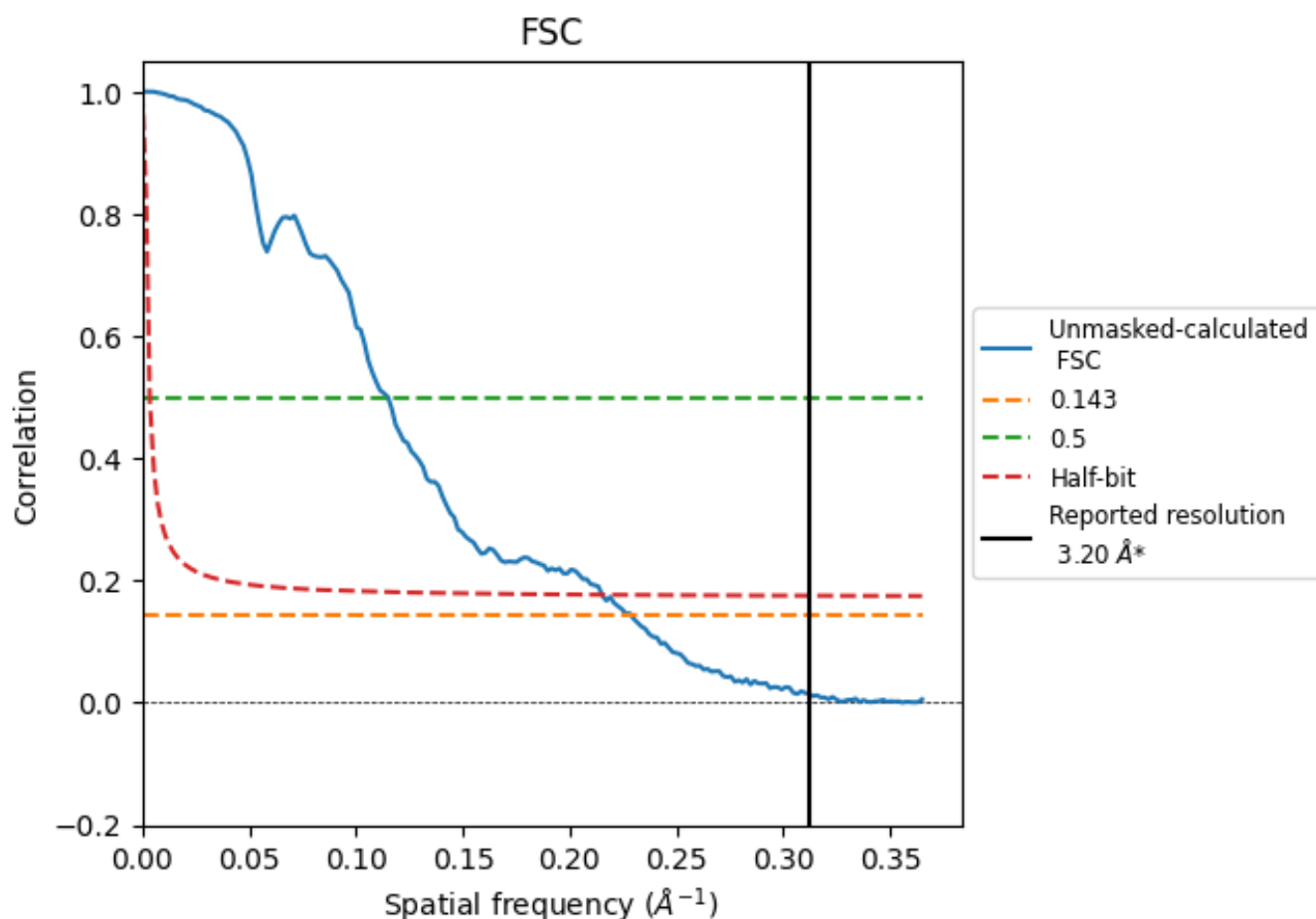


*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

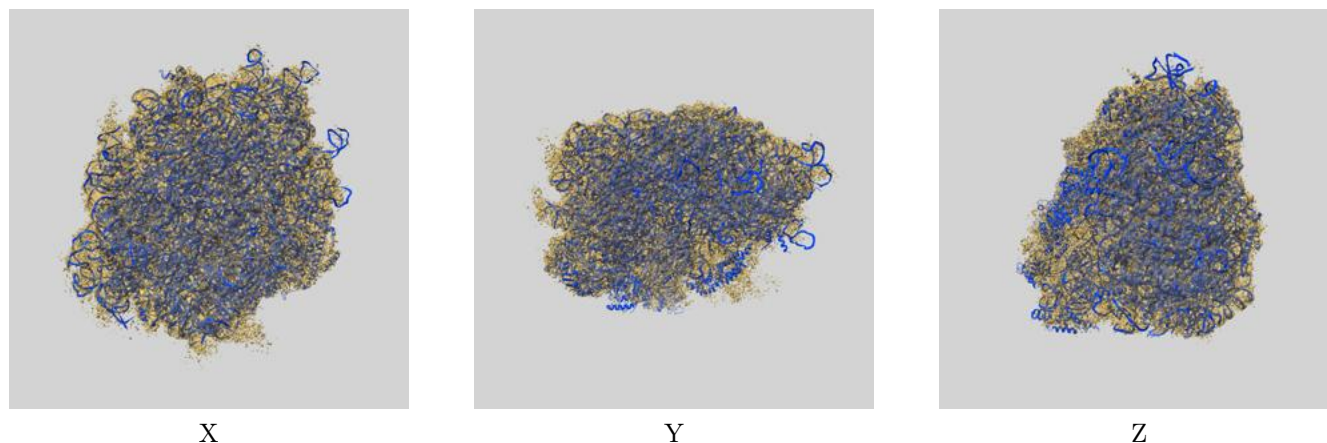
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	8.70	4.65

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

9 Map-model fit [i](#)

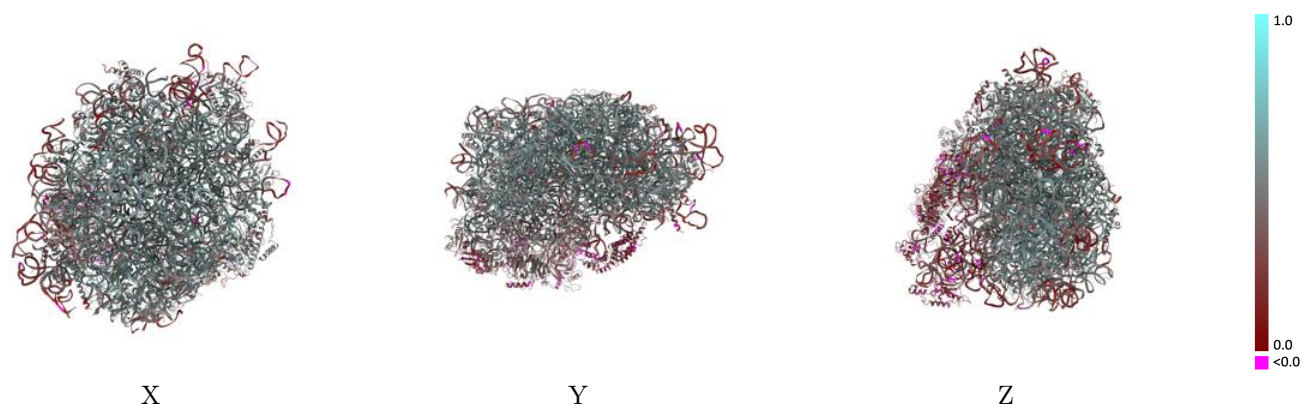
This section contains information regarding the fit between EMDB map EMD-35599 and PDB model 8INK. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



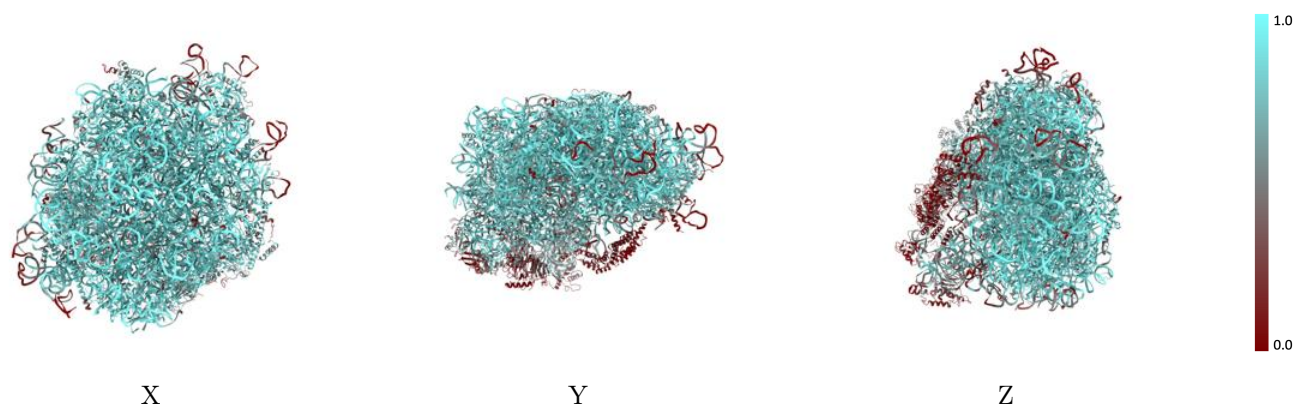
The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



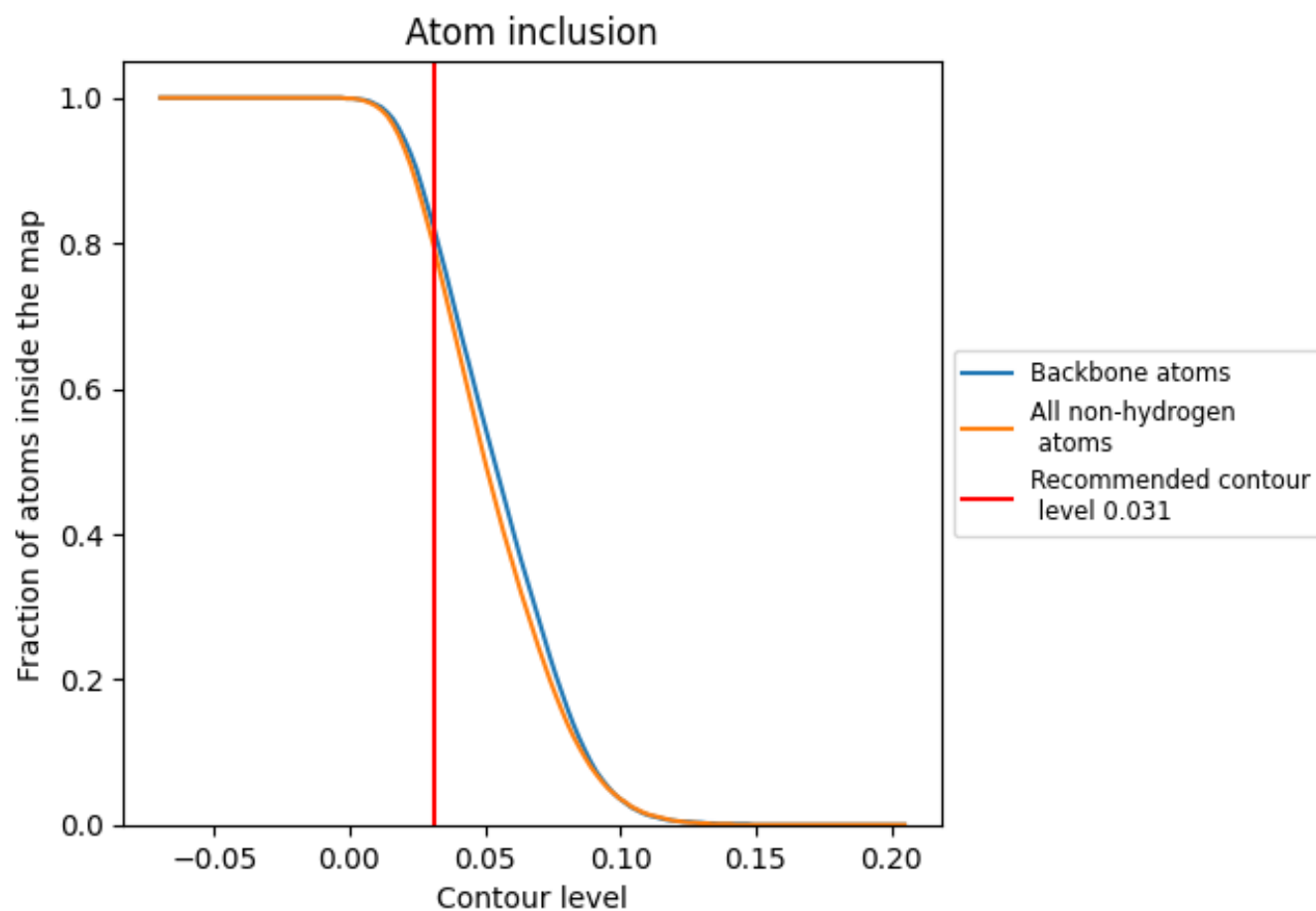
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.031).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7980	 0.4550
2	 0.8700	 0.4640
3	 0.7720	 0.3080
4	 0.6970	 0.4290
6	 0.7670	 0.4760
7	 0.8480	 0.5120
8	 0.9440	 0.5160
9	 0.3710	 0.3610
A	 0.5840	 0.3760
B	 0.9010	 0.5380
C	 0.2590	 0.2110
D	 0.9200	 0.5410
E	 0.6010	 0.4300
F	 0.8510	 0.5030
G	 0.6830	 0.4300
H	 0.8720	 0.5090
I	 0.8350	 0.5060
J	 0.7950	 0.4750
K	 0.8060	 0.4710
L	 0.9230	 0.5400
M	 0.9520	 0.5520
N	 0.1090	 0.1830
O	 0.6970	 0.4580
P	 0.9720	 0.5530
Q	 0.8090	 0.4860
R	 0.2770	 0.1820
S	 0.8970	 0.5280
T	 0.5790	 0.2680
U	 0.9180	 0.5240
V	 0.9050	 0.5400
W	 0.1950	 0.3230
X	 0.7600	 0.4670
Y	 0.8670	 0.5310
Z	 0.9220	 0.5470
a	 0.8270	 0.4890



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Chain	Atom inclusion	Q-score
b	 0.9200	 0.5510
d	 0.7800	 0.4870
e	 0.8760	 0.5210
g	 0.8830	 0.5220
h	 0.8790	 0.5250
i	 0.7230	 0.4490
j	 0.8400	 0.5090
k	 0.9470	 0.5640
l	 0.9160	 0.5490
m	 0.8320	 0.4900
n	 0.9510	 0.5700
o	 0.7960	 0.4720
p	 0.9010	 0.5320
r	 0.3640	 0.3220
u	 0.5260	 0.3660
v	 0.6020	 0.4230
w	 0.7010	 0.4360
y	 0.3620	 0.2770
z	 0.6650	 0.4280