



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 03:18 am BST

PDB ID : 9RHU / pdb_00009rhu
EMDB ID : EMD-53976
Title : Rabbit 80S ribosome in complex with eRF1-AAQ, stalled at the Stop codon in mutated F2A sequence
Authors : Li, X.; Zuber, P.K.; Loughran, G.; Bhatt, P.R.; Alquraish, F.; Ramakrishnan, V.; Firth, A.E.; Atkins, J.F.
Deposited on : 2025-06-10
Resolution : 2.65 Å (reported)
Based on initial model : 7O80

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:

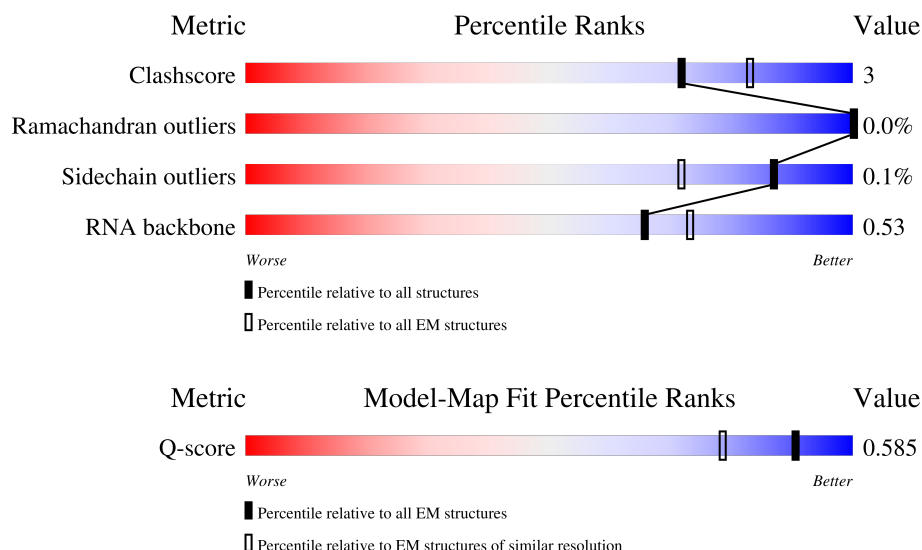
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.65 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	9050 (2.15 - 3.15)

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	MB	117	 7% 91% 6%
2	A1	1870	 11% 65% 26% 5%

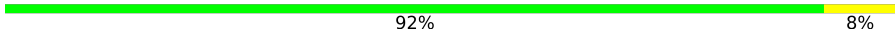
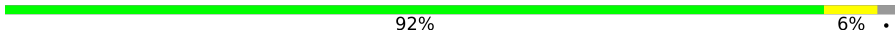
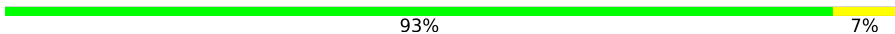
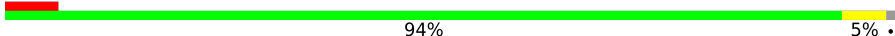
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Mol	Chain	Length	Quality of chain
3	A2	291	
4	A3	4808	
5	B1	84	
6	B2	249	
7	B3	119	
8	C1	69	
9	C2	319	
10	C3	158	
11	D1	80	
12	D2	192	
13	D3	257	
14	E1	59	
15	E2	214	
16	E3	403	
17	F1	115	
18	F2	178	
19	F3	413	
20	G1	317	
21	G2	184	
22	G3	296	
23	H1	56	
24	H2	211	
25	I1	659	
26	I2	218	
27	J1	75	

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Mol	Chain	Length	Quality of chain
28	J2	204	
29	K1	74	
30	K2	203	
31	L1	295	
32	L2	184	
33	M1	264	
34	M2	188	
35	N1	293	
36	N2	196	
37	O1	243	
38	O2	176	
39	P1	263	
40	P2	160	
41	Q1	204	
42	Q2	128	
43	R1	249	
44	R2	140	
45	S1	194	
46	S2	157	
47	T1	208	
48	T2	156	
49	U1	194	
50	U2	145	
51	V1	165	
52	V2	136	

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Mol	Chain	Length	Quality of chain
53	W1	158	
54	W2	148	
55	X1	132	
56	X2	245	
57	Y1	151	
58	Y2	115	
59	Z1	151	
60	Z2	125	
61	a1	145	
62	a2	135	
63	b1	146	
64	b2	110	
65	c1	135	
66	d1	152	
67	d2	123	
68	e1	144	
69	e2	105	
70	f1	119	
71	f2	97	
72	g1	84	
73	g2	70	
74	h1	130	
75	h2	51	
76	i1	143	
77	i2	52	

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Mol	Chain	Length	Quality of chain
78	j1	133	
79	j2	141	
80	k1	124	
81	k2	92	
82	l1	25	
83	l2	137	
84	m2	318	
85	n2	165	
86	o2	217	
87	p2	438	
88	q2	599	

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 233632 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	MB	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	1770	Total	C	N	O	P	0	0
			37833	16911	6781	12371	1770		

- Molecule 3 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A3	3764	Total	C	N	O	P	0	0
			80772	36003	14762	26243	3764		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 5 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B1	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 6 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B2	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

- Molecule 7 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B3	119	Total	C	N	O	P	0	0
			2538	1131	451	837	119		

- Molecule 8 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C1	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 9 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C2	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	86	ALA	VAL	conflict	UNP G1STW0
C2	191	GLY	CYS	conflict	UNP G1STW0

- Molecule 10 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C3	156	Total	C	N	O	P	0	0
			3319	1481	585	1097	156		

- Molecule 11 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D1	68	Total	C	N	O	S	0	0
			554	349	103	95	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D2	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 13 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D3	253	Total	C	N	O	S	0	0
			1940	1214	396	324	6		

- Molecule 14 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E1	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 15 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E2	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

- Molecule 16 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E3	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

- Molecule 17 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F1	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 18 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F2	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 19 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F3	363	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	2	ACE	-	acetylation	UNP G1SVW5

- Molecule 20 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G1	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 21 is a protein called Choriogonadotropin subunit beta variant 1,Genome polyprotein,Genome polyprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	G2	24	Total	C	N	O	0	0
			176	113	29	34		

- Molecule 22 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G3	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G3	2	MET	-	initiating methionine	UNP P19949

- Molecule 23 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	H1	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 24 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	H2	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H2	74	ARG	HIS	conflict	UNP G1TKB3
H2	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 25 is a RNA chain called mRNA containing F2A sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	I1	18	Total	C	N	O	P	0	0
			374	167	56	133	18		

- Molecule 26 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	I2	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 27 is a RNA chain called E-site tRNA-Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	J1	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 28 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	J2	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 29 is a RNA chain called P-site tRNA-Gly.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	K1	74	Total	C	N	O	P	0	0
			1582	711	273	524	74		

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K2	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 31 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L1	222	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L1	1	ACE	-	acetylation	UNP G1TLT8

- Molecule 32 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L2	159	Total	C	N	O	S	0	0
			1289	809	249	222	9		

- Molecule 33 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	M1	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 34 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M2	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M2	134	ARG	CYS	conflict	UNP F6QK19

- Molecule 35 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N1	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N1	33	ILE	VAL	conflict	UNP O18789
N1	101	ALA	SER	conflict	UNP O18789

- Molecule 36 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	N2	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N2	38	ARG	HIS	conflict	UNP G1TYL6
N2	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 37 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	O1	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 38 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O2	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

- Molecule 39 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P1	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P1	25	GLY	SER	conflict	UNP G1TK17
P1	51	ARG	LYS	conflict	UNP G1TK17
P1	78	THR	ALA	conflict	UNP G1TK17
P1	156	VAL	MET	conflict	UNP G1TK17

- Molecule 40 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	P2	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 41 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Q1	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 42 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Q2	98	Total	C	N	O	S	0	0
			797	511	139	145	2		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q2	32	GLY	ARG	conflict	UNP G1TSG1
Q2	36	ALA	GLU	conflict	UNP G1TSG1
Q2	39	PHE	SER	conflict	UNP G1TSG1
Q2	54	GLY	ARG	conflict	UNP G1TSG1
Q2	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 43 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R1	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 44 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	R2	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 45 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	S1	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 46 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S2	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 47 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	T1	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T1	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 48 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	T2	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 49 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	U1	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 50 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	U2	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 51 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	V1	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 52 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	V2	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 53 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	W1	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 54 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	W2	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 55 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	X1	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 56 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X2	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 57 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Y1	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 58 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Y2	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 59 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Z1	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Z2	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 61 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	a1	133	Total	C	N	O	S	0	0
			1091	694	205	185	7		

- Molecule 62 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	a2	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 63 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	b1	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 64 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	b2	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 65 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	c1	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 66 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	d1	146	Total	C	N	O	S	0	0
			1200	753	242	204	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d1	1	ACE	-	acetylation	UNP G1TPG3

- Molecule 67 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	d2	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 68 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	e1	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 69 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	e2	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e2	31	GLY	ARG	conflict	UNP G1TTQ5

- Molecule 70 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	f1	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 71 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	f2	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 72 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	g1	84	Total	C	N	O	S	0	0
			640	394	117	124	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g1	0	ACE	-	acetylation	UNP G1TM82

- Molecule 73 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	g2	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g2	24	LYS	ASN	conflict	UNP G1U001

- Molecule 74 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	h1	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 75 is a protein called 60S ribosomal protein L39-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	h2	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 76 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	i1	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 77 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	i2	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 78 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	j1	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 79 is a protein called Ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	j2	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 80 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	k1	74	Total	C	N	O	S	0	0
			587	376	107	103	1		

- Molecule 81 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	k2	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 82 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	l1	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 83 is a protein called [histone H4]-N-methyl-L-lysine20 N-methyltransferase KMT5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	l2	127	Total	C	N	O	S	0	0
			1014	629	209	170	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l2	1	ACE	-	acetylation	UNP A0A8C0DF35

- Molecule 84 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	m2	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 85 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	n2	156	Total	C	N	O	S	0	0
			1178	733	221	220	4		

- Molecule 86 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	o2	212	Total	C	N	O	S	0	0
			1707	1092	308	299	8		

- Molecule 87 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	p2	416	Total	C	N	O	S	0	0
			3280	2087	559	623	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p2	0	GLY	-	expression tag	UNP P62495
p2	1	PRO	-	expression tag	UNP P62495
p2	183	ALA	GLY	engineered mutation	UNP P62495
p2	184	ALA	GLY	engineered mutation	UNP P62495

- Molecule 88 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	q2	595	Total	C	N	O	S	0	0
			4668	2982	801	854	31		

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	MB	1	Total	Mg	0
			1	1	
89	A1	109	Total	Mg	0
			109	109	
89	A3	239	Total	Mg	0
			239	239	
89	B3	4	Total	Mg	0
			4	4	
89	C3	5	Total	Mg	0
			5	5	
89	E2	1	Total	Mg	0
			1	1	
89	E3	1	Total	Mg	0
			1	1	
89	I1	2	Total	Mg	0
			2	2	
89	J2	1	Total	Mg	0
			1	1	
89	L2	2	Total	Mg	0
			2	2	
89	R2	1	Total	Mg	0
			1	1	
89	i1	1	Total	Mg	0
			1	1	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
90	MB	1	Total	Zn	0
			1	1	
90	D1	1	Total	Zn	0
			1	1	
90	F1	1	Total	Zn	0
			1	1	
90	H1	1	Total	Zn	0
			1	1	
90	f2	1	Total	Zn	0
			1	1	

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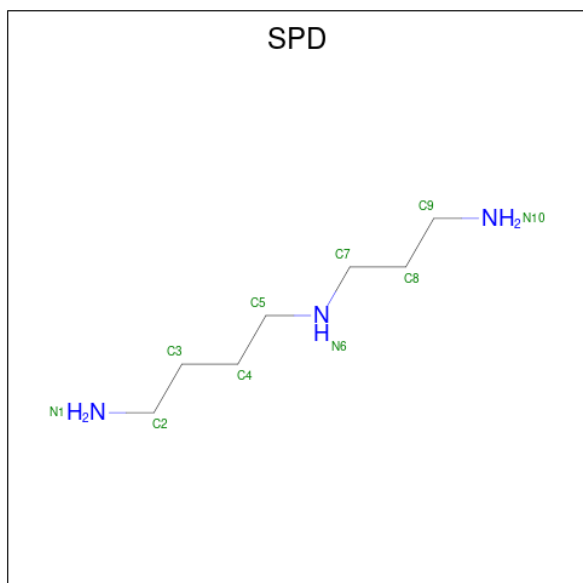
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Mol	Chain	Residues	Atoms		AltConf
90	i2	1	Total 1	Zn 1	0
90	j2	1	Total 1	Zn 1	0
90	k2	1	Total 1	Zn 1	0

- Molecule 91 is POTASSIUM ION (CCD ID: K) (formula: K).

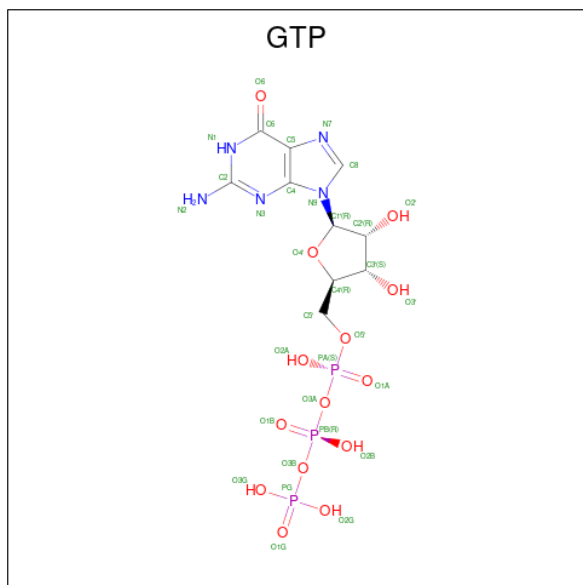
Mol	Chain	Residues	Atoms		AltConf
91	A1	9	Total 9	K 9	0
91	A3	22	Total 22	K 22	0
91	B3	2	Total 2	K 2	0
91	C3	1	Total 1	K 1	0
91	H1	1	Total 1	K 1	0
91	J2	1	Total 1	K 1	0
91	O2	1	Total 1	K 1	0

- Molecule 92 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



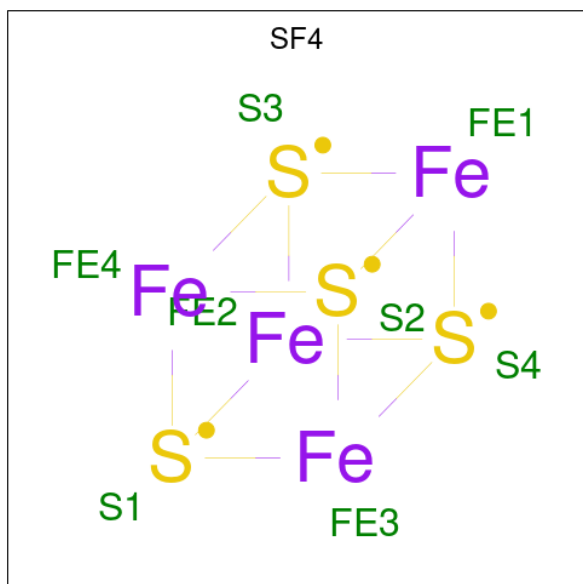
Mol	Chain	Residues	Atoms			AltConf
92	A3	1	Total	C	N	0
			10	7	3	
92	A3	1	Total	C	N	0
			10	7	3	

- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
93	B3	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 94 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
94	q2	1	Total 8	Fe 4	S 4	0
94	q2	1	Total 8	Fe 4	S 4	0

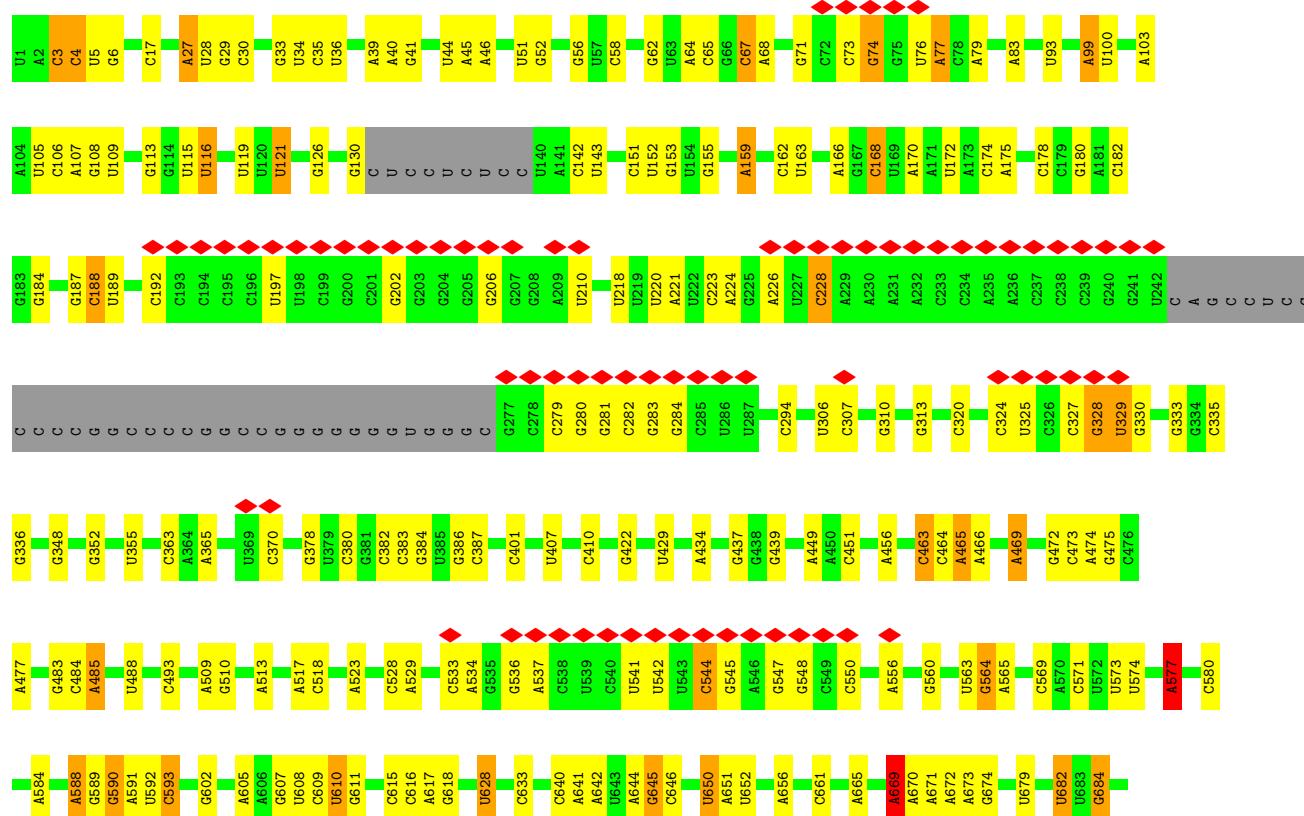
3 Residue-property plots

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

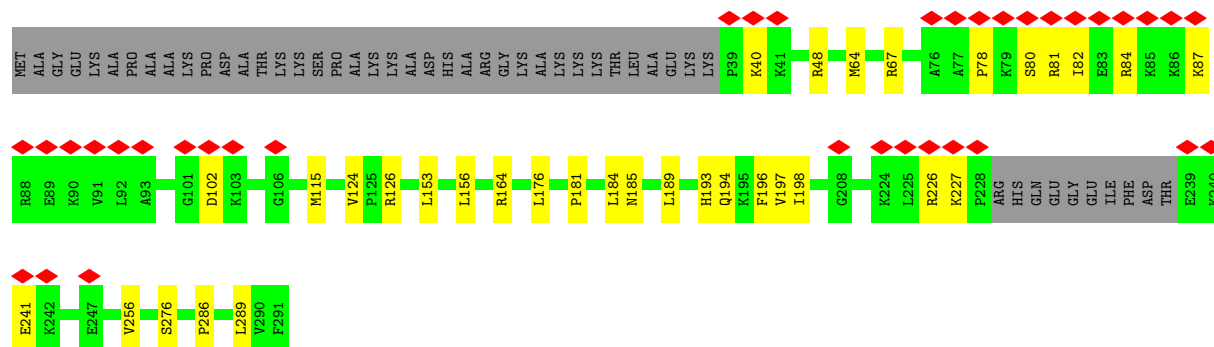
- Molecule 1: 60S ribosomal protein L34



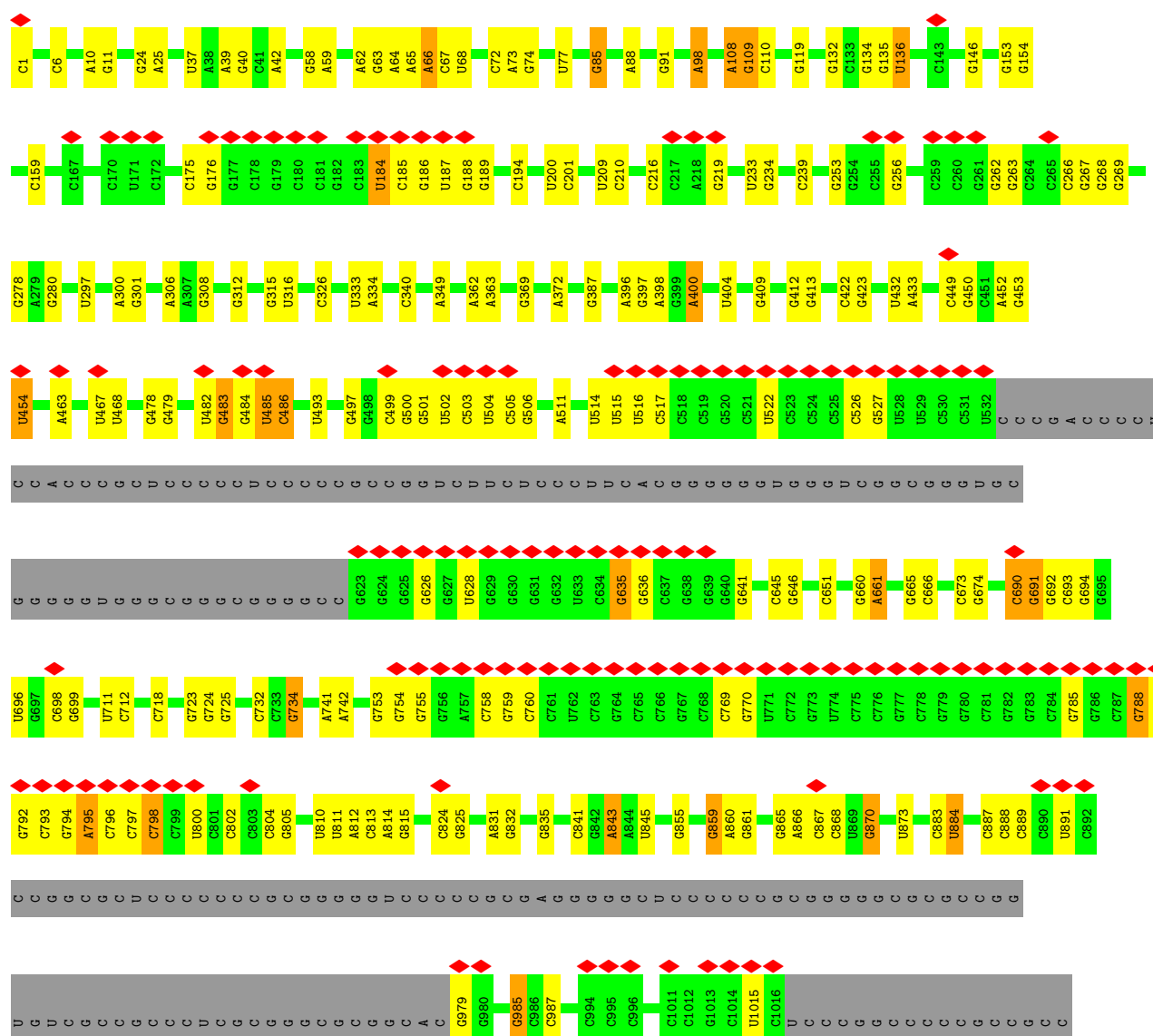
- Molecule 2: 18S rRNA

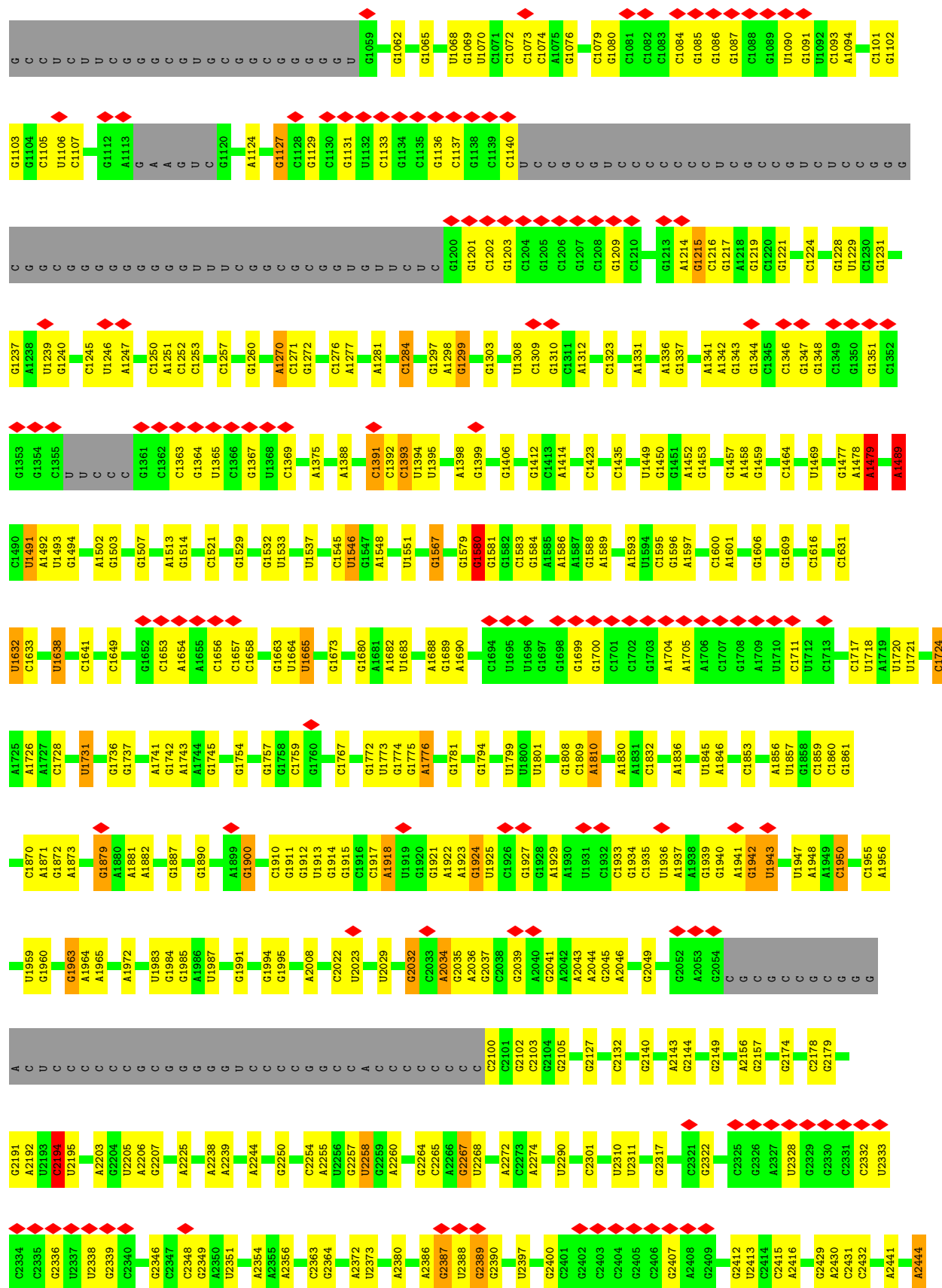




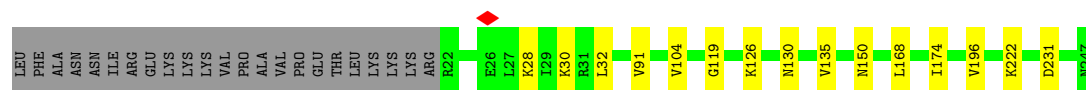


• Molecule 4: 28S rRNA

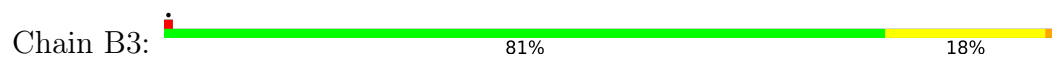




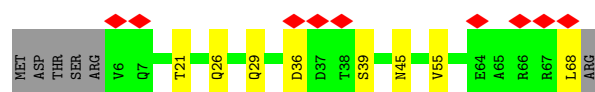
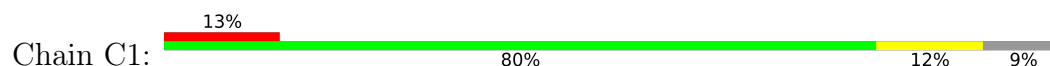




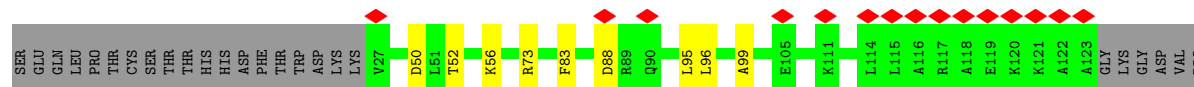
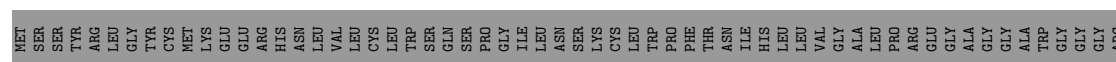
- Molecule 7: 5S rRNA



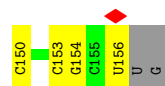
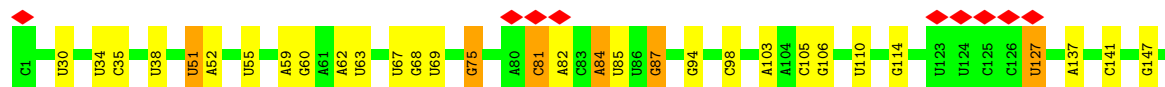
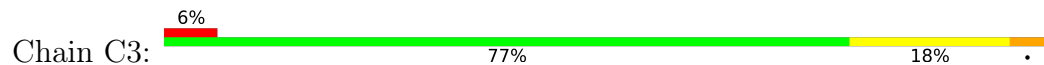
- Molecule 8: Small ribosomal subunit protein eS28



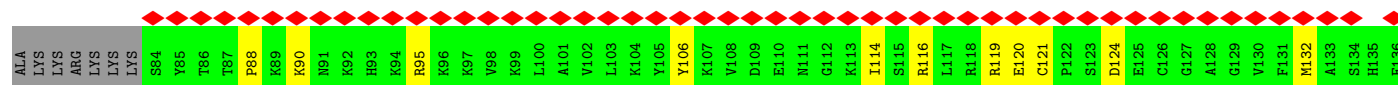
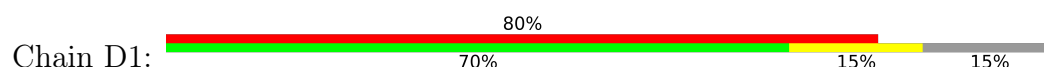
- Molecule 9: Large ribosomal subunit protein eL8

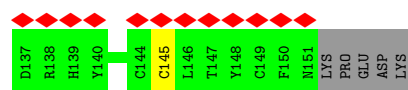


- Molecule 10: 5.8S rRNA



- Molecule 11: Ubiquitin-ribosomal protein eS31 fusion protein

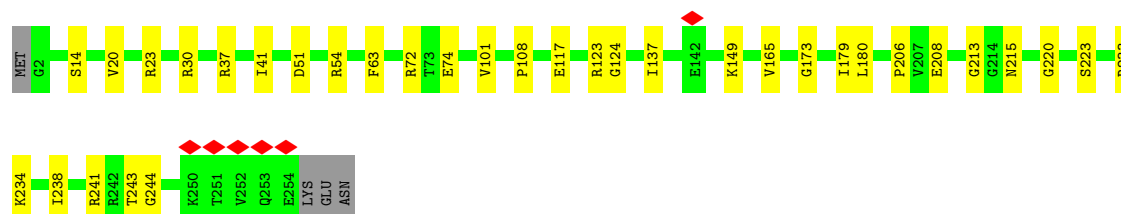




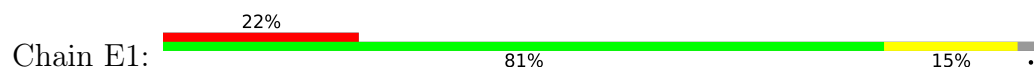
- Molecule 12: 60S ribosomal protein L9



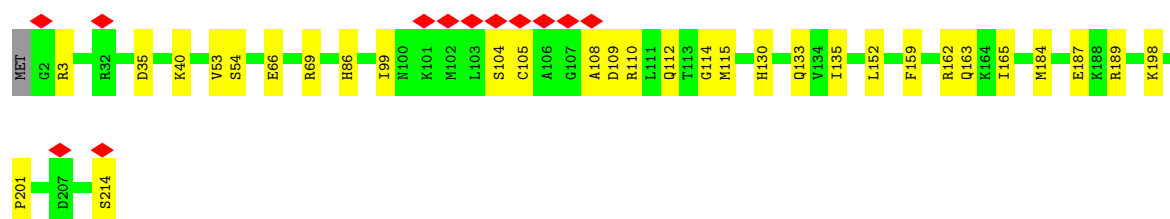
- Molecule 13: Large ribosomal subunit protein uL2



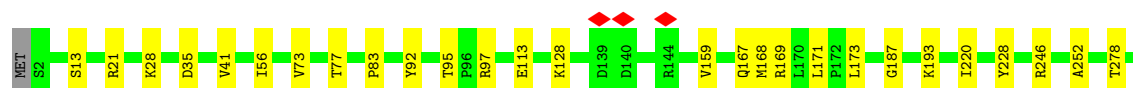
- Molecule 14: 40S ribosomal protein eS30



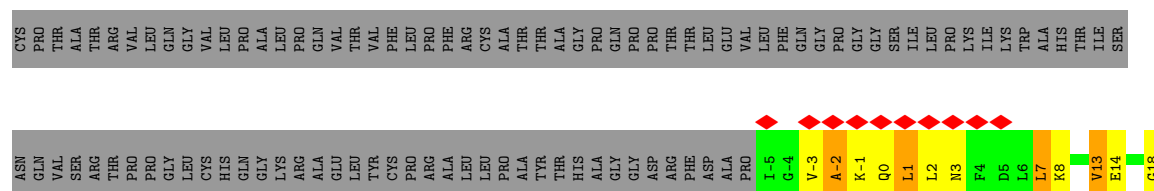
- Molecule 15: 60S ribosomal protein L10



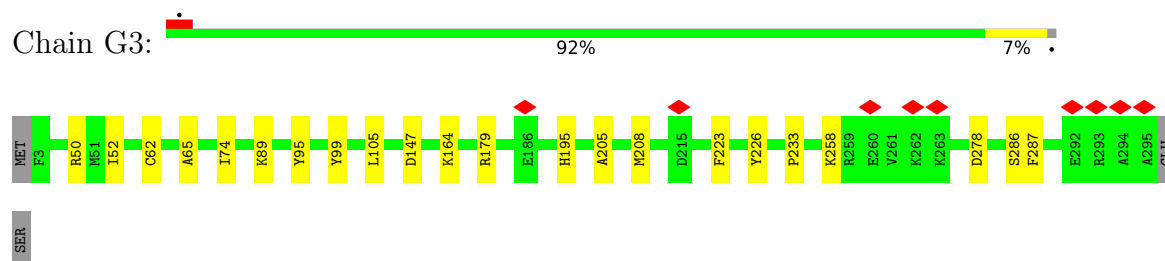
- Molecule 16: Ribosomal protein L3



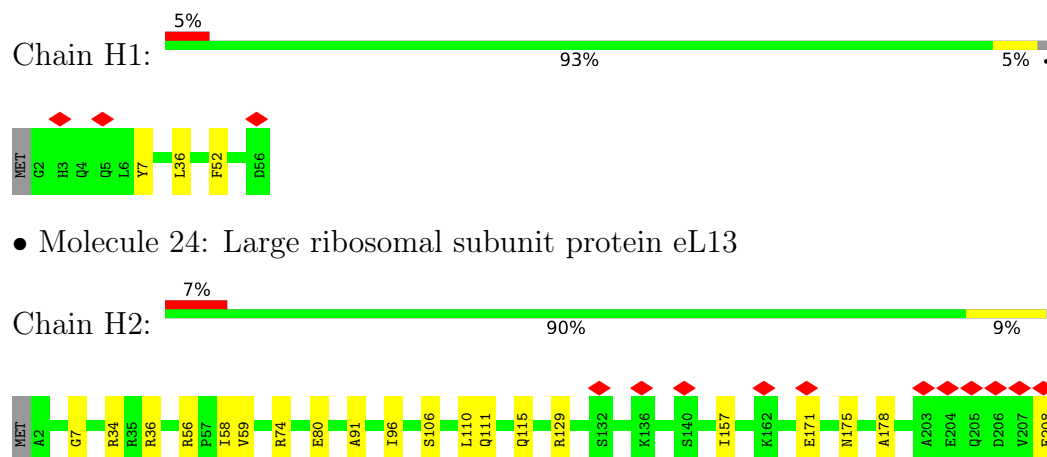




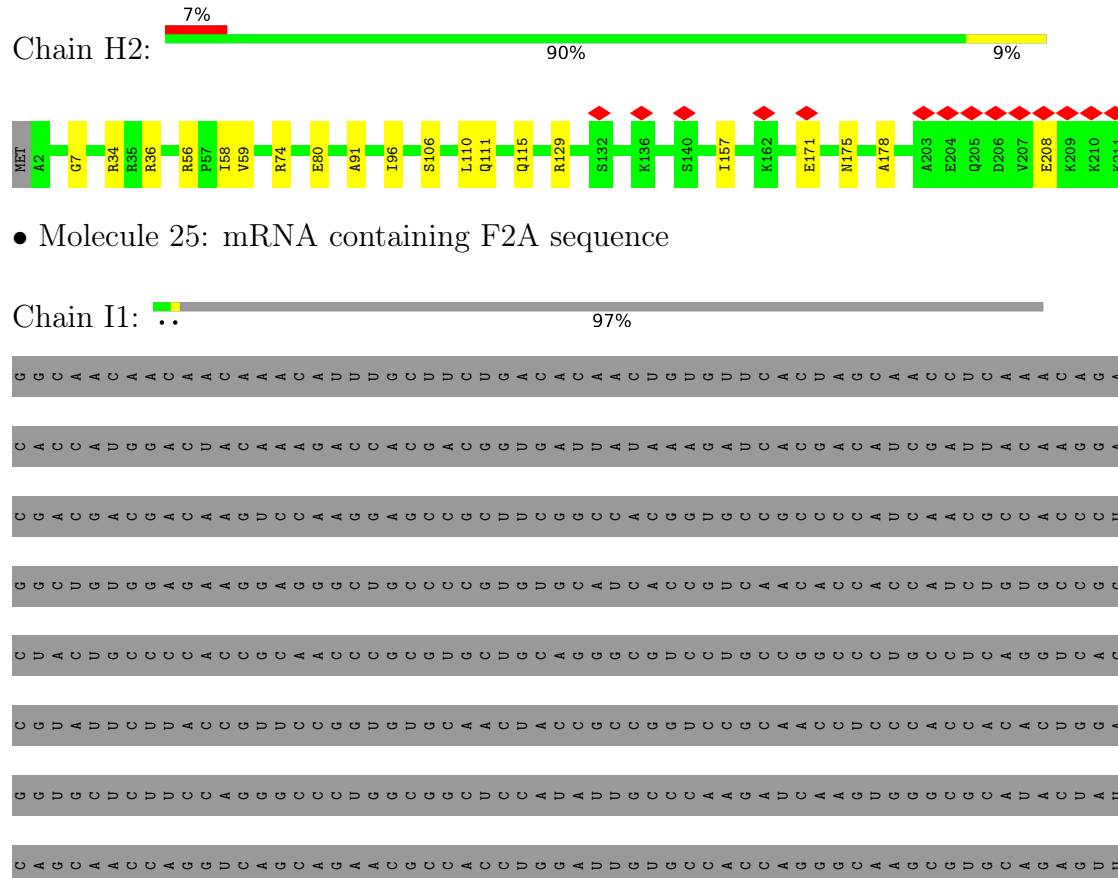
- Molecule 22: Large ribosomal subunit protein uL18



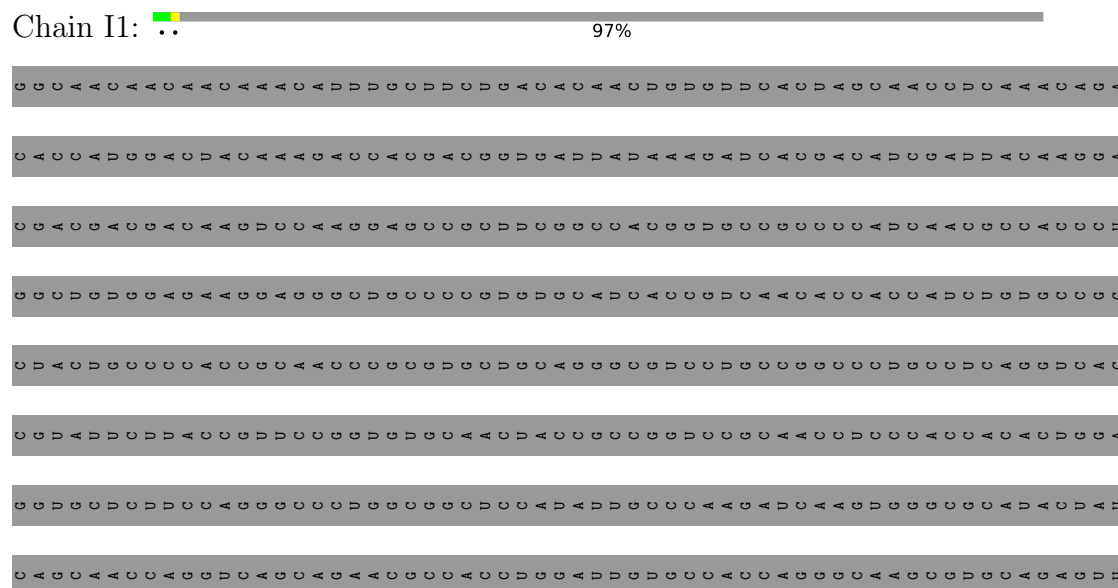
- Molecule 23: Small ribosomal subunit protein uS14



- Molecule 24: Large ribosomal subunit protein eL13

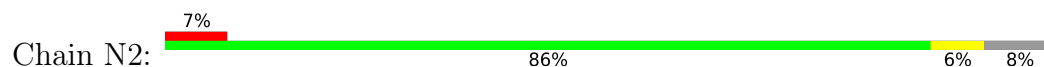


- Molecule 25: mRNA containing F2A sequence

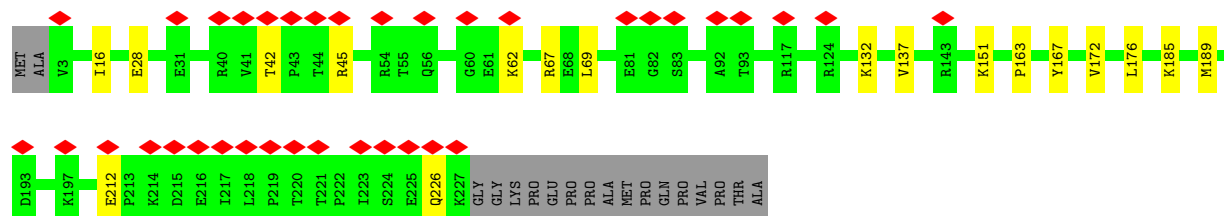
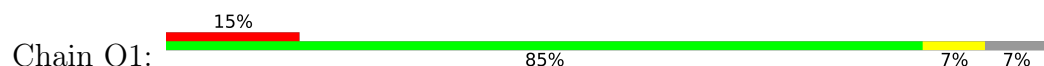




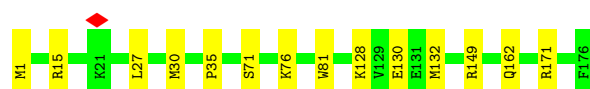
- Molecule 36: Ribosomal protein L19



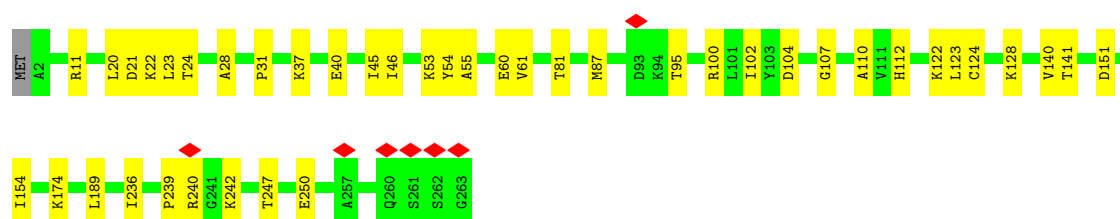
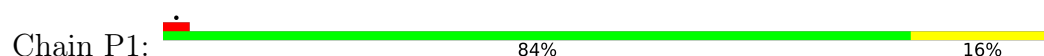
- Molecule 37: Small ribosomal subunit protein uS3



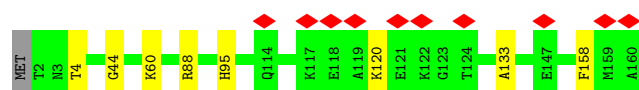
- Molecule 38: Large ribosomal subunit protein eL20



- Molecule 39: 40S ribosomal protein S4

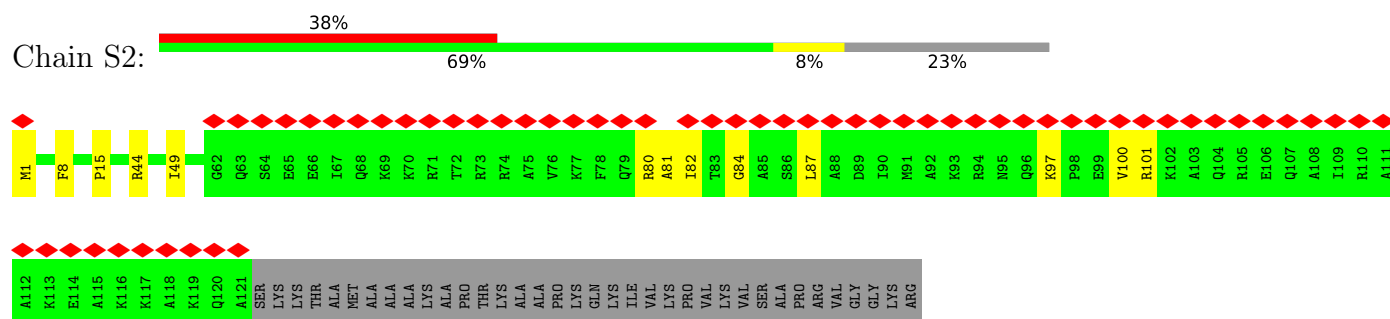


- Molecule 40: 60S ribosomal protein L21

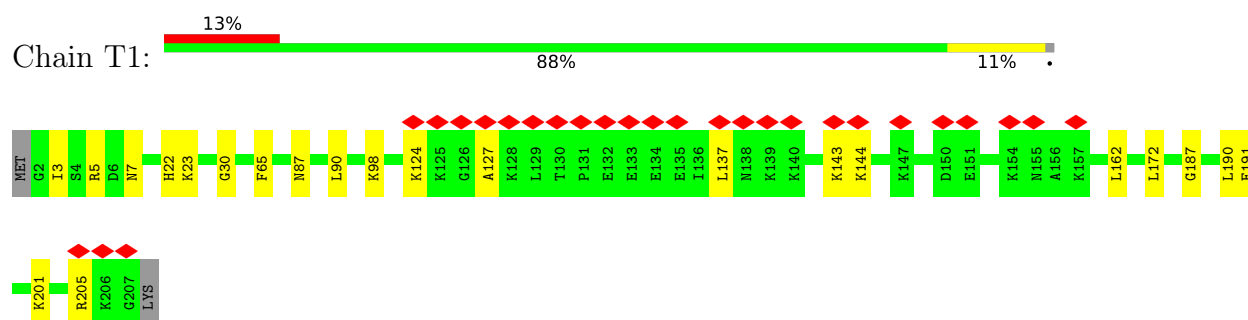


- Molecule 41: Small ribosomal subunit protein uS7

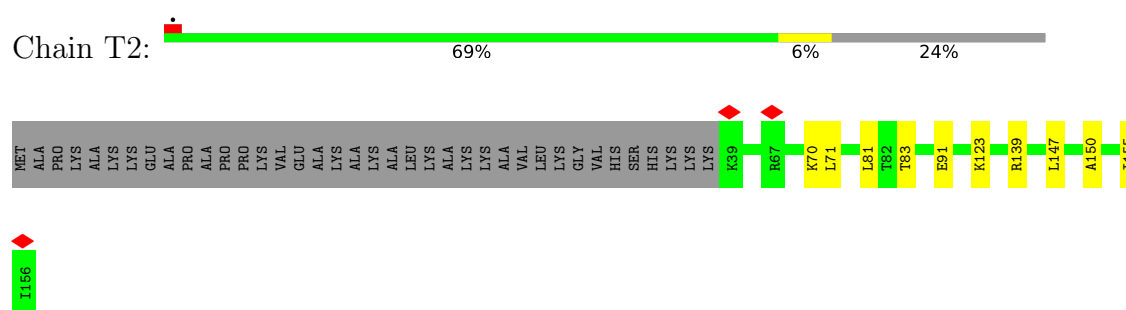
- Molecule 46: Ribosomal protein L24



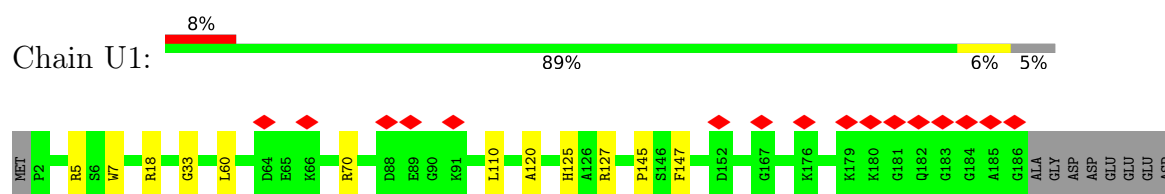
- Molecule 47: 40S ribosomal protein S8



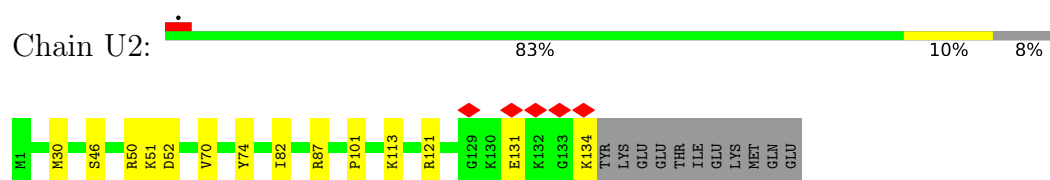
- Molecule 48: Large ribosomal subunit protein uL23



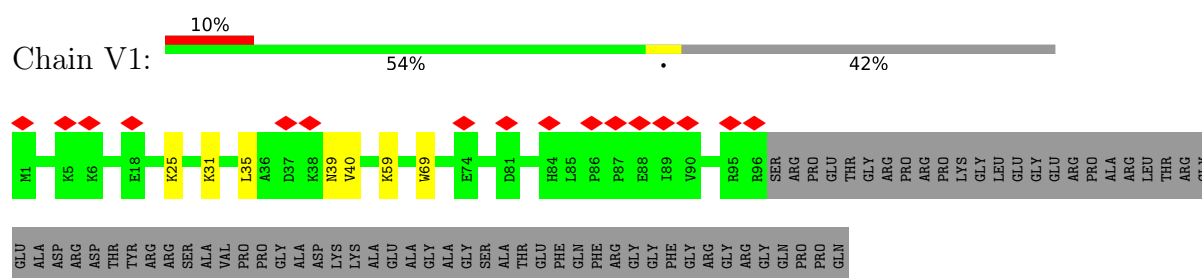
- Molecule 49: Small ribosomal subunit protein uS4



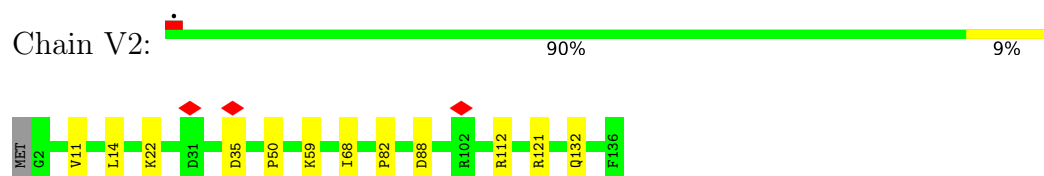
- Molecule 50: Ribosomal protein L26



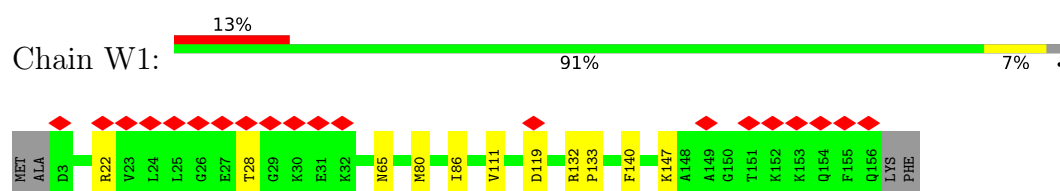
- Molecule 51: eS10



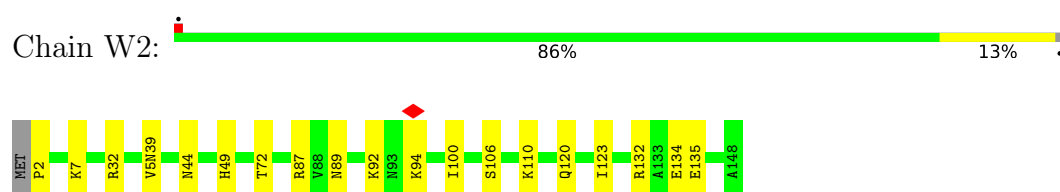
- Molecule 52: 60S ribosomal protein L27



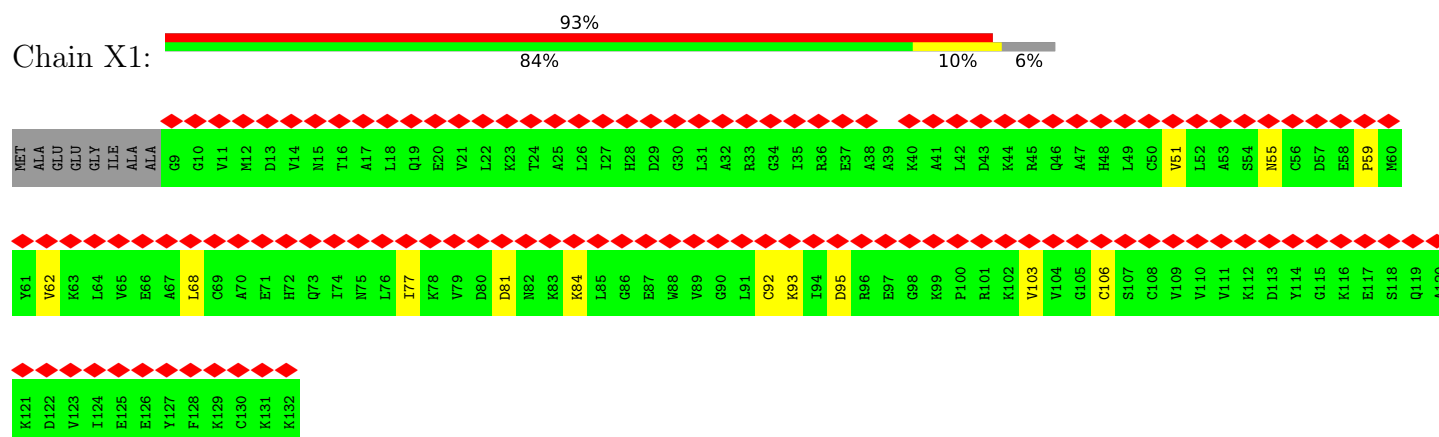
- Molecule 53: Small ribosomal subunit protein uS17



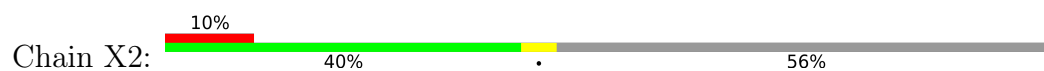
- Molecule 54: 60S ribosomal protein L27a

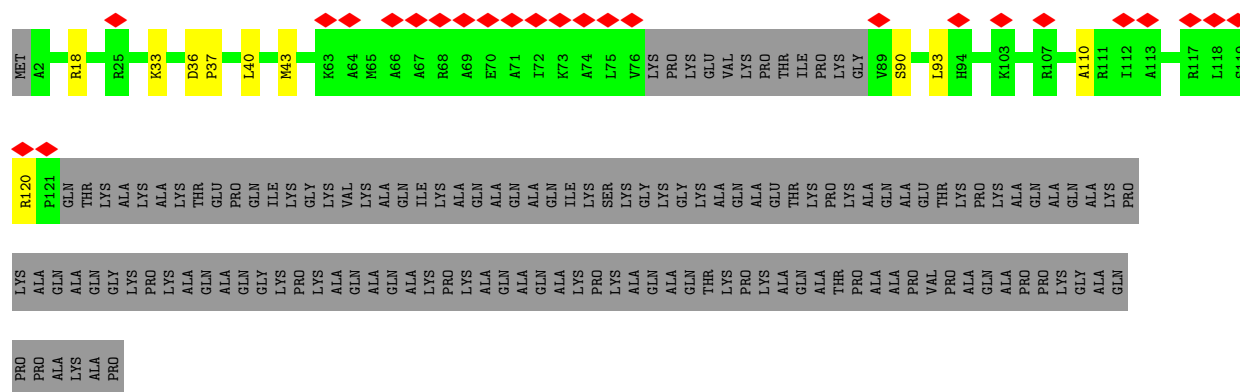


- Molecule 55: Small ribosomal subunit protein eS12



- Molecule 56: 60S ribosomal protein L29

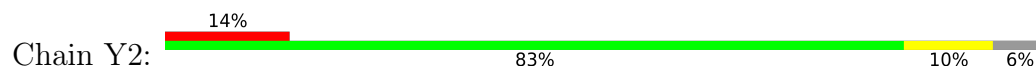




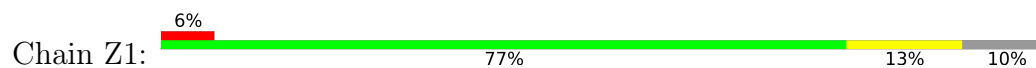
- Molecule 57: Small ribosomal subunit protein uS15



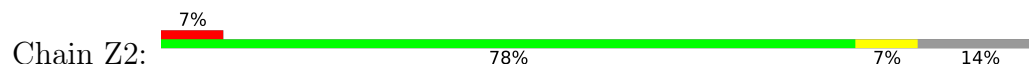
- Molecule 58: 60S ribosomal protein L30



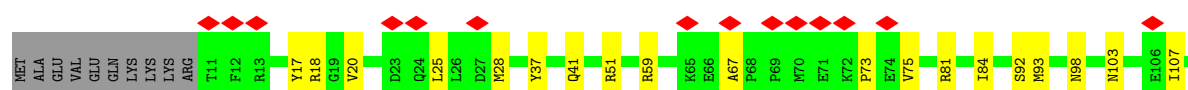
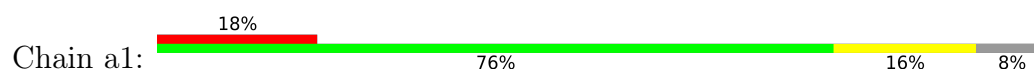
- Molecule 59: Small ribosomal subunit protein uS11

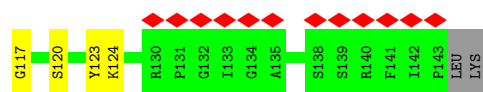


- Molecule 60: 60S ribosomal protein L31



- Molecule 61: Small ribosomal subunit protein uS19

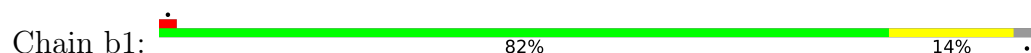




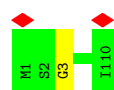
- Molecule 62: Ribosomal protein L32



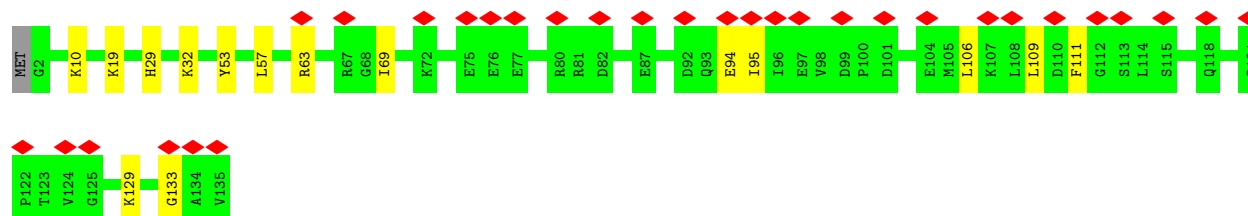
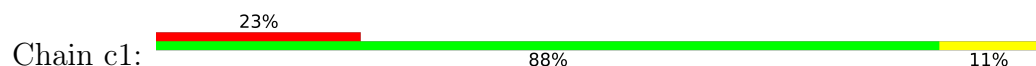
- Molecule 63: Small ribosomal subunit protein uS9



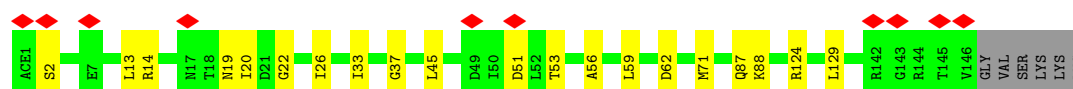
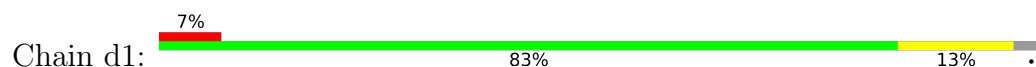
- Molecule 64: 60S ribosomal protein L35a



- Molecule 65: Small ribosomal subunit protein eS17



- Molecule 66: Small ribosomal subunit protein uS13

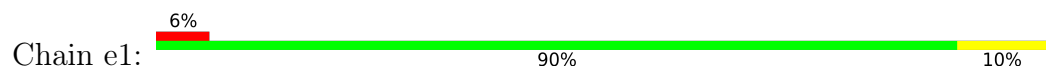


- Molecule 67: 60S ribosomal protein L35





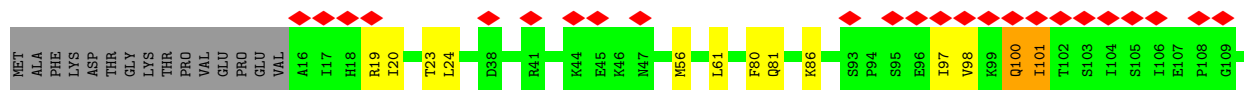
- Molecule 68: 40S ribosomal protein eS19



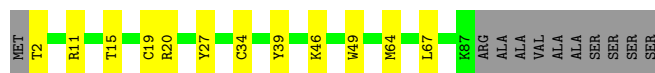
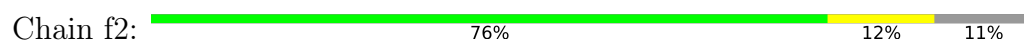
- Molecule 69: Large ribosomal subunit protein eL36



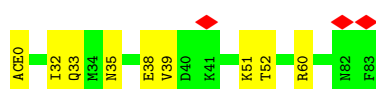
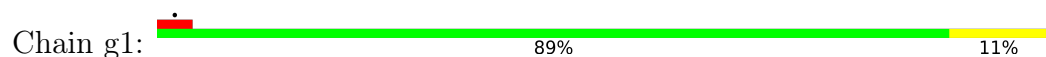
- Molecule 70: Small ribosomal subunit protein uS10



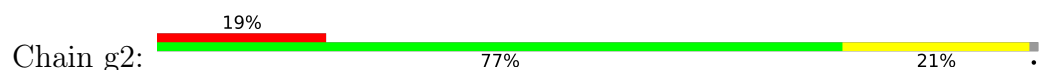
- Molecule 71: Ribosomal protein L37



- Molecule 72: Small ribosomal subunit protein eS21



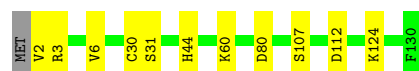
- Molecule 73: 60S ribosomal protein L38





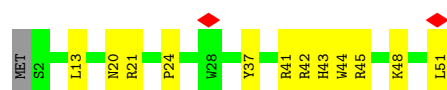
- Molecule 74: Small ribosomal subunit protein uS8

Chain h1: 91% 8%



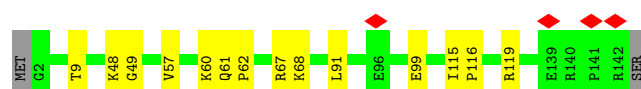
- Molecule 75: 60S ribosomal protein L39-like

Chain h2: 75% 24%



- Molecule 76: 40S ribosomal protein S23

Chain i1: 89% 10%



- Molecule 77: Ubiquitin-ribosomal protein eL40 fusion protein

Chain i2: 94% 6%



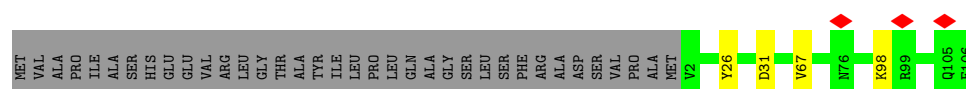
- Molecule 78: 40S ribosomal protein S24

Chain j1: 9% 80% 14% 6%

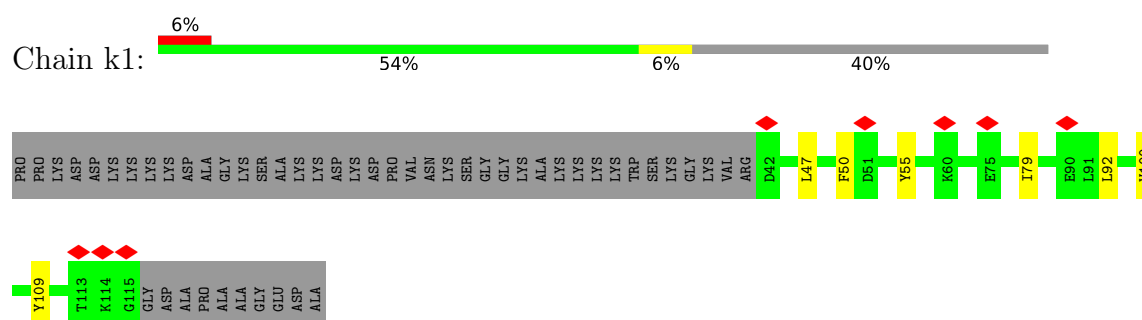


- Molecule 79: Ribosomal protein L36a

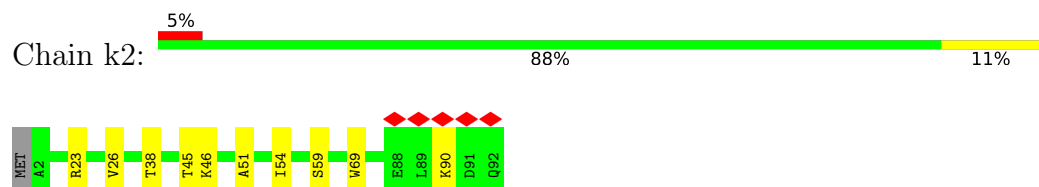
Chain j2: 72% 26%



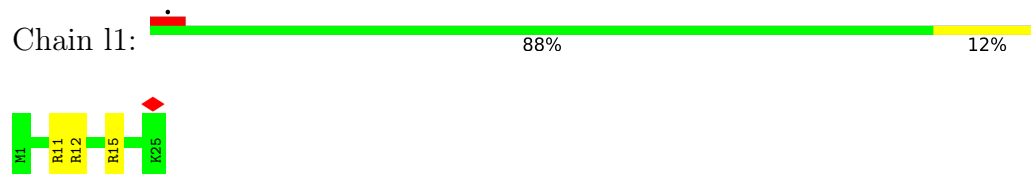
- Molecule 80: Small ribosomal subunit protein eS25



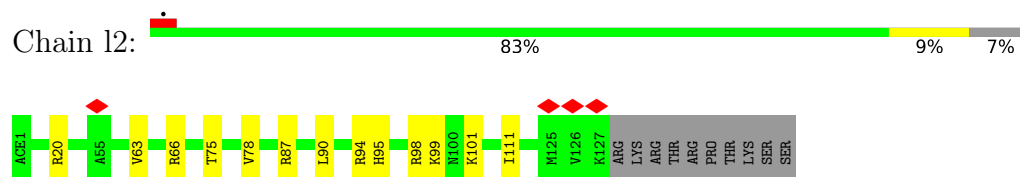
- Molecule 81: 60S ribosomal protein L37a



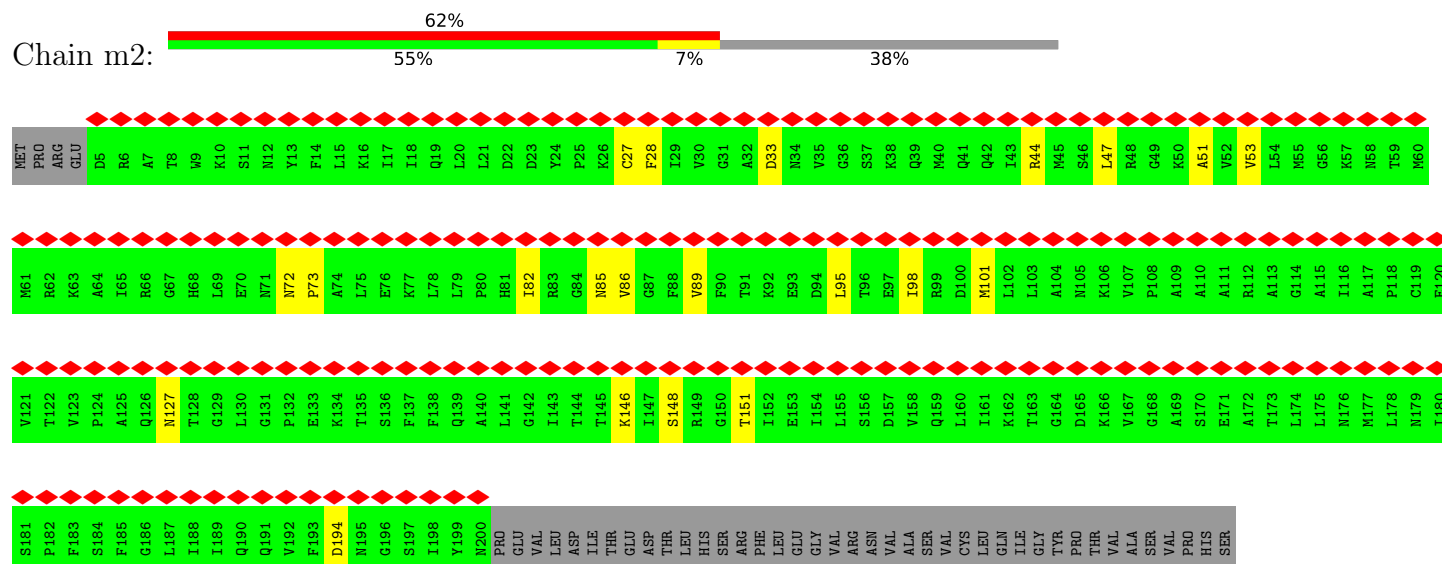
- Molecule 82: Small ribosomal subunit protein eS32

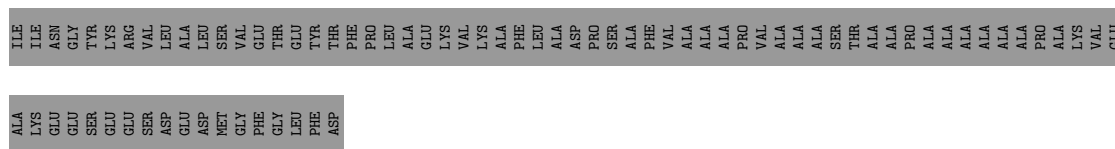


- Molecule 83: [histone H4]-N-methyl-L-lysine20 N-methyltransferase KMT5B

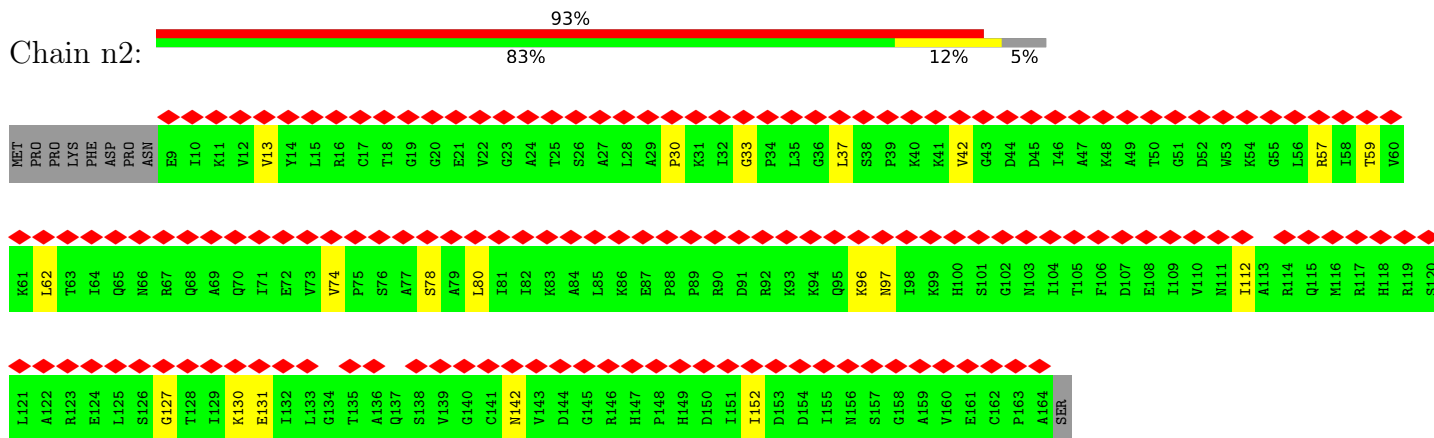


- Molecule 84: Large ribosomal subunit protein uL10

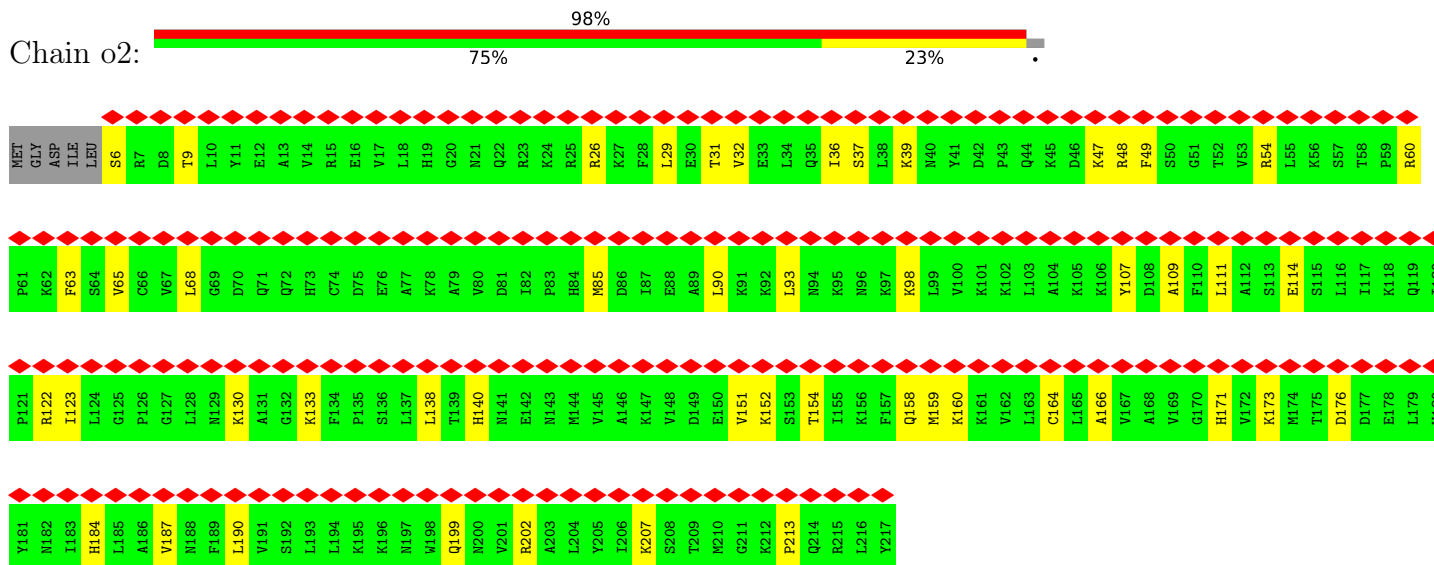




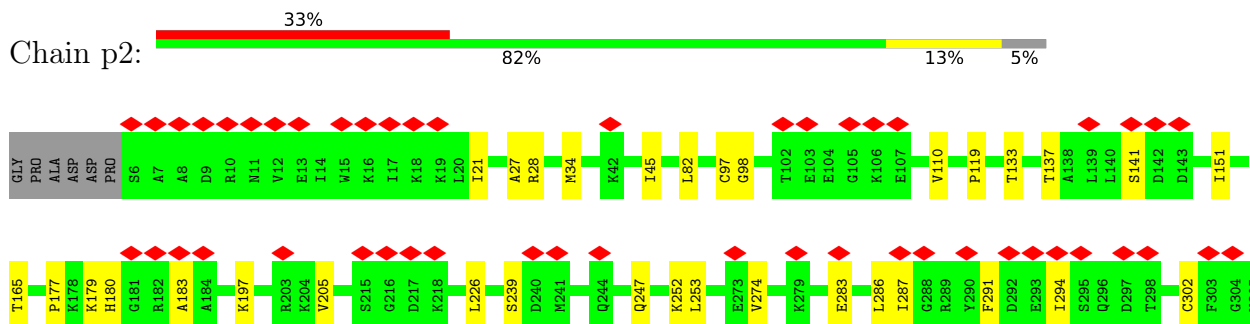
- Molecule 85: 60S ribosomal protein L12



- Molecule 86: Ribosomal protein uL1



- Molecule 87: Eukaryotic peptide chain release factor subunit 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49964	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	421.2, 421.2, 421.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.702, 0.702, 0.702	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 5MU, HY3, 4AC, HIC, SPD, SF4, K, OMG, MLZ, PSU, UR3, ACE, M3L, ZN, V5N, MG, B8N, UY1, MA6, NMM, OMC, 6MZ, H2U, 5MC, GTP, 1MA, A2M, G7M, 1MG

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	MB	0.17	0/916	0.39	0/1220
2	A1	0.25	0/40342	0.38	1/62877 (0.0%)
3	A2	0.16	0/1998	0.37	0/2673
4	A3	0.23	0/87403	0.38	0/136359
5	B1	0.16	0/665	0.43	0/891
6	B2	0.21	0/1922	0.44	0/2563
7	B3	0.22	0/2835	0.36	0/4418
8	C1	0.14	0/497	0.35	0/666
9	C2	0.19	0/1908	0.47	0/2566
10	C3	0.22	0/3635	0.36	0/5661
11	D1	0.17	0/566	0.44	0/753
12	D2	0.17	0/1535	0.43	0/2063
13	D3	0.18	0/1965	0.39	0/2633
14	E1	0.13	0/462	0.39	0/607
15	E2	0.18	0/1756	0.40	0/2346
16	E3	0.17	0/3261	0.40	0/4364
17	F1	0.20	0/828	0.48	0/1109
18	F2	0.17	0/1385	0.41	0/1852
19	F3	0.24	0/2938	0.41	0/3948
20	G1	0.22	0/2493	0.53	0/3394
21	G2	1.02	0/177	1.17	0/238
22	G3	0.15	0/2437	0.38	0/3264
23	H1	0.16	0/470	0.38	0/623
24	H2	0.17	0/1733	0.39	0/2316
25	I1	0.29	0/414	0.44	0/641
26	I2	0.19	0/1158	0.43	0/1547
27	J1	0.17	0/1779	0.39	0/2771
28	J2	0.17	0/1746	0.40	0/2338
29	K1	1.10	2/1456 (0.1%)	0.99	5/2269 (0.2%)
30	K2	0.21	0/1662	0.42	0/2222
31	L1	0.19	0/1778	0.45	0/2416

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	L2	0.18	0/1317	0.42	0/1768
33	M1	0.19	0/1841	0.45	0/2459
34	M2	0.18	0/1539	0.44	0/2054
35	N1	0.19	0/1742	0.44	0/2354
36	N2	0.18	0/1524	0.41	0/2013
37	O1	0.17	0/1779	0.43	0/2395
38	O2	0.21	0/1497	0.40	0/2008
39	P1	0.16	0/2118	0.42	0/2849
40	P2	0.16	0/1326	0.38	0/1770
41	Q1	0.20	0/1531	0.48	0/2059
42	Q2	0.18	0/811	0.46	0/1088
43	R1	0.17	0/1946	0.43	0/2590
44	R2	0.16	0/1048	0.42	0/1402
45	S1	0.27	0/1552	0.50	0/2079
46	S2	0.16	0/1006	0.39	0/1334
47	T1	0.23	0/1715	0.47	0/2287
48	T2	0.17	0/984	0.39	0/1323
49	U1	0.17	0/1550	0.42	0/2069
50	U2	0.27	0/1132	0.52	0/1504
51	V1	0.20	0/834	0.49	0/1125
52	V2	0.15	0/1130	0.33	0/1507
53	W1	0.16	0/1284	0.38	0/1717
54	W2	0.16	0/1179	0.38	0/1572
55	X1	0.23	0/968	0.57	0/1296
56	X2	0.16	0/884	0.39	0/1169
57	Y1	0.18	0/1232	0.39	0/1656
58	Y2	0.19	0/847	0.43	0/1134
59	Z1	0.18	0/1029	0.41	0/1380
60	Z2	0.19	0/903	0.43	0/1216
61	a1	0.21	0/1114	0.46	0/1490
62	a2	0.17	0/1088	0.43	0/1451
63	b1	0.22	0/1142	0.46	0/1528
64	b2	0.17	0/903	0.36	0/1208
65	c1	0.19	0/1094	0.44	0/1469
66	d1	0.19	0/1216	0.44	0/1630
67	d2	0.16	0/1021	0.37	0/1348
68	e1	0.16	0/1119	0.39	0/1498
69	e2	0.19	0/841	0.44	0/1112
70	f1	0.33	0/832	0.62	0/1117
71	f2	0.17	0/720	0.42	0/952
72	g1	0.30	1/645 (0.2%)	0.47	0/864
73	g2	0.18	0/575	0.40	0/761
74	h1	0.17	0/1051	0.40	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	h2	0.17	0/459	0.38	0/608
76	i1	0.21	0/1107	0.42	0/1475
77	i2	0.17	0/426	0.43	0/564
78	j1	0.17	0/1032	0.41	0/1371
79	j2	0.15	0/866	0.35	0/1141
80	k1	0.19	0/593	0.45	0/796
81	k2	0.20	0/718	0.49	0/953
82	l1	0.20	0/240	0.42	0/305
83	l2	0.19	0/1027	0.44	0/1376
84	m2	0.19	0/1530	0.49	0/2064
85	n2	0.20	0/1193	0.51	0/1609
86	o2	0.21	0/1735	0.51	0/2328
87	p2	0.27	0/3333	0.52	0/4483
88	q2	0.20	0/4755	0.50	0/6421
All	All	0.23	3/244743 (0.0%)	0.41	6/358113 (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
19	F3	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K1	46	A	O3'-P	22.69	1.95	1.61
29	K1	16	H2U	O3'-P	22.66	1.95	1.61
72	g1	0	ACE	C-N	6.16	1.45	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K1	16	H2U	O3'-P-O5'	-10.44	88.34	104.00
29	K1	46	A	OP2-P-O3'	9.41	136.25	108.00
29	K1	46	A	P-O3'-C3'	9.10	133.85	120.20
29	K1	16	H2U	OP2-P-O3'	8.32	132.96	108.00
29	K1	16	H2U	P-O3'-C3'	7.53	131.50	120.20
2	A1	1521	G	C2'-C3'-O3'	-5.21	105.88	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	F3	248	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	MB	906	0	998	5	0
2	A1	37833	0	19168	222	0
3	A2	1960	0	2153	24	0
4	A3	80772	0	40889	411	0
5	B1	651	0	672	4	0
6	B2	1886	0	2008	9	0
7	B3	2538	0	1284	10	0
8	C1	495	0	523	6	0
9	C2	1877	0	2023	13	0
10	C3	3319	0	1684	17	0
11	D1	554	0	556	9	0
12	D2	1516	0	1597	10	0
13	D3	1940	0	2029	25	0
14	E1	457	0	502	8	0
15	E2	1717	0	1764	24	0
16	E3	3206	0	3353	28	0
17	F1	814	0	863	12	0
18	F2	1362	0	1399	7	0
19	F3	2886	0	3057	18	0
20	G1	2436	0	2389	29	0
21	G2	176	0	186	18	0
22	G3	2391	0	2424	15	0
23	H1	459	0	448	3	0
24	H2	1702	0	1820	16	0
25	I1	374	0	191	0	0
26	I2	1137	0	1211	5	0
27	J1	1593	0	809	15	0
28	J2	1701	0	1749	13	0
29	K1	1582	0	819	18	0
30	K2	1630	0	1778	8	0
31	L1	1743	0	1748	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L2	1289	0	1329	4	0
33	M1	1815	0	1908	23	0
34	M2	1515	0	1634	10	0
35	N1	1706	0	1796	13	0
36	N2	1508	0	1664	12	0
37	O1	1751	0	1846	11	0
38	O2	1457	0	1492	9	0
39	P1	2076	0	2177	24	0
40	P2	1298	0	1366	7	0
41	Q1	1509	0	1563	11	0
42	Q2	797	0	819	7	0
43	R1	1923	0	2089	34	0
44	R2	1034	0	1097	9	0
45	S1	1529	0	1627	15	0
46	S2	991	0	1048	9	0
47	T1	1686	0	1772	16	0
48	T2	967	0	1040	6	0
49	U1	1525	0	1640	11	0
50	U2	1115	0	1205	10	0
51	V1	810	0	836	4	0
52	V2	1107	0	1182	9	0
53	W1	1262	0	1335	6	0
54	W2	1163	0	1202	14	0
55	X1	958	0	993	10	0
56	X2	881	0	957	7	0
57	Y1	1208	0	1294	10	0
58	Y2	836	0	888	7	0
59	Z1	1016	0	1039	14	0
60	Z2	888	0	930	6	0
61	a1	1091	0	1138	16	0
62	a2	1070	0	1165	5	0
63	b1	1124	0	1193	12	0
64	b2	884	0	924	1	0
65	c1	1080	0	1135	10	0
66	d1	1200	0	1262	16	0
67	d2	1013	0	1147	6	0
68	e1	1113	0	1145	10	0
69	e2	830	0	916	4	0
70	f1	822	0	887	9	0
71	f2	705	0	737	10	0
72	g1	640	0	633	5	0
73	g2	569	0	637	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	h1	1034	0	1080	8	0
75	h2	447	0	480	10	0
76	i1	1099	0	1162	9	0
77	i2	432	0	470	4	0
78	j1	1015	0	1086	12	0
79	j2	863	0	929	3	0
80	k1	587	0	643	4	0
81	k2	708	0	756	7	0
82	l1	239	0	289	2	0
83	l2	1014	0	1083	9	0
84	m2	1507	0	1564	13	0
85	n2	1178	0	1235	13	0
86	o2	1707	0	1815	36	0
87	p2	3280	0	3326	39	0
88	q2	4668	0	4784	53	0
89	A1	109	0	0	0	0
89	A3	239	0	0	0	0
89	B3	4	0	0	0	0
89	C3	5	0	0	0	0
89	E2	1	0	0	0	0
89	E3	1	0	0	0	0
89	I1	2	0	0	0	0
89	J2	1	0	0	0	0
89	L2	2	0	0	0	0
89	MB	1	0	0	0	0
89	R2	1	0	0	0	0
89	i1	1	0	0	0	0
90	D1	1	0	0	0	0
90	F1	1	0	0	0	0
90	H1	1	0	0	0	0
90	MB	1	0	0	0	0
90	f2	1	0	0	0	0
90	i2	1	0	0	0	0
90	j2	1	0	0	0	0
90	k2	1	0	0	0	0
91	A1	9	0	0	0	0
91	A3	22	0	0	0	0
91	B3	2	0	0	0	0
91	C3	1	0	0	0	0
91	H1	1	0	0	0	0
91	J2	1	0	0	0	0
91	O2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	A3	20	0	38	1	0
93	B3	32	0	11	0	0
94	q2	16	0	0	0	0
All	All	233632	0	175532	1370	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 (1370) 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)
20:G1:153:CYS:HB3	20:G1:168:CYS:O	1.60	1.00
4:A3:3703:G:H21	4:A3:3778:A:N6	1.60	0.99
2:A1:541:U:H3	2:A1:544:C:N4	1.60	0.97
4:A3:755:G:H1	4:A3:800:U:H3	1.03	0.95
19:F3:71:ARG:HH22	21:G2:1:LEU:HD11	1.33	0.93
4:A3:1015:U:H3	4:A3:1086:G:H1	1.14	0.92
86:o2:6:SER:N	86:o2:9:THR:HG1	1.68	0.91
4:A3:3703:G:H21	4:A3:3778:A:H62	0.98	0.91
4:A3:3703:G:N2	4:A3:3778:A:H62	1.67	0.91
2:A1:1758:G:H1	2:A1:1776:U:H3	1.13	0.91
29:K1:15:G:H2'	29:K1:16:H2U:H62	1.57	0.86
2:A1:324:C:H42	2:A1:328:G:H22	1.24	0.85
4:A3:1351:G:H1	4:A3:1365:U:H3	1.20	0.85
2:A1:197:U:H3	2:A1:202:G:H1	1.22	0.84
2:A1:541:U:H3	2:A1:544:C:H42	0.87	0.82
70:f1:20:ILE:HG21	70:f1:98:VAL:HG21	1.62	0.82
2:A1:324:C:N4	2:A1:328:G:H22	1.80	0.80
19:F3:67:TRP:CH2	21:G2:1:LEU:HG	2.20	0.77
27:J1:6:G:H1	27:J1:67:U:H3	1.33	0.77
4:A3:2400:G:H1	4:A3:2413:U:H3	1.30	0.77
2:A1:324:C:H42	2:A1:328:G:N2	1.83	0.76
21:G2:0:GLN:HG3	21:G2:2:LEU:HD21	1.71	0.72
4:A3:1933:C:H2'	4:A3:1934:G:H8	1.55	0.70
2:A1:941:U:H3	2:A1:1003:U:H3	1.38	0.69
19:F3:208:CYS:SG	19:F3:230:LEU:HD12	2.33	0.69
86:o2:107:TYR:O	86:o2:133:LYS:NZ	2.26	0.68
59:Z1:34:PHE:HB3	59:Z1:41:PHE:HB2	1.76	0.68
85:n2:130:LYS:HG3	85:n2:152:ILE:HD11	1.77	0.67
4:A3:522:U:H3	4:A3:635:G:H1	1.42	0.67
4:A3:3491:A:H5'	4:A3:3497:G:H22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:2205:U:H2'	4:A3:2206:A2M:H8	1.77	0.67
2:A1:1749:G:H1	2:A1:1787:U:H3	1.41	0.66
4:A3:4294:A:H1'	87:p2:179:LYS:O	1.95	0.66
86:o2:49:PHE:HB2	86:o2:159:MET:HB2	1.78	0.66
4:A3:1915:G:H1	4:A3:1929:A:H2	1.43	0.66
43:R1:2:LYS:HB2	43:R1:108:VAL:HG22	1.78	0.66
2:A1:926:G:H1	2:A1:1018:U:H3	1.44	0.66
4:A3:1879:G:H22	4:A3:4180:C:H5''	1.62	0.65
20:G1:240:CYS:H	20:G1:249:CYS:HB2	1.62	0.65
21:G2:1:LEU:O	21:G2:2:LEU:HD23	1.97	0.65
4:A3:2637:C:N3	21:G2:0:GLN:HG2	2.11	0.65
88:q2:106:LEU:HB3	88:q2:270:ILE:HG22	1.79	0.65
2:A1:1193:U:OP2	76:i1:119:ARG:NH2	2.30	0.64
2:A1:537:A:N6	2:A1:548:G:N1	2.45	0.64
44:R2:73:ARG:HG2	44:R2:74:LYS:HG3	1.79	0.64
12:D2:44:GLU:HB3	12:D2:58:ASP:HB2	1.80	0.64
28:J2:135:ILE:HG23	28:J2:142:ILE:HD13	1.80	0.64
33:M1:124:HIS:HA	33:M1:137:LEU:O	1.97	0.64
4:A3:3374:A:HO2'	71:f2:2:THR:N	1.96	0.64
29:K1:21:A:O2'	29:K1:46:A:N6	2.31	0.64
33:M1:28:LYS:HB3	33:M1:48:LEU:HD11	1.80	0.64
70:f1:19:ARG:HB2	70:f1:117:ALA:HB3	1.79	0.63
4:A3:4779:U:OP2	16:E3:396:ARG:NH2	2.32	0.63
63:b1:97:GLN:HG3	63:b1:105:LYS:HD2	1.81	0.63
4:A3:870:G:OP1	4:A3:2102:G:N2	2.32	0.63
4:A3:1297:G:N7	34:M2:104:ARG:NH2	2.46	0.63
14:E1:105:ARG:HD3	49:U1:127:ARG:HD3	1.80	0.62
14:E1:110:MET:SD	14:E1:114:ARG:NH1	2.72	0.62
39:P1:87:MET:HE2	39:P1:123:LEU:HB2	1.82	0.62
4:A3:1308:U:OP2	24:H2:36:ARG:NH2	2.32	0.62
29:K1:44:C:H2'	29:K1:45:G:C8	2.33	0.62
36:N2:39:GLN:OE1	36:N2:42:ARG:NH2	2.32	0.62
2:A1:153:G:N3	43:R1:13:GLN:NE2	2.47	0.62
2:A1:1521:G:N3	2:A1:1521:G:H2'	2.15	0.62
2:A1:1565:C:OP1	68:e1:105:GLN:NE2	2.32	0.62
87:p2:286:LEU:HD11	87:p2:319:ILE:HG21	1.82	0.61
20:G1:87:LEU:HB2	20:G1:101:PHE:HB2	1.82	0.61
66:d1:22:GLY:HA2	66:d1:56:ALA:HB3	1.82	0.61
43:R1:162:LEU:HD22	43:R1:170:ARG:HB2	1.82	0.60
85:n2:127:GLY:HA2	85:n2:130:LYS:HE2	1.83	0.60
4:A3:1398:A:H3'	4:A3:1399:G:H21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:2239:A:N7	4:A3:2657:C:H2'	2.16	0.60
2:A1:1397:A:O2'	2:A1:1399:G:N7	2.34	0.60
33:M1:183:GLU:HA	33:M1:186:ASN:HB2	1.83	0.60
85:n2:33:GLY:HA3	87:p2:420:GLN:HE21	1.67	0.60
2:A1:1092:C:HO2'	74:h1:2:VAL:N	1.99	0.60
70:f1:56:MET:HB2	70:f1:86:LYS:HB3	1.84	0.60
2:A1:1746:A:H1'	43:R1:66:GLY:HA2	1.84	0.60
10:C3:81:C:HO2'	67:d2:2:ALA:N	2.00	0.60
87:p2:34:MET:HG3	87:p2:98:GLY:HA3	1.84	0.60
15:E2:108:ALA:HA	87:p2:197:LYS:HZ1	1.66	0.59
21:G2:1:LEU:HD22	21:G2:2:LEU:N	2.17	0.59
42:Q2:41:GLN:OE1	42:Q2:44:GLN:NE2	2.35	0.59
33:M1:40:ASN:ND2	33:M1:75:GLN:OE1	2.35	0.59
63:b1:85:ARG:NH2	63:b1:118:THR:OG1	2.36	0.59
4:A3:3699:G:N2	86:o2:164:CYS:SG	2.75	0.59
2:A1:1551:G:H3'	2:A1:1580:A:H61	1.68	0.59
4:A3:3449:A:H2'	4:A3:3450:A2M:C8	2.32	0.59
4:A3:3805:A:N1	4:A3:3917:C:N4	2.51	0.58
86:o2:65:VAL:HG22	86:o2:109:ALA:HB3	1.85	0.58
4:A3:2415:C:O2'	52:V2:112:ARG:NH2	2.36	0.58
4:A3:3520:C:N4	4:A3:3544:C:OP2	2.36	0.58
88:q2:375:MET:HA	88:q2:531:ARG:O	2.04	0.58
23:H1:52:PHE:HB3	70:f1:80:PHE:HB3	1.85	0.58
45:S1:63:PHE:HA	45:S1:95:ILE:O	2.03	0.58
4:A3:396:A:H2'	4:A3:397:G:C8	2.39	0.58
2:A1:1544:U:OP1	63:b1:37:ARG:NH2	2.36	0.58
88:q2:331:PHE:HB3	88:q2:498:LEU:HD21	1.83	0.58
4:A3:753:G:H1	4:A3:802:C:H42	1.51	0.58
4:A3:1724:C:OP1	15:E2:133:GLN:NE2	2.37	0.58
4:A3:4480:A:H61	4:A3:4704:U:H3	1.52	0.58
4:A3:2022:C:OP2	34:M2:14:ARG:NH2	2.33	0.58
82:l1:12:ARG:HG2	82:l1:15:ARG:HH21	1.69	0.58
2:A1:1025:A:OP2	57:Y1:124:ARG:NH2	2.37	0.58
4:A3:2194:OMC:HM22	4:A3:2195:U:H5'	1.84	0.58
76:i1:60:LYS:HG3	76:i1:116:PRO:HG3	1.86	0.58
4:A3:67:C:OP2	4:A3:312:G:N2	2.37	0.57
4:A3:2328:U:H3	4:A3:2336:G:H1	1.52	0.57
8:C1:29:GLN:NE2	8:C1:45:ASN:OD1	2.35	0.57
2:A1:1292:A:HO2'	11:D1:145:CYS:HG	1.50	0.57
4:A3:4012:G:N3	4:A3:4012:G:H2'	2.20	0.57
15:E2:105:CYS:SG	15:E2:110:ARG:NH1	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G1:120:ILE:HB	20:G1:132:TRP:HB2	1.84	0.57
2:A1:985:C:O2'	59:Z1:138:ASP:OD2	2.23	0.57
2:A1:1758:G:N2	2:A1:1776:U:O2	2.36	0.57
18:F2:51:SER:HB2	18:F2:69:ALA:HB3	1.87	0.57
4:A3:1935:C:H42	4:A3:1939:G:N2	2.02	0.57
4:A3:4220:A:H5''	77:i2:125:LYS:HG3	1.87	0.57
4:A3:267:G:OP1	67:d2:109:ARG:NH2	2.38	0.57
31:L1:77:ILE:HG13	31:L1:99:ILE:HB	1.86	0.57
86:o2:111:LEU:HD21	86:o2:151:VAL:HG21	1.84	0.57
2:A1:903:G:H2'	2:A1:904:A:H8	1.70	0.57
13:D3:137:ILE:HD11	13:D3:149:LYS:HB2	1.86	0.57
4:A3:3782:C:HO2'	86:o2:37:SER:HG	1.53	0.57
7:B3:28:C:H2'	7:B3:29:C:H5'	1.87	0.57
10:C3:51:U:OP2	75:h2:21:ARG:NH2	2.38	0.57
13:D3:234:LYS:HG2	13:D3:238:ILE:HG12	1.87	0.57
45:S1:30:LEU:HD22	45:S1:40:LEU:HD22	1.86	0.57
4:A3:3785:C:H2'	4:A3:3786:U:H6	1.70	0.57
41:Q1:102:LEU:HD11	80:k1:100:VAL:HG21	1.87	0.57
45:S1:138:GLU:OE2	57:Y1:19:ARG:NH2	2.38	0.57
88:q2:260:ARG:NH1	88:q2:284:ASP:OD1	2.38	0.57
2:A1:65:C:H4'	43:R1:172:LYS:HD3	1.86	0.56
4:A3:108:A:N1	4:A3:333:U:O2'	2.38	0.56
4:A3:1276:C:H2'	4:A3:1277:A:H8	1.71	0.56
39:P1:247:THR:OG1	39:P1:250:GLU:OE1	2.24	0.56
2:A1:875:G:H2'	2:A1:876:A:H8	1.70	0.56
2:A1:1640:G7M:H2'	2:A1:1641:A:C8	2.41	0.56
4:A3:1911:G:N2	85:n2:131:GLU:OE1	2.38	0.56
4:A3:4292:A:N7	13:D3:215:ASN:ND2	2.53	0.56
7:B3:6:C:O2'	22:G3:50:ARG:NH2	2.38	0.56
20:G1:240:CYS:O	20:G1:249:CYS:SG	2.63	0.56
53:W1:119:ASP:O	53:W1:147:LYS:NZ	2.38	0.56
2:A1:434:A:H5''	47:T1:22:HIS:HB3	1.86	0.56
2:A1:465:A:OP1	88:q2:576:ARG:NH1	2.37	0.56
21:G2:1:LEU:C	21:G2:2:LEU:HD23	2.30	0.56
31:L1:76:VAL:HG12	31:L1:123:VAL:HB	1.87	0.56
44:R2:66:LYS:O	44:R2:73:ARG:NH1	2.38	0.56
86:o2:39:LYS:HB3	86:o2:202:ARG:HB2	1.88	0.56
2:A1:537:A:N6	2:A1:548:G:H1	2.02	0.56
4:A3:1489:A2M:N7	71:f2:15:THR:HG22	2.20	0.56
4:A3:2538:A:OP1	73:g2:35:LYS:NZ	2.38	0.56
4:A3:3812:G:O6	13:D3:72:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D1:119:ARG:NH1	11:D1:120:GLU:O	2.38	0.56
15:E2:110:ARG:HG3	15:E2:112:GLN:H	1.71	0.56
37:O1:163:PRO:O	37:O1:167:TYR:HB2	2.04	0.56
61:a1:98:ASN:ND2	61:a1:103:ASN:OD1	2.38	0.56
84:m2:28:PHE:HB2	84:m2:89:VAL:HB	1.86	0.56
4:A3:4276:UR3:O2'	87:p2:183:ALA:HA	2.05	0.56
20:G1:79:LEU:HD22	20:G1:120:ILE:HD12	1.87	0.56
47:T1:124:LYS:HB2	47:T1:127:ALA:HB2	1.86	0.56
88:q2:7:ARG:NH2	88:q2:55:CYS:O	2.38	0.56
4:A3:109:G:OP2	24:H2:74:ARG:NH2	2.36	0.56
4:A3:2250:G:N2	75:h2:51:LEU:OXT	2.38	0.56
39:P1:11:ARG:HA	39:P1:28:ALA:HB2	1.88	0.56
69:e2:99:LYS:HG2	69:e2:103:LYS:HE2	1.87	0.56
3:A2:226:ARG:HD2	4:A3:690:C:H41	1.71	0.56
4:A3:843:A:N7	6:B2:150:ASN:ND2	2.52	0.56
87:p2:315:GLY:O	87:p2:414:ARG:NH2	2.39	0.56
4:A3:3870:U:H3	4:A3:3887:G:H1	1.54	0.56
33:M1:129:THR:HB	33:M1:180:ASP:HA	1.88	0.56
49:U1:120:ALA:O	49:U1:125:HIS:ND1	2.36	0.56
4:A3:308:G:O6	28:J2:12:ARG:NH1	2.37	0.56
4:A3:4508:G:OP2	30:K2:37:ARG:NH1	2.34	0.55
16:E3:92:TYR:HB2	16:E3:159:VAL:HB	1.88	0.55
88:q2:96:ARG:HG3	88:q2:299:VAL:HB	1.89	0.55
4:A3:2301:C:H5''	28:J2:67:ARG:HD2	1.88	0.55
4:A3:3701:G:H1'	86:o2:166:ALA:HB3	1.88	0.55
17:F1:3:LYS:NZ	17:F1:8:ASN:OD1	2.39	0.55
24:H2:171:GLU:O	24:H2:175:ASN:ND2	2.39	0.55
2:A1:1229:A:H2'	2:A1:1230:G:C8	2.41	0.55
5:B1:23:ARG:O	74:h1:60:LYS:NZ	2.40	0.55
20:G1:68:ASP:HB3	20:G1:111:VAL:HG22	1.88	0.55
33:M1:9:LEU:HD13	33:M1:11:LYS:HE3	1.88	0.55
35:N1:62:PRO:HB2	35:N1:68:ARG:HG3	1.88	0.55
87:p2:307:ASP:OD2	88:q2:33:ARG:NH1	2.40	0.55
2:A1:1864:A:OP2	17:F1:4:LYS:NZ	2.40	0.55
4:A3:2274:A:OP1	75:h2:41:ARG:NH1	2.39	0.55
38:O2:71:SER:O	38:O2:76:LYS:NZ	2.40	0.54
58:Y2:9:LYS:HA	58:Y2:12:GLU:HG2	1.89	0.54
4:A3:2254:C:H2'	4:A3:2255:A:C8	2.42	0.54
4:A3:4269:A2M:O2'	16:E3:246:ARG:NH1	2.38	0.54
63:b1:90:LYS:HG2	63:b1:120:LEU:HD13	1.89	0.54
74:h1:80:ASP:OD1	74:h1:124:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A1:3:C:O2	49:U1:18:ARG:NH1	2.40	0.54
2:A1:537:A:N6	2:A1:548:G:C6	2.74	0.54
4:A3:433:A:C2	4:A3:3599:A2M:H4'	2.42	0.54
65:c1:106:LEU:HD23	65:c1:109:LEU:HD23	1.89	0.54
83:l2:66:ARG:NH1	83:l2:75:THR:O	2.40	0.54
41:Q1:127:ARG:HH12	41:Q1:134:VAL:HA	1.73	0.54
55:X1:55:ASN:ND2	55:X1:81:ASP:OD1	2.40	0.54
61:a1:41:GLN:HG3	61:a1:84:ILE:HD12	1.89	0.54
2:A1:380:C:O2	47:T1:5:ARG:NE	2.40	0.54
2:A1:746:C:O2'	45:S1:111:LYS:NZ	2.39	0.54
4:A3:40:G:N7	92:A3:5161:SPD:N1	2.55	0.54
4:A3:2178:C:H2'	4:A3:2179:G:H8	1.72	0.54
21:G2:7:LEU:HD13	21:G2:13:VAL:HG11	1.90	0.54
1:MB:88:ARG:HG3	52:V2:14:LEU:HB3	1.88	0.54
37:O1:28:GLU:HG2	37:O1:69:LEU:HD21	1.90	0.54
48:T2:91:GLU:HG2	48:T2:147:LEU:HD21	1.88	0.54
3:A2:164:ARG:NH1	3:A2:276:SER:OG	2.41	0.54
27:J1:56:C:H5'	86:o2:130:LYS:HE3	1.90	0.54
41:Q1:71:ARG:NH2	41:Q1:148:ASN:OD1	2.39	0.54
88:q2:412:LYS:HE2	88:q2:416:ILE:HD11	1.88	0.54
2:A1:617:A:OP1	76:i1:68:LYS:NZ	2.40	0.54
2:A1:914:A:OP2	45:S1:99:ARG:NH2	2.41	0.54
61:a1:81:ARG:NH1	61:a1:120:SER:OG	2.40	0.54
87:p2:332:VAL:HG13	87:p2:369:ILE:HB	1.90	0.54
88:q2:259:ILE:HD13	88:q2:262:LEU:HD12	1.90	0.54
2:A1:909:A:OP1	36:N2:172:ARG:NH2	2.41	0.54
4:A3:1215:G:H5'	56:X2:110:ALA:HB1	1.90	0.54
35:N1:267:GLN:NE2	72:g1:35:ASN:OD1	2.41	0.54
39:P1:31:PRO:HA	39:P1:81:THR:HB	1.90	0.54
2:A1:1301:U:O2'	61:a1:51:ARG:NH1	2.41	0.53
4:A3:2338:U:H2'	4:A3:2339:G:H8	1.72	0.53
4:A3:4763:C:OP1	47:T1:124:LYS:NZ	2.41	0.53
33:M1:2:ALA:N	59:Z1:62:VAL:O	2.41	0.53
2:A1:64:A:H2	2:A1:83:A:H62	1.55	0.53
4:A3:2736:U:H5''	47:T1:205:ARG:HH12	1.73	0.53
4:A3:3641:C:O2'	21:G2:18:GLY:HA3	2.09	0.53
4:A3:3678:G:H1	4:A3:3795:U:H3	1.56	0.53
27:J1:32:C:O2'	41:Q1:127:ARG:NH2	2.41	0.53
2:A1:1125:C:H5''	33:M1:150:ILE:HG12	1.90	0.53
20:G1:240:CYS:N	20:G1:249:CYS:HB2	2.23	0.53
74:h1:44:HIS:NE2	74:h1:112:ASP:OD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:4294:A:C2	87:p2:183:ALA:HB3	2.44	0.53
16:E3:113:GLU:OE2	16:E3:169:ARG:NH1	2.41	0.53
55:X1:51:VAL:HG22	55:X1:77:ILE:HB	1.91	0.53
88:q2:84:THR:HG21	88:q2:97:LEU:HG	1.89	0.53
3:A2:181:PRO:HD2	3:A2:184:LEU:HD12	1.90	0.53
4:A3:805:G:OP2	38:O2:149:ARG:NH1	2.41	0.53
6:B2:28:LYS:HE3	6:B2:32:LEU:HD11	1.90	0.53
19:F3:163:LYS:HB2	19:F3:166:GLU:HG3	1.89	0.53
30:K2:34:VAL:HG12	30:K2:103:LYS:HB2	1.91	0.53
61:a1:123:TYR:OH	66:d1:124:ARG:NH1	2.41	0.53
78:j1:4:THR:OG1	78:j1:32:LYS:NZ	2.41	0.53
87:p2:283:GLU:HG3	87:p2:392:VAL:HG23	1.90	0.53
3:A2:164:ARG:O	3:A2:185:ASN:ND2	2.41	0.53
4:A3:3396:G:H2'	4:A3:3397:G:H8	1.73	0.53
60:Z2:36:VAL:HG21	60:Z2:44:ARG:HG2	1.90	0.53
73:g2:54:GLU:O	73:g2:58:GLN:NE2	2.41	0.53
2:A1:378:G:H5'	47:T1:98:LYS:HB3	1.91	0.53
2:A1:845:U:OP1	39:P1:240:ARG:NH2	2.42	0.53
2:A1:1590:A:N3	2:A1:1654:U:O2'	2.38	0.53
4:A3:4187:A:H5''	15:E2:114:GLY:HA2	1.91	0.53
15:E2:53:VAL:HG11	40:P2:158:PHE:HZ	1.74	0.53
43:R1:21:GLU:HA	43:R1:24:LEU:HB2	1.91	0.53
2:A1:929:G:H1	2:A1:1014:U:H3	1.55	0.53
4:A3:136:U:O4	67:d2:79:LYS:NZ	2.41	0.53
4:A3:1399:G:N7	4:A3:2049:G:N1	2.53	0.53
4:A3:1503:G:O2'	4:A3:2655:A:N3	2.40	0.53
4:A3:2620:G:H5''	4:A3:2621:G:H5'	1.91	0.53
4:A3:4218:G:O2'	77:i2:100:TYR:O	2.26	0.53
6:B2:104:VAL:HG13	6:B2:135:VAL:HG12	1.91	0.53
30:K2:128:ARG:NH1	38:O2:162:GLN:OE1	2.41	0.53
51:V1:31:LYS:NZ	51:V1:39:ASN:OD1	2.41	0.53
61:a1:18:ARG:NH1	66:d1:88:LYS:O	2.41	0.53
2:A1:463:OMC:H5'	88:q2:304:SER:HB3	1.91	0.53
4:A3:194:C:O2	50:U2:121:ARG:NH2	2.41	0.53
4:A3:4099:PSU:H5'	4:A3:4100:U:H5'	1.89	0.53
43:R1:160:LYS:HA	46:S2:84:GLY:HA2	1.91	0.53
66:d1:33:ILE:HD13	66:d1:71:MET:HE1	1.90	0.53
2:A1:861:G:N2	74:h1:107:SER:OG	2.41	0.53
33:M1:5:LYS:NZ	59:Z1:65:ASP:OD2	2.42	0.53
35:N1:191:VAL:HG11	35:N1:236:PHE:HA	1.91	0.53
87:p2:394:ASP:OD1	87:p2:395:LYS:NZ	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A1:861:G:OP1	45:S1:107:LYS:NZ	2.41	0.52
2:A1:1567:G:N7	68:e1:101:ARG:NH2	2.57	0.52
4:A3:2257:G:H2'	4:A3:2258:OMU:H6	1.91	0.52
16:E3:168:MET:HA	16:E3:171:LEU:HD12	1.91	0.52
58:Y2:21:VAL:HG11	58:Y2:96:ILE:HD12	1.91	0.52
1:MB:42:PRO:HB2	1:MB:53:LEU:HD12	1.90	0.52
4:A3:734:G:OP2	26:I2:71:LYS:NZ	2.40	0.52
4:A3:3785:C:H2'	4:A3:3786:U:C6	2.44	0.52
68:e1:9:VAL:O	68:e1:11:GLN:NE2	2.42	0.52
88:q2:487:GLU:OE2	88:q2:520:HIS:ND1	2.39	0.52
88:q2:499:MET:SD	88:q2:502:ARG:NH1	2.82	0.52
1:MB:52:ARG:NH2	4:A3:2441:A:OP1	2.42	0.52
4:A3:184:U:H3	4:A3:253:G:H22	1.55	0.52
4:A3:1924:G:OP1	4:A3:1924:G:N2	2.43	0.52
87:p2:45:ILE:HD11	87:p2:82:LEU:HD22	1.92	0.52
4:A3:2254:C:H2'	4:A3:2255:A:H8	1.74	0.52
4:A3:2444:A:N6	4:A3:2587:A:OP2	2.41	0.52
4:A3:3373:U:OP2	4:A3:3378:A:N6	2.35	0.52
33:M1:103:MET:HG3	33:M1:215:VAL:HB	1.91	0.52
87:p2:335:CYS:HG	87:p2:338:THR:HG1	1.57	0.52
88:q2:128:LYS:NZ	88:q2:138:PRO:O	2.43	0.52
3:A2:40:LYS:HD2	4:A3:883:C:H5''	1.91	0.52
31:L1:8:LEU:HD11	72:g1:39:VAL:HG11	1.92	0.52
74:h1:3:ARG:HD3	74:h1:6:VAL:HG12	1.91	0.52
86:o2:26:ARG:HH21	86:o2:29:LEU:HA	1.75	0.52
2:A1:1855:U:H2'	2:A1:1856:G:H8	1.74	0.52
4:A3:404:U:O3'	50:U2:87:ARG:NH2	2.42	0.52
4:A3:1224:C:O2'	19:F3:321:ASN:OD1	2.22	0.52
4:A3:1933:C:H2'	4:A3:1934:G:C8	2.40	0.52
21:G2:1:LEU:HD22	21:G2:2:LEU:H	1.73	0.52
30:K2:55:LEU:HD23	30:K2:58:LEU:HD12	1.92	0.52
3:A2:67:ARG:NH1	4:A3:985:G:OP2	2.40	0.52
4:A3:454:U:H1'	62:a2:5:ARG:HE	1.75	0.52
88:q2:304:SER:OG	88:q2:307:GLU:OE1	2.27	0.52
4:A3:3599:A2M:H2'	4:A3:3600:G:O4'	2.10	0.52
27:J1:36:U:H1'	29:K1:40:C:H5''	1.90	0.52
85:n2:30:PRO:HD3	87:p2:314:MET:HE3	1.92	0.52
4:A3:1900:G:N2	4:A3:1963:G:O2'	2.42	0.52
4:A3:2032:G:O2'	4:A3:2100:C:N4	2.42	0.52
72:g1:33:GLN:NE2	72:g1:52:THR:OG1	2.43	0.52
85:n2:37:LEU:HD23	85:n2:42:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:q2:188:LEU:O	88:q2:192:ASP:HB2	2.10	0.52
2:A1:541:U:O2	2:A1:544:C:N3	2.43	0.52
2:A1:911:G:OP1	36:N2:176:ARG:NH1	2.43	0.52
4:A3:4721:A:OP1	32:L2:74:LYS:NZ	2.40	0.52
88:q2:497:ARG:NH1	88:q2:521:ASP:OD2	2.42	0.52
4:A3:1918:A:H61	4:A3:1922:A:H5''	1.74	0.51
88:q2:164:LEU:HD23	88:q2:237:ILE:HD11	1.92	0.51
4:A3:3449:A:H2'	4:A3:3450:A2M:H8	1.92	0.51
10:C3:84:A:N3	67:d2:3:LYS:NZ	2.58	0.51
20:G1:239:LEU:HA	20:G1:249:CYS:O	2.10	0.51
58:Y2:38:ILE:HG21	58:Y2:63:TYR:HB3	1.93	0.51
78:j1:108:LYS:O	78:j1:112:ASN:ND2	2.43	0.51
4:A3:3515:A:OP2	4:A3:3540:OMC:N4	2.43	0.51
15:E2:214:SER:HB3	22:G3:287:PHE:HZ	1.75	0.51
19:F3:218:VAL:O	19:F3:222:ARG:HB3	2.11	0.51
31:L1:108:PHE:HB2	31:L1:136:GLU:HG2	1.91	0.51
37:O1:172:VAL:HG22	37:O1:185:LYS:HG2	1.90	0.51
87:p2:239:SER:O	87:p2:247:GLN:NE2	2.43	0.51
4:A3:4328:C:OP2	16:E3:28:LYS:NZ	2.40	0.51
33:M1:44:ILE:HD12	33:M1:69:VAL:HG21	1.92	0.51
84:m2:194:ASP:OD1	84:m2:194:ASP:N	2.44	0.51
86:o2:68:LEU:HD21	86:o2:90:LEU:HD11	1.90	0.51
2:A1:1034:G:N1	2:A1:1081:A:O2'	2.41	0.51
4:A3:3455:A:H2'	4:A3:3456:A2M:H8	1.92	0.51
13:D3:108:PRO:HD3	81:k2:90:LYS:HD3	1.93	0.51
2:A1:1498:G:O6	51:V1:25:LYS:NZ	2.44	0.51
4:A3:2317:G:H22	4:A3:2346:G:H5''	1.76	0.51
31:L1:85:ARG:NH1	31:L1:203:PHE:O	2.43	0.51
87:p2:119:PRO:HB2	87:p2:165:THR:HG21	1.92	0.51
3:A2:286:PRO:HA	3:A2:289:LEU:HG	1.93	0.51
4:A3:1853:C:H4'	30:K2:89:PRO:HD3	1.92	0.51
18:F2:95:ARG:O	18:F2:98:ASN:HB2	2.11	0.51
22:G3:62:CYS:HB3	22:G3:105:LEU:HD22	1.93	0.51
35:N1:102:LEU:HD22	35:N1:130:ILE:HG12	1.92	0.51
39:P1:53:LYS:HB2	78:j1:13:MET:HE1	1.92	0.51
47:T1:162:LEU:HD11	47:T1:191:GLU:HG2	1.92	0.51
70:f1:24:LEU:HG	70:f1:112:VAL:HG22	1.93	0.51
2:A1:74:G:N1	43:R1:171:THR:OG1	2.43	0.51
2:A1:202:G:OP2	47:T1:143:LYS:NZ	2.39	0.51
4:A3:6:C:H5''	9:C2:197:LYS:HG2	1.93	0.51
4:A3:2363:C:H2'	4:A3:2364:G:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:3894:C:OP1	52:V2:59:LYS:NZ	2.40	0.51
4:A3:4294:A:H4'	4:A3:4295:G:O5'	2.09	0.51
48:T2:123:LYS:HG2	48:T2:139:ARG:HB3	1.92	0.51
2:A1:944:U:O2'	59:Z1:135:ILE:O	2.28	0.51
4:A3:4347:U:H2'	4:A3:4348:A:H8	1.75	0.51
15:E2:187:GLU:HG3	15:E2:189:ARG:HG2	1.93	0.51
17:F1:45:VAL:HG11	17:F1:53:ILE:HG13	1.91	0.51
19:F3:71:ARG:NH2	21:G2:1:LEU:HD11	2.13	0.51
20:G1:35:SER:OG	20:G1:36:ARG:N	2.43	0.51
65:c1:94:GLU:HG2	65:c1:95:ILE:HD12	1.93	0.51
2:A1:4:C:O2'	49:U1:18:ARG:NH2	2.44	0.50
4:A3:24:G:N7	71:f2:46:LYS:NZ	2.58	0.50
4:A3:62:A:OP1	28:J2:172:ARG:NH1	2.42	0.50
4:A3:1479:A2M:H62	4:A3:1606:G:H22	1.58	0.50
4:A3:3816:C:OP1	13:D3:37:ARG:NH2	2.44	0.50
4:A3:4720:G:O6	16:E3:21:ARG:NH2	2.44	0.50
43:R1:159:ARG:NH2	43:R1:171:THR:O	2.44	0.50
24:H2:129:ARG:NH1	67:d2:116:LEU:O	2.45	0.50
86:o2:63:PHE:HB2	86:o2:152:LYS:HG2	1.92	0.50
2:A1:831:A:OP2	2:A1:847:G:N2	2.45	0.50
2:A1:1832:A:H2'	2:A1:1833:6MZ:H8	1.93	0.50
3:A2:227:LYS:NZ	3:A2:241:GLU:O	2.41	0.50
4:A3:1580:OMG:N1	4:A3:3650:G:OP1	2.40	0.50
4:A3:3676:OMG:HN1	4:A3:3797:U:H3	1.58	0.50
27:J1:31:A:O2'	41:Q1:136:ARG:NH1	2.44	0.50
2:A1:99:A2M:O5'	2:A1:99:A2M:H8	2.11	0.50
3:A2:40:LYS:HB3	4:A3:883:C:H4'	1.94	0.50
4:A3:1917:C:OP2	85:n2:57:ARG:NH1	2.44	0.50
4:A3:3598:C:H2'	4:A3:3599:A2M:O4'	2.11	0.50
20:G1:130:LYS:NZ	20:G1:141:THR:OG1	2.41	0.50
39:P1:87:MET:HE1	39:P1:236:ILE:HG21	1.93	0.50
87:p2:97:CYS:HA	87:p2:110:VAL:O	2.12	0.50
88:q2:217:LEU:HD22	88:q2:221:GLU:HB3	1.94	0.50
88:q2:281:TYR:HB2	88:q2:577:ILE:HG21	1.93	0.50
88:q2:345:MET:HE3	88:q2:512:LYS:HZ2	1.77	0.50
4:A3:865:G:N2	4:A3:2035:G:O2'	2.44	0.50
4:A3:2601:G:O2'	4:A3:2608:A:N3	2.41	0.50
18:F2:35:ARG:NH1	18:F2:123:ILE:O	2.44	0.50
33:M1:28:LYS:NZ	59:Z1:51:GLU:OE1	2.44	0.50
71:f2:20:ARG:NH2	71:f2:39:TYR:OH	2.44	0.50
88:q2:441:PHE:HE2	88:q2:446:MET:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A1:1494:C:O2'	2:A1:1500:U:O4	2.28	0.50
10:C3:85:U:O4	50:U2:50:ARG:NH2	2.45	0.50
20:G1:68:ASP:O	20:G1:80:SER:HA	2.12	0.50
20:G1:223:GLU:O	37:O1:226:GLN:NE2	2.44	0.50
33:M1:152:LYS:HD3	65:c1:133:GLY:HA3	1.92	0.50
79:j2:26:TYR:HB3	79:j2:67:VAL:HB	1.93	0.50
80:k1:47:LEU:HB2	80:k1:79:ILE:HG22	1.94	0.50
84:m2:53:VAL:HG12	84:m2:89:VAL:HG22	1.93	0.50
3:A2:80:SER:OG	3:A2:81:ARG:N	2.45	0.50
4:A3:1489:A2M:N3	71:f2:11:ARG:HB2	2.26	0.50
4:A3:3599:A2M:HM'3	4:A3:3612:G:N2	2.27	0.50
4:A3:3836:G:H2'	4:A3:3837:G:H8	1.77	0.50
13:D3:101:VAL:HG22	13:D3:165:VAL:HG22	1.94	0.50
13:D3:117:GLU:HG2	13:D3:124:GLY:H	1.76	0.50
17:F1:48:ALA:O	59:Z1:117:ARG:NH1	2.44	0.50
37:O1:137:VAL:HG22	37:O1:151:LYS:HG3	1.94	0.50
38:O2:15:ARG:HB3	38:O2:27:LEU:HD23	1.94	0.50
54:W2:87:ARG:HG3	54:W2:120:GLN:HE22	1.76	0.50
87:p2:27:ALA:O	87:p2:28:ARG:NH1	2.44	0.50
4:A3:1959:U:H2'	4:A3:1960:G:H8	1.77	0.50
4:A3:3780:C:O2	86:o2:207:LYS:NZ	2.38	0.50
28:J2:159:ARG:HB3	28:J2:164:LEU:HB2	1.94	0.50
4:A3:1:C:H42	10:C3:156:U:H3	1.57	0.50
4:A3:1493:U:H2'	4:A3:1494:G:H8	1.77	0.50
10:C3:75:OMG:OP2	50:U2:74:TYR:OH	2.29	0.50
87:p2:333:LEU:HB2	87:p2:342:LYS:HG3	1.93	0.50
2:A1:1754:C:H2'	2:A1:1755:G:H8	1.77	0.49
4:A3:4287:G:N2	4:A3:4290:A:OP2	2.40	0.49
16:E3:289:GLN:O	16:E3:302:ASN:ND2	2.36	0.49
42:Q2:36:ALA:HB3	42:Q2:65:ARG:HH21	1.76	0.49
10:C3:30:U:OP1	24:H2:34:ARG:NH2	2.42	0.49
29:K1:22:U:H2'	29:K1:23:C:C6	2.46	0.49
55:X1:92:CYS:SG	55:X1:93:LYS:N	2.84	0.49
60:Z2:64:ILE:HG23	60:Z2:68:LEU:HD23	1.94	0.49
61:a1:17:TYR:HB3	61:a1:25:LEU:HD11	1.95	0.49
87:p2:287:ILE:HD11	87:p2:392:VAL:HG21	1.93	0.49
2:A1:640:C:OP1	14:E1:114:ARG:NH2	2.44	0.49
4:A3:3452:G:H22	4:A3:3465:A:H2	1.59	0.49
27:J1:15:G:N2	27:J1:48:C:C2	2.79	0.49
44:R2:92:ASP:OD1	44:R2:92:ASP:N	2.44	0.49
59:Z1:101:GLY:HA3	59:Z1:134:PRO:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A1:335:C:OP2	43:R1:190:ARG:NH2	2.44	0.49
2:A1:1651:A:H5''	63:b1:139:ALA:HB2	1.94	0.49
4:A3:522:U:O4	4:A3:635:G:O6	2.29	0.49
4:A3:4366:OMU:OP2	4:A3:4416:C:N4	2.42	0.49
10:C3:106:G:H4'	10:C3:137:A:H5'	1.95	0.49
28:J2:138:PHE:HA	28:J2:143:ARG:HD2	1.92	0.49
36:N2:105:LEU:HD22	36:N2:135:LYS:HG3	1.95	0.49
45:S1:170:VAL:HG13	45:S1:187:PHE:HB2	1.95	0.49
61:a1:37:TYR:O	66:d1:88:LYS:NZ	2.46	0.49
62:a2:99:ILE:HG21	62:a2:108:ARG:HG3	1.93	0.49
66:d1:13:LEU:HB2	66:d1:20:ILE:HB	1.93	0.49
70:f1:61:LEU:O	70:f1:81:GLN:HA	2.12	0.49
88:q2:463:SER:OG	88:q2:466:GLU:OE1	2.30	0.49
2:A1:682:PSU:H4'	76:i1:9:THR:HG22	1.95	0.49
2:A1:1093:G:OP1	57:Y1:2:GLY:N	2.45	0.49
4:A3:1911:G:H2'	4:A3:1912:G:C8	2.47	0.49
4:A3:2100:C:O2'	4:A3:2102:G:OP2	2.29	0.49
4:A3:3385:A:O2'	13:D3:179:ILE:O	2.29	0.49
20:G1:302:TYR:HE2	20:G1:308:ARG:HB2	1.76	0.49
27:J1:54:U:O3'	86:o2:48:ARG:NH2	2.46	0.49
32:L2:116:HIS:HB3	32:L2:149:ILE:HB	1.93	0.49
42:Q2:23:LEU:HD11	42:Q2:83:LEU:HD12	1.95	0.49
88:q2:412:LYS:NZ	88:q2:486:ASP:O	2.39	0.49
2:A1:39:A:OP1	49:U1:5:ARG:NH1	2.43	0.49
2:A1:1285:A:O2'	55:X1:106:CYS:SG	2.63	0.49
3:A2:82:ILE:HD11	3:A2:87:LYS:HE3	1.95	0.49
4:A3:1271:C:H2'	4:A3:1272:G:C8	2.47	0.49
17:F1:44:ILE:HD12	17:F1:65:PRO:HG2	1.93	0.49
33:M1:40:ASN:OD1	33:M1:76:ASN:ND2	2.45	0.49
38:O2:1:MET:HE3	38:O2:35:PRO:HD3	1.94	0.49
2:A1:1613:G:H1'	66:d1:87:GLN:HE21	1.78	0.49
4:A3:769:C:H2'	4:A3:770:G:H8	1.77	0.49
55:X1:93:LYS:NZ	55:X1:95:ASP:OD1	2.45	0.49
59:Z1:98:ARG:HB3	59:Z1:132:VAL:HG23	1.93	0.49
75:h2:21:ARG:HH12	75:h2:24:PRO:HG3	1.77	0.49
87:p2:177:PRO:HG3	87:p2:197:LYS:HB2	1.94	0.49
88:q2:27:LYS:O	88:q2:33:ARG:NH2	2.45	0.49
2:A1:1300:A:OP1	61:a1:59:ARG:NH1	2.46	0.49
4:A3:891:U:O2	4:A3:979:G:O6	2.31	0.49
33:M1:109:LYS:HG3	33:M1:113:MET:HE2	1.94	0.49
2:A1:1446:PSU:O2	2:A1:1447:A:N6	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:514:U:O2	4:A3:641:G:O6	2.31	0.49
4:A3:661:A:O2'	19:F3:29:LYS:NZ	2.46	0.49
4:A3:3780:C:H2'	4:A3:3781:A:C8	2.47	0.49
15:E2:54:SER:HB3	15:E2:135:ILE:HD11	1.94	0.49
86:o2:54:ARG:HA	86:o2:154:THR:HG22	1.95	0.49
17:F1:32:LYS:O	17:F1:37:LYS:NZ	2.38	0.49
18:F2:18:ARG:HG3	18:F2:135:GLY:HA3	1.94	0.49
84:m2:98:ILE:HA	84:m2:101:MET:HG2	1.94	0.49
4:A3:175:C:H2'	4:A3:176:G:H8	1.78	0.48
4:A3:1250:C:H2'	4:A3:1251:A:H8	1.78	0.48
4:A3:3979:A:H4'	79:j2:98:LYS:HD2	1.94	0.48
4:A3:4294:A:N3	87:p2:183:ALA:HB3	2.28	0.48
16:E3:220:ILE:HG12	16:E3:278:THR:HG23	1.95	0.48
19:F3:71:ARG:NH2	21:G2:1:LEU:HD21	2.28	0.48
20:G1:72:SER:OG	20:G1:74:ASP:OD1	2.27	0.48
62:a2:104:SER:O	62:a2:108:ARG:HB2	2.12	0.48
2:A1:35:C:H5''	2:A1:580:C:H5''	1.95	0.48
4:A3:3481:C:O2'	13:D3:220:GLY:O	2.30	0.48
4:A3:4735:C:OP1	60:Z2:32:ARG:NH1	2.45	0.48
87:p2:21:ILE:HD12	87:p2:133:THR:HB	1.95	0.48
87:p2:418:ASP:OD1	87:p2:418:ASP:N	2.45	0.48
2:A1:1229:A:H2'	2:A1:1230:G:H8	1.78	0.48
4:A3:2588:A:H2'	4:A3:2589:A:C8	2.49	0.48
27:J1:54:U:H4'	86:o2:47:LYS:HD2	1.95	0.48
46:S2:8:PHE:HZ	46:S2:49:ILE:HG13	1.78	0.48
87:p2:252:LYS:HD2	87:p2:274:VAL:HG21	1.95	0.48
2:A1:1118:C:O2'	2:A1:1119:C:O5'	2.31	0.48
2:A1:1537:G:H2'	2:A1:1538:A:C8	2.47	0.48
4:A3:262:G:H2'	4:A3:263:G:H8	1.78	0.48
4:A3:1276:C:H2'	4:A3:1277:A:C8	2.48	0.48
4:A3:1464:C:H5''	54:W2:2:PRO:HD2	1.94	0.48
4:A3:3811:U:OP1	13:D3:123:ARG:NH1	2.47	0.48
8:C1:36:ASP:OD1	8:C1:36:ASP:N	2.46	0.48
42:Q2:62:THR:OG1	42:Q2:73:THR:OG1	2.31	0.48
54:W2:92:LYS:O	54:W2:94:LYS:NZ	2.46	0.48
55:X1:59:PRO:HA	55:X1:62:VAL:HG22	1.95	0.48
81:k2:38:THR:HA	81:k2:45:THR:HA	1.95	0.48
2:A1:328:G:H1'	2:A1:329:U:H2'	1.96	0.48
2:A1:911:G:OP2	36:N2:173:ARG:NH2	2.46	0.48
2:A1:1465:C:OP2	65:c1:63:ARG:NH1	2.46	0.48
2:A1:1522:C:OP1	66:d1:129:LEU:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:1641:C:O2'	56:X2:18:ARG:NH1	2.46	0.48
4:A3:3649:A:H2'	4:A3:3650:G:H8	1.79	0.48
31:L1:118:GLU:HB2	35:N1:65:LYS:HD3	1.96	0.48
50:U2:51:LYS:O	50:U2:52:ASP:HB2	2.14	0.48
86:o2:85:MET:HE1	86:o2:93:LEU:HD11	1.95	0.48
87:p2:151:ILE:HD12	87:p2:205:VAL:HG11	1.94	0.48
2:A1:99:A2M:H2'	2:A1:100:U:O4'	2.14	0.48
2:A1:1031:A:H2'	2:A1:1032:A2M:H8	1.95	0.48
4:A3:63:G:OP1	28:J2:169:ARG:NH2	2.47	0.48
2:A1:1338:4AC:H2'	2:A1:1339:G:C8	2.48	0.48
4:A3:88:A:N7	34:M2:173:LYS:NZ	2.61	0.48
4:A3:2588:A:H2'	4:A3:2589:A:H8	1.79	0.48
4:A3:2678:A:O2'	16:E3:228:TYR:O	2.30	0.48
4:A3:4270:G:OP2	4:A3:4270:G:H4'	2.14	0.48
43:R1:121:ILE:HG21	43:R1:124:LEU:HD12	1.95	0.48
88:q2:462:LEU:HD13	88:q2:466:GLU:HB3	1.95	0.48
4:A3:2632:A:H1'	75:h2:45:ARG:HH22	1.78	0.48
4:A3:3391:G:OP1	13:D3:241:ARG:NH1	2.46	0.48
11:D1:121:CYS:HA	11:D1:132:MET:HE3	1.96	0.48
20:G1:256:ILE:HG23	20:G1:270:LEU:HB2	1.95	0.48
2:A1:727:C:H2'	2:A1:728:G:H8	1.79	0.48
2:A1:853:G:N3	2:A1:853:G:H2'	2.29	0.48
2:A1:920:A:OP2	57:Y1:64:ARG:NH2	2.47	0.48
2:A1:1290:U:H5	11:D1:95:ARG:HH22	1.62	0.48
2:A1:1537:G:H2'	2:A1:1538:A:H8	1.79	0.48
4:A3:3822:G:N2	4:A3:3843:G:N7	2.62	0.48
4:A3:4020:A:H2'	4:A3:4021:G:C8	2.49	0.48
14:E1:86:VAL:O	14:E1:90:THR:OG1	2.28	0.48
2:A1:5:U:H2'	2:A1:6:G:H8	1.79	0.48
2:A1:39:A:H5'	49:U1:7:TRP:HE1	1.78	0.48
4:A3:2658:A2M:H2'	4:A3:2659:G:C8	2.49	0.48
4:A3:4089:U:O2'	79:j2:31:ASP:OD1	2.32	0.48
4:A3:4486:G:H2'	4:A3:4489:G:H5'	1.96	0.48
16:E3:291:TYR:HB3	16:E3:298:LEU:HD11	1.95	0.48
20:G1:3:GLU:HG2	20:G1:314:ILE:HG12	1.96	0.48
36:N2:135:LYS:HG2	36:N2:139:MET:HE2	1.96	0.48
45:S1:79:LEU:O	45:S1:82:GLU:HG3	2.13	0.48
61:a1:75:VAL:HG22	61:a1:93:MET:HB3	1.96	0.48
3:A2:102:ASP:OD1	3:A2:102:ASP:N	2.43	0.47
4:A3:3920:U:H2'	4:A3:3921:G:H8	1.79	0.47
16:E3:56:ILE:O	16:E3:73:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:L1:145:ILE:HG12	31:L1:159:ILE:HB	1.95	0.47
34:M2:157:GLY:O	34:M2:188:ASN:ND2	2.44	0.47
88:q2:389:ILE:HG21	88:q2:484:LEU:HD22	1.96	0.47
2:A1:27:A2M:H1'	2:A1:27:A2M:HM'3	1.47	0.47
31:L1:1:ACE:O	31:L1:63:ARG:NH1	2.47	0.47
39:P1:21:ASP:OD2	39:P1:24:THR:OG1	2.28	0.47
49:U1:60:LEU:HD22	49:U1:70:ARG:HA	1.96	0.47
53:W1:111:VAL:HG12	53:W1:140:PHE:HB2	1.95	0.47
62:a2:82:VAL:HG13	62:a2:114:ARG:HG2	1.94	0.47
2:A1:352:G:OP1	47:T1:7:ASN:ND2	2.47	0.47
3:A2:48:ARG:O	3:A2:67:ARG:NH2	2.45	0.47
47:T1:3:ILE:O	47:T1:30:GLY:N	2.41	0.47
47:T1:22:HIS:ND1	47:T1:23:LYS:O	2.45	0.47
59:Z1:57:THR:HG23	59:Z1:60:MET:HE3	1.97	0.47
88:q2:111:THR:H	88:q2:114:ILE:HD11	1.79	0.47
2:A1:1508:G:N1	11:D1:88:PRO:O	2.47	0.47
4:A3:1272:G:O2'	4:A3:2192:A:OP1	2.33	0.47
4:A3:1458:A:H4'	4:A3:1459:G:H5'	1.96	0.47
4:A3:3868:C:H42	4:A3:3889:G:H22	1.61	0.47
33:M1:137:LEU:HG	33:M1:215:VAL:HG22	1.96	0.47
49:U1:110:LEU:HB2	49:U1:147:PHE:HB3	1.96	0.47
83:l2:94:ARG:HB2	83:l2:111:ILE:HD11	1.96	0.47
87:p2:137:THR:O	87:p2:141:SER:HB3	2.14	0.47
88:q2:218:SER:OG	88:q2:221:GLU:OE1	2.32	0.47
4:A3:85:G:N2	4:A3:98:A:OP2	2.43	0.47
4:A3:1394:U:H2'	6:B2:30:LYS:HG3	1.96	0.47
4:A3:1809:C:H2'	4:A3:1810:A2M:H8	1.97	0.47
8:C1:55:VAL:HB	41:Q1:34:SER:HA	1.96	0.47
39:P1:102:ILE:HD12	39:P1:112:HIS:HD2	1.80	0.47
2:A1:949:C:H2'	2:A1:950:G:H8	1.79	0.47
4:A3:741:A:H2'	4:A3:742:A:C8	2.50	0.47
4:A3:2225:A:N1	4:A3:2672:U:O2'	2.46	0.47
4:A3:4363:G:OP2	16:E3:358:ARG:NH2	2.47	0.47
16:E3:77:THR:HG21	16:E3:337:VAL:HG22	1.97	0.47
40:P2:88:ARG:NH2	56:X2:33:LYS:O	2.42	0.47
61:a1:20:VAL:HG12	61:a1:25:LEU:HG	1.97	0.47
73:g2:5:ILE:HG22	73:g2:7:GLU:H	1.80	0.47
2:A1:523:A:H5''	49:U1:145:PRO:HD2	1.95	0.47
2:A1:1500:U:H4'	37:O1:176:LEU:HD13	1.96	0.47
4:A3:73:A:OP1	24:H2:106:SER:OG	2.27	0.47
4:A3:484:G:H3'	4:A3:485:U:H2'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:1654:A:N7	4:A3:1656:C:N4	2.63	0.47
4:A3:1690:A:OP1	15:E2:40:LYS:NZ	2.48	0.47
4:A3:2658:A2M:HM'3	4:A3:2658:A2M:H1'	1.46	0.47
4:A3:3600:G:H22	4:A3:3632:G:H1'	1.80	0.47
4:A3:3892:G:H2'	4:A3:3893:G:H8	1.79	0.47
4:A3:4684:G:N1	64:b2:3:GLY:O	2.43	0.47
13:D3:41:ILE:HG12	13:D3:63:PHE:HD2	1.80	0.47
15:E2:152:LEU:HB3	15:E2:165:ILE:HD12	1.95	0.47
43:R1:129:VAL:O	46:S2:80:ARG:NH2	2.42	0.47
54:W2:72:THR:HG22	54:W2:110:LYS:HB3	1.97	0.47
65:c1:109:LEU:HG	65:c1:111:PHE:HD2	1.79	0.47
80:k1:50:PHE:HB3	80:k1:55:TYR:HB2	1.97	0.47
86:o2:176:ASP:OD1	86:o2:176:ASP:N	2.46	0.47
2:A1:921:A:O2'	2:A1:923:A:OP1	2.31	0.47
4:A3:1388:A:N6	4:A3:1406:G:O2'	2.47	0.47
4:A3:1584:G:N1	13:D3:208:GLU:OE1	2.39	0.47
13:D3:30:ARG:HB3	13:D3:74:GLU:HG2	1.96	0.47
22:G3:208:MET:HB2	22:G3:233:PRO:HG3	1.96	0.47
29:K1:16:H2U:H2'	29:K1:60:U:O2	2.14	0.47
43:R1:145:PHE:O	46:S2:101:ARG:NH2	2.46	0.47
63:b1:132:PHE:O	63:b1:140:ARG:NH1	2.46	0.47
2:A1:121:OMU:HM23	2:A1:121:OMU:H1'	1.70	0.47
2:A1:1551:G:O2'	2:A1:1559:C:O2	2.32	0.47
4:A3:3813:A:H5''	9:C2:56:LYS:HB2	1.97	0.47
13:D3:173:GLY:O	81:k2:69:TRP:NE1	2.48	0.47
31:L1:173:LEU:HD11	31:L1:177:MET:HE3	1.97	0.47
35:N1:203:GLY:O	35:N1:221:ASP:HA	2.15	0.47
42:Q2:28:PRO:HB2	42:Q2:34:MET:HG3	1.96	0.47
57:Y1:55:ARG:NH1	57:Y1:56:ASP:OD1	2.48	0.47
4:A3:1583:C:OP1	13:D3:14:SER:OG	2.33	0.47
4:A3:1741:A:O2'	4:A3:1776:A:OP1	2.29	0.47
4:A3:2363:C:H2'	4:A3:2364:G:C8	2.49	0.47
4:A3:3530:U:OP1	44:R2:73:ARG:NH2	2.48	0.47
12:D2:91:LYS:HG2	12:D2:145:VAL:HG22	1.96	0.47
61:a1:92:SER:HB2	61:a1:107:ILE:HD13	1.96	0.47
73:g2:35:LYS:HA	73:g2:43:TYR:O	2.15	0.47
85:n2:59:THR:HG23	85:n2:74:VAL:HB	1.97	0.47
88:q2:408:ASN:HB3	88:q2:481:ASP:H	1.79	0.47
2:A1:563:U:H2'	2:A1:564:G:C8	2.50	0.46
3:A2:176:LEU:HD21	3:A2:194:GLN:HG2	1.97	0.46
4:A3:62:A:N3	4:A3:77:U:O2'	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:3640:A:C2	21:G2:14:GLU:HA	2.50	0.46
4:A3:3868:C:H42	4:A3:3889:G:H1	1.63	0.46
6:B2:91:VAL:O	6:B2:119:GLY:HA2	2.15	0.46
10:C3:98:C:OP1	48:T2:70:LYS:NZ	2.42	0.46
16:E3:41:VAL:HA	16:E3:187:GLY:HA3	1.97	0.46
22:G3:65:ALA:HB2	22:G3:74:ILE:HD13	1.97	0.46
29:K1:43:G:O2'	29:K1:44:C:H5'	2.13	0.46
44:R2:13:LYS:HD2	44:R2:128:LEU:HD22	1.97	0.46
45:S1:20:GLU:HG2	45:S1:48:ALA:HB3	1.97	0.46
84:m2:146:LYS:HE3	84:m2:148:SER:HB3	1.97	0.46
2:A1:106:C:H2'	2:A1:107:A:H8	1.80	0.46
2:A1:1278:C:H2'	2:A1:1279:A:H8	1.81	0.46
4:A3:691:G:H2'	4:A3:692:G:H8	1.80	0.46
4:A3:1423:C:OP1	54:W2:132:ARG:NH2	2.43	0.46
30:K2:54:TYR:OH	30:K2:73:PHE:O	2.33	0.46
4:A3:755:G:N2	4:A3:800:U:O2	2.40	0.46
4:A3:3766:C:O2	4:A3:3778:A:O2'	2.34	0.46
9:C2:252:LYS:HD3	9:C2:255:LYS:HE3	1.96	0.46
10:C3:67:U:H2'	10:C3:68:G:H8	1.81	0.46
19:F3:67:TRP:HH2	21:G2:1:LEU:HG	1.73	0.46
32:L2:94:MET:HE1	32:L2:146:ILE:HB	1.97	0.46
43:R1:193:ALA:HA	43:R1:196:LYS:HD3	1.96	0.46
45:S1:69:LEU:HD13	45:S1:96:ALA:HB2	1.97	0.46
66:d1:26:ILE:HG13	66:d1:45:LEU:HD11	1.97	0.46
76:i1:67:ARG:HG3	76:i1:115:ILE:HG12	1.98	0.46
2:A1:484:C:OP2	76:i1:48:LYS:HB2	2.16	0.46
9:C2:52:THR:O	10:C3:150:C:N4	2.49	0.46
18:F2:78:LYS:HE3	18:F2:82:ILE:HD11	1.97	0.46
22:G3:258:LYS:HB2	22:G3:258:LYS:HE2	1.72	0.46
45:S1:76:GLN:HE21	45:S1:76:GLN:HA	1.79	0.46
65:c1:29:HIS:HA	65:c1:32:LYS:HE2	1.98	0.46
2:A1:1564:G:OP1	68:e1:121:ARG:NH1	2.46	0.46
4:A3:3781:A:H4'	86:o2:213:PRO:HG3	1.97	0.46
4:A3:4138:OMG:H2'	4:A3:4193:5MC:HM51	1.98	0.46
9:C2:50:ASP:OD1	9:C2:52:THR:OG1	2.32	0.46
38:O2:130:GLU:HB3	38:O2:132:MET:HE2	1.97	0.46
39:P1:239:PRO:O	39:P1:242:LYS:NZ	2.44	0.46
88:q2:589:LYS:HA	88:q2:594:TYR:HE1	1.81	0.46
4:A3:1947:U:H1'	4:A3:1950:C:H5	1.80	0.46
4:A3:3930:G:H5'	13:D3:233:ARG:HB2	1.97	0.46
4:A3:4741:U:OP2	16:E3:385:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:F1:60:ASP:OD1	17:F1:60:ASP:N	2.43	0.46
39:P1:54:TYR:O	78:j1:15:ASN:ND2	2.48	0.46
87:p2:177:PRO:HG3	87:p2:197:LYS:CB	2.46	0.46
2:A1:574:U:O2	2:A1:577:A2M:H8	2.15	0.46
39:P1:100:ARG:HH12	39:P1:122:LYS:HA	1.81	0.46
78:j1:83:LYS:HE2	78:j1:96:LEU:HD23	1.97	0.46
88:q2:204:LEU:HB3	88:q2:206:LEU:HD13	1.98	0.46
1:MB:56:VAL:HG13	1:MB:72:LYS:HA	1.98	0.46
2:A1:39:A:H3'	2:A1:40:A:H8	1.81	0.46
2:A1:894:U:H2'	2:A1:895:G:H8	1.81	0.46
4:A3:4340:U:H2'	4:A3:4341:G:H8	1.79	0.46
4:A3:4730:U:H2'	4:A3:4731:G:H8	1.80	0.46
20:G1:198:VAL:HA	20:G1:208:ALA:O	2.15	0.46
29:K1:2:C:H2'	29:K1:3:G:C8	2.50	0.46
31:L1:174:MET:HE3	31:L1:174:MET:HB3	1.78	0.46
88:q2:411:TYR:HD1	88:q2:484:LEU:HD23	1.81	0.46
2:A1:39:A:H5'	49:U1:7:TRP:NE1	2.31	0.46
2:A1:536:G:H2'	2:A1:537:A:H8	1.81	0.46
4:A3:3664:U:H2'	4:A3:3665:G:H8	1.81	0.46
16:E3:168:MET:HE1	16:E3:173:LEU:HD12	1.97	0.46
24:H2:208:GLU:O	86:o2:184:HIS:NE2	2.48	0.46
48:T2:81:LEU:HG	48:T2:83:THR:HG23	1.98	0.46
4:A3:1070:U:O2	22:G3:286:SER:OG	2.33	0.46
4:A3:2272:A:OP1	75:h2:43:HIS:NE2	2.41	0.46
4:A3:2469:U:O4	42:Q2:97:ARG:NH1	2.49	0.46
4:A3:2578:G:H2'	4:A3:2579:G:H8	1.80	0.46
15:E2:184:MET:HA	15:E2:187:GLU:HG2	1.98	0.46
39:P1:104:ASP:HB3	39:P1:110:ALA:HB2	1.96	0.46
70:f1:98:VAL:O	70:f1:101:ILE:HG22	2.16	0.46
85:n2:80:LEU:HB3	85:n2:112:ILE:HD11	1.98	0.46
88:q2:101:ARG:HD2	88:q2:104:GLU:HG3	1.98	0.46
2:A1:616:C:O3'	14:E1:82:ARG:NH1	2.49	0.45
2:A1:1116:U:H1'	2:A1:1117:C:H2'	1.98	0.45
4:A3:1942:G:N2	4:A3:1943:U:O4	2.48	0.45
4:A3:3984:G:H2'	4:A3:3985:A:C8	2.51	0.45
5:B1:33:MET:HE1	5:B1:73:LEU:HD11	1.98	0.45
20:G1:57:ARG:NH1	20:G1:94:THR:O	2.49	0.45
31:L1:207:PRO:HA	31:L1:210:ILE:HB	1.98	0.45
87:p2:302:CYS:O	87:p2:308:THR:OG1	2.35	0.45
2:A1:641:A:H2'	2:A1:642:A:C8	2.52	0.45
4:A3:1680:G:O6	7:B3:103:A:O2'	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:1737:G:O2'	40:P2:60:LYS:NZ	2.49	0.45
4:A3:4512:G:OP1	12:D2:23:ARG:NH1	2.49	0.45
6:B2:126:LYS:HB2	40:P2:133:ALA:HB3	1.97	0.45
24:H2:91:ALA:HB1	24:H2:96:ILE:HB	1.97	0.45
26:I2:86:TRP:O	26:I2:89:THR:OG1	2.35	0.45
35:N1:65:LYS:HG2	35:N1:273:LEU:HD22	1.99	0.45
45:S1:77:VAL:HA	45:S1:80:VAL:HG12	1.97	0.45
78:j1:82:ALA:O	78:j1:86:GLU:HB2	2.16	0.45
4:A3:795:A:O2'	4:A3:798:C:N4	2.48	0.45
4:A3:1093:C:H2'	4:A3:1094:A:H8	1.82	0.45
4:A3:1399:G:O6	4:A3:2049:G:O6	2.34	0.45
4:A3:1881:A:H2'	4:A3:1882:A:C8	2.51	0.45
4:A3:2637:C:C4	21:G2:0:GLN:HG2	2.51	0.45
4:A3:4220:A:OP2	4:A3:4222:C:N4	2.48	0.45
4:A3:4508:G:H2'	4:A3:4509:A:H8	1.81	0.45
4:A3:4610:C:N4	38:O2:171:ARG:O	2.50	0.45
24:H2:80:GLU:HG3	24:H2:110:LEU:HD12	1.99	0.45
29:K1:61:C:H2'	29:K1:62:C:C6	2.52	0.45
68:e1:104:LEU:HD22	68:e1:121:ARG:HD3	1.99	0.45
2:A1:590:G:H21	14:E1:99:LYS:HE3	1.81	0.45
3:A2:78:PRO:HD2	3:A2:84:ARG:HG3	1.98	0.45
3:A2:193:HIS:HB3	3:A2:196:PHE:HD2	1.81	0.45
4:A3:1343:G:H2'	4:A3:1344:G:H8	1.80	0.45
4:A3:4663:C:O2'	4:A3:4664:U:O4'	2.29	0.45
28:J2:165:THR:O	28:J2:169:ARG:HB2	2.16	0.45
2:A1:206:G:O6	47:T1:144:LYS:NZ	2.45	0.45
2:A1:745:G:H21	45:S1:109:ARG:HA	1.82	0.45
2:A1:1271:G:H2'	2:A1:1272:C:H5''	1.99	0.45
15:E2:109:ASP:OD1	15:E2:109:ASP:N	2.41	0.45
17:F1:44:ILE:O	59:Z1:113:GLN:NE2	2.38	0.45
55:X1:92:CYS:HB2	55:X1:103:VAL:HG23	1.98	0.45
57:Y1:34:LYS:HE2	57:Y1:74:ILE:HG12	1.99	0.45
72:g1:38:GLU:OE2	72:g1:51:LYS:NZ	2.42	0.45
76:i1:49:GLY:O	76:i1:99:GLU:HA	2.16	0.45
2:A1:279:C:H2'	2:A1:280:G:C8	2.51	0.45
2:A1:1233:PSU:H2'	2:A1:1234:G:C8	2.52	0.45
2:A1:1529:G:O2'	2:A1:1667:C:OP1	2.33	0.45
3:A2:48:ARG:HB2	3:A2:64:MET:HE1	1.98	0.45
4:A3:1079:C:H2'	4:A3:1080:G:H8	1.82	0.45
4:A3:1984:G:O6	4:A3:3602:C:O2'	2.31	0.45
4:A3:4177:PSU:OP2	15:E2:3:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D2:44:GLU:OE2	26:I2:2:VAL:N	2.49	0.45
15:E2:35:ASP:HB2	15:E2:86:HIS:HE2	1.80	0.45
19:F3:28:PHE:HA	19:F3:129:ALA:HA	1.99	0.45
45:S1:40:LEU:HD11	45:S1:79:LEU:HD21	1.97	0.45
73:g2:26:LYS:HB2	73:g2:69:LEU:HD12	1.99	0.45
2:A1:383:C:H2'	2:A1:384:G:H8	1.81	0.45
2:A1:528:C:H2'	2:A1:529:A:H8	1.82	0.45
4:A3:37:U:H4'	54:W2:32:ARG:HD2	1.98	0.45
4:A3:153:G:H2'	4:A3:154:G:H8	1.80	0.45
4:A3:1127:G:H1'	56:X2:120:ARG:HB2	1.97	0.45
4:A3:2267:OMG:HM23	4:A3:2267:OMG:H1'	1.77	0.45
4:A3:4364:OMG:H5''	44:R2:15:ARG:HB2	1.97	0.45
13:D3:20:VAL:HA	13:D3:23:ARG:HG3	1.99	0.45
16:E3:83:PRO:O	16:E3:167:GLN:NE2	2.49	0.45
20:G1:212:LYS:HA	20:G1:235:ILE:HG23	1.97	0.45
2:A1:485:A2M:O5'	2:A1:485:A2M:H8	2.16	0.45
3:A2:156:LEU:HD11	3:A2:198:ILE:HG13	1.99	0.45
4:A3:362:A:N6	75:h2:37:TYR:O	2.48	0.45
4:A3:1548:A:H5''	4:A3:2682:U:H5''	1.98	0.45
4:A3:1972:A:OP1	15:E2:162:ARG:NH2	2.46	0.45
19:F3:83:GLY:HA2	21:G2:-2:ALA:HB1	1.99	0.45
26:I2:40:GLY:HA3	26:I2:45:VAL:HB	1.98	0.45
39:P1:45:ILE:HA	39:P1:61:VAL:HG11	1.99	0.45
57:Y1:5:HIS:HB3	57:Y1:117:LEU:HD13	1.99	0.45
2:A1:1338:4AC:H2'	2:A1:1339:G:H8	1.82	0.45
4:A3:300:A:H2'	4:A3:301:G:H8	1.82	0.45
4:A3:3478:A:H5''	13:D3:244:GLY:HA3	1.99	0.45
4:A3:4135:C:H2'	4:A3:4136:A:C8	2.52	0.45
4:A3:4269:A2M:HM'3	4:A3:4269:A2M:H1'	1.71	0.45
4:A3:4650:A:OP1	16:E3:97:ARG:NH2	2.48	0.45
12:D2:115:ARG:HG2	12:D2:123:ILE:HG12	1.99	0.45
16:E3:35:ASP:OD2	16:E3:193:LYS:NZ	2.49	0.45
43:R1:3:LEU:HD13	43:R1:109:LEU:HB3	1.99	0.45
47:T1:87:ASN:HB3	47:T1:90:LEU:HG	1.98	0.45
50:U2:70:VAL:HA	50:U2:82:ILE:HG22	1.97	0.45
2:A1:1200:A:OP1	17:F1:2:THR:N	2.50	0.45
20:G1:82:SER:OG	20:G1:84:ASP:OD1	2.30	0.45
34:M2:75:ARG:HA	34:M2:78:LYS:HD3	1.99	0.45
37:O1:62:LYS:O	37:O1:67:ARG:NH2	2.48	0.45
53:W1:22:ARG:HD3	53:W1:28:THR:HB	1.98	0.45
75:h2:20:ASN:ND2	75:h2:42:ARG:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:p2:338:THR:HG23	87:p2:364:GLN:HE22	1.82	0.45
88:q2:108:LEU:HB2	88:q2:272:VAL:HG22	1.99	0.45
2:A1:1781:G:H2'	2:A1:1782:A:C8	2.52	0.44
4:A3:74:G:H5''	24:H2:59:VAL:HB	1.98	0.44
4:A3:1299:G:OP1	34:M2:108:ARG:NH2	2.38	0.44
4:A3:4456:C:H2'	4:A3:4457:C:C6	2.51	0.44
4:A3:4731:G:H2'	4:A3:4732:G:C8	2.52	0.44
6:B2:222:LYS:HA	6:B2:231:ASP:HB2	1.98	0.44
31:L1:81:ASN:OD1	31:L1:81:ASN:N	2.49	0.44
65:c1:57:LEU:HD13	65:c1:69:ILE:HD11	1.98	0.44
71:f2:19:CYS:HB3	71:f2:27:TYR:HB2	1.98	0.44
86:o2:32:VAL:HB	86:o2:171:HIS:HA	1.99	0.44
4:A3:769:C:H2'	4:A3:770:G:C8	2.53	0.44
14:E1:112:TYR:CG	49:U1:33:GLY:HA3	2.52	0.44
43:R1:67:VAL:HB	43:R1:99:GLY:HA2	1.99	0.44
53:W1:65:ASN:O	53:W1:132:ARG:NH1	2.48	0.44
55:X1:81:ASP:HB3	55:X1:84:LYS:HB2	1.97	0.44
85:n2:13:VAL:HB	85:n2:62:LEU:HB2	1.99	0.44
2:A1:77:A:H2	43:R1:175:LYS:HG3	1.80	0.44
2:A1:116:OMU:H1'	2:A1:116:OMU:HM23	1.76	0.44
4:A3:1845:U:H2'	4:A3:1846:A:H8	1.83	0.44
4:A3:3587:C:H2'	4:A3:3588:A:H8	1.82	0.44
4:A3:4337:U:H2'	4:A3:4338:C:C6	2.52	0.44
56:X2:40:LEU:HD12	56:X2:43:MET:HE3	1.99	0.44
2:A1:669:A2M:HM'3	2:A1:669:A2M:H1'	1.72	0.44
2:A1:929:G:H2'	2:A1:930:G:C8	2.53	0.44
4:A3:280:G:OP2	28:J2:44:ARG:NH2	2.48	0.44
4:A3:2250:G:H2'	75:h2:13:LEU:HD22	1.98	0.44
4:A3:3996:G:OP1	18:F2:98:ASN:ND2	2.49	0.44
9:C2:83:PHE:HA	9:C2:183:ILE:HD13	1.99	0.44
9:C2:99:ALA:HB1	9:C2:136:LEU:HD11	1.98	0.44
56:X2:90:SER:HB3	56:X2:93:LEU:HB2	2.00	0.44
62:a2:78:LEU:O	83:l2:20:ARG:NH1	2.45	0.44
66:d1:51:ASP:OD2	66:d1:53:THR:OG1	2.28	0.44
4:A3:1479:A2M:H8	4:A3:3647:U:O2	2.17	0.44
4:A3:2689:G:O2'	44:R2:19:GLY:O	2.35	0.44
4:A3:4055:G:H5'	4:A3:4084:G:H5''	1.98	0.44
6:B2:126:LYS:O	6:B2:130:ASN:ND2	2.50	0.44
38:O2:30:MET:HE2	38:O2:30:MET:HB3	1.86	0.44
63:b1:58:LEU:HB3	63:b1:62:ARG:HD2	2.00	0.44
88:q2:372:SER:N	88:q2:513:LYS:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A1:640:C:H2'	2:A1:641:A:H8	1.82	0.44
2:A1:1679:A2M:HM'3	2:A1:1679:A2M:H1'	1.48	0.44
4:A3:1935:C:H42	4:A3:1939:G:H22	1.64	0.44
4:A3:3450:A2M:HM'3	4:A3:3450:A2M:H1'	1.65	0.44
13:D3:51:ASP:HB3	13:D3:54:ARG:HB3	2.00	0.44
20:G1:199:THR:HG21	20:G1:239:LEU:O	2.18	0.44
39:P1:151:ASP:HB3	39:P1:154:ILE:HG13	2.00	0.44
46:S2:1:MET:HE3	46:S2:15:PRO:HB3	2.00	0.44
66:d1:14:ARG:HD2	66:d1:14:ARG:HA	1.70	0.44
68:e1:18:LEU:HD22	68:e1:58:ALA:HA	1.99	0.44
84:m2:33:ASP:OD1	84:m2:85:ASN:ND2	2.50	0.44
86:o2:122:ARG:HG3	86:o2:123:ILE:HG23	1.99	0.44
88:q2:76:PRO:HG2	88:q2:79:LEU:HD23	1.99	0.44
2:A1:1589:A:H2'	2:A1:1590:A:C8	2.53	0.44
4:A3:511:A:N6	54:W2:106:SER:OG	2.50	0.44
4:A3:1757:G:O2'	4:A3:1759:C:OP2	2.30	0.44
4:A3:3464:A:H2'	4:A3:3465:A:H8	1.82	0.44
9:C2:232:GLU:O	9:C2:236:HIS:HB2	2.17	0.44
36:N2:105:LEU:HD13	36:N2:135:LYS:HE3	2.00	0.44
44:R2:33:GLY:HA3	44:R2:69:LYS:HD2	2.00	0.44
71:f2:27:TYR:HA	71:f2:34:CYS:HA	2.00	0.44
87:p2:349:GLU:HA	87:p2:352:LYS:HG2	1.98	0.44
88:q2:485:ILE:O	88:q2:517:VAL:HA	2.18	0.44
2:A1:74:G:H22	43:R1:171:THR:H	1.65	0.44
4:A3:3477:U:HO2'	13:D3:243:THR:H	1.66	0.44
4:A3:3985:A:H2'	4:A3:3986:G:C8	2.53	0.44
11:D1:114:ILE:HG13	55:X1:68:LEU:HD22	2.00	0.44
16:E3:354:GLN:HB3	16:E3:359:ALA:HB1	2.00	0.44
21:G2:1:LEU:C	21:G2:1:LEU:HD13	2.43	0.44
37:O1:132:LYS:HD3	37:O1:189:MET:HE2	2.00	0.44
43:R1:39:ASP:OD1	43:R1:47:GLY:N	2.47	0.44
43:R1:85:ARG:O	43:R1:87:ARG:NH1	2.50	0.44
58:Y2:20:LEU:HA	58:Y2:23:LYS:HG2	2.00	0.44
66:d1:26:ILE:HG12	66:d1:59:LEU:HD11	1.99	0.44
73:g2:33:LYS:HG2	73:g2:46:VAL:HG22	2.00	0.44
86:o2:184:HIS:HA	86:o2:187:VAL:HG22	2.00	0.44
88:q2:449:LEU:O	88:q2:469:ARG:NH2	2.46	0.44
2:A1:751:C:H2'	2:A1:752:G:H8	1.82	0.44
2:A1:1846:A:H2'	2:A1:1847:G:C8	2.53	0.44
4:A3:1513:A:H2'	4:A3:1514:G:C8	2.53	0.44
4:A3:2034:A:H2'	4:A3:2035:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:4764:C:O2	4:A3:4767:G:N2	2.38	0.44
28:J2:20:ARG:HH22	69:e2:52:PRO:HG3	1.82	0.44
66:d1:62:ASP:OD1	66:d1:62:ASP:N	2.50	0.44
86:o2:31:THR:HB	86:o2:171:HIS:CE1	2.52	0.44
2:A1:152:U:O4'	43:R1:132:ARG:NH1	2.50	0.43
2:A1:1011:G:H2'	2:A1:1012:A:C8	2.53	0.43
2:A1:1240:U:H5''	61:a1:124:LYS:HD3	2.00	0.43
4:A3:1346:C:H2'	4:A3:1347:G:H8	1.83	0.43
4:A3:1664:U:H2'	4:A3:1665:U:H6	1.83	0.43
4:A3:1921:G:N2	4:A3:1948:A:O2'	2.51	0.43
4:A3:4384:U:OP1	4:A3:4783:A:O2'	2.36	0.43
21:G2:-3:VAL:O	21:G2:-2:ALA:C	2.60	0.43
29:K1:20:U:H4'	29:K1:21:A:H5'	2.00	0.43
29:K1:32:OMU:HM23	29:K1:32:OMU:H1'	1.79	0.43
46:S2:82:ILE:HG22	46:S2:84:GLY:H	1.83	0.43
60:Z2:33:ILE:HG22	60:Z2:44:ARG:HG3	1.99	0.43
86:o2:98:LYS:HA	86:o2:98:LYS:HD3	1.78	0.43
88:q2:351:PRO:HD2	88:q2:353:MET:HE3	1.99	0.43
2:A1:1205:A:O2'	2:A1:1701:C:OP2	2.33	0.43
2:A1:1569:C:OP1	68:e1:96:SER:OG	2.30	0.43
4:A3:2691:G:O2'	4:A3:3570:U:O4	2.30	0.43
22:G3:223:PHE:HB3	22:G3:226:TYR:HB2	1.99	0.43
34:M2:49:LYS:HB3	34:M2:49:LYS:HE2	1.72	0.43
46:S2:81:ALA:HB2	46:S2:87:LEU:HB2	2.01	0.43
63:b1:112:LEU:HD22	63:b1:119:LEU:HD13	2.00	0.43
88:q2:105:VAL:H	88:q2:284:ASP:HB2	1.82	0.43
2:A1:1514:C:H2'	2:A1:1515:G:H8	1.82	0.43
4:A3:10:A:H2'	4:A3:11:G:C8	2.52	0.43
4:A3:1688:A:H2'	4:A3:1689:G:C8	2.54	0.43
4:A3:1955:C:H2'	4:A3:1956:A:H8	1.82	0.43
34:M2:134:ARG:HE	34:M2:134:ARG:HB3	1.72	0.43
36:N2:76:MET:HE3	36:N2:76:MET:HB3	1.87	0.43
43:R1:126:ASP:OD1	43:R1:126:ASP:N	2.49	0.43
45:S1:70:LYS:O	45:S1:74:LYS:HG2	2.18	0.43
68:e1:51:ASN:HB3	68:e1:54:TYR:HD2	1.83	0.43
2:A1:67:C:OP2	43:R1:172:LYS:NZ	2.49	0.43
2:A1:384:G:O2'	53:W1:133:PRO:O	2.33	0.43
4:A3:268:G:H2'	4:A3:269:G:H8	1.83	0.43
4:A3:400:A2M:HM'3	4:A3:400:A2M:H1'	1.80	0.43
4:A3:483:G:O2'	4:A3:486:C:OP2	2.33	0.43
4:A3:1414:A:OP1	34:M2:65:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:1638:PSU:OP1	54:W2:44:ASN:ND2	2.47	0.43
4:A3:3480:A:O2'	13:D3:223:SER:OG	2.35	0.43
4:A3:4117:G:N2	27:J1:76:A:O2'	2.51	0.43
4:A3:4383:OMG:HM23	4:A3:4383:OMG:H1'	1.63	0.43
4:A3:4706:A:H2'	4:A3:4707:A:C8	2.53	0.43
7:B3:3:C:H2'	7:B3:4:U:H6	1.83	0.43
7:B3:92:C:H2'	7:B3:93:G:H8	1.83	0.43
11:D1:124:ASP:OD1	11:D1:124:ASP:N	2.45	0.43
27:J1:35:U:H2'	27:J1:36:U:H6	1.82	0.43
39:P1:124:CYS:HB3	39:P1:141:THR:HB	2.00	0.43
63:b1:34:VAL:HG22	63:b1:70:VAL:HB	2.00	0.43
86:o2:158:GLN:HG3	86:o2:160:LYS:HG3	2.00	0.43
2:A1:159:A2M:H8	2:A1:159:A2M:O5'	2.19	0.43
2:A1:1384:A2M:H1'	2:A1:1384:A2M:HM'3	1.61	0.43
2:A1:1414:G:H2'	2:A1:1415:A:H8	1.83	0.43
4:A3:68:U:OP1	28:J2:178:HIS:ND1	2.40	0.43
4:A3:1252:C:H2'	4:A3:1253:C:C6	2.54	0.43
4:A3:4506:C:H2'	4:A3:4507:G:C8	2.53	0.43
6:B2:168:LEU:HD13	6:B2:174:ILE:HD11	2.00	0.43
32:L2:112:LEU:HD13	32:L2:150:LEU:HD13	2.01	0.43
41:Q1:50:PRO:HG2	41:Q1:90:VAL:HG22	2.00	0.43
43:R1:181:THR:HG22	43:R1:183:ARG:H	1.84	0.43
71:f2:64:MET:HE3	71:f2:67:LEU:HD23	2.00	0.43
81:k2:46:LYS:HD3	81:k2:59:SER:HB2	2.00	0.43
2:A1:997:A:H2'	2:A1:998:A:C8	2.54	0.43
4:A3:478:G:H2'	4:A3:479:G:H8	1.83	0.43
4:A3:3779:C:H2'	4:A3:3780:C:C6	2.53	0.43
4:A3:4017:A:OP1	4:A3:4018:G:N2	2.51	0.43
7:B3:3:C:H2'	7:B3:4:U:C6	2.54	0.43
9:C2:96:LEU:HD11	9:C2:189:ARG:HD2	2.00	0.43
22:G3:52:ILE:HA	22:G3:147:ASP:HB3	2.01	0.43
35:N1:272:HIS:CD2	35:N1:275:LYS:HE3	2.54	0.43
37:O1:212:GLU:OE1	65:c1:19:LYS:NZ	2.44	0.43
52:V2:35:ASP:OD1	52:V2:35:ASP:N	2.52	0.43
87:p2:372:MET:HA	87:p2:373:PRO:HD3	1.90	0.43
2:A1:1419:C:O2'	2:A1:1421:G:OP2	2.30	0.43
4:A3:1343:G:H2'	4:A3:1344:G:C8	2.54	0.43
4:A3:2105:G:OP2	83:l2:98:ARG:NH1	2.41	0.43
4:A3:3511:A:H2'	4:A3:3512:G:O4'	2.18	0.43
4:A3:3664:U:H2'	4:A3:3665:G:C8	2.53	0.43
4:A3:3954:U:OP1	4:A3:4080:U:O2'	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:4357:A:H2	12:D2:120:GLU:HG2	1.82	0.43
15:E2:198:LYS:HB2	15:E2:198:LYS:HE3	1.87	0.43
19:F3:156:ASP:OD2	19:F3:255:SER:OG	2.33	0.43
24:H2:111:GLN:O	24:H2:115:GLN:OE1	2.37	0.43
35:N1:196:ILE:HB	35:N1:223:TYR:HB2	1.99	0.43
44:R2:3:LYS:HD3	44:R2:3:LYS:HA	1.83	0.43
68:e1:111:LYS:HE2	68:e1:111:LYS:HB2	1.75	0.43
78:j1:10:ARG:HG3	78:j1:11:LYS:HG3	2.01	0.43
83:l2:63:VAL:HA	83:l2:78:VAL:O	2.18	0.43
86:o2:36:ILE:HG21	86:o2:190:LEU:HD21	1.99	0.43
2:A1:228:C:H4'	43:R1:231:ARG:HH12	1.83	0.43
7:B3:63:C:H5'	7:B3:64:G:H5''	2.00	0.43
19:F3:171:LEU:HD21	19:F3:227:ILE:HD11	2.00	0.43
54:W2:132:ARG:HA	54:W2:135:GLU:HG2	2.01	0.43
84:m2:44:ARG:HA	84:m2:47:LEU:HG	2.01	0.43
4:A3:1513:A:H2'	4:A3:1514:G:H8	1.84	0.43
4:A3:4006:U:H2'	4:A3:4007:C:C6	2.54	0.43
12:D2:95:VAL:HG22	77:i2:82:LEU:HB3	2.01	0.43
23:H1:36:LEU:HD23	37:O1:16:ILE:HD11	2.00	0.43
88:q2:486:ASP:OD1	88:q2:486:ASP:N	2.46	0.43
3:A2:124:VAL:HG21	4:A3:696:U:H5'	2.01	0.43
4:A3:1076:G:O2'	22:G3:278:ASP:OD2	2.26	0.43
4:A3:1449:U:H2'	4:A3:1450:G:H8	1.84	0.43
4:A3:1546:U:OP2	4:A3:2699:C:O2'	2.27	0.43
4:A3:2140:G:H4'	19:F3:242:PRO:HB2	2.01	0.43
4:A3:2400:G:O6	4:A3:2413:U:O4	2.37	0.43
4:A3:2592:C:H2'	4:A3:2593:G:H8	1.84	0.43
4:A3:4283:C:H2'	4:A3:4284:G:C8	2.54	0.43
4:A3:4635:G:H2'	4:A3:4636:G:C8	2.54	0.43
7:B3:15:C:H2'	7:B3:16:A:H8	1.84	0.43
9:C2:88:ASP:OD1	9:C2:88:ASP:N	2.50	0.43
10:C3:153:C:H2'	10:C3:154:G:H8	1.84	0.43
24:H2:56:ARG:NH1	24:H2:74:ARG:O	2.46	0.43
26:I2:38:VAL:O	26:I2:47:ARG:HA	2.19	0.43
57:Y1:132:LYS:HA	57:Y1:132:LYS:HD3	1.78	0.43
61:a1:81:ARG:NH2	61:a1:117:GLY:O	2.52	0.43
84:m2:47:LEU:HB2	84:m2:51:ALA:HB3	2.00	0.43
86:o2:6:SER:N	86:o2:9:THR:OG1	2.42	0.43
12:D2:59:LYS:HE3	12:D2:66:GLU:HB3	2.01	0.42
13:D3:180:LEU:HD11	81:k2:26:VAL:HG11	2.01	0.42
22:G3:179:ARG:HA	22:G3:179:ARG:HD3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:P1:128:LYS:HG2	39:P1:140:VAL:HB	2.00	0.42
43:R1:67:VAL:HG12	43:R1:69:THR:HG22	2.01	0.42
47:T1:65:PHE:HA	47:T1:187:GLY:O	2.18	0.42
2:A1:1101:A:OP1	65:c1:129:LYS:NZ	2.42	0.42
2:A1:1148:C:OP1	17:F1:6:ARG:NH1	2.52	0.42
2:A1:1289:OMU:HN3	2:A1:1312:C:H42	1.65	0.42
2:A1:1770:C:H2'	2:A1:1771:G:C8	2.53	0.42
4:A3:2545:C:O3'	42:Q2:113:ARG:NH1	2.52	0.42
19:F3:116:ASN:HB2	19:F3:119:GLN:HG3	2.02	0.42
20:G1:42:MET:HE2	20:G1:92:LEU:HD22	2.01	0.42
46:S2:97:LYS:HB2	46:S2:100:VAL:HG23	2.01	0.42
52:V2:11:VAL:HG12	52:V2:82:PRO:HA	2.01	0.42
60:Z2:50:ARG:HG2	60:Z2:54:MET:HE3	2.00	0.42
2:A1:5:U:H2'	2:A1:6:G:C8	2.54	0.42
2:A1:151:C:OP1	78:j1:120:THR:OG1	2.31	0.42
2:A1:1233:PSU:H2'	2:A1:1234:G:H8	1.84	0.42
4:A3:1699:G:H2'	4:A3:1700:G:C8	2.54	0.42
4:A3:4429:U:H2'	4:A3:4430:A:C8	2.54	0.42
4:A3:4786:C:O2'	4:A3:4789:C:OP2	2.31	0.42
14:E1:83:VAL:HG11	76:i1:91:LEU:HB3	2.01	0.42
15:E2:189:ARG:HH21	15:E2:201:PRO:HA	1.84	0.42
20:G1:146:SER:HA	20:G1:177:TRP:HH2	1.85	0.42
33:M1:25:PHE:HA	33:M1:28:LYS:HG3	2.00	0.42
35:N1:65:LYS:HE3	35:N1:273:LEU:HD13	2.01	0.42
36:N2:96:MET:HE3	36:N2:96:MET:HB2	1.83	0.42
54:W2:89:ASN:HA	54:W2:92:LYS:HG2	2.00	0.42
85:n2:96:LYS:NZ	85:n2:97:ASN:OD1	2.42	0.42
88:q2:36:LYS:HB3	88:q2:54:LEU:HD21	2.01	0.42
2:A1:99:A2M:HM'3	2:A1:99:A2M:H1'	1.81	0.42
2:A1:571:C:O2'	78:j1:34:THR:O	2.35	0.42
4:A3:1250:C:H2'	4:A3:1251:A:C8	2.55	0.42
4:A3:3816:C:H2'	4:A3:3817:G:C8	2.54	0.42
4:A3:4508:G:H2'	4:A3:4509:A:C8	2.55	0.42
12:D2:111:LEU:HD13	12:D2:127:ARG:HE	1.84	0.42
15:E2:109:ASP:HB2	29:K1:74:C:OP2	2.19	0.42
20:G1:124:SER:OG	20:G1:126:ASP:OD1	2.29	0.42
33:M1:131:ASP:OD1	33:M1:131:ASP:N	2.50	0.42
38:O2:81:TRP:HB2	38:O2:128:LYS:HB3	2.00	0.42
39:P1:107:GLY:HA2	39:P1:189:LEU:HG	2.02	0.42
61:a1:67:ALA:HB2	61:a1:73:PRO:HB3	2.02	0.42
88:q2:424:VAL:HB	88:q2:455:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A1:1099:C:H2'	2:A1:1100:G:C8	2.54	0.42
2:A1:1185:G:OP1	82:l1:11:ARG:NH2	2.50	0.42
3:A2:115:MET:O	83:l2:87:ARG:NH1	2.42	0.42
4:A3:10:A:H2'	4:A3:11:G:H8	1.85	0.42
4:A3:673:C:H2'	4:A3:674:G:H8	1.84	0.42
4:A3:2387:G:H4'	4:A3:2389:G:C8	2.54	0.42
4:A3:3920:U:H2'	4:A3:3921:G:C8	2.54	0.42
4:A3:4635:G:H2'	4:A3:4636:G:H8	1.85	0.42
8:C1:21:THR:HB	8:C1:68:LEU:HD11	2.00	0.42
8:C1:26:GLN:NE2	41:Q1:127:ARG:O	2.52	0.42
15:E2:115:MET:HE3	15:E2:115:MET:HB3	1.87	0.42
24:H2:58:ILE:HG12	24:H2:157:ILE:HG12	2.01	0.42
35:N1:166:ARG:HD3	35:N1:181:PRO:HG3	2.01	0.42
54:W2:100:ILE:HG12	54:W2:123:ILE:HB	2.01	0.42
70:f1:97:ILE:O	70:f1:100:GLN:HG3	2.20	0.42
83:l2:90:LEU:HG	83:l2:111:ILE:HG23	2.00	0.42
4:A3:66:A:O2'	4:A3:326:C:O2	2.37	0.42
4:A3:1601:A:O2'	71:f2:49:TRP:O	2.31	0.42
4:A3:2206:A2M:H2'	4:A3:2207:OMG:O4'	2.19	0.42
4:A3:3347:G:H1'	46:S2:44:ARG:HE	1.84	0.42
4:A3:3593:A:H2'	4:A3:3594:A:H8	1.85	0.42
4:A3:4138:OMG:HM21	4:A3:4140:A:H2'	2.02	0.42
15:E2:54:SER:OG	15:E2:130:HIS:O	2.38	0.42
20:G1:153:CYS:O	20:G1:167:SER:HA	2.20	0.42
22:G3:99:TYR:HE1	22:G3:164:LYS:HG3	1.85	0.42
63:b1:86:GLN:HE22	63:b1:122:ALA:HB2	1.83	0.42
70:f1:23:THR:OG1	70:f1:113:GLU:OE1	2.38	0.42
88:q2:29:CYS:HB3	88:q2:32:VAL:HG12	2.02	0.42
2:A1:106:C:H2'	2:A1:107:A:C8	2.54	0.42
2:A1:168:C:O2'	43:R1:133:LEU:O	2.35	0.42
2:A1:795:A:H2'	2:A1:796:A:H8	1.84	0.42
2:A1:935:G:H22	2:A1:1009:A:H2	1.68	0.42
2:A1:1122:G:O2'	33:M1:204:ILE:O	2.36	0.42
2:A1:1842:C:H2'	2:A1:1843:4AC:H6	2.01	0.42
4:A3:1391:C:H4'	4:A3:1393:C:H5'	2.02	0.42
4:A3:1507:G:O2'	4:A3:1529:G:N2	2.43	0.42
4:A3:1545:C:H3'	4:A3:1546:U:H4'	2.02	0.42
5:B1:67:THR:OG1	5:B1:70:LYS:O	2.30	0.42
12:D2:92:MET:HG2	12:D2:181:VAL:HA	2.00	0.42
27:J1:41:U:H2'	27:J1:42:G:C8	2.54	0.42
41:Q1:19:LEU:HD21	41:Q1:69:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:g2:49:ASP:OD2	73:g2:52:LYS:NZ	2.48	0.42
86:o2:111:LEU:HB3	86:o2:138:LEU:HD11	2.00	0.42
87:p2:291:PHE:HA	87:p2:294:ILE:HG22	2.02	0.42
2:A1:65:C:N4	43:R1:134:GLY:O	2.40	0.42
2:A1:188:C:H2'	2:A1:189:U:C6	2.55	0.42
2:A1:1760:G:H2'	2:A1:1761:G:H8	1.85	0.42
2:A1:1783:G:H5'	2:A1:1784:C:H4'	2.01	0.42
3:A2:189:LEU:HD21	3:A2:256:VAL:HG11	2.01	0.42
4:A3:306:A:O3'	69:e2:86:LYS:NZ	2.51	0.42
4:A3:1068:U:H2'	4:A3:1069:G:H8	1.85	0.42
4:A3:1600:C:H2'	4:A3:1601:A:C8	2.55	0.42
27:J1:43:A:H2'	27:J1:44:G:C8	2.55	0.42
63:b1:109:LYS:HB3	63:b1:109:LYS:HE2	1.85	0.42
2:A1:642:A:O2'	2:A1:646:C:OP1	2.37	0.42
2:A1:1652:A:H2'	2:A1:1653:G:H8	1.84	0.42
4:A3:1872:G:H2'	4:A3:1873:A:C8	2.55	0.42
4:A3:3897:G:H2'	4:A3:3898:G:H8	1.85	0.42
4:A3:3954:U:H2'	4:A3:3955:G:H8	1.85	0.42
7:B3:112:U:H2'	7:B3:113:G:H8	1.85	0.42
11:D1:106:TYR:HE1	11:D1:116:ARG:HG3	1.83	0.42
29:K1:39:OMU:HM23	29:K1:39:OMU:H1'	1.82	0.42
33:M1:136:ARG:HB2	33:M1:218:LEU:HD11	2.02	0.42
39:P1:174:LYS:HB3	39:P1:174:LYS:HE3	1.83	0.42
40:P2:44:GLY:HA2	40:P2:95:HIS:HB3	2.02	0.42
50:U2:30:MET:HB3	50:U2:101:PRO:HG2	2.02	0.42
63:b1:47:LEU:HB2	63:b1:81:ILE:HD13	2.01	0.42
81:k2:51:ALA:HB3	81:k2:54:ILE:HD12	2.02	0.42
84:m2:27:CYS:SG	84:m2:28:PHE:N	2.93	0.42
2:A1:1038:G:H4'	2:A1:1846:A:H4'	2.02	0.42
4:A3:1336:A:H2'	4:A3:1337:G:C8	2.55	0.42
4:A3:3612:G:H2'	4:A3:3613:G:C8	2.55	0.42
4:A3:3983:C:H2'	4:A3:3984:G:C8	2.55	0.42
4:A3:4705:A:H5'	16:E3:128:LYS:HG3	2.02	0.42
15:E2:66:GLU:OE1	15:E2:69:ARG:NH1	2.53	0.42
33:M1:48:LEU:O	33:M1:65:ARG:NH1	2.53	0.42
43:R1:32:MET:HE3	43:R1:54:GLY:HA2	2.01	0.42
58:Y2:29:LEU:HD23	58:Y2:94:LEU:HD13	2.02	0.42
65:c1:10:LYS:HD3	65:c1:53:TYR:CE2	2.55	0.42
74:h1:30:CYS:SG	74:h1:31:SER:N	2.93	0.42
84:m2:95:LEU:HA	84:m2:98:ILE:HG22	2.01	0.42
87:p2:226:LEU:O	87:p2:253:LEU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A1:333:G:O6	43:R1:189:ARG:NH2	2.44	0.41
2:A1:547:G:H2'	2:A1:548:G:C8	2.55	0.41
2:A1:665:A:O2'	2:A1:671:A:N1	2.51	0.41
2:A1:1102:U:H2'	2:A1:1103:G:H8	1.85	0.41
4:A3:422:C:H2'	4:A3:423:G:H8	1.84	0.41
4:A3:693:C:H2'	4:A3:694:G:H8	1.85	0.41
4:A3:788:G:H2'	4:A3:789:G:H8	1.84	0.41
4:A3:3439:U:H2'	4:A3:3440:C:C6	2.55	0.41
4:A3:3782:C:O2'	86:o2:37:SER:OG	2.30	0.41
9:C2:95:LEU:HD23	9:C2:184:LEU:HD13	2.02	0.41
11:D1:90:LYS:HE2	11:D1:90:LYS:HB2	1.92	0.41
30:K2:81:TRP:HB2	30:K2:104:VAL:HG21	2.01	0.41
35:N1:202:THR:HG22	35:N1:221:ASP:HB3	2.02	0.41
39:P1:95:THR:HG22	78:j1:16:ARG:HB2	2.01	0.41
51:V1:59:LYS:O	51:V1:69:TRP:HA	2.20	0.41
84:m2:127:ASN:HD21	84:m2:151:THR:HG21	1.85	0.41
2:A1:469:A2M:H1'	2:A1:469:A2M:HM'3	1.77	0.41
4:A3:1915:G:O2'	85:m2:78:SER:OG	2.34	0.41
4:A3:4383:OMG:OP1	60:Z2:30:HIS:NE2	2.36	0.41
4:A3:4649:A:H4'	16:E3:95:THR:HG22	2.02	0.41
27:J1:41:U:H2'	27:J1:42:G:H8	1.85	0.41
41:Q1:192:LYS:HA	41:Q1:192:LYS:HD3	1.92	0.41
51:V1:35:LEU:HD22	51:V1:40:VAL:HG11	2.02	0.41
52:V2:50:PRO:HD3	52:V2:68:ILE:HG12	2.02	0.41
55:X1:55:ASN:OD1	55:X1:55:ASN:N	2.53	0.41
75:h2:44:TRP:O	75:h2:48:LYS:NZ	2.52	0.41
87:p2:177:PRO:HG3	87:p2:197:LYS:HG3	2.02	0.41
2:A1:1008:C:H2'	2:A1:1009:A:C8	2.55	0.41
4:A3:308:G:OP2	4:A3:308:G:N2	2.43	0.41
4:A3:2310:U:H4'	4:A3:2311:U:H5'	2.01	0.41
4:A3:2706:G:O2'	36:N2:82:LYS:O	2.34	0.41
4:A3:2712:U:O2'	4:A3:2724:A:N7	2.48	0.41
4:A3:3386:G:O2'	4:A3:3425:U:OP1	2.32	0.41
4:A3:3625:C:H2'	4:A3:3626:A:C8	2.56	0.41
4:A3:3984:G:H2'	4:A3:3985:A:H8	1.85	0.41
16:E3:285:TYR:N	16:E3:332:MET:O	2.53	0.41
16:E3:356:LYS:HA	16:E3:356:LYS:HD3	1.83	0.41
27:J1:4:C:H2'	27:J1:5:G:H8	1.84	0.41
31:L1:102:ARG:HA	31:L1:102:ARG:HD2	1.75	0.41
34:M2:154:LYS:NZ	34:M2:159:PRO:O	2.48	0.41
36:N2:105:LEU:HD23	36:N2:138:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:V2:121:ARG:HA	52:V2:121:ARG:HD3	1.87	0.41
53:W1:80:MET:HA	53:W1:86:ILE:HG22	2.01	0.41
57:Y1:78:LYS:HG3	57:Y1:80:LEU:HD13	2.01	0.41
86:o2:114:GLU:OE2	86:o2:140:HIS:ND1	2.53	0.41
2:A1:429:OMU:H6	2:A1:429:OMU:H2'	1.85	0.41
2:A1:1749:G:O6	2:A1:1787:U:O4	2.38	0.41
3:A2:40:LYS:NZ	4:A3:884:U:O5'	2.49	0.41
4:A3:526:C:H2'	4:A3:527:G:C8	2.56	0.41
4:A3:3954:U:OP2	40:P2:4:THR:OG1	2.33	0.41
5:B1:36:LYS:HE2	5:B1:41:TYR:HA	2.01	0.41
22:G3:205:ALA:HB1	22:G3:233:PRO:HB3	2.02	0.41
28:J2:135:ILE:HG21	28:J2:151:ILE:HG21	2.02	0.41
29:K1:11:U:H2'	29:K1:12:G:O4'	2.20	0.41
88:q2:254:LYS:HD3	88:q2:254:LYS:HA	1.91	0.41
2:A1:223:C:H2'	2:A1:224:A:C8	2.55	0.41
2:A1:640:C:H2'	2:A1:641:A:C8	2.55	0.41
2:A1:1172:G:O2'	2:A1:1188:G:O6	2.31	0.41
2:A1:1439:A:H2'	2:A1:1440:A:C8	2.56	0.41
4:A3:369:G:N2	4:A3:372:A:OP2	2.40	0.41
4:A3:711:U:H2'	4:A3:712:C:C6	2.56	0.41
4:A3:1245:C:H2'	4:A3:1246:U:C2	2.55	0.41
4:A3:3697:A:N7	4:A3:3775:A:N6	2.69	0.41
4:A3:4135:C:H2'	4:A3:4136:A:H8	1.86	0.41
4:A3:4445:U:H1'	4:A3:4446:A:H5''	2.01	0.41
10:C3:87:G:O6	50:U2:113:LYS:NZ	2.54	0.41
31:L1:176:TRP:HE1	31:L1:197:VAL:HG23	1.86	0.41
2:A1:27:A2M:H2'	2:A1:28:U:O4'	2.21	0.41
2:A1:29:G:H2'	2:A1:30:C:C6	2.56	0.41
2:A1:650:PSU:H2'	2:A1:651:A:C8	2.56	0.41
2:A1:1355:G:N2	2:A1:1358:A:OP2	2.43	0.41
2:A1:1522:C:P	66:d1:124:ARG:HH22	2.43	0.41
4:A3:2592:C:H2'	4:A3:2593:G:C8	2.56	0.41
8:C1:39:SER:HB2	17:F1:51:ARG:HH12	1.85	0.41
15:E2:99:ILE:HG12	15:E2:104:SER:HB3	2.03	0.41
24:H2:178:ALA:N	54:W2:134:GLU:OE2	2.43	0.41
33:M1:68:GLU:OE1	33:M1:85:LYS:NZ	2.48	0.41
37:O1:42:THR:OG1	37:O1:45:ARG:O	2.28	0.41
43:R1:231:ARG:HH21	43:R1:232:ARG:HH12	1.69	0.41
52:V2:22:LYS:NZ	52:V2:132:GLN:O	2.46	0.41
61:a1:25:LEU:HA	61:a1:28:MET:HE3	2.01	0.41
66:d1:14:ARG:NH1	66:d1:19:ASN:OD1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:q2:121:LYS:HD3	88:q2:127:GLN:HB2	2.01	0.41
1:MB:40:LYS:NZ	4:A3:2444:A:OP1	2.47	0.41
2:A1:1706:C:H2'	2:A1:1707:G:C8	2.56	0.41
4:A3:239:C:OP1	50:U2:46:SER:OG	2.32	0.41
4:A3:2239:A:C8	4:A3:2657:C:H2'	2.56	0.41
4:A3:2737:A:H2'	4:A3:2738:A:C8	2.56	0.41
4:A3:4203:PSU:H1'	16:E3:252:ALA:HB3	2.03	0.41
4:A3:4340:U:H2'	4:A3:4341:G:C8	2.55	0.41
10:C3:141:C:H5''	28:J2:60:VAL:HG11	2.02	0.41
18:F2:64:ARG:HE	18:F2:64:ARG:HB3	1.75	0.41
27:J1:49:C:H2'	27:J1:50:A:H8	1.86	0.41
35:N1:169:TYR:OH	35:N1:175:GLY:O	2.33	0.41
39:P1:37:LYS:HB2	39:P1:40:GLU:HG2	2.03	0.41
84:m2:82:ILE:HG23	84:m2:86:VAL:HG21	2.02	0.41
2:A1:533:C:H2'	2:A1:534:A:H8	1.86	0.41
2:A1:1064:C:O2'	59:Z1:150:ARG:O	2.35	0.41
2:A1:1222:G:H2'	2:A1:1223:G:C8	2.55	0.41
2:A1:1513:C:O2'	23:H1:7:TYR:O	2.31	0.41
2:A1:1809:U:H2'	2:A1:1810:A:C8	2.55	0.41
3:A2:126:ARG:HG2	4:A3:859:G:C8	2.56	0.41
4:A3:887:C:H2'	4:A3:888:C:H6	1.86	0.41
4:A3:2470:C:H2'	4:A3:2471:U:C6	2.56	0.41
4:A3:2727:G:H2'	4:A3:2728:A:H8	1.86	0.41
4:A3:3908:C:H5	9:C2:73:ARG:HH12	1.68	0.41
22:G3:95:TYR:OH	22:G3:195:HIS:NE2	2.45	0.41
24:H2:7:GLY:O	54:W2:49:HIS:NE2	2.48	0.41
50:U2:131:GLU:HA	50:U2:134:LYS:HG2	2.03	0.41
59:Z1:124:MET:HE3	59:Z1:124:MET:HB3	1.86	0.41
2:A1:679:U:OP2	2:A1:1027:C:N4	2.43	0.41
2:A1:751:C:H2'	2:A1:752:G:C8	2.56	0.41
2:A1:894:U:H2'	2:A1:895:G:C8	2.56	0.41
2:A1:1013:A:OP1	57:Y1:3:ARG:NH1	2.48	0.41
2:A1:1014:U:OP1	2:A1:1130:G:O2'	2.38	0.41
4:A3:645:C:H2'	4:A3:646:G:C8	2.56	0.41
4:A3:2587:A:H2'	4:A3:2588:A:C8	2.55	0.41
4:A3:2727:G:H2'	4:A3:2728:A:C8	2.56	0.41
4:A3:3593:A:H2'	4:A3:3594:A:C8	2.56	0.41
4:A3:3602:C:H2'	4:A3:3603:A:H8	1.86	0.41
4:A3:3674:A:H2'	4:A3:3675:A:C8	2.56	0.41
9:C2:157:ILE:HA	9:C2:201:THR:HG22	2.02	0.41
10:C3:127:U:H6	10:C3:127:U:H2'	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E2:159:PHE:HB2	15:E2:163:GLN:HE22	1.86	0.41
20:G1:86:THR:HG22	20:G1:102:VAL:HG12	2.03	0.41
20:G1:163:PRO:HB2	20:G1:179:LEU:HB3	2.01	0.41
20:G1:292:SER:OG	20:G1:293:ALA:N	2.52	0.41
29:K1:4:OMC:HM23	29:K1:4:OMC:H1'	1.71	0.41
31:L1:137:ALA:HB1	31:L1:142:LEU:HB3	2.02	0.41
39:P1:55:ALA:HB1	39:P1:60:GLU:HB2	2.03	0.41
59:Z1:16:SER:OG	59:Z1:17:LEU:N	2.54	0.41
69:e2:45:ARG:HA	69:e2:45:ARG:HD3	1.97	0.41
72:g1:32:ILE:HG12	72:g1:60:ARG:HD2	2.02	0.41
73:g2:70:LYS:HE3	73:g2:70:LYS:HB3	1.96	0.41
76:i1:57:VAL:HG23	76:i1:67:ARG:HB2	2.02	0.41
81:k2:23:ARG:HA	81:k2:26:VAL:HG12	2.03	0.41
83:l2:101:LYS:HE2	83:l2:101:LYS:HB3	1.85	0.41
88:q2:140:TRP:HB3	88:q2:160:LEU:HD11	2.03	0.41
2:A1:51:U:H2'	2:A1:52:G:C8	2.55	0.41
2:A1:610:PSU:H2'	2:A1:611:G:H8	1.86	0.41
2:A1:1102:U:H2'	2:A1:1103:G:C8	2.55	0.41
2:A1:1654:U:H2'	2:A1:1655:G:C8	2.56	0.41
2:A1:1754:C:H2'	2:A1:1755:G:C8	2.55	0.41
4:A3:2127:G:OP1	54:W2:7:LYS:NZ	2.45	0.41
4:A3:2453:G:H2'	4:A3:2454:A:H8	1.85	0.41
4:A3:2553:C:H2'	4:A3:2555:G:H5'	2.02	0.41
4:A3:3774:A:H2'	4:A3:3775:A:C8	2.56	0.41
10:C3:67:U:H2'	10:C3:68:G:C8	2.56	0.41
71:f2:67:LEU:HD12	71:f2:67:LEU:HA	1.92	0.41
73:g2:24:LYS:HA	73:g2:67:LYS:O	2.20	0.41
80:k1:92:LEU:HD22	80:k1:109:TYR:HE1	1.85	0.41
86:o2:111:LEU:HD22	86:o2:138:LEU:HD21	2.02	0.41
88:q2:168:ILE:HG13	88:q2:239:MET:HB2	2.03	0.41
2:A1:577:A2M:HM'3	2:A1:577:A2M:H1'	1.69	0.40
2:A1:588:A:H5'	2:A1:593:C:H41	1.86	0.40
4:A3:1491:PSU:H2'	4:A3:1492:A:H8	1.86	0.40
4:A3:3456:A2M:H1'	4:A3:3456:A2M:HM'3	1.85	0.40
4:A3:3954:U:H2'	4:A3:3955:G:C8	2.56	0.40
7:B3:28:C:H2'	7:B3:29:C:C5'	2.51	0.40
19:F3:9:SER:OG	19:F3:149:GLU:OE1	2.37	0.40
30:K2:183:LYS:HB2	30:K2:183:LYS:HE2	1.82	0.40
39:P1:20:LEU:HD21	39:P1:46:ILE:HD12	2.02	0.40
43:R1:20:ASP:HB3	43:R1:23:LYS:HE2	2.04	0.40
48:T2:71:LEU:HD12	48:T2:71:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:V2:88:ASP:OD1	52:V2:88:ASP:N	2.54	0.40
68:e1:144:LYS:HE2	68:e1:144:LYS:HB2	1.84	0.40
84:m2:72:ASN:HA	84:m2:73:PRO:HD3	1.89	0.40
87:p2:318:GLU:HB2	87:p2:414:ARG:HD2	2.03	0.40
88:q2:248:ASP:HB2	88:q2:251:GLN:HG2	2.03	0.40
88:q2:378:LEU:HB3	88:q2:558:PHE:CG	2.56	0.40
2:A1:159:A2M:HM'2	2:A1:159:A2M:H1'	1.51	0.40
2:A1:982:A:H2'	2:A1:983:G:C8	2.56	0.40
2:A1:1392:OMC:HM22	2:A1:1393:U:H5'	2.02	0.40
2:A1:1863:G:N2	17:F1:76:SER:OG	2.54	0.40
3:A2:153:LEU:HD13	3:A2:197:VAL:HG11	2.03	0.40
4:A3:1093:C:H2'	4:A3:1094:A:C8	2.57	0.40
4:A3:1284:OMC:HM23	4:A3:1284:OMC:H1'	1.95	0.40
4:A3:1532:G:O2'	4:A3:1567:G:H4'	2.22	0.40
4:A3:2450:C:H2'	4:A3:2451:G:C8	2.55	0.40
4:A3:3331:A:H2'	4:A3:3332:G:C8	2.56	0.40
4:A3:3816:C:H2'	4:A3:3817:G:H8	1.86	0.40
4:A3:4693:G:H2'	4:A3:4694:A:C8	2.56	0.40
4:A3:4706:A:H2'	4:A3:4707:A:H8	1.85	0.40
10:C3:82:A:N1	67:d2:45:SER:OG	2.46	0.40
29:K1:75:C:O2'	29:K1:76:A:OP1	2.38	0.40
47:T1:201:LYS:HA	47:T1:201:LYS:HD3	1.84	0.40
48:T2:150:ALA:HB1	48:T2:155:ILE:HB	2.04	0.40
58:Y2:29:LEU:HD22	58:Y2:91:VAL:HG21	2.02	0.40
83:l2:95:HIS:O	83:l2:99:LYS:HB2	2.21	0.40
87:p2:319:ILE:HB	87:p2:412:ILE:HB	2.03	0.40
2:A1:942:C:H2'	2:A1:943:G:C8	2.56	0.40
4:A3:1308:U:H5''	24:H2:36:ARG:HH22	1.85	0.40
4:A3:2654:G:N1	4:A3:2657:C:OP2	2.40	0.40
4:A3:3464:A:H2'	4:A3:3465:A:C8	2.57	0.40
4:A3:4221:G:O6	77:i2:125:LYS:NZ	2.54	0.40
4:A3:4368:A:H4'	16:E3:13:SER:HB2	2.04	0.40
29:K1:24:A:H3'	29:K1:25:U:H6	1.85	0.40
43:R1:136:LYS:NZ	43:R1:175:LYS:O	2.52	0.40
56:X2:36:ASP:HA	56:X2:37:PRO:HD3	1.95	0.40
87:p2:318:GLU:OE1	87:p2:414:ARG:NH1	2.44	0.40
2:A1:107:A:H2'	2:A1:108:G:C8	2.56	0.40
2:A1:863:A:C8	74:h1:107:SER:HA	2.56	0.40
2:A1:1278:C:H2'	2:A1:1279:A:C8	2.56	0.40
2:A1:1631:A:H5''	66:d1:37:GLY:H	1.87	0.40
4:A3:268:G:H2'	4:A3:269:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:2450:C:H2'	4:A3:2451:G:H8	1.86	0.40
16:E3:396:ARG:HA	16:E3:399:LYS:HD2	2.04	0.40
39:P1:22:LYS:HG3	39:P1:23:LEU:HD12	2.01	0.40
43:R1:49:VAL:HG22	43:R1:115:LYS:HG2	2.03	0.40
47:T1:172:LEU:HB3	47:T1:190:LEU:HD12	2.04	0.40
78:j1:44:LEU:HD13	78:j1:75:ILE:HD11	2.03	0.40
78:j1:86:GLU:OE1	78:j1:90:ARG:NE	2.39	0.40
88:q2:106:LEU:O	88:q2:270:ILE:HA	2.21	0.40
2:A1:220:U:H2'	2:A1:221:A:H8	1.86	0.40
2:A1:930:G:OP1	58:Y2:5:LYS:NZ	2.47	0.40
4:A3:718:C:H1'	19:F3:343:GLN:HG2	2.04	0.40
4:A3:1068:U:H2'	4:A3:1069:G:C8	2.57	0.40
4:A3:1682:A:N1	4:A3:1728:C:O2'	2.48	0.40
4:A3:3457:G:H5''	86:o2:199:GLN:HG2	2.04	0.40
4:A3:3457:G:OP1	86:o2:39:LYS:NZ	2.54	0.40
4:A3:3490:PSU:H2'	4:A3:3497:G:N2	2.36	0.40
4:A3:3580:U:H2'	4:A3:3581:A:H8	1.86	0.40
4:A3:3657:OMU:HM23	4:A3:3657:OMU:H1'	1.78	0.40
13:D3:206:PRO:HG3	13:D3:213:GLY:HA3	2.04	0.40
22:G3:89:LYS:HA	22:G3:89:LYS:HD3	1.91	0.40
29:K1:43:G:C2'	29:K1:44:C:H5'	2.51	0.40
31:L1:57:LYS:HA	31:L1:57:LYS:HD2	1.89	0.40
33:M1:33:VAL:HB	33:M1:44:ILE:HB	2.04	0.40
36:N2:82:LYS:HA	36:N2:82:LYS:HD2	1.95	0.40
40:P2:120:LYS:HE2	40:P2:120:LYS:HB3	1.95	0.40
41:Q1:176:GLU:OE2	41:Q1:188:TYR:N	2.54	0.40
85:n2:142:ASN:OD1	85:n2:142:ASN:N	2.55	0.40
86:o2:60:ARG:HH21	86:o2:173:LYS:HG2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	MB	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
3	A2	239/291 (82%)	233 (98%)	6 (2%)	0	100	100
5	B1	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
6	B2	224/249 (90%)	216 (96%)	7 (3%)	1 (0%)	30	45
8	C1	61/69 (88%)	60 (98%)	1 (2%)	0	100	100
9	C2	229/319 (72%)	224 (98%)	5 (2%)	0	100	100
11	D1	66/80 (82%)	62 (94%)	4 (6%)	0	100	100
12	D2	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
13	D3	250/257 (97%)	247 (99%)	3 (1%)	0	100	100
14	E1	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
15	E2	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
16	E3	395/403 (98%)	390 (99%)	5 (1%)	0	100	100
17	F1	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
18	F2	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
19	F3	361/413 (87%)	354 (98%)	7 (2%)	0	100	100
20	G1	311/317 (98%)	294 (94%)	17 (6%)	0	100	100
21	G2	22/184 (12%)	19 (86%)	1 (4%)	2 (9%)	0	0
22	G3	291/296 (98%)	287 (99%)	4 (1%)	0	100	100
23	H1	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
24	H2	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
26	I2	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
28	J2	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
30	K2	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
31	L1	220/295 (75%)	215 (98%)	5 (2%)	0	100	100
32	L2	157/184 (85%)	154 (98%)	3 (2%)	0	100	100
33	M1	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
34	M2	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
35	N1	218/293 (74%)	216 (99%)	2 (1%)	0	100	100
36	N2	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
37	O1	223/243 (92%)	222 (100%)	1 (0%)	0	100	100
38	O2	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
39	P1	260/263 (99%)	255 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	P2	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
41	Q1	189/204 (93%)	183 (97%)	6 (3%)	0	100	100
42	Q2	96/128 (75%)	92 (96%)	4 (4%)	0	100	100
43	R1	235/249 (94%)	229 (97%)	6 (3%)	0	100	100
44	R2	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
45	S1	188/194 (97%)	178 (95%)	10 (5%)	0	100	100
46	S2	119/157 (76%)	117 (98%)	2 (2%)	0	100	100
47	T1	204/208 (98%)	203 (100%)	1 (0%)	0	100	100
48	T2	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
49	U1	183/194 (94%)	178 (97%)	5 (3%)	0	100	100
50	U2	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
51	V1	94/165 (57%)	93 (99%)	1 (1%)	0	100	100
52	V2	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
53	W1	152/158 (96%)	145 (95%)	7 (5%)	0	100	100
54	W2	144/148 (97%)	140 (97%)	4 (3%)	0	100	100
55	X1	122/132 (92%)	115 (94%)	7 (6%)	0	100	100
56	X2	103/245 (42%)	100 (97%)	3 (3%)	0	100	100
57	Y1	148/151 (98%)	148 (100%)	0	0	100	100
58	Y2	106/115 (92%)	104 (98%)	2 (2%)	0	100	100
59	Z1	134/151 (89%)	127 (95%)	7 (5%)	0	100	100
60	Z2	105/125 (84%)	105 (100%)	0	0	100	100
61	a1	131/145 (90%)	129 (98%)	2 (2%)	0	100	100
62	a2	128/135 (95%)	126 (98%)	2 (2%)	0	100	100
63	b1	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
64	b2	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
65	c1	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
66	d1	144/152 (95%)	137 (95%)	7 (5%)	0	100	100
67	d2	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
68	e1	140/144 (97%)	139 (99%)	1 (1%)	0	100	100
69	e2	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
70	f1	102/119 (86%)	99 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	f2	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
72	g1	82/84 (98%)	82 (100%)	0	0	100	100
73	g2	67/70 (96%)	67 (100%)	0	0	100	100
74	h1	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
75	h2	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
76	i1	138/143 (96%)	133 (96%)	5 (4%)	0	100	100
77	i2	49/52 (94%)	49 (100%)	0	0	100	100
78	j1	123/133 (92%)	121 (98%)	2 (2%)	0	100	100
79	j2	102/141 (72%)	100 (98%)	2 (2%)	0	100	100
80	k1	72/124 (58%)	71 (99%)	1 (1%)	0	100	100
81	k2	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
82	l1	23/25 (92%)	23 (100%)	0	0	100	100
83	l2	125/137 (91%)	122 (98%)	3 (2%)	0	100	100
84	m2	194/318 (61%)	181 (93%)	13 (7%)	0	100	100
85	n2	154/165 (93%)	146 (95%)	8 (5%)	0	100	100
86	o2	210/217 (97%)	202 (96%)	8 (4%)	0	100	100
87	p2	414/438 (94%)	397 (96%)	16 (4%)	1 (0%)	43	60
88	q2	593/599 (99%)	574 (97%)	18 (3%)	1 (0%)	43	60
All	All	12928/14622 (88%)	12619 (98%)	304 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
88	q2	96	ARG
21	G2	-1	LYS
87	p2	180	HIS
21	G2	-2	ALA
6	B2	196	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	MB	98/100 (98%)	98 (100%)	0	100	100
3	A2	216/251 (86%)	216 (100%)	0	100	100
5	B1	75/76 (99%)	75 (100%)	0	100	100
6	B2	197/218 (90%)	197 (100%)	0	100	100
8	C1	56/62 (90%)	56 (100%)	0	100	100
9	C2	199/271 (73%)	199 (100%)	0	100	100
11	D1	61/72 (85%)	61 (100%)	0	100	100
12	D2	169/171 (99%)	169 (100%)	0	100	100
13	D3	194/198 (98%)	194 (100%)	0	100	100
14	E1	47/49 (96%)	47 (100%)	0	100	100
15	E2	180/181 (99%)	180 (100%)	0	100	100
16	E3	344/347 (99%)	344 (100%)	0	100	100
17	F1	88/98 (90%)	88 (100%)	0	100	100
18	F2	143/149 (96%)	143 (100%)	0	100	100
19	F3	302/336 (90%)	302 (100%)	0	100	100
20	G1	272/275 (99%)	272 (100%)	0	100	100
21	G2	19/154 (12%)	14 (74%)	5 (26%)	0	0
22	G3	247/250 (99%)	247 (100%)	0	100	100
23	H1	48/49 (98%)	48 (100%)	0	100	100
24	H2	175/176 (99%)	175 (100%)	0	100	100
26	I2	117/161 (73%)	117 (100%)	0	100	100
28	J2	171/172 (99%)	171 (100%)	0	100	100
30	K2	171/173 (99%)	171 (100%)	0	100	100
31	L1	183/243 (75%)	183 (100%)	0	100	100
32	L2	140/163 (86%)	140 (100%)	0	100	100
33	M1	203/231 (88%)	203 (100%)	0	100	100
34	M2	164/165 (99%)	164 (100%)	0	100	100
35	N1	185/223 (83%)	185 (100%)	0	100	100
36	N2	159/175 (91%)	159 (100%)	0	100	100
37	O1	189/202 (94%)	189 (100%)	0	100	100
38	O2	154/154 (100%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	P1	224/225 (100%)	224 (100%)	0	100	100
40	P2	139/140 (99%)	139 (100%)	0	100	100
41	Q1	161/170 (95%)	161 (100%)	0	100	100
42	Q2	87/113 (77%)	87 (100%)	0	100	100
43	R1	207/218 (95%)	207 (100%)	0	100	100
44	R2	106/107 (99%)	106 (100%)	0	100	100
45	S1	170/174 (98%)	167 (98%)	3 (2%)	51	72
46	S2	100/126 (79%)	100 (100%)	0	100	100
47	T1	178/180 (99%)	177 (99%)	1 (1%)	78	88
48	T2	106/134 (79%)	106 (100%)	0	100	100
49	U1	161/168 (96%)	161 (100%)	0	100	100
50	U2	124/135 (92%)	124 (100%)	0	100	100
51	V1	87/136 (64%)	87 (100%)	0	100	100
52	V2	117/118 (99%)	117 (100%)	0	100	100
53	W1	139/142 (98%)	139 (100%)	0	100	100
54	W2	118/119 (99%)	118 (100%)	0	100	100
55	X1	104/108 (96%)	104 (100%)	0	100	100
56	X2	87/183 (48%)	87 (100%)	0	100	100
57	Y1	130/131 (99%)	130 (100%)	0	100	100
58	Y2	92/98 (94%)	92 (100%)	0	100	100
59	Z1	106/119 (89%)	106 (100%)	0	100	100
60	Z2	98/110 (89%)	98 (100%)	0	100	100
61	a1	119/130 (92%)	119 (100%)	0	100	100
62	a2	116/121 (96%)	116 (100%)	0	100	100
63	b1	117/121 (97%)	117 (100%)	0	100	100
64	b2	89/89 (100%)	89 (100%)	0	100	100
65	c1	120/121 (99%)	120 (100%)	0	100	100
66	d1	126/131 (96%)	125 (99%)	1 (1%)	73	85
67	d2	109/110 (99%)	109 (100%)	0	100	100
68	e1	112/113 (99%)	112 (100%)	0	100	100
69	e2	86/89 (97%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	f1	94/107 (88%)	92 (98%)	2 (2%)	47	69
71	f2	73/80 (91%)	73 (100%)	0	100	100
72	g1	68/68 (100%)	68 (100%)	0	100	100
73	g2	64/65 (98%)	64 (100%)	0	100	100
74	h1	112/113 (99%)	112 (100%)	0	100	100
75	h2	47/48 (98%)	47 (100%)	0	100	100
76	i1	112/114 (98%)	111 (99%)	1 (1%)	70	82
77	i2	47/47 (100%)	47 (100%)	0	100	100
78	j1	107/115 (93%)	107 (100%)	0	100	100
79	j2	92/120 (77%)	92 (100%)	0	100	100
80	k1	65/102 (64%)	65 (100%)	0	100	100
81	k2	74/75 (99%)	74 (100%)	0	100	100
82	l1	24/24 (100%)	24 (100%)	0	100	100
83	l2	110/120 (92%)	110 (100%)	0	100	100
84	m2	164/258 (64%)	164 (100%)	0	100	100
85	n2	128/137 (93%)	128 (100%)	0	100	100
86	o2	191/195 (98%)	191 (100%)	0	100	100
87	p2	358/376 (95%)	358 (100%)	0	100	100
88	q2	516/526 (98%)	516 (100%)	0	100	100
All	All	11247/12414 (91%)	11234 (100%)	13 (0%)	87	95

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	G2	1	LEU
21	G2	3	ASN
21	G2	7	LEU
21	G2	8	LYS
21	G2	13	VAL
45	S1	76	GLN
45	S1	77	VAL
45	S1	79	LEU
47	T1	137	LEU
66	d1	2	SER
70	f1	100	GLN

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Mol	Chain	Res	Type
70	f1	101	ILE
76	i1	61	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
6	B2	62	GLN
6	B2	118	ASN
6	B2	205	ASN
9	C2	153	GLN
9	C2	236	HIS
11	D1	91	ASN
11	D1	151	ASN
13	D3	22	HIS
15	E2	73	ASN
16	E3	184	GLN
16	E3	203	GLN
16	E3	376	HIS
17	F1	25	ASN
18	F2	46	GLN
19	F3	89	GLN
19	F3	212	ASN
19	F3	329	ASN
20	G1	26	GLN
20	G1	56	GLN
20	G1	285	GLN
22	G3	45	ASN
22	G3	138	GLN
22	G3	191	ASN
22	G3	202	GLN
24	H2	175	ASN
26	I2	34	ASN
26	I2	70	GLN
26	I2	131	GLN
28	J2	32	GLN
30	K2	26	GLN
30	K2	167	HIS
31	L1	9	GLN
31	L1	36	GLN
31	L1	141	ASN
32	L2	21	ASN
32	L2	28	ASN

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Mol	Chain	Res	Type
32	L2	56	GLN
33	M1	92	GLN
33	M1	124	HIS
33	M1	158	HIS
33	M1	208	HIS
34	M2	57	ASN
39	P1	67	GLN
39	P1	161	GLN
39	P1	214	ASN
41	Q1	137	GLN
42	Q2	38	ASN
42	Q2	105	ASN
43	R1	146	ASN
45	S1	97	GLN
47	T1	116	HIS
48	T2	57	GLN
50	U2	18	HIS
50	U2	61	HIS
50	U2	96	HIS
50	U2	127	GLN
51	V1	28	HIS
53	W1	19	ASN
53	W1	94	HIS
53	W1	100	ASN
53	W1	121	GLN
54	W2	34	ASN
54	W2	120	GLN
55	X1	28	HIS
56	X2	6	ASN
56	X2	60	ASN
57	Y1	58	HIS
58	Y2	72	HIS
60	Z2	28	ASN
61	a1	54	HIS
62	a2	34	ASN
62	a2	52	GLN
67	d2	108	GLN
71	f2	30	GLN
73	g2	31	ASN
75	h2	17	GLN
75	h2	33	ASN
76	i1	31	HIS

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Mol	Chain	Res	Type
80	k1	112	ASN
84	m2	105	ASN
84	m2	127	ASN
84	m2	179	ASN
84	m2	195	ASN
85	n2	68	GLN
86	o2	19	HIS
86	o2	44	GLN
86	o2	94	ASN
86	o2	197	ASN
87	p2	266	GLN
87	p2	420	GLN
88	q2	310	ASN
88	q2	429	HIS
88	q2	438	HIS
88	q2	440	GLN
88	q2	460	GLN
88	q2	542	ASN
88	q2	578	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	C3	155/158 (98%)	19 (12%)	0
2	A1	1764/1870 (94%)	285 (16%)	4 (0%)
25	I1	17/659 (2%)	5 (29%)	0
27	J1	74/75 (98%)	18 (24%)	1 (1%)
29	K1	73/74 (98%)	21 (28%)	4 (5%)
4	A3	3752/4808 (78%)	599 (15%)	8 (0%)
7	B3	118/119 (99%)	11 (9%)	0
All	All	5953/7763 (76%)	958 (16%)	17 (0%)

All (958) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A1	3	C
2	A1	4	C
2	A1	17	C
2	A1	33	G
2	A1	41	G
2	A1	44	U

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Mol	Chain	Res	Type
2	A1	45	A
2	A1	46	A
2	A1	56	G
2	A1	58	C
2	A1	62	G
2	A1	67	C
2	A1	68	A
2	A1	71	G
2	A1	73	C
2	A1	74	G
2	A1	76	U
2	A1	77	A
2	A1	79	A
2	A1	103	A
2	A1	113	G
2	A1	115	U
2	A1	126	G
2	A1	130	G
2	A1	142	C
2	A1	143	U
2	A1	155	G
2	A1	162	C
2	A1	163	U
2	A1	168	C
2	A1	170	A
2	A1	175	A
2	A1	178	C
2	A1	180	G
2	A1	182	C
2	A1	184	G
2	A1	187	G
2	A1	188	C
2	A1	192	C
2	A1	226	A
2	A1	228	C
2	A1	281	G
2	A1	282	C
2	A1	283	G
2	A1	284	G
2	A1	306	U
2	A1	307	C
2	A1	310	G

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Mol	Chain	Res	Type
2	A1	313	G
2	A1	320	C
2	A1	325	U
2	A1	327	C
2	A1	328	G
2	A1	329	U
2	A1	330	G
2	A1	336	G
2	A1	348	G
2	A1	363	C
2	A1	365	A
2	A1	370	C
2	A1	382	C
2	A1	386	G
2	A1	387	C
2	A1	401	C
2	A1	410	C
2	A1	422	G
2	A1	439	G
2	A1	449	A
2	A1	451	C
2	A1	456	A
2	A1	464	C
2	A1	465	A
2	A1	466	A
2	A1	472	G
2	A1	473	C
2	A1	474	A
2	A1	475	G
2	A1	477	A
2	A1	483	G
2	A1	488	U
2	A1	493	C
2	A1	509	A
2	A1	517	A
2	A1	542	U
2	A1	544	C
2	A1	545	G
2	A1	550	C
2	A1	556	A
2	A1	560	G
2	A1	564	G

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Mol	Chain	Res	Type
2	A1	565	A
2	A1	569	C
2	A1	577	A2M
2	A1	584	A
2	A1	588	A
2	A1	589	G
2	A1	590	G
2	A1	592	U
2	A1	593	C
2	A1	605	A
2	A1	607	G
2	A1	608	U
2	A1	609	C
2	A1	615	C
2	A1	618	G
2	A1	628	OMU
2	A1	633	C
2	A1	644	A
2	A1	645	OMG
2	A1	656	A
2	A1	661	C
2	A1	669	A2M
2	A1	670	A
2	A1	672	A
2	A1	673	A
2	A1	674	G
2	A1	684	OMG
2	A1	699	G
2	A1	731	C
2	A1	734	C
2	A1	735	C
2	A1	748	U
2	A1	749	C
2	A1	750	U
2	A1	753	G
2	A1	755	G
2	A1	758	C
2	A1	790	G
2	A1	795	A
2	A1	800	U
2	A1	812	A
2	A1	822	G

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Mol	Chain	Res	Type
2	A1	828	A
2	A1	831	A
2	A1	832	G
2	A1	837	G
2	A1	838	A
2	A1	839	G
2	A1	840	C
2	A1	841	C
2	A1	842	G
2	A1	848	A
2	A1	868	OMG
2	A1	871	A
2	A1	873	A
2	A1	892	G
2	A1	911	G
2	A1	914	A
2	A1	915	U
2	A1	918	U
2	A1	921	A
2	A1	923	A
2	A1	934	G
2	A1	944	U
2	A1	956	A
2	A1	964	A
2	A1	972	G
2	A1	991	A
2	A1	993	A
2	A1	1000	G
2	A1	1018	U
2	A1	1024	A
2	A1	1081	A
2	A1	1084	A
2	A1	1086	C
2	A1	1090	G
2	A1	1116	U
2	A1	1117	C
2	A1	1118	C
2	A1	1119	C
2	A1	1122	G
2	A1	1124	C
2	A1	1134	A
2	A1	1145	A

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Mol	Chain	Res	Type
2	A1	1154	C
2	A1	1155	U
2	A1	1196	A
2	A1	1204	G
2	A1	1208	G
2	A1	1216	C
2	A1	1225	G
2	A1	1243	U
2	A1	1252	A
2	A1	1254	A
2	A1	1257	G
2	A1	1258	G
2	A1	1260	A
2	A1	1272	C
2	A1	1275	G
2	A1	1276	G
2	A1	1285	A
2	A1	1286	G
2	A1	1287	G
2	A1	1294	A
2	A1	1295	G
2	A1	1298	U
2	A1	1302	A
2	A1	1303	G
2	A1	1304	C
2	A1	1309	U
2	A1	1321	G
2	A1	1343	U
2	A1	1349	G
2	A1	1359	U
2	A1	1364	C
2	A1	1365	U
2	A1	1372	U
2	A1	1373	U
2	A1	1376	G
2	A1	1379	A
2	A1	1383	A
2	A1	1398	U
2	A1	1406	A
2	A1	1407	G
2	A1	1419	C
2	A1	1420	C

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Mol	Chain	Res	Type
2	A1	1422	A
2	A1	1424	C
2	A1	1425	G
2	A1	1429	G
2	A1	1435	C
2	A1	1436	C
2	A1	1448	OMG
2	A1	1455	A
2	A1	1463	U
2	A1	1464	U
2	A1	1481	A
2	A1	1488	A
2	A1	1490	A
2	A1	1491	OMG
2	A1	1495	U
2	A1	1496	G
2	A1	1498	G
2	A1	1508	G
2	A1	1521	G
2	A1	1522	C
2	A1	1523	A
2	A1	1524	C
2	A1	1534	A
2	A1	1553	G
2	A1	1554	C
2	A1	1556	U
2	A1	1561	U
2	A1	1571	G
2	A1	1579	U
2	A1	1581	A
2	A1	1586	U
2	A1	1589	A
2	A1	1602	A
2	A1	1603	U
2	A1	1622	U
2	A1	1624	A
2	A1	1640	G7M
2	A1	1642	A
2	A1	1655	G
2	A1	1662	A
2	A1	1665	A
2	A1	1666	G

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Mol	Chain	Res	Type
2	A1	1680	A
2	A1	1681	G
2	A1	1699	C
2	A1	1700	A
2	A1	1722	U
2	A1	1723	G
2	A1	1745	G
2	A1	1768	C
2	A1	1769	A
2	A1	1778	G
2	A1	1784	C
2	A1	1785	G
2	A1	1820	A
2	A1	1826	A
2	A1	1827	G
2	A1	1830	G
2	A1	1832	A
2	A1	1836	A
2	A1	1837	G
2	A1	1839	U
2	A1	1850	G
2	A1	1852	MA6
2	A1	1862	G
2	A1	1863	G
2	A1	1864	A
2	A1	1865	U
2	A1	1866	C
4	A3	25	A
4	A3	39	A
4	A3	42	A
4	A3	58	G
4	A3	59	A
4	A3	64	A
4	A3	65	A
4	A3	66	A
4	A3	72	C
4	A3	85	G
4	A3	91	G
4	A3	98	A
4	A3	108	A
4	A3	109	G
4	A3	110	C

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Mol	Chain	Res	Type
4	A3	119	G
4	A3	132	G
4	A3	134	G
4	A3	135	G
4	A3	136	U
4	A3	146	G
4	A3	159	C
4	A3	184	U
4	A3	185	C
4	A3	186	G
4	A3	187	U
4	A3	188	G
4	A3	189	G
4	A3	200	U
4	A3	201	C
4	A3	209	U
4	A3	210	C
4	A3	216	C
4	A3	219	G
4	A3	233	U
4	A3	234	G
4	A3	256	G
4	A3	266	C
4	A3	278	G
4	A3	297	U
4	A3	315	G
4	A3	316	U
4	A3	334	A
4	A3	340	C
4	A3	349	A
4	A3	363	A
4	A3	387	G
4	A3	409	G
4	A3	412	G
4	A3	413	G
4	A3	432	U
4	A3	449	C
4	A3	450	G
4	A3	452	A
4	A3	453	G
4	A3	454	U
4	A3	463	A

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Mol	Chain	Res	Type
4	A3	467	U
4	A3	468	U
4	A3	482	U
4	A3	483	G
4	A3	485	U
4	A3	486	C
4	A3	493	U
4	A3	497	G
4	A3	499	C
4	A3	500	G
4	A3	501	G
4	A3	502	U
4	A3	503	C
4	A3	504	U
4	A3	505	C
4	A3	506	G
4	A3	515	U
4	A3	516	U
4	A3	517	C
4	A3	626	G
4	A3	628	U
4	A3	635	G
4	A3	636	G
4	A3	651	C
4	A3	660	G
4	A3	661	A
4	A3	665	G
4	A3	666	C
4	A3	690	C
4	A3	691	G
4	A3	698	C
4	A3	699	G
4	A3	723	G
4	A3	724	G
4	A3	725	G
4	A3	732	C
4	A3	734	G
4	A3	754	G
4	A3	758	C
4	A3	759	G
4	A3	760	C
4	A3	785	G

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Mol	Chain	Res	Type
4	A3	788	G
4	A3	790	G
4	A3	791	C
4	A3	792	G
4	A3	793	C
4	A3	794	G
4	A3	795	A
4	A3	796	C
4	A3	797	C
4	A3	798	C
4	A3	804	C
4	A3	810	U
4	A3	811	U
4	A3	812	A
4	A3	813	C
4	A3	814	A
4	A3	815	G
4	A3	824	C
4	A3	825	G
4	A3	831	A
4	A3	832	G
4	A3	835	G
4	A3	841	C
4	A3	843	A
4	A3	845	U
4	A3	859	G
4	A3	860	A
4	A3	861	G
4	A3	866	A
4	A3	867	C
4	A3	868	C
4	A3	870	G
4	A3	873	U
4	A3	884	U
4	A3	889	C
4	A3	985	G
4	A3	987	C
4	A3	1062	G
4	A3	1065	G
4	A3	1072	C
4	A3	1073	C
4	A3	1074	C

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Mol	Chain	Res	Type
4	A3	1084	C
4	A3	1085	G
4	A3	1087	G
4	A3	1090	U
4	A3	1091	G
4	A3	1101	C
4	A3	1102	G
4	A3	1103	G
4	A3	1105	C
4	A3	1106	U
4	A3	1107	C
4	A3	1124	A
4	A3	1127	G
4	A3	1129	G
4	A3	1131	G
4	A3	1133	C
4	A3	1136	G
4	A3	1137	C
4	A3	1140	C
4	A3	1201	G
4	A3	1202	C
4	A3	1203	G
4	A3	1209	G
4	A3	1214	A
4	A3	1215	G
4	A3	1216	C
4	A3	1217	G
4	A3	1219	G
4	A3	1221	G
4	A3	1228	G
4	A3	1229	U
4	A3	1231	G
4	A3	1237	G
4	A3	1239	U
4	A3	1240	G
4	A3	1247	A
4	A3	1257	C
4	A3	1270	A2M
4	A3	1281	A
4	A3	1298	A
4	A3	1299	G
4	A3	1303	G

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Mol	Chain	Res	Type
4	A3	1309	C
4	A3	1310	G
4	A3	1312	A
4	A3	1323	C
4	A3	1331	A
4	A3	1341	A
4	A3	1342	A
4	A3	1348	G
4	A3	1363	C
4	A3	1364	G
4	A3	1367	G
4	A3	1369	C
4	A3	1375	A
4	A3	1391	C
4	A3	1392	C
4	A3	1393	C
4	A3	1395	U
4	A3	1412	G
4	A3	1435	C
4	A3	1452	A
4	A3	1453	G
4	A3	1457	G
4	A3	1469	U
4	A3	1478	A
4	A3	1479	A2M
4	A3	1489	A2M
4	A3	1502	A
4	A3	1521	C
4	A3	1533	U
4	A3	1546	U
4	A3	1551	U
4	A3	1567	G
4	A3	1579	G
4	A3	1580	OMG
4	A3	1581	G
4	A3	1586	A
4	A3	1588	G
4	A3	1589	A
4	A3	1593	A
4	A3	1595	C
4	A3	1596	G
4	A3	1597	A

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Mol	Chain	Res	Type
4	A3	1609	G
4	A3	1616	C
4	A3	1631	C
4	A3	1632	PSU
4	A3	1633	C
4	A3	1649	C
4	A3	1653	C
4	A3	1657	C
4	A3	1658	C
4	A3	1663	G
4	A3	1665	U
4	A3	1673	G
4	A3	1704	A
4	A3	1705	A
4	A3	1711	C
4	A3	1717	C
4	A3	1724	C
4	A3	1726	A
4	A3	1731	PSU
4	A3	1736	G
4	A3	1742	G
4	A3	1743	A
4	A3	1745	G
4	A3	1754	G
4	A3	1767	C
4	A3	1772	G
4	A3	1773	U
4	A3	1774	G
4	A3	1775	G
4	A3	1776	A
4	A3	1781	G
4	A3	1794	G
4	A3	1808	G
4	A3	1830	A
4	A3	1832	C
4	A3	1836	A
4	A3	1856	A
4	A3	1857	U
4	A3	1859	C
4	A3	1860	C
4	A3	1861	G
4	A3	1870	C

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Mol	Chain	Res	Type
4	A3	1871	A
4	A3	1879	G
4	A3	1887	G
4	A3	1890	G
4	A3	1900	G
4	A3	1910	C
4	A3	1913	U
4	A3	1914	G
4	A3	1918	A
4	A3	1923	A
4	A3	1924	G
4	A3	1925	U
4	A3	1927	G
4	A3	1936	U
4	A3	1937	A
4	A3	1940	G
4	A3	1941	A
4	A3	1942	G
4	A3	1943	U
4	A3	1950	C
4	A3	1963	G
4	A3	1964	A
4	A3	1965	A
4	A3	1983	U
4	A3	1985	G
4	A3	1987	U
4	A3	1991	G
4	A3	1994	G
4	A3	1995	G
4	A3	2008	A
4	A3	2023	U
4	A3	2029	U
4	A3	2032	G
4	A3	2034	A
4	A3	2036	A
4	A3	2037	G
4	A3	2039	G
4	A3	2041	G
4	A3	2043	A
4	A3	2044	A
4	A3	2045	G
4	A3	2046	A

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Mol	Chain	Res	Type
4	A3	2103	C
4	A3	2132	C
4	A3	2143	A
4	A3	2144	G
4	A3	2149	G
4	A3	2156	A
4	A3	2157	G
4	A3	2174	G
4	A3	2191	G
4	A3	2194	OMC
4	A3	2203	A
4	A3	2238	A
4	A3	2260	A
4	A3	2264	G
4	A3	2268	U
4	A3	2290	U
4	A3	2322	G
4	A3	2332	C
4	A3	2333	U
4	A3	2348	C
4	A3	2349	G
4	A3	2354	A
4	A3	2356	A
4	A3	2372	A
4	A3	2373	U
4	A3	2380	A
4	A3	2386	A
4	A3	2387	G
4	A3	2388	U
4	A3	2389	G
4	A3	2390	G
4	A3	2397	U
4	A3	2407	G
4	A3	2412	G
4	A3	2416	A
4	A3	2429	G
4	A3	2430	A
4	A3	2431	C
4	A3	2432	C
4	A3	2444	A
4	A3	2496	C
4	A3	2503	A

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Mol	Chain	Res	Type
4	A3	2512	C
4	A3	2513	C
4	A3	2530	U
4	A3	2537	G
4	A3	2538	A
4	A3	2539	A
4	A3	2546	G
4	A3	2550	U
4	A3	2551	U
4	A3	2552	C
4	A3	2553	C
4	A3	2554	G
4	A3	2567	G
4	A3	2569	G
4	A3	2586	A
4	A3	2606	U
4	A3	2631	U
4	A3	2633	U
4	A3	2641	A
4	A3	2657	C
4	A3	2669	U
4	A3	2670	G
4	A3	2672	U
4	A3	2698	G
4	A3	2745	G
4	A3	3328	A
4	A3	3346	G
4	A3	3347	G
4	A3	3350	C
4	A3	3358	G
4	A3	3362	A
4	A3	3367	A
4	A3	3376	U
4	A3	3380	A
4	A3	3394	A
4	A3	3405	C
4	A3	3412	U
4	A3	3428	C
4	A3	3442	G
4	A3	3444	A
4	A3	3461	U
4	A3	3485	G

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Mol	Chain	Res	Type
4	A3	3491	A
4	A3	3492	A2M
4	A3	3508	G
4	A3	3509	G
4	A3	3510	U
4	A3	3517	A2M
4	A3	3518	U
4	A3	3522	U
4	A3	3543	G
4	A3	3544	C
4	A3	3546	U
4	A3	3549	A
4	A3	3551	G
4	A3	3570	U
4	A3	3571	G
4	A3	3572	U
4	A3	3599	A2M
4	A3	3609	A
4	A3	3610	C
4	A3	3611	G
4	A3	3624	U
4	A3	3629	G
4	A3	3633	A
4	A3	3638	A
4	A3	3639	G
4	A3	3640	A
4	A3	3641	C
4	A3	3647	U
4	A3	3670	G
4	A3	3676	OMG
4	A3	3687	G
4	A3	3688	G
4	A3	3689	U
4	A3	3695	A
4	A3	3698	A
4	A3	3704	A
4	A3	3706	G
4	A3	3766	C
4	A3	3767	G
4	A3	3783	U
4	A3	3784	A
4	A3	3804	G

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Mol	Chain	Res	Type
4	A3	3812	G
4	A3	3823	G
4	A3	3824	C
4	A3	3825	G
4	A3	3832	G
4	A3	3833	A
4	A3	3834	G
4	A3	3843	G
4	A3	3846	U
4	A3	3847	C
4	A3	3849	G
4	A3	3850	G
4	A3	3855	A
4	A3	3869	G
4	A3	3875	C
4	A3	3886	G
4	A3	3887	G
4	A3	3891	C
4	A3	3892	G
4	A3	3896	G
4	A3	3904	C
4	A3	3908	C
4	A3	3909	U
4	A3	3916	A
4	A3	3929	G
4	A3	3930	G
4	A3	3937	G
4	A3	3949	A
4	A3	3958	A
4	A3	3971	G
4	A3	3975	U
4	A3	3979	A
4	A3	3989	C
4	A3	3997	A
4	A3	4000	G
4	A3	4012	G
4	A3	4013	G
4	A3	4014	A
4	A3	4017	A
4	A3	4019	A
4	A3	4027	A
4	A3	4028	A

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Mol	Chain	Res	Type
4	A3	4035	U
4	A3	4037	G
4	A3	4043	G
4	A3	4050	A
4	A3	4051	G
4	A3	4052	OMU
4	A3	4060	C
4	A3	4075	G
4	A3	4076	G
4	A3	4078	C
4	A3	4096	C
4	A3	4100	U
4	A3	4119	G
4	A3	4123	G
4	A3	4124	A
4	A3	4126	A
4	A3	4133	C
4	A3	4137	G
4	A3	4140	A
4	A3	4167	C
4	A3	4168	A
4	A3	4172	C
4	A3	4179	G
4	A3	4190	C
4	A3	4194	G
4	A3	4210	A
4	A3	4212	C
4	A3	4221	G
4	A3	4246	PSU
4	A3	4258	U
4	A3	4259	A
4	A3	4261	G
4	A3	4265	C
4	A3	4270	G
4	A3	4275	G
4	A3	4277	U
4	A3	4294	A
4	A3	4295	G
4	A3	4306	C
4	A3	4313	G
4	A3	4315	U
4	A3	4321	G

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Mol	Chain	Res	Type
4	A3	4336	A2M
4	A3	4347	U
4	A3	4373	U
4	A3	4382	PSU
4	A3	4383	OMG
4	A3	4398	G
4	A3	4402	A
4	A3	4416	C
4	A3	4418	A
4	A3	4423	U
4	A3	4433	A
4	A3	4437	A
4	A3	4446	A
4	A3	4454	A
4	A3	4455	U
4	A3	4465	G
4	A3	4475	A
4	A3	4476	C
4	A3	4478	G
4	A3	4482	C
4	A3	4486	G
4	A3	4487	A
4	A3	4488	A
4	A3	4489	G
4	A3	4490	G
4	A3	4492	G
4	A3	4501	G
4	A3	4504	C
4	A3	4506	C
4	A3	4508	G
4	A3	4512	G
4	A3	4518	C
4	A3	4609	G
4	A3	4610	C
4	A3	4614	G
4	A3	4621	U
4	A3	4622	C
4	A3	4634	U
4	A3	4637	G
4	A3	4638	G
4	A3	4639	C
4	A3	4640	G

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Mol	Chain	Res	Type
4	A3	4643	G
4	A3	4645	C
4	A3	4646	G
4	A3	4647	G
4	A3	4649	A
4	A3	4651	G
4	A3	4652	G
4	A3	4653	G
4	A3	4657	C
4	A3	4663	C
4	A3	4670	G
4	A3	4674	C
4	A3	4676	C
4	A3	4682	A
4	A3	4683	C
4	A3	4690	G
4	A3	4705	A
4	A3	4714	G
4	A3	4715	U
4	A3	4718	A
4	A3	4724	U
4	A3	4728	U
4	A3	4729	C
4	A3	4753	A
4	A3	4756	G
4	A3	4761	U
4	A3	4762	C
4	A3	4763	C
4	A3	4764	C
4	A3	4766	C
4	A3	4767	G
4	A3	4780	G
4	A3	4789	C
4	A3	4792	U
4	A3	4793	C
4	A3	4800	A
4	A3	4801	G
4	A3	4808	U
7	B3	7	G
7	B3	25	G
7	B3	27	G
7	B3	33	U

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Mol	Chain	Res	Type
7	B3	53	U
7	B3	54	A
7	B3	63	C
7	B3	64	G
7	B3	97	G
7	B3	110	G
7	B3	120	U
10	C3	34	U
10	C3	35	C
10	C3	38	U
10	C3	51	U
10	C3	52	A
10	C3	59	A
10	C3	60	G
10	C3	62	A
10	C3	63	U
10	C3	81	C
10	C3	84	A
10	C3	87	G
10	C3	94	G
10	C3	103	A
10	C3	105	C
10	C3	110	U
10	C3	114	G
10	C3	127	U
10	C3	147	G
25	I1	2	C
25	I1	8	U
25	I1	13	C
25	I1	14	U
25	I1	18	U
27	J1	7	A
27	J1	10	G
27	J1	13	C
27	J1	16	C
27	J1	18	U
27	J1	19	G
27	J1	20	U
27	J1	21	A
27	J1	31	A
27	J1	34	U
27	J1	35	U

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Mol	Chain	Res	Type
27	J1	49	C
27	J1	58	A
27	J1	59	G
27	J1	69	G
27	J1	70	G
27	J1	71	G
27	J1	76	A
29	K1	5	C
29	K1	6	G
29	K1	9	1MG
29	K1	12	G
29	K1	14	1MA
29	K1	18	G
29	K1	20	U
29	K1	21	A
29	K1	22	U
29	K1	24	A
29	K1	43	G
29	K1	44	C
29	K1	48	C
29	K1	49	5MC
29	K1	59	U
29	K1	65	G
29	K1	66	G
29	K1	68	G
29	K1	73	A
29	K1	75	C
29	K1	76	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A1	294	C
2	A1	1118	C
2	A1	1521	G
2	A1	1680	A
4	A3	855	G
4	A3	1588	G
4	A3	2372	A
4	A3	2431	C
4	A3	4012	G
4	A3	4124	A

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Mol	Chain	Res	Type
4	A3	4294	A
4	A3	4445	U
27	J1	19	G
29	K1	4	OMC
29	K1	16	H2U
29	K1	48	C
29	K1	75	C

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

230 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	$\# Z > 2$
4	PSU	A3	3494	4	18,21,22	1.07	1 (5%)	22,30,33	1.62	4 (18%)
2	PSU	A1	823	2	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
4	A2M	A3	398	4	22,25,26	1.25	1 (4%)	31,36,39	1.54	7 (22%)
2	PSU	A1	218	2	18,21,22	1.05	1 (5%)	22,30,33	1.65	4 (18%)
2	A2M	A1	485	2	22,25,26	1.27	1 (4%)	31,36,39	1.43	6 (19%)
2	OMC	A1	1704	2	19,22,23	2.99	8 (42%)	26,31,34	0.83	1 (3%)
4	A2M	A3	4317	4	22,25,26	1.36	2 (9%)	31,36,39	1.59	9 (29%)
29	1MA	K1	14	29	21,25,26	0.36	0	31,37,40	0.77	0
56	MLZ	X2	5	56	8,9,10	0.76	0	4,9,11	0.61	0
4	PSU	A3	3466	4	18,21,22	1.01	1 (5%)	22,30,33	1.66	5 (22%)
2	G7M	A1	1640	2,29	23,26,27	2.60	8 (34%)	35,39,42	2.45	10 (28%)
29	1MG	K1	9	29	22,26,27	0.61	0	33,39,42	0.67	0
54	V5N	W2	39	54	9,11,12	0.77	0	9,14,16	1.14	1 (11%)
2	PSU	A1	1245	2	18,21,22	1.08	1 (5%)	22,30,33	1.67	4 (18%)
4	PSU	A3	1731	4	18,21,22	1.02	1 (5%)	22,30,33	1.63	4 (18%)
2	OMC	A1	1392	2	19,22,23	3.03	8 (42%)	26,31,34	1.03	2 (7%)
2	A2M	A1	669	89,2	22,25,26	1.42	2 (9%)	31,36,39	1.58	9 (29%)
2	OMU	A1	628	2	19,22,23	3.05	8 (42%)	26,31,34	1.68	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A1	967	2	18,21,22	0.89	1 (5%)	22,30,33	0.60	0
2	OMG	A1	1448	2	23,26,27	2.32	6 (26%)	33,38,41	2.34	10 (30%)
2	PSU	A1	1644	89,2	18,21,22	1.09	1 (5%)	22,30,33	1.68	4 (18%)
4	PSU	A3	4382	4	18,21,22	1.04	1 (5%)	22,30,33	1.67	5 (22%)
2	4AC	A1	1338	2	21,24,25	3.34	10 (47%)	29,34,37	1.81	6 (20%)
4	PSU	A3	2351	4	18,21,22	1.05	1 (5%)	22,30,33	1.66	4 (18%)
4	PSU	A3	4203	4	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
2	6MZ	A1	1833	89,2	22,25,26	2.67	4 (18%)	30,36,39	2.28	7 (23%)
4	PSU	A3	3462	4	18,21,22	1.05	1 (5%)	22,30,33	1.65	4 (18%)
2	OMU	A1	1327	89,2	19,22,23	3.04	8 (42%)	26,31,34	1.72	5 (19%)
4	PSU	A3	1638	4	18,21,22	1.10	1 (5%)	22,30,33	1.66	4 (18%)
2	OMU	A1	1805	2	19,22,23	3.07	8 (42%)	26,31,34	1.71	4 (15%)
77	M3L	i2	98	77	10,11,12	0.39	0	9,14,16	0.29	0
4	PSU	A3	3616	4	18,21,22	1.07	1 (5%)	22,30,33	1.69	4 (18%)
2	PSU	A1	682	2	18,21,22	1.07	1 (5%)	22,30,33	1.65	4 (18%)
2	OMU	A1	1289	2	19,22,23	3.05	8 (42%)	26,31,34	1.67	4 (15%)
4	A2M	A3	3517	4	22,25,26	3.18	11 (50%)	31,36,39	3.72	13 (41%)
4	OMC	A3	2265	89,4	19,22,23	3.03	8 (42%)	26,31,34	0.80	1 (3%)
2	OMG	A1	437	2	23,26,27	2.30	6 (26%)	33,38,41	2.29	12 (36%)
4	OMC	A3	2647	4	19,22,23	2.98	8 (42%)	26,31,34	0.67	0
4	PSU	A3	3576	4	18,21,22	1.09	1 (5%)	22,30,33	1.61	4 (18%)
4	OMG	A3	3631	89,4	23,26,27	2.27	6 (26%)	33,38,41	2.25	11 (33%)
2	PSU	A1	573	2	18,21,22	1.04	1 (5%)	22,30,33	1.60	4 (18%)
2	PSU	A1	109	2	18,21,22	1.08	1 (5%)	22,30,33	1.75	5 (22%)
4	OMC	A3	3433	4,91	19,22,23	2.92	8 (42%)	26,31,34	0.75	0
2	PSU	A1	1693	2	18,21,22	1.08	1 (5%)	22,30,33	1.65	4 (18%)
4	OMG	A3	4364	4	23,26,27	2.26	7 (30%)	33,38,41	2.25	12 (36%)
4	OMG	A3	2267	4	23,26,27	2.32	6 (26%)	33,38,41	2.41	9 (27%)
2	PSU	A1	864	2	18,21,22	1.00	1 (5%)	22,30,33	1.60	4 (18%)
4	A2M	A3	4336	4	22,25,26	1.22	1 (4%)	31,36,39	1.54	7 (22%)
10	OMG	C3	75	10	23,26,27	2.28	7 (30%)	33,38,41	2.29	12 (36%)
4	OMU	A3	3973	4	19,22,23	3.04	8 (42%)	26,31,34	1.75	5 (19%)
29	5MU	K1	54	29	19,22,23	0.23	0	28,32,35	0.31	0
4	OMG	A3	2719	4	23,26,27	2.30	6 (26%)	33,38,41	2.45	10 (30%)
2	A2M	A1	469	2	22,25,26	1.42	1 (4%)	31,36,39	1.55	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMG	A3	4245	4	23,26,27	2.28	6 (26%)	33,38,41	2.35	10 (30%)
2	A2M	A1	27	89,2	22,25,26	1.32	1 (4%)	31,36,39	1.51	7 (22%)
2	OMG	A1	684	2	23,26,27	2.31	6 (26%)	33,38,41	2.26	10 (30%)
4	OMC	A3	2208	4	19,22,23	0.27	0	26,31,34	0.40	0
4	PSU	A3	4149	4	18,21,22	1.00	1 (5%)	22,30,33	1.72	5 (22%)
2	A2M	A1	1384	2	22,25,26	1.33	1 (4%)	31,36,39	1.62	8 (25%)
2	PSU	A1	1348	2	18,21,22	1.07	1 (5%)	22,30,33	1.68	4 (18%)
2	PSU	A1	1046	2	18,21,22	1.02	1 (5%)	22,30,33	1.64	4 (18%)
4	PSU	A3	4039	4	18,21,22	1.12	1 (5%)	22,30,33	1.73	4 (18%)
2	OMU	A1	121	2	19,22,23	3.00	8 (42%)	26,31,34	1.61	5 (19%)
4	PSU	A3	3502	4	18,21,22	1.10	1 (5%)	22,30,33	1.61	4 (18%)
4	A2M	A3	1810	4	22,25,26	1.32	1 (4%)	31,36,39	1.66	8 (25%)
4	A2M	A3	2658	4	22,25,26	1.29	1 (4%)	31,36,39	1.51	8 (25%)
4	PSU	A3	4042	4	18,21,22	1.03	1 (5%)	22,30,33	1.66	4 (18%)
2	A2M	A1	159	2	22,25,26	1.37	1 (4%)	31,36,39	1.56	8 (25%)
4	A2M	A3	3557	4	22,25,26	1.28	1 (4%)	31,36,39	1.57	7 (22%)
4	A2M	A3	3492	4	22,25,26	1.33	1 (4%)	31,36,39	1.51	7 (22%)
16	HIC	E3	245	16	10,11,12	0.52	0	8,14,16	0.48	0
4	PSU	A3	4217	4	18,21,22	1.07	1 (5%)	22,30,33	1.57	4 (18%)
4	OMG	A3	3524	4	23,26,27	2.28	6 (26%)	33,38,41	2.24	11 (33%)
2	OMG	A1	510	89,2	23,26,27	2.23	6 (26%)	33,38,41	2.29	10 (30%)
2	PSU	A1	105	2	18,21,22	1.06	1 (5%)	22,30,33	1.67	4 (18%)
4	PSU	A3	3369	89,4	18,21,22	0.89	1 (5%)	22,30,33	0.79	0
2	PSU	A1	93	2	18,21,22	1.08	1 (5%)	22,30,33	1.58	4 (18%)
79	MLZ	j2	53	79	8,9,10	0.71	0	4,9,11	0.57	0
2	PSU	A1	1233	2	18,21,22	1.14	1 (5%)	22,30,33	1.65	4 (18%)
2	MA6	A1	1851	2	23,26,27	1.29	4 (17%)	34,38,41	2.68	13 (38%)
2	PSU	A1	650	2	18,21,22	1.10	1 (5%)	22,30,33	1.67	4 (18%)
2	MA6	A1	1852	2	23,26,27	1.25	4 (17%)	34,38,41	2.71	13 (38%)
29	5MC	K1	50	29	18,22,23	0.31	0	26,32,35	0.51	0
4	OMC	A3	3601	4	19,22,23	2.98	8 (42%)	26,31,34	0.77	0
4	OMC	A3	2667	4	19,22,23	3.02	8 (42%)	26,31,34	0.74	0
4	OMG	A3	1580	4	23,26,27	2.32	6 (26%)	33,38,41	2.36	9 (27%)
2	OMG	A1	602	2	23,26,27	2.29	6 (26%)	33,38,41	2.34	12 (36%)
4	A2M	A3	2244	4	22,25,26	1.34	1 (4%)	31,36,39	1.55	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	A1	99	89,2	22,25,26	1.26	1 (4%)	31,36,39	1.46	6 (19%)
4	PSU	A3	4435	4	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
4	PSU	A3	4246	4	18,21,22	1.00	1 (5%)	22,30,33	1.79	4 (18%)
2	PSU	A1	1446	2	18,21,22	1.07	1 (5%)	22,30,33	1.81	4 (18%)
2	OMC	A1	518	2	19,22,23	3.05	8 (42%)	26,31,34	0.88	1 (3%)
29	H2U	K1	16	29	18,21,22	0.71	1 (5%)	21,30,33	0.77	0
4	A2M	A3	3450	4	22,25,26	1.28	1 (4%)	31,36,39	1.58	6 (19%)
4	OMG	A3	1260	4	23,26,27	2.29	6 (26%)	33,38,41	2.31	11 (33%)
2	PSU	A1	36	2	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
4	A2M	A3	3456	4	22,25,26	1.31	1 (4%)	31,36,39	1.52	7 (22%)
4	PSU	A3	4099	4	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
4	PSU	A3	3585	89,4	18,21,22	1.05	1 (5%)	22,30,33	1.60	4 (18%)
4	PSU	A3	1632	4	18,21,22	1.07	1 (5%)	22,30,33	1.78	5 (22%)
2	OMU	A1	172	2	19,22,23	3.02	8 (42%)	26,31,34	1.74	5 (19%)
2	OMU	A1	355	2	19,22,23	3.02	8 (42%)	26,31,34	1.75	5 (19%)
2	OMG	A1	1491	89,2	23,26,27	2.32	6 (26%)	33,38,41	2.35	9 (27%)
2	PSU	A1	816	2	18,21,22	1.08	1 (5%)	22,30,33	1.67	4 (18%)
4	PSU	A3	3500	4	18,21,22	0.88	1 (5%)	22,30,33	0.60	0
4	OMC	A3	3540	4	19,22,23	2.96	8 (42%)	26,31,34	0.79	1 (3%)
4	A2M	A3	1489	89,4	22,25,26	1.39	3 (13%)	31,36,39	1.55	9 (29%)
4	OMC	A3	3619	4	19,22,23	3.02	8 (42%)	26,31,34	0.88	1 (3%)
4	OMG	A3	4383	4,91	23,26,27	2.27	6 (26%)	33,38,41	2.32	11 (33%)
29	PSU	K1	13	29	18,21,22	0.85	1 (5%)	22,30,33	0.72	0
4	PSU	A3	4107	4	18,21,22	1.05	1 (5%)	22,30,33	1.59	4 (18%)
2	OMG	A1	1329	91,2	23,26,27	2.29	6 (26%)	33,38,41	2.32	11 (33%)
2	OMG	A1	645	2	23,26,27	2.26	6 (26%)	33,38,41	2.30	11 (33%)
29	OMC	K1	34	25,29	19,22,23	4.09	13 (68%)	26,31,34	0.89	1 (3%)
4	UR3	A3	4276	4	19,22,23	2.85	7 (36%)	26,32,35	1.35	3 (11%)
4	PSU	A3	1683	4	18,21,22	1.07	1 (5%)	22,30,33	1.66	4 (18%)
4	PSU	A3	4045	4	18,21,22	1.04	1 (5%)	22,30,33	1.65	4 (18%)
4	PSU	A3	4374	4	18,21,22	1.09	1 (5%)	22,30,33	1.82	4 (18%)
29	OMU	K1	32	29	19,22,23	0.21	0	26,31,34	0.40	0
29	1MA	K1	58	29	21,25,26	1.41	2 (9%)	31,37,40	1.33	5 (16%)
4	5MC	A3	4193	4,91	18,22,23	3.52	7 (38%)	26,32,35	1.23	2 (7%)
29	OMU	K1	39	29	19,22,23	0.20	0	26,31,34	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	A3	3496	4	18,21,22	1.05	1 (5%)	22,30,33	1.67	4 (18%)
4	OMG	A3	4138	4	23,26,27	2.27	6 (26%)	33,38,41	2.30	12 (36%)
4	OMG	A3	4369	4	23,26,27	2.27	6 (26%)	33,38,41	2.27	11 (33%)
4	A2M	A3	3599	4	22,25,26	1.33	1 (4%)	31,36,39	1.50	8 (25%)
4	OMC	A3	2194	89,4	19,22,23	2.97	8 (42%)	26,31,34	1.40	4 (15%)
4	A2M	A3	4269	89,4	22,25,26	1.33	1 (4%)	31,36,39	1.58	7 (22%)
4	OMU	A3	2680	4	19,22,23	3.04	8 (42%)	26,31,34	1.77	5 (19%)
4	PSU	A3	1537	4	18,21,22	1.08	1 (5%)	22,30,33	1.57	5 (22%)
4	OMG	A3	1477	4	23,26,27	2.25	6 (26%)	33,38,41	2.26	11 (33%)
4	PSU	A3	4278	4	18,21,22	1.10	1 (5%)	22,30,33	1.63	4 (18%)
2	PSU	A1	1057	2	18,21,22	1.05	1 (5%)	22,30,33	1.70	4 (18%)
4	OMC	A3	2704	4	19,22,23	3.03	8 (42%)	26,31,34	0.82	1 (3%)
4	OMG	A3	3942	89,4,29	23,26,27	2.30	6 (26%)	33,38,41	2.32	10 (30%)
2	PSU	A1	687	2	18,21,22	1.06	1 (5%)	22,30,33	1.68	4 (18%)
4	PSU	A3	4325	4	18,21,22	1.00	1 (5%)	22,30,33	1.62	4 (18%)
4	PSU	A3	1721	4	18,21,22	1.08	1 (5%)	22,30,33	1.62	4 (18%)
4	PSU	A3	4298	4	18,21,22	1.09	1 (5%)	22,30,33	1.70	4 (18%)
2	OMC	A1	463	2	19,22,23	3.03	8 (42%)	26,31,34	0.91	1 (3%)
2	PSU	A1	1178	2	18,21,22	1.11	1 (5%)	22,30,33	1.67	4 (18%)
29	5MC	K1	49	29	18,22,23	0.32	0	26,32,35	0.46	0
4	A2M	A3	1479	4	22,25,26	1.38	2 (9%)	31,36,39	1.49	8 (25%)
4	PSU	A3	1801	4	18,21,22	1.06	1 (5%)	22,30,33	1.67	4 (18%)
2	PSU	A1	1005	2	18,21,22	1.12	1 (5%)	22,30,33	1.64	4 (18%)
2	PSU	A1	210	2	18,21,22	1.08	1 (5%)	22,30,33	1.71	4 (18%)
4	A2M	A3	400	4	22,25,26	1.34	1 (4%)	31,36,39	1.54	9 (29%)
4	5MC	A3	3514	89,4	18,22,23	3.53	7 (38%)	26,32,35	1.12	3 (11%)
2	PSU	A1	1175	91,2	18,21,22	1.10	1 (5%)	22,30,33	1.67	4 (18%)
4	OMC	A3	4202	4	19,22,23	2.97	8 (42%)	26,31,34	0.92	2 (7%)
4	OMG	A3	3974	4	23,26,27	0.31	0	33,38,41	0.45	0
29	5MC	K1	72	29	18,22,23	0.32	0	26,32,35	0.43	0
4	PSU	A3	4711	4	18,21,22	1.04	1 (5%)	22,30,33	1.66	4 (18%)
4	A2M	A3	2630	89,4	22,25,26	1.27	1 (4%)	31,36,39	1.55	8 (25%)
2	A2M	A1	166	2	22,25,26	1.35	1 (4%)	31,36,39	1.56	8 (25%)
4	OMC	A3	1820	89,4	19,22,23	0.29	0	26,31,34	0.73	0
2	PSU	A1	407	2	18,21,22	1.09	1 (5%)	22,30,33	1.68	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	A3	2475	4	18,21,22	1.07	1 (5%)	22,30,33	1.58	4 (18%)
4	OMC	A3	3573	4	19,22,23	3.00	8 (42%)	26,31,34	0.74	0
4	PSU	A3	3554	4	18,21,22	1.07	1 (5%)	22,30,33	1.70	4 (18%)
4	PSU	A3	4169	4	18,21,22	1.10	1 (5%)	22,30,33	1.66	4 (18%)
2	A2M	A1	1032	2	22,25,26	1.30	1 (4%)	31,36,39	1.50	7 (22%)
2	PSU	A1	119	2	18,21,22	1.04	1 (5%)	22,30,33	1.55	4 (18%)
4	OMC	A3	4282	4	19,22,23	3.01	8 (42%)	26,31,34	0.88	1 (3%)
2	PSU	A1	34	2	18,21,22	1.04	1 (5%)	22,30,33	1.65	4 (18%)
4	PSU	A3	3490	4	18,21,22	0.88	1 (5%)	22,30,33	0.61	0
4	OMG	A3	4240	4	23,26,27	2.28	6 (26%)	33,38,41	2.31	10 (30%)
4	A2M	A3	2206	89,4	22,25,26	0.18	0	31,36,39	0.32	0
2	A2M	A1	513	2	22,25,26	1.46	1 (4%)	31,36,39	1.61	6 (19%)
2	4AC	A1	1843	2	21,24,25	3.24	10 (47%)	29,34,37	1.16	3 (10%)
2	A2M	A1	591	2	22,25,26	1.40	1 (4%)	31,36,39	1.48	7 (22%)
4	UY1	A3	3550	89,4	19,22,23	0.85	1 (5%)	22,31,34	0.65	0
76	HY3	i1	62	76	6,8,9	1.84	1 (16%)	5,10,12	1.00	0
4	OMC	A3	1284	4	19,22,23	2.90	8 (42%)	26,31,34	0.81	0
2	OMC	A1	174	89,2	19,22,23	3.05	8 (42%)	26,31,34	0.73	0
4	OMU	A3	4244	89,4	19,22,23	3.04	8 (42%)	26,31,34	1.73	5 (19%)
10	PSU	C3	55	10	18,21,22	1.08	1 (5%)	22,30,33	1.69	4 (18%)
2	PSU	A1	802	2	18,21,22	1.10	1 (5%)	22,30,33	1.64	4 (18%)
4	PSU	A3	4188	4	18,21,22	1.05	1 (5%)	22,30,33	1.69	5 (22%)
29	OMC	K1	4	29	19,22,23	4.10	13 (68%)	26,31,34	1.33	3 (11%)
2	PSU	A1	1047	2	18,21,22	1.08	1 (5%)	22,30,33	1.63	4 (18%)
2	A2M	A1	1679	2	22,25,26	1.33	2 (9%)	31,36,39	1.53	9 (29%)
10	PSU	C3	69	10	18,21,22	1.06	1 (5%)	22,30,33	1.66	5 (22%)
4	OMG	A3	2207	4	23,26,27	0.29	0	33,38,41	0.37	0
2	OMG	A1	868	2	23,26,27	2.36	6 (26%)	33,38,41	2.41	10 (30%)
2	B8N	A1	1249	2	24,29,30	2.89	5 (20%)	29,42,45	1.76	6 (20%)
4	6MZ	A3	3966	4	22,25,26	2.59	4 (18%)	30,36,39	2.23	8 (26%)
4	PSU	A3	4177	4	18,21,22	1.10	1 (5%)	22,30,33	1.65	4 (18%)
4	OMG	A3	3359	4	23,26,27	2.26	7 (30%)	33,38,41	2.23	13 (39%)
4	PSU	A3	3652	89,4	18,21,22	1.03	1 (5%)	22,30,33	1.64	4 (18%)
2	PSU	A1	1626	2	18,21,22	1.08	1 (5%)	22,30,33	1.60	4 (18%)
4	PSU	A3	4419	4	18,21,22	1.10	1 (5%)	22,30,33	1.65	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A1	1239	2	18,21,22	1.08	1 (5%)	22,30,33	1.67	4 (18%)
4	PSU	A3	1718	4	18,21,22	1.08	1 (5%)	22,30,33	1.69	4 (18%)
2	OMU	A1	1443	89,2	19,22,23	3.05	8 (42%)	26,31,34	1.68	4 (15%)
4	OMU	A3	4366	4	19,22,23	2.95	8 (42%)	26,31,34	1.63	4 (15%)
4	PSU	A3	4740	4	18,21,22	1.10	1 (5%)	22,30,33	1.62	4 (18%)
4	1MA	A3	1266	89,4	21,25,26	0.45	0	31,37,40	0.59	0
4	OMG	A3	4116	4	23,26,27	2.29	6 (26%)	33,38,41	2.30	10 (30%)
4	OMU	A3	2258	4	19,22,23	3.05	8 (42%)	26,31,34	1.69	4 (15%)
4	OMU	A3	3657	4	19,22,23	3.01	8 (42%)	26,31,34	1.77	5 (19%)
4	PSU	A3	4166	4	18,21,22	1.04	1 (5%)	22,30,33	1.56	5 (22%)
4	OMU	A3	4052	4	19,22,23	3.01	8 (42%)	26,31,34	1.72	5 (19%)
2	PSU	A1	610	2	18,21,22	1.08	1 (5%)	22,30,33	1.66	4 (18%)
2	PSU	A1	815	2	18,21,22	1.02	1 (5%)	22,30,33	1.59	4 (18%)
2	A2M	A1	577	2	22,25,26	1.33	1 (4%)	31,36,39	1.52	7 (22%)
4	OMG	A3	3476	4	23,26,27	2.29	6 (26%)	33,38,41	2.31	11 (33%)
4	PSU	A3	4749	4	18,21,22	1.12	1 (5%)	22,30,33	1.66	4 (18%)
4	PSU	A3	1799	4	18,21,22	1.06	1 (5%)	22,30,33	1.65	4 (18%)
4	PSU	A3	1720	4	18,21,22	1.08	1 (5%)	22,30,33	1.59	4 (18%)
4	PSU	A3	1491	4	18,21,22	1.11	1 (5%)	22,30,33	1.76	4 (18%)
4	A2M	A3	3562	4	22,25,26	1.31	1 (4%)	31,36,39	1.58	6 (19%)
4	PSU	A3	3583	4	18,21,22	1.07	1 (5%)	22,30,33	1.62	4 (18%)
2	OMU	A1	429	2	19,22,23	0.22	0	26,31,34	0.44	0
2	PSU	A1	1082	2	18,21,22	1.06	1 (5%)	22,30,33	1.67	4 (18%)
2	PSU	A1	1368	2	18,21,22	1.04	1 (5%)	22,30,33	1.66	4 (18%)
4	PSU	A3	3427	4	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
2	OMU	A1	116	2	19,22,23	3.01	8 (42%)	26,31,34	1.57	4 (15%)
4	PSU	A3	4267	89,4,91	18,21,22	1.13	1 (5%)	22,30,33	1.77	4 (18%)
4	A2M	A3	1270	4	22,25,26	1.29	1 (4%)	31,36,39	1.53	9 (29%)
4	PSU	A3	3371	4	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)
2	PSU	A1	652	2	18,21,22	1.12	1 (5%)	22,30,33	1.68	4 (18%)
4	PSU	A3	4322	4	18,21,22	1.08	1 (5%)	22,30,33	1.66	4 (18%)
68	NMM	e1	67	68	9,11,12	0.65	0	6,12,14	2.31	2 (33%)
2	PSU	A1	867	2	18,21,22	1.13	1 (5%)	22,30,33	1.66	4 (18%)
4	OMG	A3	3676	4	23,26,27	2.32	6 (26%)	33,38,41	2.25	10 (30%)
4	PSU	A3	3447	4	18,21,22	1.09	1 (5%)	22,30,33	1.67	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	V5N	D3	216	13	9,11,12	0.80	0	9,14,16	0.99	0
4	PSU	A3	4058	4	18,21,22	1.07	1 (5%)	22,30,33	1.66	4 (18%)

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
4	PSU	A3	3494	4	-	2/7/25/26	0/2/2/2
2	PSU	A1	823	2	-	0/7/25/26	0/2/2/2
4	A2M	A3	398	4	-	1/9/27/28	0/3/3/3
2	PSU	A1	218	2	-	0/7/25/26	0/2/2/2
2	A2M	A1	485	2	-	0/9/27/28	0/3/3/3
2	OMC	A1	1704	2	-	0/9/27/28	0/2/2/2
4	A2M	A3	4317	4	-	0/9/27/28	0/3/3/3
29	1MA	K1	14	29	-	1/7/25/26	0/3/3/3
56	MLZ	X2	5	56	-	4/7/8/10	-
4	PSU	A3	3466	4	-	1/7/25/26	0/2/2/2
2	G7M	A1	1640	2,29	-	2/7/25/26	0/3/3/3
29	1MG	K1	9	29	-	1/7/25/26	0/3/3/3
54	V5N	W2	39	54	-	2/9/10/12	0/1/1/1
2	PSU	A1	1245	2	-	2/7/25/26	0/2/2/2
4	PSU	A3	1731	4	-	2/7/25/26	0/2/2/2
2	OMC	A1	1392	2	-	2/9/27/28	0/2/2/2
2	A2M	A1	669	89,2	-	4/9/27/28	0/3/3/3
2	OMU	A1	628	2	-	1/9/27/28	0/2/2/2
2	PSU	A1	967	2	-	0/7/25/26	0/2/2/2
2	OMG	A1	1448	2	-	2/9/27/28	0/3/3/3
2	PSU	A1	1644	89,2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4382	4	-	3/7/25/26	0/2/2/2
2	4AC	A1	1338	2	-	1/11/29/30	0/2/2/2
4	PSU	A3	2351	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4203	4	-	0/7/25/26	0/2/2/2
2	6MZ	A1	1833	89,2	-	0/9/27/28	0/3/3/3
4	PSU	A3	3462	4	-	0/7/25/26	0/2/2/2
2	OMU	A1	1327	89,2	-	0/9/27/28	0/2/2/2
4	PSU	A3	1638	4	-	0/7/25/26	0/2/2/2
2	OMU	A1	1805	2	-	0/9/27/28	0/2/2/2
77	M3L	i2	98	77	-	0/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	A3	3616	4	-	0/7/25/26	0/2/2/2
2	PSU	A1	682	2	-	0/7/25/26	0/2/2/2
2	OMU	A1	1289	2	-	0/9/27/28	0/2/2/2
4	A2M	A3	3517	4	-	3/9/27/28	0/3/3/3
4	OMC	A3	2265	89,4	-	2/9/27/28	0/2/2/2
2	OMG	A1	437	2	-	2/9/27/28	0/3/3/3
4	OMC	A3	2647	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	3576	4	-	1/7/25/26	0/2/2/2
4	OMG	A3	3631	89,4	-	2/9/27/28	0/3/3/3
2	PSU	A1	573	2	-	0/7/25/26	0/2/2/2
2	PSU	A1	109	2	-	0/7/25/26	0/2/2/2
4	OMC	A3	3433	4,91	-	4/9/27/28	0/2/2/2
2	PSU	A1	1693	2	-	0/7/25/26	0/2/2/2
4	OMG	A3	4364	4	-	2/9/27/28	0/3/3/3
4	OMG	A3	2267	4	-	1/9/27/28	0/3/3/3
2	PSU	A1	864	2	-	0/7/25/26	0/2/2/2
4	A2M	A3	4336	4	-	1/9/27/28	0/3/3/3
10	OMG	C3	75	10	-	1/9/27/28	0/3/3/3
4	OMU	A3	3973	4	-	0/9/27/28	0/2/2/2
29	5MU	K1	54	29	-	0/7/25/26	0/2/2/2
4	OMG	A3	2719	4	-	0/9/27/28	0/3/3/3
2	A2M	A1	469	2	-	2/9/27/28	0/3/3/3
4	OMG	A3	4245	4	-	0/9/27/28	0/3/3/3
2	A2M	A1	27	89,2	-	1/9/27/28	0/3/3/3
2	OMG	A1	684	2	-	2/9/27/28	0/3/3/3
4	OMC	A3	2208	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	4149	4	-	0/7/25/26	0/2/2/2
2	A2M	A1	1384	2	-	1/9/27/28	0/3/3/3
2	PSU	A1	1348	2	-	0/7/25/26	0/2/2/2
2	PSU	A1	1046	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4039	4	-	0/7/25/26	0/2/2/2
2	OMU	A1	121	2	-	1/9/27/28	0/2/2/2
4	PSU	A3	3502	4	-	0/7/25/26	0/2/2/2
4	A2M	A3	1810	4	-	0/9/27/28	0/3/3/3
4	A2M	A3	2658	4	-	1/9/27/28	0/3/3/3
4	PSU	A3	4042	4	-	0/7/25/26	0/2/2/2
2	A2M	A1	159	2	-	1/9/27/28	0/3/3/3
4	A2M	A3	3557	4	-	0/9/27/28	0/3/3/3
4	A2M	A3	3492	4	-	0/9/27/28	0/3/3/3
16	HIC	E3	245	16	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	A3	4217	4	-	1/7/25/26	0/2/2/2
4	OMG	A3	3524	4	-	0/9/27/28	0/3/3/3
2	OMG	A1	510	89,2	-	1/9/27/28	0/3/3/3
2	PSU	A1	105	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	3369	89,4	-	0/7/25/26	0/2/2/2
2	PSU	A1	93	2	-	0/7/25/26	0/2/2/2
79	MLZ	j2	53	79	-	1/7/8/10	-
2	PSU	A1	1233	2	-	0/7/25/26	0/2/2/2
2	MA6	A1	1851	2	-	0/11/29/30	0/3/3/3
2	PSU	A1	650	2	-	0/7/25/26	0/2/2/2
2	MA6	A1	1852	2	-	1/11/29/30	0/3/3/3
29	5MC	K1	50	29	-	0/7/25/26	0/2/2/2
4	OMC	A3	3601	4	-	2/9/27/28	0/2/2/2
4	OMC	A3	2667	4	-	0/9/27/28	0/2/2/2
4	OMG	A3	1580	4	-	0/9/27/28	0/3/3/3
2	OMG	A1	602	2	-	0/9/27/28	0/3/3/3
4	A2M	A3	2244	4	-	0/9/27/28	0/3/3/3
2	A2M	A1	99	89,2	-	0/9/27/28	0/3/3/3
4	PSU	A3	4435	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4246	4	-	1/7/25/26	0/2/2/2
2	PSU	A1	1446	2	-	0/7/25/26	0/2/2/2
2	OMC	A1	518	2	-	0/9/27/28	0/2/2/2
29	H2U	K1	16	29	-	0/7/38/39	0/2/2/2
4	A2M	A3	3450	4	-	1/9/27/28	0/3/3/3
4	OMG	A3	1260	4	-	0/9/27/28	0/3/3/3
2	PSU	A1	36	2	-	0/7/25/26	0/2/2/2
4	A2M	A3	3456	4	-	0/9/27/28	0/3/3/3
4	PSU	A3	4099	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	3585	89,4	-	0/7/25/26	0/2/2/2
4	PSU	A3	1632	4	-	3/7/25/26	0/2/2/2
2	OMU	A1	172	2	-	0/9/27/28	0/2/2/2
2	OMU	A1	355	2	-	0/9/27/28	0/2/2/2
2	OMG	A1	1491	89,2	-	1/9/27/28	0/3/3/3
2	PSU	A1	816	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	3500	4	-	0/7/25/26	0/2/2/2
4	OMC	A3	3540	4	-	0/9/27/28	0/2/2/2
4	A2M	A3	1489	89,4	-	2/9/27/28	0/3/3/3
4	OMC	A3	3619	4	-	1/9/27/28	0/2/2/2
4	OMG	A3	4383	4,91	-	1/9/27/28	0/3/3/3
29	PSU	K1	13	29	-	2/7/25/26	0/2/2/2
4	PSU	A3	4107	4	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	A1	1329	91,2	-	0/9/27/28	0/3/3/3
2	OMG	A1	645	2	-	3/9/27/28	0/3/3/3
29	OMC	K1	34	25,29	-	0/9/27/28	0/2/2/2
4	UR3	A3	4276	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	1683	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4045	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4374	4	-	0/7/25/26	0/2/2/2
29	OMU	K1	32	29	-	1/9/27/28	0/2/2/2
29	1MA	K1	58	29	-	0/7/25/26	0/3/3/3
4	5MC	A3	4193	4,91	-	4/7/25/26	0/2/2/2
29	OMU	K1	39	29	-	1/9/27/28	0/2/2/2
4	PSU	A3	3496	4	-	0/7/25/26	0/2/2/2
4	OMG	A3	4138	4	-	0/9/27/28	0/3/3/3
4	OMG	A3	4369	4	-	0/9/27/28	0/3/3/3
4	A2M	A3	3599	4	-	2/9/27/28	0/3/3/3
4	OMC	A3	2194	89,4	-	3/9/27/28	0/2/2/2
4	A2M	A3	4269	89,4	-	1/9/27/28	0/3/3/3
4	OMU	A3	2680	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	1537	4	-	0/7/25/26	0/2/2/2
4	OMG	A3	1477	4	-	0/9/27/28	0/3/3/3
4	PSU	A3	4278	4	-	0/7/25/26	0/2/2/2
2	PSU	A1	1057	2	-	0/7/25/26	0/2/2/2
4	OMC	A3	2704	4	-	0/9/27/28	0/2/2/2
4	OMG	A3	3942	89,4,29	-	0/9/27/28	0/3/3/3
2	PSU	A1	687	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4325	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	1721	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4298	4	-	0/7/25/26	0/2/2/2
2	OMC	A1	463	2	-	1/9/27/28	0/2/2/2
2	PSU	A1	1178	2	-	0/7/25/26	0/2/2/2
29	5MC	K1	49	29	-	2/7/25/26	0/2/2/2
4	A2M	A3	1479	4	-	1/9/27/28	0/3/3/3
4	PSU	A3	1801	4	-	0/7/25/26	0/2/2/2
2	PSU	A1	1005	2	-	0/7/25/26	0/2/2/2
2	PSU	A1	210	2	-	2/7/25/26	0/2/2/2
4	A2M	A3	400	4	-	0/9/27/28	0/3/3/3
4	5MC	A3	3514	89,4	-	0/7/25/26	0/2/2/2
2	PSU	A1	1175	91,2	-	0/7/25/26	0/2/2/2
4	OMC	A3	4202	4	-	0/9/27/28	0/2/2/2
4	OMG	A3	3974	4	-	0/9/27/28	0/3/3/3
29	5MC	K1	72	29	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	A3	4711	4	-	0/7/25/26	0/2/2/2
4	A2M	A3	2630	89,4	-	3/9/27/28	0/3/3/3
2	A2M	A1	166	2	-	0/9/27/28	0/3/3/3
4	OMC	A3	1820	89,4	-	0/9/27/28	0/2/2/2
2	PSU	A1	407	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	2475	4	-	0/7/25/26	0/2/2/2
4	OMC	A3	3573	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	3554	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4169	4	-	0/7/25/26	0/2/2/2
2	A2M	A1	1032	2	-	0/9/27/28	0/3/3/3
2	PSU	A1	119	2	-	0/7/25/26	0/2/2/2
4	OMC	A3	4282	4	-	0/9/27/28	0/2/2/2
2	PSU	A1	34	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	3490	4	-	0/7/25/26	0/2/2/2
4	OMG	A3	4240	4	-	0/9/27/28	0/3/3/3
4	A2M	A3	2206	89,4	-	0/9/27/28	0/3/3/3
2	A2M	A1	513	2	-	2/9/27/28	0/3/3/3
2	4AC	A1	1843	2	-	0/11/29/30	0/2/2/2
2	A2M	A1	591	2	-	1/9/27/28	0/3/3/3
4	UY1	A3	3550	89,4	-	3/9/27/28	0/2/2/2
76	HY3	i1	62	76	-	1/1/12/14	0/1/1/1
4	OMC	A3	1284	4	-	0/9/27/28	0/2/2/2
2	OMC	A1	174	89,2	-	2/9/27/28	0/2/2/2
4	OMU	A3	4244	89,4	-	1/9/27/28	0/2/2/2
10	PSU	C3	55	10	-	0/7/25/26	0/2/2/2
2	PSU	A1	802	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4188	4	-	0/7/25/26	0/2/2/2
29	OMC	K1	4	29	-	1/9/27/28	0/2/2/2
2	PSU	A1	1047	2	-	0/7/25/26	0/2/2/2
2	A2M	A1	1679	2	-	1/9/27/28	0/3/3/3
10	PSU	C3	69	10	-	0/7/25/26	0/2/2/2
4	OMG	A3	2207	4	-	1/9/27/28	0/3/3/3
2	OMG	A1	868	2	-	2/9/27/28	0/3/3/3
2	B8N	A1	1249	2	-	3/16/34/35	0/2/2/2
4	6MZ	A3	3966	4	-	0/9/27/28	0/3/3/3
4	PSU	A3	4177	4	-	0/7/25/26	0/2/2/2
4	OMG	A3	3359	4	-	1/9/27/28	0/3/3/3
4	PSU	A3	3652	89,4	-	0/7/25/26	0/2/2/2
2	PSU	A1	1626	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4419	4	-	0/7/25/26	0/2/2/2
2	PSU	A1	1239	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	A3	1718	4	-	0/7/25/26	0/2/2/2
2	OMU	A1	1443	89,2	-	1/9/27/28	0/2/2/2
4	OMU	A3	4366	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	4740	4	-	0/7/25/26	0/2/2/2
4	1MA	A3	1266	89,4	-	0/7/25/26	0/3/3/3
4	OMG	A3	4116	4	-	1/9/27/28	0/3/3/3
4	OMU	A3	2258	4	-	0/9/27/28	0/2/2/2
4	OMU	A3	3657	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	4166	4	-	4/7/25/26	0/2/2/2
4	OMU	A3	4052	4	-	0/9/27/28	0/2/2/2
2	PSU	A1	610	2	-	0/7/25/26	0/2/2/2
2	PSU	A1	815	2	-	0/7/25/26	0/2/2/2
2	A2M	A1	577	2	-	3/9/27/28	0/3/3/3
4	OMG	A3	3476	4	-	0/9/27/28	0/3/3/3
4	PSU	A3	4749	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	1799	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	1720	4	-	2/7/25/26	0/2/2/2
4	PSU	A3	1491	4	-	0/7/25/26	0/2/2/2
4	A2M	A3	3562	4	-	0/9/27/28	0/3/3/3
4	PSU	A3	3583	4	-	2/7/25/26	0/2/2/2
2	OMU	A1	429	2	-	4/9/27/28	0/2/2/2
2	PSU	A1	1082	2	-	0/7/25/26	0/2/2/2
2	PSU	A1	1368	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	3427	4	-	0/7/25/26	0/2/2/2
2	OMU	A1	116	2	-	1/9/27/28	0/2/2/2
4	PSU	A3	4267	89,4,91	-	0/7/25/26	0/2/2/2
4	A2M	A3	1270	4	-	3/9/27/28	0/3/3/3
4	PSU	A3	3371	4	-	0/7/25/26	0/2/2/2
2	PSU	A1	652	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4322	4	-	0/7/25/26	0/2/2/2
68	NMM	e1	67	68	-	1/9/11/13	-
2	PSU	A1	867	2	-	0/7/25/26	0/2/2/2
4	OMG	A3	3676	4	-	2/9/27/28	0/3/3/3
4	PSU	A3	3447	4	-	0/7/25/26	0/2/2/2
13	V5N	D3	216	13	-	1/9/10/12	0/1/1/1
4	PSU	A3	4058	4	-	0/7/25/26	0/2/2/2

All (689) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A1	1833	6MZ	C6-N6	11.13	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A3	3966	6MZ	C6-N6	10.73	1.45	1.34
4	A3	4193	5MC	C6-C5	9.53	1.50	1.34
4	A3	3514	5MC	C6-C5	9.09	1.49	1.34
4	A3	3517	A2M	C3'-C4'	-8.36	1.31	1.53
2	A1	1249	B8N	C6-N1	8.21	1.56	1.36
4	A3	3517	A2M	O4'-C4'	7.76	1.62	1.45
4	A3	4276	UR3	C2-N1	7.67	1.49	1.38
29	K1	34	OMC	C3'-C4'	-7.50	1.33	1.53
2	A1	1338	4AC	C4-N3	7.49	1.45	1.32
29	K1	4	OMC	O4'-C4'	7.22	1.61	1.45
29	K1	4	OMC	C3'-C4'	-7.20	1.34	1.53
2	A1	1805	OMU	C2-N1	7.20	1.50	1.38
4	A3	2258	OMU	C2-N1	7.17	1.50	1.38
29	K1	34	OMC	O4'-C4'	7.17	1.61	1.45
4	A3	3973	OMU	C2-N1	7.15	1.49	1.38
2	A1	1289	OMU	C2-N1	7.11	1.49	1.38
4	A3	3657	OMU	C2-N1	7.08	1.49	1.38
2	A1	1443	OMU	C2-N1	7.08	1.49	1.38
4	A3	4244	OMU	C2-N1	7.07	1.49	1.38
4	A3	2680	OMU	C2-N1	7.07	1.49	1.38
2	A1	1249	B8N	C4-N3	-7.06	1.27	1.40
2	A1	1327	OMU	C2-N1	7.00	1.49	1.38
2	A1	628	OMU	C2-N1	6.99	1.49	1.38
2	A1	355	OMU	C2-N1	6.99	1.49	1.38
2	A1	172	OMU	C2-N1	6.97	1.49	1.38
2	A1	116	OMU	C2-N3	6.95	1.50	1.38
4	A3	2258	OMU	C2-N3	6.94	1.50	1.38
2	A1	172	OMU	C2-N3	6.93	1.50	1.38
2	A1	628	OMU	C2-N3	6.92	1.50	1.38
2	A1	116	OMU	C2-N1	6.91	1.49	1.38
2	A1	1805	OMU	C2-N3	6.88	1.50	1.38
2	A1	121	OMU	C2-N3	6.85	1.50	1.38
2	A1	1443	OMU	C2-N3	6.85	1.50	1.38
4	A3	4052	OMU	C2-N1	6.85	1.49	1.38
2	A1	121	OMU	C2-N1	6.84	1.49	1.38
4	A3	4052	OMU	C2-N3	6.84	1.50	1.38
2	A1	1327	OMU	C2-N3	6.83	1.50	1.38
2	A1	1843	4AC	C4-N3	6.83	1.44	1.32
2	A1	355	OMU	C2-N3	6.82	1.50	1.38
4	A3	3973	OMU	C2-N3	6.81	1.50	1.38
4	A3	4244	OMU	C2-N3	6.80	1.50	1.38
2	A1	1289	OMU	C2-N3	6.79	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A3	2680	OMU	C2-N3	6.77	1.50	1.38
4	A3	4366	OMU	C2-N1	6.74	1.49	1.38
4	A3	3657	OMU	C2-N3	6.69	1.49	1.38
4	A3	4366	OMU	C2-N3	6.65	1.49	1.38
2	A1	1338	4AC	C2-N3	6.59	1.49	1.36
2	A1	868	OMG	C4-N3	6.52	1.49	1.34
4	A3	2267	OMG	C4-N3	6.43	1.49	1.34
2	A1	518	OMC	C2-N3	6.40	1.49	1.36
4	A3	1580	OMG	C4-N3	6.40	1.49	1.34
4	A3	2265	OMC	C2-N3	6.38	1.49	1.36
2	A1	1491	OMG	C4-N3	6.38	1.49	1.34
4	A3	3573	OMC	C2-N3	6.37	1.49	1.36
4	A3	4282	OMC	C2-N3	6.36	1.49	1.36
2	A1	1392	OMC	C2-N3	6.36	1.49	1.36
4	A3	3676	OMG	C4-N3	6.35	1.49	1.34
4	A3	3619	OMC	C2-N3	6.35	1.49	1.36
2	A1	1640	G7M	C4-N3	6.35	1.49	1.34
4	A3	3942	OMG	C4-N3	6.34	1.49	1.34
2	A1	174	OMC	C2-N3	6.33	1.49	1.36
4	A3	2704	OMC	C2-N3	6.33	1.49	1.36
4	A3	4202	OMC	C2-N3	6.32	1.49	1.36
2	A1	1448	OMG	C4-N3	6.32	1.49	1.34
4	A3	2647	OMC	C2-N3	6.32	1.49	1.36
2	A1	463	OMC	C2-N3	6.31	1.49	1.36
2	A1	684	OMG	C4-N3	6.31	1.49	1.34
4	A3	2719	OMG	C4-N3	6.31	1.49	1.34
4	A3	3524	OMG	C4-N3	6.29	1.49	1.34
2	A1	437	OMG	C4-N3	6.29	1.49	1.34
4	A3	2667	OMC	C2-N3	6.28	1.49	1.36
2	A1	1329	OMG	C4-N3	6.27	1.49	1.34
4	A3	4245	OMG	C4-N3	6.27	1.49	1.34
4	A3	4116	OMG	C4-N3	6.26	1.49	1.34
4	A3	3476	OMG	C4-N3	6.25	1.49	1.34
4	A3	3601	OMC	C2-N3	6.25	1.49	1.36
2	A1	602	OMG	C4-N3	6.23	1.49	1.34
4	A3	4240	OMG	C4-N3	6.23	1.49	1.34
4	A3	3514	5MC	C4-N3	6.22	1.44	1.34
4	A3	4383	OMG	C4-N3	6.21	1.49	1.34
4	A3	1260	OMG	C4-N3	6.21	1.49	1.34
2	A1	1704	OMC	C2-N3	6.21	1.48	1.36
10	C3	75	OMG	C4-N3	6.20	1.49	1.34
4	A3	3540	OMC	C2-N3	6.18	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A3	4138	OMG	C4-N3	6.17	1.48	1.34
4	A3	2194	OMC	C2-N3	6.16	1.48	1.36
2	A1	645	OMG	C4-N3	6.16	1.48	1.34
29	K1	34	OMC	C2-N3	6.15	1.48	1.36
4	A3	4276	UR3	C6-C5	6.14	1.49	1.35
2	A1	1843	4AC	C6-C5	6.12	1.49	1.35
4	A3	1284	OMC	C2-N3	6.12	1.48	1.36
2	A1	510	OMG	C4-N3	6.12	1.48	1.34
2	A1	174	OMC	C6-C5	6.10	1.49	1.35
4	A3	3433	OMC	C2-N3	6.09	1.48	1.36
4	A3	4369	OMG	C4-N3	6.07	1.48	1.34
29	K1	4	OMC	C2-N3	6.06	1.48	1.36
4	A3	3631	OMG	C4-N3	6.04	1.48	1.34
4	A3	2667	OMC	C6-C5	6.02	1.49	1.35
4	A3	2265	OMC	C6-C5	6.01	1.49	1.35
2	A1	463	OMC	C6-C5	6.01	1.49	1.35
4	A3	4364	OMG	C4-N3	6.01	1.48	1.34
4	A3	3359	OMG	C4-N3	6.01	1.48	1.34
4	A3	1477	OMG	C4-N3	6.00	1.48	1.34
4	A3	3433	OMC	C6-C5	5.99	1.49	1.35
4	A3	3514	5MC	C2-N3	5.99	1.48	1.36
4	A3	2704	OMC	C6-C5	5.98	1.48	1.35
2	A1	518	OMC	C6-C5	5.97	1.48	1.35
4	A3	3601	OMC	C6-C5	5.96	1.48	1.35
4	A3	3540	OMC	C6-C5	5.95	1.48	1.35
2	A1	1704	OMC	C6-C5	5.95	1.48	1.35
2	A1	1392	OMC	C6-C5	5.94	1.48	1.35
4	A3	3573	OMC	C6-C5	5.94	1.48	1.35
4	A3	3619	OMC	C6-C5	5.94	1.48	1.35
4	A3	4282	OMC	C6-C5	5.93	1.48	1.35
2	A1	1338	4AC	C6-C5	5.92	1.48	1.35
4	A3	2647	OMC	C6-C5	5.91	1.48	1.35
2	A1	1843	4AC	C2-N3	5.91	1.48	1.36
4	A3	1284	OMC	C6-C5	5.86	1.48	1.35
4	A3	2194	OMC	C6-C5	5.85	1.48	1.35
4	A3	4202	OMC	C6-C5	5.82	1.48	1.35
2	A1	628	OMU	C6-C5	5.81	1.48	1.35
2	A1	1327	OMU	C6-C5	5.81	1.48	1.35
29	K1	4	OMC	C6-C5	5.80	1.48	1.35
29	K1	34	OMC	C6-C5	5.79	1.48	1.35
2	A1	1805	OMU	C6-C5	5.78	1.48	1.35
4	A3	3973	OMU	C6-C5	5.77	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A3	2680	OMU	C6-C5	5.76	1.48	1.35
2	A1	121	OMU	C6-C5	5.74	1.48	1.35
2	A1	1289	OMU	C6-C5	5.74	1.48	1.35
4	A3	4244	OMU	C6-C5	5.73	1.48	1.35
4	A3	4193	5MC	C2-N3	5.73	1.48	1.36
2	A1	1443	OMU	C6-C5	5.73	1.48	1.35
2	A1	172	OMU	C6-C5	5.71	1.48	1.35
2	A1	1249	B8N	C2-N1	5.70	1.56	1.39
2	A1	116	OMU	C6-C5	5.69	1.48	1.35
4	A3	2258	OMU	C6-C5	5.69	1.48	1.35
4	A3	4193	5MC	C4-N3	5.67	1.43	1.34
4	A3	4052	OMU	C6-C5	5.67	1.48	1.35
4	A3	3657	OMU	C6-C5	5.67	1.48	1.35
2	A1	355	OMU	C6-C5	5.64	1.48	1.35
4	A3	4366	OMU	C6-C5	5.60	1.48	1.35
2	A1	1640	G7M	C2-N3	5.45	1.46	1.33
4	A3	4276	UR3	C2-N3	5.27	1.49	1.39
2	A1	174	OMC	C4-N3	5.22	1.45	1.34
2	A1	518	OMC	C4-N3	5.15	1.44	1.34
4	A3	2704	OMC	C4-N3	5.13	1.44	1.34
4	A3	2667	OMC	C4-N3	5.13	1.44	1.34
2	A1	463	OMC	C4-N3	5.10	1.44	1.34
4	A3	2265	OMC	C4-N3	5.08	1.44	1.34
4	A3	2647	OMC	C4-N3	5.08	1.44	1.34
4	A3	3573	OMC	C4-N3	5.08	1.44	1.34
2	A1	1392	OMC	C4-N3	5.07	1.44	1.34
2	A1	1704	OMC	C4-N3	5.06	1.44	1.34
2	A1	1249	B8N	C6-C5	5.05	1.42	1.34
4	A3	3619	OMC	C4-N3	5.01	1.44	1.34
2	A1	868	OMG	C2-N2	5.00	1.46	1.34
4	A3	3601	OMC	C4-N3	5.00	1.44	1.34
4	A3	3676	OMG	C2-N2	4.99	1.46	1.34
29	K1	34	OMC	O4'-C1'	-4.99	1.30	1.42
2	A1	868	OMG	C2-N3	4.99	1.45	1.33
4	A3	4202	OMC	C4-N3	4.99	1.44	1.34
4	A3	2194	OMC	C2-N1	4.99	1.50	1.40
29	K1	4	OMC	C4-N3	4.98	1.44	1.34
2	A1	1448	OMG	C2-N2	4.97	1.46	1.34
4	A3	4282	OMC	C4-N3	4.97	1.44	1.34
2	A1	684	OMG	C2-N2	4.94	1.45	1.34
29	K1	34	OMC	C4-N3	4.94	1.44	1.34
2	A1	513	A2M	O5'-C5'	-4.94	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A3	1284	OMC	C4-N3	4.93	1.44	1.34
4	A3	1580	OMG	C2-N2	4.92	1.45	1.34
4	A3	3517	A2M	O4'-C1'	-4.91	1.30	1.42
2	A1	463	OMC	C4-N4	4.91	1.45	1.33
4	A3	4245	OMG	C2-N2	4.91	1.45	1.34
4	A3	3942	OMG	C2-N2	4.91	1.45	1.34
4	A3	3433	OMC	C4-N3	4.90	1.44	1.34
2	A1	437	OMG	C2-N2	4.90	1.45	1.34
2	A1	463	OMC	C2-N1	4.90	1.50	1.40
4	A3	2704	OMC	C4-N4	4.90	1.45	1.33
2	A1	1491	OMG	C2-N2	4.90	1.45	1.34
2	A1	1392	OMC	C2-N1	4.90	1.50	1.40
4	A3	2267	OMG	C2-N3	4.90	1.45	1.33
4	A3	3540	OMC	C4-N3	4.89	1.44	1.34
4	A3	2267	OMG	C2-N2	4.89	1.45	1.34
2	A1	602	OMG	C2-N2	4.89	1.45	1.34
4	A3	4116	OMG	C2-N2	4.88	1.45	1.34
4	A3	3524	OMG	C2-N2	4.88	1.45	1.34
2	A1	518	OMC	C4-N4	4.88	1.45	1.33
4	A3	1260	OMG	C2-N2	4.87	1.45	1.34
4	A3	1580	OMG	C2-N3	4.87	1.44	1.33
2	A1	174	OMC	C4-N4	4.87	1.45	1.33
2	A1	1329	OMG	C2-N2	4.86	1.45	1.34
2	A1	1392	OMC	C4-N4	4.86	1.45	1.33
4	A3	3476	OMG	C2-N2	4.86	1.45	1.34
4	A3	4282	OMC	C4-N4	4.85	1.45	1.33
4	A3	2667	OMC	C4-N4	4.85	1.45	1.33
29	K1	4	OMC	O4'-C1'	-4.85	1.30	1.42
2	A1	1843	4AC	C7-N4	4.85	1.46	1.37
4	A3	3619	OMC	C4-N4	4.85	1.45	1.33
4	A3	3631	OMG	C2-N2	4.85	1.45	1.34
2	A1	518	OMC	C2-N1	4.85	1.50	1.40
2	A1	1448	OMG	C2-N3	4.85	1.44	1.33
4	A3	2265	OMC	C4-N4	4.84	1.45	1.33
4	A3	3573	OMC	C4-N4	4.84	1.45	1.33
4	A3	3540	OMC	C4-N4	4.84	1.45	1.33
4	A3	4364	OMG	C2-N2	4.84	1.45	1.34
2	A1	1704	OMC	C4-N4	4.84	1.45	1.33
4	A3	2719	OMG	C2-N2	4.83	1.45	1.34
4	A3	4240	OMG	C2-N2	4.83	1.45	1.34
4	A3	2647	OMC	C4-N4	4.83	1.45	1.33
4	A3	3601	OMC	C4-N4	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C3	75	OMG	C2-N2	4.82	1.45	1.34
4	A3	4138	OMG	C2-N2	4.81	1.45	1.34
4	A3	3359	OMG	C2-N2	4.80	1.45	1.34
4	A3	1284	OMC	C4-N4	4.80	1.45	1.33
4	A3	4202	OMC	C4-N4	4.79	1.45	1.33
4	A3	2244	A2M	O5'-C5'	-4.79	1.33	1.44
2	A1	1640	G7M	C5-N7	-4.79	1.33	1.39
2	A1	1491	OMG	C2-N3	4.78	1.44	1.33
4	A3	4369	OMG	C2-N2	4.78	1.45	1.34
29	K1	4	OMC	C4-N4	4.77	1.45	1.33
4	A3	2194	OMC	C4-N3	4.77	1.44	1.34
4	A3	4202	OMC	C2-N1	4.76	1.50	1.40
4	A3	2704	OMC	C2-N1	4.75	1.50	1.40
4	A3	3676	OMG	C2-N3	4.75	1.44	1.33
4	A3	3619	OMC	C2-N1	4.75	1.50	1.40
4	A3	2719	OMG	C2-N3	4.74	1.44	1.33
4	A3	2265	OMC	C2-N1	4.73	1.50	1.40
4	A3	1477	OMG	C2-N2	4.72	1.45	1.34
2	A1	437	OMG	C2-N3	4.71	1.44	1.33
4	A3	3942	OMG	C2-N3	4.70	1.44	1.33
29	K1	34	OMC	C4-N4	4.70	1.45	1.33
2	A1	1704	OMC	C2-N1	4.70	1.50	1.40
4	A3	4245	OMG	C2-N3	4.70	1.44	1.33
4	A3	4193	5MC	C6-N1	4.69	1.46	1.38
4	A3	4116	OMG	C2-N3	4.69	1.44	1.33
2	A1	684	OMG	C2-N3	4.69	1.44	1.33
4	A3	3476	OMG	C2-N3	4.68	1.44	1.33
2	A1	602	OMG	C2-N3	4.67	1.44	1.33
4	A3	2194	OMC	C4-N4	4.67	1.44	1.33
2	A1	1329	OMG	C2-N3	4.67	1.44	1.33
2	A1	1640	G7M	C2-N2	4.66	1.45	1.34
2	A1	645	OMG	C2-N2	4.66	1.45	1.34
4	A3	4240	OMG	C2-N3	4.66	1.44	1.33
4	A3	3524	OMG	C2-N3	4.65	1.44	1.33
4	A3	4383	OMG	C2-N3	4.63	1.44	1.33
4	A3	4282	OMC	C2-N1	4.63	1.50	1.40
4	A3	1260	OMG	C2-N3	4.63	1.44	1.33
2	A1	174	OMC	C2-N1	4.62	1.50	1.40
4	A3	4383	OMG	C2-N2	4.62	1.45	1.34
2	A1	645	OMG	C2-N3	4.62	1.44	1.33
10	C3	75	OMG	C2-N3	4.60	1.44	1.33
2	A1	469	A2M	O5'-C5'	-4.60	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A3	2667	OMC	C2-N1	4.60	1.50	1.40
2	A1	1843	4AC	C4-N4	4.59	1.46	1.39
4	A3	3433	OMC	C4-N4	4.59	1.44	1.33
2	A1	510	OMG	C2-N3	4.56	1.44	1.33
4	A3	3540	OMC	C2-N1	4.54	1.49	1.40
4	A3	3573	OMC	C2-N1	4.52	1.49	1.40
29	K1	34	OMC	C2-N1	4.51	1.49	1.40
2	A1	1338	4AC	C4-N4	4.51	1.46	1.39
2	A1	1338	4AC	C7-N4	4.51	1.45	1.37
4	A3	4138	OMG	C2-N3	4.51	1.44	1.33
4	A3	4369	OMG	C2-N3	4.49	1.44	1.33
4	A3	3601	OMC	C2-N1	4.48	1.49	1.40
2	A1	510	OMG	C2-N2	4.48	1.44	1.34
2	A1	1338	4AC	C2-N1	4.47	1.49	1.40
4	A3	4364	OMG	C2-N3	4.44	1.43	1.33
4	A3	3631	OMG	C2-N3	4.43	1.43	1.33
4	A3	3514	5MC	C2-N1	4.42	1.49	1.40
4	A3	2647	OMC	C2-N1	4.41	1.49	1.40
4	A3	3514	5MC	C6-N1	4.40	1.45	1.38
4	A3	1479	A2M	O5'-C5'	-4.37	1.34	1.44
4	A3	1477	OMG	C2-N3	4.37	1.43	1.33
4	A3	3359	OMG	C2-N3	4.36	1.43	1.33
4	A3	400	A2M	O5'-C5'	-4.36	1.34	1.44
4	A3	3562	A2M	O5'-C5'	-4.35	1.34	1.44
29	K1	4	OMC	C2-N1	4.35	1.49	1.40
4	A3	1810	A2M	O5'-C5'	-4.32	1.34	1.44
4	A3	3433	OMC	C2-N1	4.29	1.49	1.40
2	A1	1289	OMU	C4-N3	4.29	1.46	1.38
4	A3	4193	5MC	C4-N4	4.29	1.45	1.34
29	K1	58	1MA	O5'-C5'	-4.29	1.34	1.44
4	A3	3557	A2M	O5'-C5'	-4.27	1.34	1.44
2	A1	27	A2M	O5'-C5'	-4.27	1.34	1.44
2	A1	669	A2M	O5'-C5'	-4.26	1.34	1.44
4	A3	3456	A2M	O5'-C5'	-4.26	1.34	1.44
4	A3	3514	5MC	C4-N4	4.26	1.45	1.34
2	A1	485	A2M	O5'-C5'	-4.26	1.34	1.44
2	A1	591	A2M	O5'-C5'	-4.23	1.34	1.44
2	A1	1679	A2M	O5'-C5'	-4.23	1.34	1.44
4	A3	2630	A2M	O5'-C5'	-4.23	1.34	1.44
4	A3	2658	A2M	O5'-C5'	-4.23	1.34	1.44
2	A1	1384	A2M	O5'-C5'	-4.22	1.34	1.44
4	A3	4317	A2M	O5'-C5'	-4.22	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A1	577	A2M	O5'-C5'	-4.21	1.34	1.44
2	A1	628	OMU	C4-N3	4.21	1.46	1.38
4	A3	3450	A2M	O5'-C5'	-4.21	1.34	1.44
4	A3	1270	A2M	O5'-C5'	-4.20	1.34	1.44
2	A1	99	A2M	O5'-C5'	-4.20	1.34	1.44
4	A3	3492	A2M	O5'-C5'	-4.19	1.34	1.44
2	A1	159	A2M	O5'-C5'	-4.19	1.34	1.44
4	A3	4269	A2M	O5'-C5'	-4.18	1.34	1.44
4	A3	3599	A2M	O5'-C5'	-4.17	1.34	1.44
4	A3	3517	A2M	C6-N6	4.16	1.44	1.34
2	A1	1443	OMU	C4-N3	4.16	1.46	1.38
2	A1	1805	OMU	C4-N3	4.15	1.46	1.38
2	A1	172	OMU	C4-N3	4.15	1.46	1.38
4	A3	1284	OMC	C2-N1	4.14	1.49	1.40
2	A1	1032	A2M	O5'-C5'	-4.14	1.34	1.44
2	A1	166	A2M	O5'-C5'	-4.14	1.34	1.44
2	A1	355	OMU	C4-N3	4.11	1.45	1.38
2	A1	116	OMU	C4-N3	4.11	1.45	1.38
2	A1	1327	OMU	C4-N3	4.11	1.45	1.38
2	A1	1843	4AC	C2-N1	4.11	1.48	1.40
4	A3	398	A2M	O5'-C5'	-4.09	1.34	1.44
4	A3	4244	OMU	C4-N3	4.07	1.45	1.38
4	A3	4052	OMU	C4-N3	4.07	1.45	1.38
4	A3	1489	A2M	O5'-C5'	-4.07	1.34	1.44
4	A3	3973	OMU	C4-N3	4.06	1.45	1.38
4	A3	2258	OMU	C4-N3	4.05	1.45	1.38
4	A3	2680	OMU	C4-N3	4.04	1.45	1.38
2	A1	121	OMU	C4-N3	3.99	1.45	1.38
4	A3	4366	OMU	C4-N3	3.98	1.45	1.38
2	A1	1843	4AC	C5-C4	3.94	1.49	1.40
4	A3	3657	OMU	C4-N3	3.90	1.45	1.38
4	A3	4193	5MC	C2-N1	3.89	1.48	1.40
2	A1	1233	PSU	C6-C5	3.88	1.39	1.35
2	A1	867	PSU	C6-C5	3.86	1.39	1.35
2	A1	1640	G7M	C5-C6	3.83	1.54	1.43
76	i1	62	HY3	C5-N	3.81	1.62	1.49
29	K1	4	OMC	O3'-C3'	3.81	1.51	1.43
4	A3	3576	PSU	C6-C5	3.79	1.39	1.35
2	A1	93	PSU	C6-C5	3.79	1.39	1.35
2	A1	1005	PSU	C6-C5	3.78	1.39	1.35
4	A3	1638	PSU	C6-C5	3.75	1.39	1.35
2	A1	407	PSU	C6-C5	3.74	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A1	652	PSU	C6-C5	3.73	1.39	1.35
4	A3	4749	PSU	C6-C5	3.73	1.39	1.35
4	A3	3502	PSU	C6-C5	3.73	1.39	1.35
4	A3	1537	PSU	C6-C5	3.73	1.39	1.35
2	A1	1178	PSU	C6-C5	3.72	1.39	1.35
2	A1	802	PSU	C6-C5	3.72	1.39	1.35
4	A3	4177	PSU	C6-C5	3.71	1.39	1.35
4	A3	4169	PSU	C6-C5	3.71	1.39	1.35
2	A1	650	PSU	C6-C5	3.70	1.39	1.35
2	A1	1626	PSU	C6-C5	3.70	1.39	1.35
2	A1	1175	PSU	C6-C5	3.70	1.39	1.35
2	A1	1338	4AC	C5-C4	3.69	1.48	1.40
4	A3	1720	PSU	C6-C5	3.68	1.39	1.35
4	A3	4419	PSU	C6-C5	3.66	1.39	1.35
4	A3	1721	PSU	C6-C5	3.66	1.39	1.35
4	A3	2475	PSU	C6-C5	3.65	1.39	1.35
4	A3	3494	PSU	C6-C5	3.65	1.39	1.35
4	A3	4298	PSU	C6-C5	3.65	1.39	1.35
4	A3	4217	PSU	C6-C5	3.64	1.39	1.35
10	C3	55	PSU	C6-C5	3.64	1.39	1.35
4	A3	4039	PSU	C6-C5	3.63	1.39	1.35
4	A3	4278	PSU	C6-C5	3.63	1.39	1.35
2	A1	816	PSU	C6-C5	3.63	1.39	1.35
2	A1	1693	PSU	C6-C5	3.63	1.39	1.35
2	A1	610	PSU	C6-C5	3.62	1.39	1.35
2	A1	119	PSU	C6-C5	3.61	1.39	1.35
4	A3	4267	PSU	C6-C5	3.61	1.39	1.35
4	A3	4166	PSU	C6-C5	3.61	1.39	1.35
2	A1	1348	PSU	C6-C5	3.60	1.39	1.35
4	A3	1718	PSU	C6-C5	3.59	1.39	1.35
4	A3	3583	PSU	C6-C5	3.59	1.39	1.35
2	A1	105	PSU	C6-C5	3.59	1.39	1.35
4	A3	4374	PSU	C6-C5	3.58	1.39	1.35
2	A1	1245	PSU	C6-C5	3.58	1.39	1.35
4	A3	1491	PSU	C6-C5	3.58	1.39	1.35
2	A1	210	PSU	C6-C5	3.58	1.39	1.35
4	A3	4740	PSU	C6-C5	3.58	1.39	1.35
4	A3	4336	A2M	O5'-C5'	-3.58	1.36	1.44
4	A3	4058	PSU	C6-C5	3.57	1.39	1.35
2	A1	1239	PSU	C6-C5	3.57	1.39	1.35
4	A3	1801	PSU	C6-C5	3.56	1.39	1.35
4	A3	1683	PSU	C6-C5	3.56	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A3	1799	PSU	C6-C5	3.56	1.39	1.35
4	A3	4322	PSU	C6-C5	3.55	1.39	1.35
2	A1	687	PSU	C6-C5	3.55	1.39	1.35
4	A3	4107	PSU	C6-C5	3.55	1.39	1.35
2	A1	1047	PSU	C6-C5	3.52	1.39	1.35
4	A3	4099	PSU	C6-C5	3.52	1.39	1.35
2	A1	1082	PSU	C6-C5	3.51	1.39	1.35
4	A3	2194	OMC	C6-N1	3.51	1.46	1.38
4	A3	3616	PSU	C6-C5	3.51	1.39	1.35
4	A3	3371	PSU	C6-C5	3.51	1.39	1.35
4	A3	3447	PSU	C6-C5	3.51	1.39	1.35
4	A3	1731	PSU	C6-C5	3.49	1.39	1.35
4	A3	2351	PSU	C6-C5	3.49	1.39	1.35
4	A3	3585	PSU	C6-C5	3.49	1.39	1.35
2	A1	218	PSU	C6-C5	3.49	1.39	1.35
2	A1	34	PSU	C6-C5	3.48	1.39	1.35
2	A1	109	PSU	C6-C5	3.48	1.39	1.35
2	A1	1644	PSU	C6-C5	3.48	1.39	1.35
4	A3	4711	PSU	C6-C5	3.48	1.39	1.35
2	A1	573	PSU	C6-C5	3.48	1.39	1.35
4	A3	3462	PSU	C6-C5	3.48	1.39	1.35
4	A3	4045	PSU	C6-C5	3.48	1.39	1.35
2	A1	682	PSU	C6-C5	3.45	1.39	1.35
2	A1	1851	MA6	C6-N6	3.45	1.47	1.36
2	A1	1368	PSU	C6-C5	3.45	1.39	1.35
2	A1	967	PSU	C6-C5	3.45	1.39	1.35
4	A3	3554	PSU	C6-C5	3.44	1.39	1.35
2	A1	36	PSU	C6-C5	3.44	1.39	1.35
4	A3	4382	PSU	C6-C5	3.44	1.39	1.35
2	A1	1446	PSU	C6-C5	3.43	1.39	1.35
10	C3	69	PSU	C6-C5	3.43	1.39	1.35
4	A3	4435	PSU	C6-C5	3.43	1.39	1.35
4	A3	4042	PSU	C6-C5	3.41	1.39	1.35
2	A1	823	PSU	C6-C5	3.41	1.39	1.35
4	A3	3500	PSU	C6-C5	3.41	1.39	1.35
4	A3	3619	OMC	C6-N1	3.41	1.46	1.38
4	A3	3652	PSU	C6-C5	3.40	1.39	1.35
2	A1	1852	MA6	C6-N6	3.40	1.46	1.36
2	A1	1046	PSU	C6-C5	3.40	1.39	1.35
4	A3	3490	PSU	C6-C5	3.39	1.39	1.35
4	A3	3496	PSU	C6-C5	3.39	1.39	1.35
2	A1	815	PSU	C6-C5	3.39	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A1	518	OMC	C6-N1	3.38	1.46	1.38
4	A3	3601	OMC	C6-N1	3.37	1.46	1.38
4	A3	3369	PSU	C6-C5	3.37	1.39	1.35
4	A3	3427	PSU	C6-C5	3.37	1.39	1.35
4	A3	3550	UY1	C6-C5	3.35	1.39	1.35
2	A1	174	OMC	C6-N1	3.35	1.46	1.38
2	A1	1057	PSU	C6-C5	3.35	1.39	1.35
4	A3	4188	PSU	C6-C5	3.33	1.39	1.35
29	K1	13	PSU	C6-C5	3.32	1.39	1.35
4	A3	4282	OMC	C6-N1	3.31	1.46	1.38
4	A3	2265	OMC	C6-N1	3.30	1.46	1.38
4	A3	4203	PSU	C6-C5	3.29	1.39	1.35
4	A3	2667	OMC	C6-N1	3.29	1.45	1.38
4	A3	4325	PSU	C6-C5	3.29	1.39	1.35
2	A1	1704	OMC	C6-N1	3.28	1.45	1.38
2	A1	1392	OMC	C6-N1	3.28	1.45	1.38
2	A1	463	OMC	C6-N1	3.27	1.45	1.38
2	A1	1491	OMG	O6-C6	-3.27	1.17	1.23
2	A1	1843	4AC	C6-N1	3.26	1.45	1.38
29	K1	4	OMC	C6-N1	3.26	1.45	1.38
4	A3	2647	OMC	C6-N1	3.25	1.45	1.38
4	A3	3466	PSU	C6-C5	3.25	1.39	1.35
4	A3	2704	OMC	C6-N1	3.25	1.45	1.38
4	A3	3433	OMC	C6-N1	3.25	1.45	1.38
4	A3	3573	OMC	C6-N1	3.24	1.45	1.38
2	A1	864	PSU	C6-C5	3.24	1.39	1.35
2	A1	510	OMG	O6-C6	-3.21	1.17	1.23
4	A3	4149	PSU	C6-C5	3.19	1.39	1.35
4	A3	4138	OMG	O6-C6	-3.19	1.17	1.23
4	A3	1632	PSU	C6-C5	3.18	1.39	1.35
4	A3	3540	OMC	C6-N1	3.17	1.45	1.38
4	A3	3517	A2M	C5-C4	-3.15	1.33	1.39
4	A3	1284	OMC	C6-N1	3.14	1.45	1.38
4	A3	1260	OMG	O6-C6	-3.11	1.17	1.23
2	A1	1338	4AC	C6-N1	3.10	1.45	1.38
4	A3	4202	OMC	C6-N1	3.10	1.45	1.38
29	K1	34	OMC	C6-N1	3.10	1.45	1.38
4	A3	4246	PSU	C6-C5	3.09	1.38	1.35
4	A3	4369	OMG	O6-C6	-3.08	1.17	1.23
4	A3	3942	OMG	O6-C6	-3.08	1.17	1.23
4	A3	4276	UR3	C6-N1	3.08	1.45	1.38
4	A3	3657	OMU	O4-C4	-3.07	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A3	4366	OMU	O4-C4	-3.06	1.18	1.24
4	A3	3476	OMG	O6-C6	-3.06	1.17	1.23
4	A3	2680	OMU	O4-C4	-3.05	1.18	1.24
2	A1	355	OMU	O4-C4	-3.05	1.18	1.24
4	A3	3359	OMG	O6-C6	-3.05	1.17	1.23
4	A3	1477	OMG	O6-C6	-3.05	1.17	1.23
4	A3	3631	OMG	O6-C6	-3.05	1.17	1.23
4	A3	4383	OMG	O6-C6	-3.05	1.17	1.23
4	A3	4116	OMG	O6-C6	-3.05	1.17	1.23
4	A3	4052	OMU	O4-C4	-3.04	1.18	1.24
2	A1	645	OMG	O6-C6	-3.04	1.17	1.23
4	A3	1580	OMG	O6-C6	-3.03	1.17	1.23
2	A1	121	OMU	O4-C4	-3.02	1.18	1.24
4	A3	2719	OMG	O6-C6	-3.02	1.17	1.23
4	A3	2258	OMU	O4-C4	-3.01	1.18	1.24
2	A1	1329	OMG	O6-C6	-3.01	1.17	1.23
2	A1	602	OMG	O6-C6	-3.01	1.17	1.23
2	A1	1327	OMU	O4-C4	-3.00	1.18	1.24
2	A1	437	OMG	O6-C6	-3.00	1.17	1.23
4	A3	4245	OMG	O6-C6	-3.00	1.17	1.23
2	A1	1443	OMU	O4-C4	-3.00	1.18	1.24
4	A3	4364	OMG	O6-C6	-2.99	1.17	1.23
10	C3	75	OMG	O6-C6	-2.99	1.17	1.23
4	A3	3676	OMG	O6-C6	-2.98	1.17	1.23
4	A3	4240	OMG	O6-C6	-2.98	1.17	1.23
4	A3	3524	OMG	O6-C6	-2.98	1.17	1.23
2	A1	116	OMU	O4-C4	-2.98	1.18	1.24
2	A1	1805	OMU	O4-C4	-2.98	1.18	1.24
4	A3	4244	OMU	O4-C4	-2.98	1.18	1.24
4	A3	2267	OMG	O6-C6	-2.98	1.17	1.23
2	A1	684	OMG	O6-C6	-2.97	1.17	1.23
2	A1	868	OMG	O6-C6	-2.97	1.17	1.23
4	A3	3973	OMU	O4-C4	-2.96	1.18	1.24
2	A1	1448	OMG	O6-C6	-2.96	1.18	1.23
2	A1	1289	OMU	O4-C4	-2.96	1.18	1.24
29	K1	4	OMC	O2-C2	-2.95	1.18	1.23
2	A1	172	OMU	O4-C4	-2.94	1.18	1.24
4	A3	3517	A2M	O3'-C3'	2.93	1.49	1.43
2	A1	1289	OMU	C6-N1	2.92	1.45	1.38
2	A1	628	OMU	O4-C4	-2.91	1.18	1.24
29	K1	34	OMC	O2-C2	-2.90	1.18	1.23
2	A1	628	OMU	C6-N1	2.90	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A1	355	OMU	C6-N1	2.86	1.44	1.38
2	A1	1805	OMU	C6-N1	2.84	1.44	1.38
4	A3	3966	6MZ	C5-C4	-2.84	1.33	1.39
4	A3	4244	OMU	C6-N1	2.83	1.44	1.38
2	A1	1443	OMU	C6-N1	2.82	1.44	1.38
4	A3	2680	OMU	C6-N1	2.82	1.44	1.38
29	K1	4	OMC	O2'-C2'	-2.82	1.35	1.42
2	A1	1327	OMU	C6-N1	2.82	1.44	1.38
2	A1	1833	6MZ	C5-N7	-2.80	1.33	1.39
4	A3	4052	OMU	C6-N1	2.77	1.44	1.38
4	A3	3657	OMU	C6-N1	2.77	1.44	1.38
4	A3	3966	6MZ	C5-N7	-2.76	1.33	1.39
2	A1	1833	6MZ	C5-C4	-2.76	1.33	1.39
4	A3	4193	5MC	O2-C2	-2.74	1.18	1.23
4	A3	3433	OMC	O2-C2	-2.74	1.18	1.23
4	A3	3973	OMU	C6-N1	2.74	1.44	1.38
4	A3	2258	OMU	C6-N1	2.73	1.44	1.38
2	A1	1338	4AC	O2-C2	-2.73	1.18	1.23
2	A1	121	OMU	C6-N1	2.73	1.44	1.38
4	A3	3573	OMC	O2-C2	-2.73	1.18	1.23
29	K1	34	OMC	O2'-C2'	-2.73	1.35	1.42
4	A3	2647	OMC	O2-C2	-2.72	1.18	1.23
4	A3	4364	OMG	C2-N1	2.71	1.44	1.37
4	A3	3540	OMC	O2-C2	-2.70	1.18	1.23
4	A3	1284	OMC	O2-C2	-2.70	1.18	1.23
4	A3	4282	OMC	O2-C2	-2.70	1.18	1.23
2	A1	174	OMC	O2-C2	-2.70	1.18	1.23
4	A3	3359	OMG	C2-N1	2.70	1.44	1.37
4	A3	2667	OMC	O2-C2	-2.70	1.18	1.23
4	A3	4366	OMU	C6-N1	2.70	1.44	1.38
4	A3	3514	5MC	O2-C2	-2.70	1.18	1.23
2	A1	116	OMU	C6-N1	2.69	1.44	1.38
2	A1	1704	OMC	O2-C2	-2.69	1.18	1.23
2	A1	602	OMG	C2-N1	2.68	1.44	1.37
2	A1	1448	OMG	C2-N1	2.68	1.44	1.37
4	A3	1477	OMG	C2-N1	2.67	1.44	1.37
2	A1	1843	4AC	O2-C2	-2.67	1.18	1.23
4	A3	4369	OMG	C2-N1	2.67	1.44	1.37
4	A3	2704	OMC	O2-C2	-2.66	1.18	1.23
4	A3	3631	OMG	C2-N1	2.66	1.44	1.37
4	A3	2265	OMC	O2-C2	-2.66	1.18	1.23
2	A1	437	OMG	C2-N1	2.66	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A1	172	OMU	C6-N1	2.66	1.44	1.38
4	A3	3601	OMC	O2-C2	-2.66	1.18	1.23
2	A1	1640	G7M	C2-N1	2.66	1.44	1.37
10	C3	75	OMG	C2-N1	2.66	1.44	1.37
2	A1	669	A2M	O4'-C4'	-2.66	1.39	1.45
2	A1	868	OMG	C2-N1	2.65	1.44	1.37
2	A1	1491	OMG	C2-N1	2.65	1.44	1.37
4	A3	3476	OMG	C2-N1	2.65	1.44	1.37
4	A3	3517	A2M	O2'-C2'	-2.64	1.35	1.42
4	A3	3676	OMG	C2-N1	2.64	1.44	1.37
2	A1	684	OMG	C2-N1	2.64	1.44	1.37
4	A3	2719	OMG	C2-N1	2.64	1.44	1.37
4	A3	3942	OMG	C2-N1	2.63	1.44	1.37
4	A3	4240	OMG	C2-N1	2.63	1.44	1.37
2	A1	518	OMC	O2-C2	-2.63	1.18	1.23
4	A3	2267	OMG	C2-N1	2.63	1.44	1.37
4	A3	4138	OMG	C5-C6	2.63	1.54	1.44
2	A1	1329	OMG	C2-N1	2.62	1.44	1.37
4	A3	4364	OMG	C5-C6	2.62	1.54	1.44
2	A1	645	OMG	C2-N1	2.61	1.44	1.37
4	A3	4369	OMG	C5-C6	2.61	1.54	1.44
4	A3	3359	OMG	C5-C6	2.61	1.54	1.44
4	A3	3619	OMC	O2-C2	-2.61	1.18	1.23
4	A3	2194	OMC	O2-C2	-2.60	1.18	1.23
4	A3	4116	OMG	C2-N1	2.60	1.44	1.37
4	A3	1580	OMG	C2-N1	2.60	1.44	1.37
4	A3	1477	OMG	C5-C6	2.60	1.54	1.44
4	A3	1260	OMG	C2-N1	2.60	1.44	1.37
2	A1	602	OMG	C5-C6	2.60	1.54	1.44
2	A1	1851	MA6	C5-C4	-2.59	1.34	1.39
4	A3	4383	OMG	C5-C6	2.59	1.54	1.44
10	C3	75	OMG	C5-C6	2.59	1.54	1.44
2	A1	1329	OMG	C5-C6	2.59	1.54	1.44
4	A3	4202	OMC	O2-C2	-2.58	1.18	1.23
4	A3	3631	OMG	C5-C6	2.58	1.54	1.44
4	A3	4383	OMG	C2-N1	2.58	1.44	1.37
4	A3	4138	OMG	C2-N1	2.58	1.44	1.37
4	A3	3476	OMG	C5-C6	2.58	1.54	1.44
4	A3	3676	OMG	C5-C6	2.57	1.54	1.44
2	A1	510	OMG	C5-C6	2.57	1.53	1.44
2	A1	645	OMG	C5-C6	2.57	1.53	1.44
4	A3	3524	OMG	C2-N1	2.56	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A1	1448	OMG	C5-C6	2.56	1.53	1.44
2	A1	174	OMC	C5-C4	2.56	1.48	1.42
2	A1	868	OMG	C5-C6	2.56	1.53	1.44
4	A3	2719	OMG	C5-C6	2.55	1.53	1.44
2	A1	684	OMG	C5-C6	2.55	1.53	1.44
4	A3	4240	OMG	C5-C6	2.54	1.53	1.44
4	A3	3433	OMC	C5-C4	2.54	1.48	1.42
29	K1	34	OMC	O3'-C3'	2.53	1.48	1.43
2	A1	437	OMG	C5-C6	2.52	1.53	1.44
2	A1	510	OMG	C2-N1	2.52	1.43	1.37
2	A1	1392	OMC	O2-C2	-2.52	1.19	1.23
4	A3	1260	OMG	C5-C6	2.52	1.53	1.44
2	A1	1852	MA6	C5-C4	-2.51	1.34	1.39
2	A1	1851	MA6	C8-N9	-2.50	1.33	1.37
4	A3	2667	OMC	C5-C4	2.50	1.48	1.42
2	A1	463	OMC	O2-C2	-2.50	1.19	1.23
4	A3	3942	OMG	C5-C6	2.50	1.53	1.44
4	A3	1580	OMG	C5-C6	2.49	1.53	1.44
4	A3	4245	OMG	C2-N1	2.49	1.43	1.37
2	A1	1640	G7M	O6-C6	-2.48	1.18	1.23
4	A3	2267	OMG	C5-C6	2.48	1.53	1.44
4	A3	4116	OMG	C5-C6	2.47	1.53	1.44
4	A3	1489	A2M	O4'-C4'	-2.46	1.39	1.45
4	A3	3524	OMG	C5-C6	2.45	1.53	1.44
29	K1	4	OMC	C5-C4	2.45	1.48	1.42
4	A3	2265	OMC	C5-C4	2.44	1.48	1.42
4	A3	2704	OMC	C5-C4	2.43	1.48	1.42
4	A3	3540	OMC	C5-C4	2.43	1.48	1.42
4	A3	1479	A2M	O4'-C4'	-2.42	1.39	1.45
2	A1	518	OMC	C5-C4	2.39	1.48	1.42
2	A1	463	OMC	C5-C4	2.38	1.48	1.42
2	A1	1338	4AC	O7-C7	-2.38	1.17	1.23
4	A3	3619	OMC	C5-C4	2.38	1.48	1.42
2	A1	1491	OMG	C5-C6	2.37	1.53	1.44
4	A3	3573	OMC	C5-C4	2.37	1.48	1.42
2	A1	1289	OMU	C5-C4	2.37	1.48	1.43
4	A3	3973	OMU	C5-C4	2.36	1.48	1.43
2	A1	628	OMU	C5-C4	2.36	1.48	1.43
2	A1	1327	OMU	C5-C4	2.35	1.48	1.43
2	A1	1852	MA6	C5-N7	-2.35	1.34	1.39
4	A3	2680	OMU	C5-C4	2.35	1.48	1.43
4	A3	3601	OMC	C5-C4	2.35	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A3	2647	OMC	C5-C4	2.35	1.48	1.42
2	A1	1704	OMC	C5-C4	2.34	1.48	1.42
2	A1	1805	OMU	C5-C4	2.34	1.48	1.43
4	A3	2258	OMU	O2-C2	-2.34	1.18	1.23
29	K1	58	1MA	C2-N1	2.33	1.40	1.35
29	K1	34	OMC	C5-C4	2.33	1.48	1.42
4	A3	4282	OMC	C5-C4	2.32	1.48	1.42
4	A3	3657	OMU	O2-C2	-2.31	1.18	1.23
4	A3	4244	OMU	C5-C4	2.31	1.48	1.43
4	A3	4052	OMU	O2-C2	-2.30	1.18	1.23
4	A3	4244	OMU	O2-C2	-2.29	1.18	1.23
4	A3	4052	OMU	C5-C4	2.29	1.48	1.43
2	A1	1640	G7M	C6-N1	2.29	1.43	1.38
2	A1	1852	MA6	C8-N9	-2.28	1.33	1.37
2	A1	1679	A2M	O4'-C4'	-2.28	1.39	1.45
2	A1	1443	OMU	C5-C4	2.28	1.48	1.43
2	A1	172	OMU	C5-C4	2.28	1.48	1.43
4	A3	2680	OMU	O2-C2	-2.27	1.18	1.23
2	A1	1392	OMC	C5-C4	2.27	1.48	1.42
4	A3	3657	OMU	C5-C4	2.26	1.48	1.43
2	A1	1327	OMU	O2-C2	-2.26	1.18	1.23
4	A3	4245	OMG	C5-C6	2.26	1.52	1.44
2	A1	121	OMU	O2-C2	-2.26	1.18	1.23
4	A3	4366	OMU	O2-C2	-2.25	1.18	1.23
2	A1	355	OMU	O2-C2	-2.24	1.18	1.23
2	A1	355	OMU	C5-C4	2.24	1.48	1.43
4	A3	4202	OMC	C5-C4	2.24	1.48	1.42
2	A1	1833	6MZ	C8-N9	-2.23	1.33	1.37
2	A1	1443	OMU	O2-C2	-2.23	1.19	1.23
2	A1	628	OMU	O2-C2	-2.22	1.19	1.23
4	A3	3973	OMU	O2-C2	-2.22	1.19	1.23
2	A1	1805	OMU	O2-C2	-2.21	1.19	1.23
2	A1	116	OMU	O2-C2	-2.21	1.19	1.23
4	A3	3517	A2M	C5-N7	-2.21	1.34	1.39
2	A1	1851	MA6	C5-N7	-2.21	1.34	1.39
4	A3	4317	A2M	O4'-C4'	-2.20	1.40	1.45
4	A3	4276	UR3	C5-C4	2.20	1.49	1.43
4	A3	2258	OMU	C5-C4	2.19	1.48	1.43
2	A1	172	OMU	O2-C2	-2.19	1.19	1.23
29	K1	16	H2U	C2-N3	-2.18	1.34	1.38
2	A1	116	OMU	C5-C4	2.17	1.48	1.43
4	A3	4276	UR3	O4-C4	-2.16	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A1	121	OMU	C5-C4	2.16	1.48	1.43
2	A1	1289	OMU	O2-C2	-2.14	1.19	1.23
4	A3	4276	UR3	C4-N3	2.13	1.45	1.40
4	A3	4366	OMU	C5-C4	2.11	1.48	1.43
4	A3	1284	OMC	C5-C4	2.11	1.47	1.42
4	A3	3517	A2M	C8-N9	-2.10	1.33	1.37
4	A3	3517	A2M	C4-N9	-2.10	1.33	1.37
2	A1	1843	4AC	O7-C7	-2.07	1.18	1.23
4	A3	1489	A2M	O3'-C3'	-2.07	1.38	1.43
4	A3	4364	OMG	C6-N1	2.07	1.42	1.38
4	A3	3517	A2M	O5'-C5'	-2.05	1.39	1.44
4	A3	3359	OMG	C6-N1	2.05	1.42	1.38
2	A1	1249	B8N	O2-C2	-2.05	1.18	1.22
4	A3	2194	OMC	C5-C4	2.04	1.47	1.42
4	A3	3966	6MZ	C8-N9	-2.01	1.33	1.37
10	C3	75	OMG	C6-N1	2.00	1.42	1.38

All (1098) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	3517	A2M	C1'-N9-C8	-9.64	105.36	127.14
2	A1	1852	MA6	N1-C6-N6	-7.55	108.83	117.08
2	A1	1851	MA6	N1-C6-N6	-7.39	109.00	117.08
4	A3	2719	OMG	C1'-N9-C8	-7.26	106.02	126.70
4	A3	2267	OMG	C1'-N9-C8	-6.97	106.84	126.70
4	A3	3517	A2M	C4-N9-C1'	6.80	142.80	126.59
2	A1	868	OMG	C1'-N9-C8	-6.76	107.44	126.70
2	A1	1338	4AC	N4-C4-N3	6.68	125.06	113.85
4	A3	4245	OMG	C1'-N9-C8	-6.66	107.75	126.70
2	A1	1491	OMG	C1'-N9-C8	-6.57	107.99	126.70
4	A3	3517	A2M	N6-C6-N1	-6.57	103.97	118.35
4	A3	1580	OMG	C1'-N9-C8	-6.54	108.09	126.70
4	A3	2267	OMG	C1'-N9-C4	6.51	145.83	126.50
2	A1	1448	OMG	C1'-N9-C8	-6.47	108.29	126.70
4	A3	3517	A2M	N9-C8-N7	-6.43	105.11	113.91
4	A3	2719	OMG	C1'-N9-C4	6.37	145.41	126.50
2	A1	602	OMG	C1'-N9-C8	-6.36	108.61	126.70
2	A1	1329	OMG	C1'-N9-C8	-6.35	108.61	126.70
4	A3	3942	OMG	C1'-N9-C8	-6.35	108.61	126.70
4	A3	4116	OMG	C1'-N9-C8	-6.35	108.63	126.70
4	A3	4240	OMG	C1'-N9-C8	-6.30	108.76	126.70
4	A3	3524	OMG	C1'-N9-C8	-6.28	108.81	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A1	1640	G7M	C1'-N9-C4	-6.28	107.84	126.50
2	A1	645	OMG	C1'-N9-C8	-6.28	108.83	126.70
4	A3	4383	OMG	C1'-N9-C8	-6.27	108.86	126.70
4	A3	3476	OMG	C1'-N9-C8	-6.25	108.90	126.70
2	A1	868	OMG	C1'-N9-C4	6.18	144.85	126.50
2	A1	510	OMG	C1'-N9-C8	-6.15	109.19	126.70
4	A3	1260	OMG	C1'-N9-C8	-6.14	109.22	126.70
4	A3	4138	OMG	C1'-N9-C8	-6.13	109.25	126.70
4	A3	4245	OMG	C1'-N9-C4	6.12	144.69	126.50
2	A1	684	OMG	C1'-N9-C8	-6.09	109.36	126.70
2	A1	437	OMG	C1'-N9-C8	-6.08	109.38	126.70
10	C3	75	OMG	C1'-N9-C8	-6.07	109.43	126.70
4	A3	3676	OMG	C1'-N9-C8	-6.06	109.45	126.70
4	A3	1580	OMG	C1'-N9-C4	6.00	144.33	126.50
2	A1	1448	OMG	C1'-N9-C4	5.90	144.01	126.50
2	A1	1491	OMG	C1'-N9-C4	5.87	143.95	126.50
2	A1	1640	G7M	CN7-N7-C5	5.87	134.06	126.77
4	A3	4369	OMG	C1'-N9-C8	-5.86	110.03	126.70
4	A3	3966	6MZ	N1-C2-N3	-5.84	119.46	128.60
4	A3	1477	OMG	C1'-N9-C8	-5.83	110.09	126.70
4	A3	3517	A2M	N3-C2-N1	-5.82	119.49	128.60
2	A1	1851	MA6	N1-C2-N3	-5.76	119.59	128.60
2	A1	1852	MA6	N1-C2-N3	-5.75	119.60	128.60
2	A1	602	OMG	C1'-N9-C4	5.74	143.57	126.50
4	A3	3631	OMG	C1'-N9-C8	-5.73	110.38	126.70
2	A1	1329	OMG	C1'-N9-C4	5.71	143.45	126.50
4	A3	3942	OMG	C1'-N9-C4	5.68	143.36	126.50
2	A1	1833	6MZ	C5-C4-N3	-5.64	119.39	126.75
4	A3	3517	A2M	C4-N9-C8	5.64	111.84	105.73
4	A3	4240	OMG	C1'-N9-C4	5.63	143.23	126.50
2	A1	645	OMG	C1'-N9-C4	5.63	143.21	126.50
4	A3	3476	OMG	C1'-N9-C4	5.61	143.17	126.50
4	A3	4364	OMG	C1'-N9-C8	-5.59	110.77	126.70
2	A1	510	OMG	C1'-N9-C4	5.59	143.10	126.50
4	A3	4116	OMG	C1'-N9-C4	5.58	143.09	126.50
4	A3	4383	OMG	C1'-N9-C4	5.54	142.94	126.50
4	A3	3524	OMG	C1'-N9-C4	5.52	142.89	126.50
4	A3	3973	OMU	C4-N3-C2	-5.48	119.35	126.58
4	A3	3657	OMU	C4-N3-C2	-5.48	119.35	126.58
4	A3	4138	OMG	C1'-N9-C4	5.46	142.72	126.50
4	A3	2680	OMU	C4-N3-C2	-5.46	119.38	126.58
4	A3	3517	A2M	C5-C6-N6	5.45	135.29	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	4244	OMU	C4-N3-C2	-5.40	119.46	126.58
2	A1	1833	6MZ	N1-C2-N3	-5.39	120.16	128.60
2	A1	172	OMU	C4-N3-C2	-5.38	119.48	126.58
10	C3	75	OMG	C1'-N9-C4	5.37	142.47	126.50
2	A1	1327	OMU	C4-N3-C2	-5.35	119.52	126.58
4	A3	1260	OMG	C1'-N9-C4	5.33	142.32	126.50
4	A3	4052	OMU	C4-N3-C2	-5.32	119.56	126.58
2	A1	437	OMG	C1'-N9-C4	5.32	142.30	126.50
2	A1	1805	OMU	C4-N3-C2	-5.32	119.57	126.58
2	A1	355	OMU	C4-N3-C2	-5.29	119.60	126.58
2	A1	628	OMU	C4-N3-C2	-5.29	119.61	126.58
2	A1	684	OMG	C1'-N9-C4	5.27	142.17	126.50
2	A1	868	OMG	C5-C4-N3	-5.23	119.97	128.46
2	A1	1443	OMU	C4-N3-C2	-5.23	119.69	126.58
4	A3	3359	OMG	C1'-N9-C8	-5.22	111.83	126.70
4	A3	2267	OMG	C5-C4-N3	-5.21	120.00	128.46
2	A1	1852	MA6	C5-C4-N3	-5.19	119.98	126.75
4	A3	3676	OMG	C1'-N9-C4	5.18	141.87	126.50
4	A3	1580	OMG	C5-C4-N3	-5.11	120.17	128.46
4	A3	2258	OMU	C4-N3-C2	-5.11	119.84	126.58
2	A1	1289	OMU	C4-N3-C2	-5.11	119.84	126.58
4	A3	4369	OMG	C1'-N9-C4	5.08	141.59	126.50
4	A3	1477	OMG	C1'-N9-C4	5.02	141.42	126.50
2	A1	1249	B8N	C5-C4-N3	5.01	125.45	116.17
2	A1	1851	MA6	N9-C8-N7	-5.01	107.06	113.91
2	A1	1448	OMG	C5-C4-N3	-4.99	120.37	128.46
2	A1	1833	6MZ	C4-C5-C6	4.92	120.62	116.81
4	A3	3631	OMG	C1'-N9-C4	4.88	141.01	126.50
4	A3	4383	OMG	C5-C4-N3	-4.86	120.57	128.46
4	A3	4245	OMG	C5-C4-N3	-4.85	120.59	128.46
2	A1	1491	OMG	C5-C4-N3	-4.85	120.59	128.46
2	A1	1852	MA6	N9-C8-N7	-4.85	107.28	113.91
4	A3	3966	6MZ	C5-C4-N3	-4.85	120.43	126.75
2	A1	602	OMG	C5-C4-N3	-4.84	120.60	128.46
2	A1	1640	G7M	CN7-N7-C8	-4.84	117.36	124.84
68	e1	67	NMM	NE-CZ-NH2	-4.84	115.04	119.48
4	A3	3942	OMG	C5-C4-N3	-4.82	120.64	128.46
2	A1	1329	OMG	C5-C4-N3	-4.82	120.65	128.46
2	A1	510	OMG	C5-C4-N3	-4.80	120.67	128.46
4	A3	3476	OMG	C5-C4-N3	-4.80	120.68	128.46
4	A3	4366	OMU	C4-N3-C2	-4.79	120.26	126.58
2	A1	1640	G7M	C1'-N9-C8	4.79	142.90	126.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	2719	OMG	C5-C4-N3	-4.79	120.70	128.46
4	A3	4364	OMG	C1'-N9-C4	4.78	140.69	126.50
4	A3	4374	PSU	N1-C2-N3	4.77	120.54	115.13
2	A1	645	OMG	C5-C4-N3	-4.75	120.76	128.46
2	A1	121	OMU	C4-N3-C2	-4.75	120.32	126.58
4	A3	4240	OMG	C5-C4-N3	-4.74	120.77	128.46
2	A1	1446	PSU	C4-N3-C2	-4.68	119.59	126.34
4	A3	1632	PSU	C4-N3-C2	-4.68	119.60	126.34
4	A3	1810	A2M	C3'-C2'-C1'	-4.67	94.11	102.89
2	A1	1446	PSU	N1-C2-N3	4.65	120.40	115.13
4	A3	4138	OMG	C5-C4-N3	-4.65	120.92	128.46
4	A3	4203	PSU	C4-N3-C2	-4.64	119.65	126.34
10	C3	75	OMG	C5-C4-N3	-4.63	120.95	128.46
2	A1	823	PSU	C4-N3-C2	-4.62	119.68	126.34
4	A3	4116	OMG	C5-C4-N3	-4.61	120.98	128.46
4	A3	1632	PSU	N1-C2-N3	4.61	120.35	115.13
4	A3	1260	OMG	C5-C4-N3	-4.61	120.99	128.46
2	A1	437	OMG	C5-C4-N3	-4.58	121.02	128.46
4	A3	3427	PSU	N1-C2-N3	4.58	120.32	115.13
4	A3	4267	PSU	C4-N3-C2	-4.58	119.75	126.34
2	A1	1851	MA6	C5-C4-N3	-4.57	120.79	126.75
4	A3	4246	PSU	N1-C2-N3	4.57	120.30	115.13
4	A3	4138	OMG	C2-N3-C4	4.56	120.42	112.30
4	A3	4246	PSU	C4-N3-C2	-4.56	119.78	126.34
4	A3	4203	PSU	N1-C2-N3	4.55	120.28	115.13
4	A3	4435	PSU	N1-C2-N3	4.55	120.28	115.13
4	A3	1491	PSU	N1-C2-N3	4.54	120.28	115.13
2	A1	1249	B8N	C4-N3-C2	-4.54	119.72	125.46
4	A3	4374	PSU	C4-N3-C2	-4.53	119.81	126.34
2	A1	684	OMG	C5-C4-N3	-4.53	121.11	128.46
4	A3	4099	PSU	N1-C2-N3	4.52	120.25	115.13
4	A3	3427	PSU	C4-N3-C2	-4.52	119.82	126.34
2	A1	868	OMG	C2-N3-C4	4.51	120.34	112.30
2	A1	823	PSU	N1-C2-N3	4.50	120.23	115.13
4	A3	4267	PSU	N1-C2-N3	4.50	120.22	115.13
2	A1	116	OMU	C4-N3-C2	-4.49	120.65	126.58
4	A3	1491	PSU	C4-N3-C2	-4.49	119.87	126.34
4	A3	4099	PSU	C4-N3-C2	-4.49	119.87	126.34
2	A1	36	PSU	C4-N3-C2	-4.48	119.88	126.34
4	A3	3371	PSU	N1-C2-N3	4.48	120.21	115.13
2	A1	109	PSU	C4-N3-C2	-4.48	119.88	126.34
4	A3	3524	OMG	C5-C4-N3	-4.47	121.21	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	4039	PSU	N1-C2-N3	4.46	120.19	115.13
4	A3	3676	OMG	C5-C4-N3	-4.45	121.23	128.46
2	A1	602	OMG	C2-N3-C4	4.45	120.23	112.30
10	C3	75	OMG	C2-N3-C4	4.44	120.21	112.30
4	A3	4039	PSU	C4-N3-C2	-4.44	119.95	126.34
4	A3	4149	PSU	C4-N3-C2	-4.44	119.95	126.34
4	A3	4298	PSU	N1-C2-N3	4.43	120.15	115.13
2	A1	105	PSU	N1-C2-N3	4.43	120.15	115.13
4	A3	4193	5MC	C5-C6-N1	-4.42	118.79	123.34
4	A3	3554	PSU	N1-C2-N3	4.42	120.14	115.13
4	A3	4149	PSU	N1-C2-N3	4.42	120.14	115.13
2	A1	36	PSU	N1-C2-N3	4.42	120.13	115.13
4	A3	1580	OMG	C2-N3-C4	4.42	120.17	112.30
4	A3	4276	UR3	C4-N3-C2	-4.41	120.41	124.56
4	A3	4245	OMG	C2-N3-C4	4.41	120.16	112.30
4	A3	3942	OMG	C2-N3-C4	4.41	120.16	112.30
2	A1	109	PSU	N1-C2-N3	4.41	120.12	115.13
2	A1	210	PSU	C4-N3-C2	-4.40	119.99	126.34
10	C3	55	PSU	C4-N3-C2	-4.40	120.00	126.34
4	A3	3966	6MZ	C9-N6-C6	-4.40	119.08	122.87
4	A3	3476	OMG	C2-N3-C4	4.40	120.14	112.30
2	A1	1057	PSU	C4-N3-C2	-4.39	120.01	126.34
2	A1	687	PSU	C4-N3-C2	-4.39	120.01	126.34
2	A1	1348	PSU	C4-N3-C2	-4.39	120.01	126.34
2	A1	816	PSU	C4-N3-C2	-4.39	120.01	126.34
4	A3	3371	PSU	C4-N3-C2	-4.39	120.02	126.34
4	A3	2719	OMG	C2-N3-C4	4.38	120.11	112.30
4	A3	4188	PSU	C4-N3-C2	-4.38	120.03	126.34
2	A1	1329	OMG	C2-N3-C4	4.38	120.10	112.30
4	A3	3496	PSU	N1-C2-N3	4.38	120.09	115.13
4	A3	2351	PSU	C4-N3-C2	-4.37	120.04	126.34
2	A1	1491	OMG	C2-N3-C4	4.37	120.09	112.30
4	A3	1718	PSU	C4-N3-C2	-4.37	120.04	126.34
4	A3	1801	PSU	N1-C2-N3	4.37	120.08	115.13
4	A3	3616	PSU	C4-N3-C2	-4.37	120.04	126.34
4	A3	1260	OMG	C2-N3-C4	4.37	120.08	112.30
4	A3	4382	PSU	N1-C2-N3	4.37	120.08	115.13
2	A1	1178	PSU	C4-N3-C2	-4.36	120.05	126.34
4	A3	4298	PSU	C4-N3-C2	-4.36	120.05	126.34
4	A3	3616	PSU	N1-C2-N3	4.36	120.07	115.13
2	A1	1082	PSU	N1-C2-N3	4.36	120.07	115.13
4	A3	4240	OMG	C2-N3-C4	4.36	120.06	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A1	652	PSU	N1-C2-N3	4.36	120.07	115.13
4	A3	1683	PSU	C4-N3-C2	-4.36	120.06	126.34
4	A3	3517	A2M	C5-C4-N3	-4.35	121.08	126.75
4	A3	4042	PSU	C4-N3-C2	-4.35	120.07	126.34
4	A3	4188	PSU	N1-C2-N3	4.35	120.06	115.13
2	A1	1245	PSU	N1-C2-N3	4.35	120.06	115.13
2	A1	1057	PSU	N1-C2-N3	4.35	120.06	115.13
4	A3	3447	PSU	N1-C2-N3	4.34	120.05	115.13
2	A1	802	PSU	N1-C2-N3	4.34	120.05	115.13
2	A1	1239	PSU	N1-C2-N3	4.34	120.05	115.13
2	A1	1239	PSU	C4-N3-C2	-4.34	120.09	126.34
4	A3	4364	OMG	C2-N3-C4	4.34	120.03	112.30
4	A3	1718	PSU	N1-C2-N3	4.34	120.04	115.13
2	A1	687	PSU	N1-C2-N3	4.34	120.04	115.13
4	A3	1799	PSU	N1-C2-N3	4.34	120.04	115.13
2	A1	1245	PSU	C4-N3-C2	-4.33	120.09	126.34
2	A1	650	PSU	N1-C2-N3	4.33	120.04	115.13
4	A3	4749	PSU	C4-N3-C2	-4.33	120.10	126.34
2	A1	210	PSU	N1-C2-N3	4.33	120.04	115.13
4	A3	1638	PSU	N1-C2-N3	4.33	120.03	115.13
10	C3	55	PSU	N1-C2-N3	4.33	120.03	115.13
4	A3	4177	PSU	N1-C2-N3	4.33	120.03	115.13
4	A3	4169	PSU	N1-C2-N3	4.33	120.03	115.13
2	A1	1348	PSU	N1-C2-N3	4.32	120.03	115.13
4	A3	3554	PSU	C4-N3-C2	-4.32	120.11	126.34
2	A1	610	PSU	N1-C2-N3	4.32	120.03	115.13
2	A1	1644	PSU	N1-C2-N3	4.32	120.03	115.13
4	A3	4045	PSU	N1-C2-N3	4.32	120.02	115.13
2	A1	1644	PSU	C4-N3-C2	-4.32	120.12	126.34
2	A1	1178	PSU	N1-C2-N3	4.32	120.02	115.13
4	A3	2267	OMG	C2-N3-C4	4.31	119.99	112.30
2	A1	867	PSU	N1-C2-N3	4.31	120.02	115.13
4	A3	3462	PSU	C4-N3-C2	-4.31	120.12	126.34
4	A3	4369	OMG	C5-C4-N3	-4.31	121.46	128.46
4	A3	4419	PSU	N1-C2-N3	4.31	120.02	115.13
2	A1	407	PSU	N1-C2-N3	4.31	120.01	115.13
2	A1	652	PSU	C4-N3-C2	-4.31	120.13	126.34
4	A3	4058	PSU	N1-C2-N3	4.31	120.01	115.13
4	A3	4058	PSU	C4-N3-C2	-4.31	120.13	126.34
4	A3	1683	PSU	N1-C2-N3	4.31	120.01	115.13
2	A1	1448	OMG	C2-N3-C4	4.31	119.97	112.30
4	A3	4369	OMG	C2-N3-C4	4.30	119.97	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	3652	PSU	C4-N3-C2	-4.30	120.14	126.34
2	A1	1175	PSU	N1-C2-N3	4.30	120.00	115.13
2	A1	437	OMG	C2-N3-C4	4.30	119.96	112.30
2	A1	34	PSU	N1-C2-N3	4.30	120.00	115.13
2	A1	682	PSU	N1-C2-N3	4.30	120.00	115.13
4	A3	4116	OMG	C2-N3-C4	4.30	119.96	112.30
4	A3	4322	PSU	N1-C2-N3	4.30	120.00	115.13
2	A1	1175	PSU	C4-N3-C2	-4.30	120.15	126.34
2	A1	1368	PSU	N1-C2-N3	4.30	120.00	115.13
2	A1	650	PSU	C4-N3-C2	-4.29	120.15	126.34
2	A1	218	PSU	C4-N3-C2	-4.29	120.16	126.34
2	A1	1640	G7M	C2-N3-C4	4.29	119.94	112.30
4	A3	3652	PSU	N1-C2-N3	4.29	119.99	115.13
4	A3	4042	PSU	N1-C2-N3	4.29	119.99	115.13
4	A3	2351	PSU	N1-C2-N3	4.29	119.99	115.13
4	A3	4711	PSU	N1-C2-N3	4.29	119.99	115.13
2	A1	407	PSU	C4-N3-C2	-4.29	120.16	126.34
4	A3	3496	PSU	C4-N3-C2	-4.28	120.17	126.34
2	A1	1082	PSU	C4-N3-C2	-4.28	120.17	126.34
4	A3	1801	PSU	C4-N3-C2	-4.28	120.17	126.34
4	A3	4278	PSU	N1-C2-N3	4.28	119.98	115.13
2	A1	816	PSU	N1-C2-N3	4.28	119.98	115.13
2	A1	1368	PSU	C4-N3-C2	-4.28	120.17	126.34
2	A1	1046	PSU	C4-N3-C2	-4.28	120.17	126.34
4	A3	4711	PSU	C4-N3-C2	-4.28	120.17	126.34
2	A1	34	PSU	C4-N3-C2	-4.28	120.17	126.34
4	A3	4749	PSU	N1-C2-N3	4.28	119.98	115.13
2	A1	1047	PSU	C4-N3-C2	-4.27	120.18	126.34
10	C3	69	PSU	C4-N3-C2	-4.27	120.18	126.34
10	C3	69	PSU	N1-C2-N3	4.27	119.97	115.13
2	A1	1693	PSU	C4-N3-C2	-4.27	120.19	126.34
4	A3	3494	PSU	N1-C2-N3	4.27	119.97	115.13
4	A3	1477	OMG	C2-N3-C4	4.27	119.91	112.30
4	A3	3631	OMG	C2-N3-C4	4.27	119.90	112.30
4	A3	3583	PSU	N1-C2-N3	4.27	119.96	115.13
2	A1	610	PSU	C4-N3-C2	-4.27	120.19	126.34
4	A3	4177	PSU	C4-N3-C2	-4.26	120.19	126.34
2	A1	1693	PSU	N1-C2-N3	4.26	119.96	115.13
4	A3	1638	PSU	C4-N3-C2	-4.26	120.20	126.34
4	A3	4169	PSU	C4-N3-C2	-4.26	120.20	126.34
4	A3	3576	PSU	N1-C2-N3	4.26	119.95	115.13
2	A1	1233	PSU	C4-N3-C2	-4.26	120.21	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	1731	PSU	N1-C2-N3	4.26	119.95	115.13
4	A3	3462	PSU	N1-C2-N3	4.25	119.95	115.13
2	A1	218	PSU	N1-C2-N3	4.25	119.95	115.13
2	A1	1047	PSU	N1-C2-N3	4.25	119.95	115.13
2	A1	1233	PSU	N1-C2-N3	4.25	119.95	115.13
4	A3	3359	OMG	C1'-N9-C4	4.25	139.12	126.50
4	A3	4419	PSU	C4-N3-C2	-4.24	120.22	126.34
4	A3	3676	OMG	C2-N3-C4	4.24	119.86	112.30
4	A3	4322	PSU	C4-N3-C2	-4.24	120.23	126.34
4	A3	4364	OMG	C5-C4-N3	-4.24	121.58	128.46
4	A3	4045	PSU	C4-N3-C2	-4.24	120.23	126.34
2	A1	867	PSU	C4-N3-C2	-4.23	120.24	126.34
4	A3	3447	PSU	C4-N3-C2	-4.23	120.24	126.34
4	A3	4383	OMG	C2-N3-C4	4.23	119.83	112.30
2	A1	1046	PSU	N1-C2-N3	4.23	119.92	115.13
4	A3	3631	OMG	C5-C4-N3	-4.23	121.61	128.46
4	A3	3502	PSU	C4-N3-C2	-4.22	120.26	126.34
4	A3	1721	PSU	N1-C2-N3	4.22	119.91	115.13
4	A3	4740	PSU	N1-C2-N3	4.22	119.91	115.13
4	A3	4740	PSU	C4-N3-C2	-4.21	120.27	126.34
2	A1	105	PSU	C4-N3-C2	-4.21	120.27	126.34
2	A1	1005	PSU	C4-N3-C2	-4.21	120.27	126.34
2	A1	684	OMG	C2-N3-C4	4.21	119.80	112.30
2	A1	1005	PSU	N1-C2-N3	4.21	119.90	115.13
4	A3	4278	PSU	C4-N3-C2	-4.21	120.28	126.34
2	A1	645	OMG	C2-N3-C4	4.21	119.80	112.30
4	A3	3517	A2M	O4'-C1'-N9	4.21	116.35	108.06
4	A3	1721	PSU	C4-N3-C2	-4.20	120.28	126.34
4	A3	3466	PSU	N1-C2-N3	4.20	119.89	115.13
4	A3	3502	PSU	N1-C2-N3	4.20	119.88	115.13
4	A3	3359	OMG	C2-N3-C4	4.19	119.77	112.30
4	A3	1799	PSU	C4-N3-C2	-4.19	120.30	126.34
4	A3	4325	PSU	N1-C2-N3	4.19	119.88	115.13
4	A3	1477	OMG	C5-C4-N3	-4.19	121.67	128.46
4	A3	1731	PSU	C4-N3-C2	-4.18	120.31	126.34
4	A3	3524	OMG	C2-N3-C4	4.18	119.75	112.30
4	A3	3466	PSU	C4-N3-C2	-4.18	120.32	126.34
2	A1	682	PSU	C4-N3-C2	-4.18	120.32	126.34
2	A1	1626	PSU	N1-C2-N3	4.17	119.86	115.13
2	A1	573	PSU	N1-C2-N3	4.17	119.86	115.13
4	A3	1720	PSU	N1-C2-N3	4.16	119.84	115.13
4	A3	3583	PSU	C4-N3-C2	-4.16	120.35	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	3585	PSU	N1-C2-N3	4.16	119.84	115.13
2	A1	864	PSU	C4-N3-C2	-4.16	120.35	126.34
2	A1	802	PSU	C4-N3-C2	-4.15	120.35	126.34
4	A3	4107	PSU	C4-N3-C2	-4.15	120.36	126.34
4	A3	4325	PSU	C4-N3-C2	-4.14	120.37	126.34
4	A3	2475	PSU	N1-C2-N3	4.13	119.81	115.13
4	A3	4217	PSU	N1-C2-N3	4.13	119.81	115.13
4	A3	4107	PSU	N1-C2-N3	4.13	119.81	115.13
2	A1	93	PSU	N1-C2-N3	4.12	119.80	115.13
2	A1	510	OMG	C2-N3-C4	4.12	119.64	112.30
4	A3	4435	PSU	C4-N3-C2	-4.11	120.42	126.34
4	A3	3585	PSU	C4-N3-C2	-4.09	120.44	126.34
2	A1	1384	A2M	C3'-C2'-C1'	-4.08	95.21	102.89
2	A1	815	PSU	N1-C2-N3	4.08	119.75	115.13
2	A1	815	PSU	C4-N3-C2	-4.06	120.48	126.34
2	A1	1626	PSU	C4-N3-C2	-4.06	120.49	126.34
4	A3	3576	PSU	C4-N3-C2	-4.05	120.50	126.34
2	A1	864	PSU	N1-C2-N3	4.04	119.70	115.13
2	A1	573	PSU	C4-N3-C2	-4.03	120.53	126.34
4	A3	2680	OMU	N3-C2-N1	4.03	120.24	114.89
4	A3	3562	A2M	C3'-C2'-C1'	-4.02	95.34	102.89
4	A3	3973	OMU	N3-C2-N1	4.01	120.22	114.89
2	A1	1851	MA6	C2-N1-C6	4.01	121.23	111.75
2	A1	1640	G7M	C5-C4-N3	-4.01	120.46	128.15
4	A3	3657	OMU	N3-C2-N1	4.00	120.20	114.89
4	A3	1537	PSU	N1-C2-N3	4.00	119.66	115.13
4	A3	4382	PSU	C4-N3-C2	-4.00	120.58	126.34
4	A3	4244	OMU	N3-C2-N1	3.99	120.19	114.89
4	A3	1720	PSU	C4-N3-C2	-3.99	120.60	126.34
4	A3	1489	A2M	C3'-C2'-C1'	-3.97	95.42	102.89
4	A3	2475	PSU	C4-N3-C2	-3.97	120.62	126.34
2	A1	1833	6MZ	N3-C4-N9	3.96	133.61	127.08
4	A3	3494	PSU	C4-N3-C2	-3.96	120.64	126.34
2	A1	93	PSU	C4-N3-C2	-3.95	120.65	126.34
4	A3	3557	A2M	C3'-C2'-C1'	-3.95	95.47	102.89
4	A3	4269	A2M	C3'-C2'-C1'	-3.94	95.49	102.89
2	A1	1852	MA6	C5-N7-C8	3.94	109.10	103.51
2	A1	355	OMU	N3-C2-N1	3.91	120.08	114.89
4	A3	4217	PSU	C4-N3-C2	-3.91	120.70	126.34
4	A3	3359	OMG	C5-C4-N3	-3.91	122.12	128.46
2	A1	119	PSU	N1-C2-N3	3.91	119.56	115.13
4	A3	3517	A2M	N3-C4-N9	3.90	133.50	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	2258	OMU	N3-C2-N1	3.90	120.06	114.89
2	A1	1805	OMU	N3-C2-N1	3.89	120.06	114.89
2	A1	1640	G7M	C5-C6-N1	3.88	119.90	111.79
2	A1	1327	OMU	N3-C2-N1	3.87	120.03	114.89
2	A1	1852	MA6	C2-N1-C6	3.87	120.90	111.75
2	A1	172	OMU	N3-C2-N1	3.86	120.01	114.89
2	A1	1338	4AC	C5-C4-N4	-3.86	116.22	122.92
4	A3	3966	6MZ	N9-C8-N7	-3.85	108.65	113.91
2	A1	1851	MA6	C5-N7-C8	3.82	108.94	103.51
4	A3	3450	A2M	C3'-C2'-C1'	-3.80	95.74	102.89
2	A1	119	PSU	C4-N3-C2	-3.78	120.89	126.34
2	A1	1443	OMU	N3-C2-N1	3.76	119.89	114.89
2	A1	1852	MA6	C2-N3-C4	3.75	120.60	111.75
2	A1	1833	6MZ	N9-C8-N7	-3.74	108.80	113.91
4	A3	2630	A2M	O3'-C3'-C2'	3.73	121.75	111.17
4	A3	4166	PSU	N1-C2-N3	3.72	119.35	115.13
2	A1	1851	MA6	C5-C6-N6	3.72	131.77	125.30
2	A1	628	OMU	N3-C2-N1	3.71	119.81	114.89
4	A3	1537	PSU	C4-N3-C2	-3.70	121.00	126.34
2	A1	513	A2M	C3'-C2'-C1'	-3.69	95.95	102.89
4	A3	3359	OMG	N9-C8-N7	-3.68	106.47	113.39
2	A1	1852	MA6	C5-C6-N6	3.67	131.70	125.30
4	A3	2194	OMC	O2-C2-N3	-3.66	116.38	122.33
4	A3	4052	OMU	N3-C2-N1	3.66	119.75	114.89
4	A3	4166	PSU	C4-N3-C2	-3.64	121.10	126.34
2	A1	1289	OMU	N3-C2-N1	3.61	119.68	114.89
4	A3	3517	A2M	C5-N7-C8	3.59	108.62	103.51
2	A1	99	A2M	C3'-C2'-C1'	-3.57	96.18	102.89
2	A1	121	OMU	N3-C2-N1	3.57	119.63	114.89
4	A3	3966	6MZ	C4-C5-C6	3.57	119.57	116.81
4	A3	2194	OMC	C1'-N1-C2	3.55	126.35	118.42
2	A1	1833	6MZ	C2-N3-C4	3.53	120.09	111.75
4	A3	4366	OMU	N3-C2-N1	3.51	119.55	114.89
4	A3	3657	OMU	C5-C4-N3	3.49	120.07	114.84
29	K1	4	OMC	O3'-C3'-C2'	3.49	121.07	111.17
4	A3	398	A2M	C3'-C2'-C1'	-3.48	96.34	102.89
2	A1	1851	MA6	C2-N3-C4	3.47	119.96	111.75
4	A3	2244	A2M	O3'-C3'-C2'	3.47	121.03	111.17
4	A3	3966	6MZ	C2-N3-C4	3.46	119.93	111.75
2	A1	116	OMU	N3-C2-N1	3.45	119.47	114.89
4	A3	4052	OMU	C5-C4-N3	3.45	120.00	114.84
4	A3	3631	OMG	N9-C8-N7	-3.40	106.99	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	3517	A2M	C2-N3-C4	3.39	119.77	111.75
4	A3	4435	PSU	O2-C2-N1	-3.39	119.06	122.79
2	A1	166	A2M	C3'-C2'-C1'	-3.39	96.51	102.89
2	A1	628	OMU	C5-C4-N3	3.38	119.89	114.84
4	A3	2680	OMU	C5-C4-N3	3.38	119.89	114.84
4	A3	4244	OMU	C5-C4-N3	3.38	119.89	114.84
2	A1	355	OMU	C5-C4-N3	3.37	119.89	114.84
2	A1	1327	OMU	C5-C4-N3	3.36	119.87	114.84
4	A3	4364	OMG	N9-C8-N7	-3.36	107.06	113.39
2	A1	1289	OMU	C5-C4-N3	3.36	119.86	114.84
4	A3	4336	A2M	C3'-C2'-C1'	-3.35	96.59	102.89
2	A1	1851	MA6	C4-N9-C8	3.34	109.34	105.73
2	A1	513	A2M	O3'-C3'-C2'	3.32	120.60	111.17
2	A1	1805	OMU	C5-C4-N3	3.32	119.81	114.84
4	A3	3517	A2M	C4'-O4'-C1'	-3.32	102.15	109.47
2	A1	1443	OMU	C5-C4-N3	3.32	119.80	114.84
4	A3	3973	OMU	C5-C4-N3	3.31	119.80	114.84
4	A3	1477	OMG	N9-C8-N7	-3.31	107.15	113.39
4	A3	3676	OMG	N9-C8-N7	-3.30	107.18	113.39
4	A3	4369	OMG	N9-C8-N7	-3.29	107.19	113.39
4	A3	4317	A2M	O3'-C3'-C2'	3.29	120.51	111.17
2	A1	1852	MA6	N3-C4-N9	3.29	132.50	127.08
4	A3	398	A2M	O3'-C3'-C2'	3.27	120.45	111.17
2	A1	172	OMU	C5-C4-N3	3.26	119.71	114.84
4	A3	4366	OMU	C5-C4-N3	3.25	119.70	114.84
2	A1	510	OMG	C2-N1-C6	-3.24	119.19	125.10
2	A1	27	A2M	C3'-C2'-C1'	-3.24	96.81	102.89
2	A1	159	A2M	O4'-C1'-C2'	3.22	112.22	106.57
2	A1	684	OMG	N9-C8-N7	-3.20	107.36	113.39
2	A1	1852	MA6	C4-C5-C6	3.20	119.46	115.88
4	A3	1260	OMG	N9-C8-N7	-3.20	107.37	113.39
29	K1	58	1MA	C6-C5-N7	-3.19	126.39	132.20
2	A1	469	A2M	C3'-C2'-C1'	-3.19	96.89	102.89
4	A3	3450	A2M	O3'-C3'-C2'	3.19	120.23	111.17
4	A3	4383	OMG	N9-C8-N7	-3.18	107.41	113.39
2	A1	121	OMU	C5-C4-N3	3.17	119.58	114.84
4	A3	3456	A2M	C3'-C2'-C1'	-3.17	96.94	102.89
2	A1	1032	A2M	C3'-C2'-C1'	-3.17	96.94	102.89
4	A3	400	A2M	O3'-C3'-C2'	3.16	120.15	111.17
4	A3	3562	A2M	O3'-C3'-C2'	3.15	120.12	111.17
4	A3	2719	OMG	N9-C8-N7	-3.15	107.46	113.39
4	A3	2258	OMU	C5-C4-N3	3.14	119.54	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	4435	PSU	C6-N1-C2	-3.14	119.48	122.68
4	A3	1479	A2M	O3'-C3'-C2'	3.13	120.06	111.17
4	A3	4374	PSU	O2-C2-N1	-3.12	119.35	122.79
2	A1	437	OMG	N9-C8-N7	-3.12	107.52	113.39
4	A3	400	A2M	C3'-C2'-C1'	-3.12	97.03	102.89
2	A1	1249	B8N	N3-C2-N1	3.11	121.16	116.76
2	A1	1384	A2M	O3'-C3'-C2'	3.11	119.98	111.17
2	A1	577	A2M	O3'-C3'-C2'	3.10	119.96	111.17
2	A1	1640	G7M	N9-C4-N3	3.10	132.16	125.94
2	A1	645	OMG	C2-N1-C6	-3.09	119.46	125.10
4	A3	4383	OMG	C2-N1-C6	-3.09	119.47	125.10
4	A3	4269	A2M	O3'-C3'-C2'	3.09	119.94	111.17
2	A1	159	A2M	O3'-C3'-C2'	3.08	119.92	111.17
2	A1	1640	G7M	O6-C6-C5	-3.08	121.12	128.06
29	K1	58	1MA	N1-C6-N6	3.07	127.59	119.77
2	A1	469	A2M	O3'-C3'-C2'	3.07	119.88	111.17
10	C3	75	OMG	N9-C8-N7	-3.06	107.62	113.39
2	A1	669	A2M	C4-N9-C1'	-3.06	119.30	126.59
4	A3	3514	5MC	C5-C6-N1	-3.06	120.19	123.34
4	A3	3557	A2M	O3'-C3'-C2'	3.05	119.82	111.17
4	A3	3524	OMG	N9-C8-N7	-3.05	107.65	113.39
29	K1	58	1MA	CM1-N1-C6	-3.04	115.66	120.27
2	A1	1491	OMG	C2-N1-C6	-3.04	119.55	125.10
4	A3	4116	OMG	N9-C8-N7	-3.04	107.66	113.39
4	A3	4138	OMG	N9-C8-N7	-3.04	107.67	113.39
2	A1	1679	A2M	O3'-C3'-C2'	3.03	119.77	111.17
2	A1	1851	MA6	C4-N9-C1'	-3.03	119.38	126.59
2	A1	116	OMU	C5-C4-N3	3.02	119.36	114.84
2	A1	645	OMG	N9-C8-N7	-3.02	107.71	113.39
4	A3	1810	A2M	O3'-C3'-C2'	3.02	119.73	111.17
2	A1	868	OMG	N9-C4-N3	3.01	131.99	125.94
2	A1	577	A2M	C3'-C2'-C1'	-3.01	97.23	102.89
2	A1	591	A2M	O3'-C3'-C2'	3.01	119.70	111.17
2	A1	1448	OMG	C2-N1-C6	-3.00	119.62	125.10
4	A3	2267	OMG	N9-C4-N3	3.00	131.97	125.94
4	A3	4276	UR3	C6-N1-C2	-2.99	119.11	121.79
2	A1	602	OMG	C2-N1-C6	-2.99	119.65	125.10
2	A1	1851	MA6	C4-C5-C6	2.98	119.22	115.88
4	A3	3966	6MZ	N3-C4-N9	2.98	132.00	127.08
4	A3	4240	OMG	N9-C8-N7	-2.97	107.80	113.39
4	A3	1491	PSU	O2-C2-N1	-2.97	119.52	122.79
2	A1	166	A2M	O3'-C3'-C2'	2.97	119.59	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A1	1329	OMG	C2-N1-C6	-2.96	119.70	125.10
4	A3	2267	OMG	C2-N1-C6	-2.96	119.70	125.10
2	A1	602	OMG	N9-C8-N7	-2.96	107.82	113.39
4	A3	3942	OMG	N9-C8-N7	-2.96	107.82	113.39
2	A1	868	OMG	C2-N1-C6	-2.95	119.71	125.10
4	A3	4369	OMG	C2-N1-C6	-2.95	119.72	125.10
2	A1	1329	OMG	N9-C8-N7	-2.95	107.84	113.39
4	A3	2719	OMG	C2-N1-C6	-2.95	119.73	125.10
4	A3	3476	OMG	N9-C8-N7	-2.94	107.85	113.39
4	A3	4364	OMG	C2-N1-C6	-2.94	119.74	125.10
10	C3	75	OMG	C2-N1-C6	-2.93	119.75	125.10
4	A3	4052	OMU	O4-C4-C5	-2.93	120.00	125.16
4	A3	4240	OMG	C2-N1-C6	-2.93	119.75	125.10
4	A3	2244	A2M	C3'-C2'-C1'	-2.93	97.39	102.89
4	A3	4317	A2M	C3'-C2'-C1'	-2.92	97.39	102.89
4	A3	4269	A2M	C4-N9-C1'	-2.92	119.64	126.59
4	A3	4138	OMG	C2-N1-C6	-2.91	119.79	125.10
4	A3	3476	OMG	C2-N1-C6	-2.91	119.79	125.10
4	A3	4116	OMG	C2-N1-C6	-2.91	119.80	125.10
2	A1	172	OMU	O4-C4-C5	-2.91	120.05	125.16
2	A1	1384	A2M	C4-N9-C1'	-2.91	119.67	126.59
4	A3	4336	A2M	O3'-C3'-C2'	2.90	119.41	111.17
4	A3	2658	A2M	O3'-C3'-C2'	2.90	119.41	111.17
4	A3	1810	A2M	C4-N9-C1'	-2.90	119.68	126.59
2	A1	1852	MA6	C4-N9-C8	2.89	108.86	105.73
2	A1	437	OMG	C2-N1-C6	-2.89	119.83	125.10
4	A3	3450	A2M	C4-N9-C1'	-2.89	119.71	126.59
2	A1	669	A2M	O3'-C3'-C2'	2.88	119.34	111.17
2	A1	1289	OMU	O4-C4-C5	-2.87	120.11	125.16
2	A1	355	OMU	O4-C4-C5	-2.87	120.11	125.16
4	A3	1580	OMG	C2-N1-C6	-2.87	119.87	125.10
4	A3	1477	OMG	C2-N1-C6	-2.87	119.87	125.10
2	A1	1640	G7M	C2-N1-C6	-2.86	119.88	125.10
4	A3	3631	OMG	C2-N1-C6	-2.86	119.88	125.10
4	A3	3657	OMU	O4-C4-C5	-2.86	120.13	125.16
2	A1	1491	OMG	N9-C8-N7	-2.85	108.01	113.39
4	A3	2258	OMU	O4-C4-C5	-2.85	120.14	125.16
4	A3	3359	OMG	C2-N1-C6	-2.85	119.90	125.10
2	A1	27	A2M	C4-N9-C1'	-2.85	119.80	126.59
4	A3	1580	OMG	N9-C4-N3	2.85	131.66	125.94
2	A1	1443	OMU	O4-C4-C5	-2.84	120.16	125.16
4	A3	3942	OMG	C2-N1-C6	-2.83	119.93	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	1270	A2M	C2'-C1'-N9	2.83	118.30	113.53
2	A1	1327	OMU	O4-C4-C5	-2.83	120.18	125.16
2	A1	1851	MA6	N3-C4-N9	2.83	131.75	127.08
4	A3	3492	A2M	C4-N9-C1'	-2.83	119.86	126.59
4	A3	2194	OMC	O2-C2-N1	2.82	124.73	118.89
4	A3	1260	OMG	C2-N1-C6	-2.82	119.95	125.10
2	A1	510	OMG	N9-C8-N7	-2.82	108.08	113.39
2	A1	628	OMU	O4-C4-C5	-2.82	120.20	125.16
4	A3	4245	OMG	N9-C4-N3	2.82	131.59	125.94
2	A1	1851	MA6	C4-C5-N7	-2.82	107.19	110.62
2	A1	1032	A2M	O3'-C3'-C2'	2.81	119.15	111.17
4	A3	4244	OMU	O4-C4-C5	-2.81	120.22	125.16
4	A3	3557	A2M	C4-N9-C1'	-2.81	119.90	126.59
4	A3	3562	A2M	C4-N9-C1'	-2.80	119.92	126.59
2	A1	669	A2M	C1'-N9-C8	2.80	133.45	127.14
4	A3	1270	A2M	O3'-C3'-C2'	2.80	119.11	111.17
2	A1	1491	OMG	C5-C6-N1	2.79	120.28	113.19
2	A1	684	OMG	C2-N1-C6	-2.79	120.01	125.10
2	A1	1491	OMG	O6-C6-C5	-2.79	119.21	126.60
2	A1	1679	A2M	C3'-C2'-C1'	-2.78	97.66	102.89
2	A1	1852	MA6	C4-C5-N7	-2.78	107.23	110.62
2	A1	1491	OMG	N9-C4-N3	2.78	131.53	125.94
2	A1	116	OMU	O4-C4-C5	-2.78	120.27	125.16
2	A1	1448	OMG	N9-C8-N7	-2.78	108.15	113.39
4	A3	3450	A2M	C1'-N9-C8	2.78	133.41	127.14
2	A1	513	A2M	C4-N9-C1'	-2.78	119.98	126.59
2	A1	121	OMU	O4-C4-C5	-2.78	120.28	125.16
4	A3	3456	A2M	O3'-C3'-C2'	2.77	119.03	111.17
2	A1	1805	OMU	O4-C4-C5	-2.77	120.30	125.16
4	A3	3973	OMU	O4-C4-C5	-2.76	120.30	125.16
4	A3	4366	OMU	O4-C4-C5	-2.75	120.32	125.16
4	A3	3456	A2M	C4-N9-C1'	-2.73	120.08	126.59
2	A1	166	A2M	C4-N9-C1'	-2.73	120.09	126.59
29	K1	58	1MA	O3'-C3'-C4'	-2.72	103.18	111.05
4	A3	3359	OMG	N2-C2-N1	2.72	122.50	116.71
2	A1	1833	6MZ	C5-N7-C8	2.71	107.36	103.51
4	A3	3676	OMG	C2-N1-C6	-2.71	120.16	125.10
4	A3	4317	A2M	C4-N9-C1'	-2.71	120.14	126.59
4	A3	2680	OMU	O4-C4-C5	-2.71	120.40	125.16
4	A3	1270	A2M	C3'-C2'-C1'	-2.71	97.80	102.89
2	A1	99	A2M	O3'-C3'-C2'	2.70	118.84	111.17
4	A3	2719	OMG	N9-C4-N3	2.70	131.35	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A1	1392	OMC	O2-C2-N3	-2.70	117.95	122.33
4	A3	2630	A2M	C3'-C2'-C1'	-2.70	97.82	102.89
2	A1	485	A2M	C4-N9-C1'	-2.69	120.17	126.59
2	A1	868	OMG	N9-C8-N7	-2.69	108.32	113.39
4	A3	3599	A2M	C4-N9-C1'	-2.69	120.17	126.59
4	A3	4138	OMG	C5-C6-N1	2.69	120.02	113.19
2	A1	1032	A2M	C4-N9-C1'	-2.69	120.19	126.59
2	A1	1384	A2M	C1'-N9-C8	2.69	133.20	127.14
2	A1	1843	4AC	C5-C4-N3	-2.68	118.27	122.59
4	A3	4374	PSU	C6-N1-C2	-2.68	119.94	122.68
4	A3	1810	A2M	C1'-N9-C8	2.68	133.18	127.14
4	A3	1580	OMG	N9-C8-N7	-2.67	108.35	113.39
4	A3	4245	OMG	C2-N1-C6	-2.67	120.22	125.10
4	A3	1718	PSU	O2-C2-N1	-2.67	119.85	122.79
2	A1	27	A2M	O3'-C3'-C2'	2.67	118.74	111.17
2	A1	485	A2M	C1'-N9-C8	2.66	133.15	127.14
2	A1	159	A2M	O4'-C4'-C3'	2.66	110.38	105.11
4	A3	4116	OMG	C5-C6-N1	2.66	119.94	113.19
2	A1	1448	OMG	N9-C4-N3	2.65	131.27	125.94
2	A1	669	A2M	C2'-C1'-N9	2.65	118.00	113.53
4	A3	3494	PSU	O2-C2-N1	-2.65	119.87	122.79
2	A1	868	OMG	C5-C6-N1	2.65	119.92	113.19
2	A1	577	A2M	C4-N9-C1'	-2.65	120.28	126.59
2	A1	510	OMG	C5-C6-N1	2.65	119.92	113.19
4	A3	4245	OMG	O6-C6-C5	-2.65	119.58	126.60
4	A3	2244	A2M	C4-N9-C1'	-2.64	120.29	126.59
4	A3	2719	OMG	C5-C6-N1	2.64	119.91	113.19
4	A3	3966	6MZ	C5-N7-C8	2.64	107.26	103.51
4	A3	4269	A2M	C1'-N9-C8	2.64	133.10	127.14
4	A3	4369	OMG	C5-C6-N1	2.64	119.89	113.19
10	C3	75	OMG	C5-C6-N1	2.64	119.89	113.19
4	A3	1632	PSU	O2-C2-N1	-2.64	119.89	122.79
2	A1	437	OMG	C5-C6-N1	2.64	119.89	113.19
2	A1	1175	PSU	O2-C2-N1	-2.63	119.89	122.79
4	A3	4336	A2M	C4-N9-C1'	-2.63	120.33	126.59
4	A3	4149	PSU	O2-C2-N1	-2.63	119.90	122.79
2	A1	1446	PSU	O2-C2-N1	-2.63	119.90	122.79
2	A1	36	PSU	O2-C2-N1	-2.62	119.90	122.79
2	A1	210	PSU	O2-C2-N1	-2.62	119.90	122.79
4	A3	3942	OMG	C5-C6-N1	2.62	119.85	113.19
2	A1	602	OMG	C5-C6-N1	2.62	119.85	113.19
4	A3	4240	OMG	C5-C6-N1	2.62	119.84	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	3562	A2M	C1'-N9-C8	2.62	133.05	127.14
2	A1	1329	OMG	C5-C6-N1	2.62	119.84	113.19
4	A3	4364	OMG	C5-C6-N1	2.62	119.84	113.19
2	A1	27	A2M	C1'-N9-C8	2.62	133.04	127.14
4	A3	4364	OMG	N2-C2-N1	2.61	122.27	116.71
4	A3	3359	OMG	C5-C6-N1	2.60	119.80	113.19
2	A1	469	A2M	C4-N9-C1'	-2.59	120.41	126.59
4	A3	3476	OMG	C5-C6-N1	2.59	119.77	113.19
4	A3	3554	PSU	O2-C2-N1	-2.59	119.94	122.79
4	A3	1260	OMG	C5-C6-N1	2.59	119.77	113.19
2	A1	1644	PSU	O2-C2-N1	-2.59	119.94	122.79
2	A1	159	A2M	C4-N9-C1'	-2.59	120.42	126.59
2	A1	645	OMG	C5-C6-N1	2.59	119.76	113.19
4	A3	3492	A2M	O4'-C1'-C2'	2.59	111.10	106.57
4	A3	3631	OMG	C5-C6-N1	2.59	119.76	113.19
4	A3	4278	PSU	O2-C2-N1	-2.59	119.94	122.79
4	A3	3942	OMG	N9-C4-N3	2.58	131.13	125.94
4	A3	4383	OMG	C5-C6-N1	2.58	119.75	113.19
2	A1	109	PSU	O2-C2-N1	-2.58	119.95	122.79
2	A1	687	PSU	O2-C2-N1	-2.58	119.95	122.79
4	A3	1489	A2M	C4-N9-C1'	-2.58	120.44	126.59
4	A3	4246	PSU	O2-C2-N1	-2.58	119.95	122.79
4	A3	1477	OMG	N2-C2-N1	2.57	122.19	116.71
4	A3	1477	OMG	C5-C6-N1	2.57	119.72	113.19
4	A3	1580	OMG	C5-C6-N1	2.57	119.72	113.19
2	A1	513	A2M	C1'-N9-C8	2.57	132.94	127.14
4	A3	3557	A2M	C1'-N9-C8	2.57	132.93	127.14
68	e1	67	NMM	NE-CZ-NH1	2.56	125.06	120.26
2	A1	105	PSU	O2-C2-N1	-2.56	119.97	122.79
4	A3	3676	OMG	C5-C6-N1	2.56	119.70	113.19
2	A1	1679	A2M	C4-N9-C1'	-2.56	120.49	126.59
4	A3	398	A2M	C4-N9-C1'	-2.56	120.50	126.59
2	A1	591	A2M	C4'-O4'-C1'	-2.56	103.83	109.47
4	A3	2267	OMG	C5-C6-N1	2.56	119.68	113.19
2	A1	1448	OMG	C5-C6-N1	2.56	119.68	113.19
2	A1	684	OMG	C5-C6-N1	2.55	119.67	113.19
2	A1	610	PSU	O2-C2-N1	-2.55	119.99	122.79
2	A1	1047	PSU	O2-C2-N1	-2.55	119.99	122.79
4	A3	4245	OMG	C5-C6-N1	2.54	119.65	113.19
4	A3	4382	PSU	C6-N1-C2	-2.54	120.08	122.68
4	A3	3466	PSU	O2-C2-N1	-2.54	119.99	122.79
4	A3	3492	A2M	O3'-C3'-C2'	2.54	118.38	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	4099	PSU	O2-C2-N1	-2.54	120.00	122.79
4	A3	1638	PSU	O2-C2-N1	-2.54	120.00	122.79
4	A3	4245	OMG	N9-C8-N7	-2.54	108.61	113.39
4	A3	4336	A2M	C1'-N9-C8	2.54	132.86	127.14
2	A1	166	A2M	C1'-N9-C8	2.53	132.86	127.14
4	A3	4039	PSU	O2-C2-N1	-2.53	120.00	122.79
2	A1	407	PSU	O2-C2-N1	-2.53	120.00	122.79
2	A1	1338	4AC	C6-C5-C4	2.53	120.06	116.96
4	A3	4325	PSU	O2-C2-N1	-2.53	120.01	122.79
4	A3	4419	PSU	O2-C2-N1	-2.53	120.01	122.79
4	A3	3456	A2M	C1'-N9-C8	2.52	132.84	127.14
4	A3	398	A2M	C1'-N9-C8	2.52	132.83	127.14
2	A1	485	A2M	O3'-C3'-C2'	2.52	118.33	111.17
4	A3	3492	A2M	C3'-C2'-C1'	-2.52	98.15	102.89
4	A3	3427	PSU	O2-C2-N1	-2.52	120.02	122.79
4	A3	3494	PSU	C6-N1-C2	-2.52	120.11	122.68
4	A3	1479	A2M	C4-N9-C1'	-2.52	120.59	126.59
4	A3	3492	A2M	C1'-N9-C8	2.52	132.82	127.14
2	A1	1348	PSU	O2-C2-N1	-2.52	120.02	122.79
2	A1	437	OMG	O6-C6-C5	-2.51	119.93	126.60
4	A3	1799	PSU	O2-C2-N1	-2.51	120.02	122.79
4	A3	3599	A2M	C1'-N9-C8	2.51	132.81	127.14
2	A1	669	A2M	O4'-C1'-C2'	2.51	110.97	106.57
4	A3	4749	PSU	O2-C2-N1	-2.51	120.03	122.79
4	A3	1810	A2M	C5-C6-N1	2.51	122.78	117.39
2	A1	1693	PSU	O2-C2-N1	-2.51	120.03	122.79
4	A3	398	A2M	C5-C6-N1	2.51	122.78	117.39
4	A3	3599	A2M	O3'-C3'-C2'	2.51	118.29	111.17
4	A3	3462	PSU	O2-C2-N1	-2.51	120.03	122.79
2	A1	1032	A2M	C1'-N9-C8	2.51	132.79	127.14
2	A1	99	A2M	C4-N9-C1'	-2.50	120.63	126.59
4	A3	4383	OMG	N9-C4-N3	2.50	130.96	125.94
2	A1	652	PSU	O2-C2-N1	-2.50	120.04	122.79
2	A1	1679	A2M	C2'-C1'-N9	2.50	117.74	113.53
4	A3	4369	OMG	N2-C2-N1	2.50	122.03	116.71
2	A1	823	PSU	O2-C2-N1	-2.50	120.04	122.79
4	A3	4188	PSU	O2-C2-N1	-2.49	120.04	122.79
2	A1	1032	A2M	C5-C6-N1	2.49	122.74	117.39
2	A1	868	OMG	O6-C6-C5	-2.49	119.98	126.60
4	A3	3562	A2M	C5-C6-N1	2.49	122.74	117.39
2	A1	1057	PSU	O2-C2-N1	-2.49	120.05	122.79
4	A3	400	A2M	C5-C6-N1	2.49	122.74	117.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	1479	A2M	O4'-C1'-C2'	2.49	110.93	106.57
4	A3	4166	PSU	O4-C4-N3	-2.49	115.34	120.12
4	A3	1489	A2M	C1'-N9-C8	2.49	132.75	127.14
4	A3	1537	PSU	C6-N1-C2	-2.49	120.14	122.68
2	A1	513	A2M	C5-C6-N1	2.49	122.73	117.39
2	A1	591	A2M	C4-N9-C1'	-2.49	120.67	126.59
2	A1	650	PSU	O2-C2-N1	-2.49	120.05	122.79
4	A3	3447	PSU	C6-N1-C2	-2.48	120.14	122.68
2	A1	166	A2M	C5-C6-N1	2.48	122.72	117.39
4	A3	4322	PSU	O2-C2-N1	-2.48	120.06	122.79
2	A1	27	A2M	C5-C6-N1	2.48	122.72	117.39
4	A3	3456	A2M	C5-C6-N1	2.48	122.72	117.39
2	A1	1384	A2M	C5-C6-N1	2.48	122.72	117.39
4	A3	3371	PSU	O2-C2-N1	-2.48	120.06	122.79
4	A3	4317	A2M	C1'-N9-C8	2.48	132.73	127.14
4	A3	4382	PSU	O2-C2-N1	-2.48	120.06	122.79
10	C3	55	PSU	O2-C2-N1	-2.48	120.06	122.79
2	A1	1843	4AC	C6-C5-C4	2.48	119.99	116.96
4	A3	4116	OMG	O6-C6-C5	-2.48	120.03	126.60
2	A1	1626	PSU	O2-C2-N1	-2.47	120.07	122.79
4	A3	4336	A2M	C5-C6-N1	2.47	122.70	117.39
4	A3	3447	PSU	O2-C2-N1	-2.47	120.07	122.79
2	A1	99	A2M	C5-C6-N1	2.47	122.70	117.39
2	A1	577	A2M	C5-C6-N1	2.47	122.70	117.39
4	A3	2630	A2M	C5-C6-N1	2.47	122.70	117.39
4	A3	3599	A2M	C3'-C2'-C1'	-2.47	98.24	102.89
2	A1	1245	PSU	O2-C2-N1	-2.47	120.07	122.79
4	A3	2244	A2M	C5-C6-N1	2.47	122.69	117.39
4	A3	2244	A2M	C1'-N9-C8	2.47	132.71	127.14
4	A3	3359	OMG	C2'-C1'-N9	-2.47	109.43	114.22
2	A1	802	PSU	C6-N1-C2	-2.47	120.16	122.68
4	A3	3616	PSU	O2-C2-N1	-2.46	120.08	122.79
4	A3	3599	A2M	C2'-C1'-N9	2.46	117.68	113.53
4	A3	3476	OMG	N9-C4-N3	2.46	130.88	125.94
2	A1	591	A2M	C5-C6-N1	2.46	122.67	117.39
4	A3	3576	PSU	O2-C2-N1	-2.46	120.08	122.79
4	A3	4169	PSU	O2-C2-N1	-2.46	120.09	122.79
4	A3	4042	PSU	O2-C2-N1	-2.46	120.09	122.79
2	A1	469	A2M	C5-C6-N1	2.45	122.66	117.39
4	A3	3557	A2M	C5-C6-N1	2.45	122.66	117.39
4	A3	1270	A2M	C5-C6-N1	2.45	122.65	117.39
4	A3	4298	PSU	O2-C2-N1	-2.45	120.09	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	3427	PSU	C6-N1-C2	-2.45	120.18	122.68
4	A3	2719	OMG	O6-C6-C5	-2.45	120.10	126.60
2	A1	485	A2M	C5-C6-N1	2.45	122.65	117.39
4	A3	3599	A2M	C5-C6-N1	2.45	122.65	117.39
4	A3	2267	OMG	O6-C6-C5	-2.45	120.11	126.60
4	A3	2658	A2M	C5-C6-N1	2.45	122.64	117.39
4	A3	1479	A2M	C5-C6-N1	2.44	122.64	117.39
4	A3	4269	A2M	C5-C6-N1	2.44	122.63	117.39
4	A3	2658	A2M	C4-N9-C1'	-2.44	120.78	126.59
4	A3	3359	OMG	C8-N7-C5	2.44	108.66	104.24
4	A3	400	A2M	C4-N9-C1'	-2.44	120.79	126.59
10	C3	69	PSU	O2-C2-N1	-2.44	120.11	122.79
2	A1	34	PSU	O2-C2-N1	-2.44	120.11	122.79
2	A1	577	A2M	C1'-N9-C8	2.44	132.63	127.14
2	A1	463	OMC	O2-C2-N3	-2.44	118.37	122.33
4	A3	1580	OMG	O6-C6-C5	-2.43	120.14	126.60
4	A3	3450	A2M	C5-C6-N1	2.43	122.62	117.39
2	A1	669	A2M	C5-C6-N1	2.43	122.62	117.39
4	A3	4116	OMG	N9-C4-N3	2.43	130.82	125.94
2	A1	1329	OMG	N9-C4-N3	2.43	130.82	125.94
4	A3	4039	PSU	C6-N1-C2	-2.43	120.20	122.68
4	A3	2658	A2M	C2'-C1'-N9	2.43	117.62	113.53
4	A3	3492	A2M	C5-C6-N1	2.43	122.61	117.39
4	A3	1491	PSU	C6-N1-C2	-2.43	120.20	122.68
4	A3	1260	OMG	O6-C6-C5	-2.43	120.16	126.60
2	A1	573	PSU	C6-N1-C2	-2.43	120.20	122.68
2	A1	867	PSU	C6-N1-C2	-2.43	120.20	122.68
4	A3	3942	OMG	O6-C6-C5	-2.43	120.16	126.60
4	A3	3524	OMG	C5-C6-N1	2.42	119.35	113.19
2	A1	159	A2M	C5-C6-N1	2.42	122.59	117.39
2	A1	1679	A2M	C5-C6-N1	2.42	122.59	117.39
2	A1	1233	PSU	O2-C2-N1	-2.42	120.12	122.79
4	A3	4317	A2M	C5-C6-N1	2.42	122.59	117.39
2	A1	591	A2M	O4'-C1'-C2'	2.42	110.81	106.57
4	A3	2267	OMG	N9-C8-N7	-2.42	108.83	113.39
4	A3	4711	PSU	O2-C2-N1	-2.42	120.13	122.79
2	A1	864	PSU	O2-C2-N1	-2.42	120.13	122.79
2	A1	1338	4AC	CM7-C7-N4	2.41	119.47	115.29
2	A1	469	A2M	C1'-N9-C8	2.41	132.58	127.14
2	A1	1239	PSU	O2-C2-N1	-2.41	120.14	122.79
4	A3	4240	OMG	N9-C4-N3	2.41	130.78	125.94
2	A1	1338	4AC	C5-C4-N3	-2.41	118.72	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	4298	PSU	C6-N1-C2	-2.41	120.22	122.68
4	A3	4058	PSU	O2-C2-N1	-2.41	120.14	122.79
4	A3	4267	PSU	O2-C2-N1	-2.41	120.14	122.79
2	A1	652	PSU	C6-N1-C2	-2.41	120.22	122.68
4	A3	3524	OMG	C2-N1-C6	-2.40	120.71	125.10
4	A3	4276	UR3	C1'-N1-C2	2.40	121.05	116.99
10	C3	75	OMG	O6-C6-C5	-2.40	120.22	126.60
2	A1	602	OMG	O6-C6-C5	-2.40	120.22	126.60
4	A3	3496	PSU	O2-C2-N1	-2.40	120.15	122.79
2	A1	119	PSU	O2-C2-N1	-2.40	120.15	122.79
4	A3	2475	PSU	O2-C2-N1	-2.40	120.15	122.79
2	A1	1329	OMG	O6-C6-C5	-2.40	120.23	126.60
4	A3	3359	OMG	O6-C6-C5	-2.40	120.23	126.60
2	A1	1005	PSU	O2-C2-N1	-2.40	120.15	122.79
2	A1	591	A2M	C1'-N9-C8	2.40	132.55	127.14
4	A3	3619	OMC	O2-C2-N3	-2.40	118.43	122.33
4	A3	3631	OMG	N2-C2-N1	2.40	121.82	116.71
2	A1	1448	OMG	O6-C6-C5	-2.40	120.24	126.60
4	A3	3585	PSU	O2-C2-N1	-2.40	120.15	122.79
2	A1	1046	PSU	O2-C2-N1	-2.40	120.15	122.79
2	A1	1178	PSU	O2-C2-N1	-2.39	120.16	122.79
2	A1	105	PSU	C6-N1-C2	-2.39	120.24	122.68
2	A1	573	PSU	O2-C2-N1	-2.39	120.16	122.79
2	A1	1679	A2M	O4'-C1'-C2'	2.39	110.76	106.57
2	A1	99	A2M	C1'-N9-C8	2.39	132.53	127.14
2	A1	1005	PSU	C6-N1-C2	-2.39	120.24	122.68
4	A3	3631	OMG	O6-C6-C5	-2.39	120.27	126.60
4	A3	4240	OMG	O6-C6-C5	-2.38	120.28	126.60
2	A1	602	OMG	N9-C4-N3	2.38	130.73	125.94
4	A3	3359	OMG	C4-C5-N7	-2.38	106.95	110.72
4	A3	1801	PSU	O2-C2-N1	-2.38	120.17	122.79
4	A3	4203	PSU	O2-C2-N1	-2.38	120.17	122.79
4	A3	3476	OMG	O6-C6-C5	-2.38	120.28	126.60
4	A3	1683	PSU	O2-C2-N1	-2.38	120.17	122.79
2	A1	159	A2M	C1'-N9-C8	2.38	132.51	127.14
4	A3	3496	PSU	C6-N1-C2	-2.38	120.25	122.68
4	A3	1479	A2M	C4'-O4'-C1'	-2.38	104.22	109.47
4	A3	3676	OMG	O6-C6-C5	-2.38	120.29	126.60
4	A3	4177	PSU	O2-C2-N1	-2.38	120.17	122.79
29	K1	34	OMC	O2-C2-N3	-2.37	118.47	122.33
4	A3	1537	PSU	O2-C2-N1	-2.37	120.18	122.79
4	A3	3616	PSU	C6-N1-C2	-2.37	120.26	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	4364	OMG	O6-C6-C5	-2.37	120.31	126.60
4	A3	4169	PSU	C6-N1-C2	-2.37	120.26	122.68
4	A3	1260	OMG	N9-C4-N3	2.37	130.70	125.94
2	A1	437	OMG	N9-C4-N3	2.37	130.70	125.94
4	A3	3576	PSU	C6-N1-C2	-2.37	120.26	122.68
2	A1	1626	PSU	C6-N1-C2	-2.37	120.26	122.68
4	A3	4325	PSU	C6-N1-C2	-2.36	120.27	122.68
4	A3	3514	5MC	O2-C2-N3	-2.36	118.49	122.33
2	A1	682	PSU	C6-N1-C2	-2.36	120.27	122.68
4	A3	4419	PSU	C6-N1-C2	-2.36	120.27	122.68
4	A3	2658	A2M	C1'-N9-C8	2.36	132.47	127.14
2	A1	1368	PSU	O2-C2-N1	-2.36	120.19	122.79
4	A3	3466	PSU	C6-N1-C2	-2.36	120.27	122.68
2	A1	1679	A2M	C1'-N9-C8	2.35	132.45	127.14
2	A1	816	PSU	O2-C2-N1	-2.35	120.20	122.79
2	A1	802	PSU	O2-C2-N1	-2.35	120.20	122.79
4	A3	2475	PSU	C6-N1-C2	-2.35	120.28	122.68
4	A3	4217	PSU	C6-N1-C2	-2.35	120.28	122.68
2	A1	485	A2M	O4'-C1'-C2'	2.35	110.69	106.57
4	A3	1489	A2M	C5-C6-N1	2.35	122.44	117.39
4	A3	3583	PSU	O2-C2-N1	-2.35	120.20	122.79
2	A1	119	PSU	C6-N1-C2	-2.35	120.28	122.68
2	A1	1852	MA6	C4-N9-C1'	-2.35	121.00	126.59
2	A1	1249	B8N	C31-N3-C4	2.35	120.77	117.31
2	A1	684	OMG	O6-C6-C5	-2.35	120.37	126.60
2	A1	682	PSU	O2-C2-N1	-2.35	120.21	122.79
4	A3	4383	OMG	C8-N7-C5	2.34	108.48	104.24
4	A3	4278	PSU	C6-N1-C2	-2.34	120.29	122.68
2	A1	864	PSU	C6-N1-C2	-2.34	120.29	122.68
2	A1	518	OMC	O2-C2-N3	-2.34	118.52	122.33
4	A3	4383	OMG	O6-C6-C5	-2.34	120.39	126.60
4	A3	1720	PSU	O2-C2-N1	-2.34	120.22	122.79
4	A3	4369	OMG	O6-C6-C5	-2.34	120.40	126.60
4	A3	1810	A2M	C6-C5-C4	-2.34	114.04	117.18
2	A1	1175	PSU	C6-N1-C2	-2.33	120.30	122.68
2	A1	867	PSU	O2-C2-N1	-2.33	120.22	122.79
4	A3	4246	PSU	C6-N1-C2	-2.33	120.30	122.68
2	A1	218	PSU	O2-C2-N1	-2.33	120.22	122.79
4	A3	1799	PSU	C6-N1-C2	-2.33	120.30	122.68
2	A1	510	OMG	N9-C4-N3	2.33	130.61	125.94
4	A3	2630	A2M	C4-N9-C1'	-2.33	121.05	126.59
2	A1	1047	PSU	C6-N1-C2	-2.33	120.31	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A1	684	OMG	N9-C4-N3	2.33	130.61	125.94
4	A3	1720	PSU	C6-N1-C2	-2.32	120.31	122.68
4	A3	3554	PSU	C6-N1-C2	-2.32	120.31	122.68
4	A3	3631	OMG	C8-N7-C5	2.32	108.44	104.24
2	A1	645	OMG	O6-C6-C5	-2.32	120.45	126.60
4	A3	4317	A2M	O4'-C1'-C2'	2.32	110.63	106.57
4	A3	4138	OMG	O6-C6-C5	-2.32	120.45	126.60
4	A3	3502	PSU	O2-C2-N1	-2.32	120.24	122.79
2	A1	1233	PSU	C6-N1-C2	-2.32	120.31	122.68
4	A3	2351	PSU	O2-C2-N1	-2.32	120.24	122.79
4	A3	1479	A2M	C1'-N9-C8	2.31	132.36	127.14
4	A3	3676	OMG	N9-C4-N3	2.31	130.59	125.94
2	A1	93	PSU	C6-N1-C2	-2.31	120.32	122.68
2	A1	650	PSU	C6-N1-C2	-2.31	120.32	122.68
4	A3	1632	PSU	C6-C5-C4	2.31	119.81	118.20
4	A3	4138	OMG	N2-C2-N1	2.30	121.62	116.71
54	W2	39	V5N	O2-CB-CA	2.30	112.14	107.28
2	A1	1693	PSU	C6-N1-C2	-2.30	120.33	122.68
2	A1	645	OMG	N9-C4-N3	2.30	130.56	125.94
2	A1	166	A2M	O4'-C1'-C2'	2.30	110.59	106.57
4	A3	4177	PSU	C6-N1-C2	-2.29	120.34	122.68
4	A3	4322	PSU	C6-N1-C2	-2.29	120.34	122.68
4	A3	400	A2M	C1'-N9-C8	2.29	132.31	127.14
4	A3	4166	PSU	O2-C2-N1	-2.29	120.27	122.79
4	A3	1638	PSU	C6-N1-C2	-2.29	120.34	122.68
2	A1	610	PSU	C6-N1-C2	-2.29	120.34	122.68
4	A3	1718	PSU	C6-N1-C2	-2.29	120.34	122.68
2	A1	815	PSU	C6-N1-C2	-2.29	120.34	122.68
4	A3	4202	OMC	O2-C2-N3	-2.28	118.62	122.33
4	A3	4740	PSU	O2-C2-N1	-2.28	120.28	122.79
4	A3	3371	PSU	C6-N1-C2	-2.28	120.35	122.68
4	A3	1477	OMG	O6-C6-C5	-2.28	120.55	126.60
2	A1	815	PSU	O2-C2-N1	-2.28	120.28	122.79
2	A1	93	PSU	O2-C2-N1	-2.28	120.28	122.79
2	A1	1392	OMC	C1'-N1-C2	2.28	123.50	118.42
4	A3	3524	OMG	N9-C4-N3	2.27	130.50	125.94
2	A1	407	PSU	C6-N1-C2	-2.27	120.36	122.68
4	A3	4217	PSU	O2-C2-N1	-2.27	120.29	122.79
4	A3	4749	PSU	C6-N1-C2	-2.27	120.36	122.68
2	A1	1178	PSU	C6-N1-C2	-2.27	120.36	122.68
2	A1	1249	B8N	O4'-C1'-C2'	2.26	108.34	105.14
4	A3	4364	OMG	C8-N7-C5	2.26	108.33	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	4269	A2M	O4'-C1'-C2'	2.26	110.53	106.57
2	A1	669	A2M	C6-C5-C4	-2.26	114.15	117.18
10	C3	75	OMG	N2-C2-N1	2.26	121.52	116.71
2	A1	1245	PSU	C6-N1-C2	-2.25	120.38	122.68
4	A3	4369	OMG	C8-N7-C5	2.25	108.32	104.24
4	A3	3524	OMG	O6-C6-C5	-2.25	120.63	126.60
4	A3	4045	PSU	O2-C2-N1	-2.25	120.31	122.79
4	A3	2658	A2M	O4'-C1'-C2'	2.25	110.51	106.57
4	A3	3359	OMG	C6-C5-N7	2.25	134.43	130.25
2	A1	1644	PSU	C6-N1-C2	-2.25	120.39	122.68
2	A1	1704	OMC	O2-C2-N3	-2.25	118.68	122.33
4	A3	1477	OMG	C8-N7-C5	2.24	108.30	104.24
4	A3	4336	A2M	O4'-C1'-C2'	2.24	110.49	106.57
4	A3	1721	PSU	O2-C2-N1	-2.23	120.33	122.79
4	A3	4364	OMG	C4-C5-N7	-2.23	107.19	110.72
4	A3	1683	PSU	C6-N1-C2	-2.23	120.40	122.68
2	A1	687	PSU	C6-N1-C2	-2.23	120.40	122.68
4	A3	1801	PSU	C6-N1-C2	-2.23	120.40	122.68
2	A1	1446	PSU	C6-N1-C2	-2.23	120.40	122.68
2	A1	1384	A2M	C6-C5-C4	-2.23	114.18	117.18
2	A1	1368	PSU	C6-N1-C2	-2.23	120.40	122.68
4	A3	4193	5MC	C1'-N1-C6	2.23	124.83	121.12
2	A1	27	A2M	O4'-C1'-C2'	2.23	110.47	106.57
4	A3	3652	PSU	O2-C2-N1	-2.23	120.34	122.79
4	A3	4740	PSU	C6-N1-C2	-2.22	120.41	122.68
2	A1	510	OMG	O6-C6-C5	-2.22	120.70	126.60
10	C3	75	OMG	N9-C4-N3	2.22	130.40	125.94
4	A3	1477	OMG	C4-C5-N7	-2.22	107.21	110.72
4	A3	3492	A2M	C6-C5-C4	-2.22	114.20	117.18
10	C3	69	PSU	C6-N1-C2	-2.21	120.42	122.68
4	A3	1260	OMG	C8-N7-C5	2.21	108.24	104.24
2	A1	1082	PSU	O2-C2-N1	-2.21	120.36	122.79
4	A3	4058	PSU	C6-N1-C2	-2.21	120.43	122.68
4	A3	2658	A2M	C3'-C2'-C1'	-2.21	98.74	102.89
4	A3	2630	A2M	C1'-N9-C8	2.21	132.12	127.14
2	A1	36	PSU	C6-N1-C2	-2.21	120.43	122.68
4	A3	3562	A2M	C6-C5-C4	-2.21	114.22	117.18
4	A3	3514	5MC	CM5-C5-C6	-2.21	119.90	122.85
4	A3	1721	PSU	C6-N1-C2	-2.20	120.43	122.68
4	A3	4336	A2M	C6-C5-C4	-2.20	114.23	117.18
4	A3	2719	OMG	C8-N7-C5	2.20	108.22	104.24
4	A3	3676	OMG	C8-N7-C5	2.20	108.22	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A1	684	OMG	C8-N7-C5	2.20	108.22	104.24
4	A3	3456	A2M	O4'-C1'-C2'	2.20	110.42	106.57
4	A3	4369	OMG	C4-C5-N7	-2.20	107.25	110.72
4	A3	3450	A2M	C6-C5-C4	-2.20	114.23	117.18
4	A3	4099	PSU	C6-N1-C2	-2.19	120.44	122.68
4	A3	1479	A2M	C6-C5-C4	-2.19	114.24	117.18
4	A3	3599	A2M	C6-C5-C4	-2.19	114.24	117.18
2	A1	109	PSU	C6-N1-C2	-2.19	120.45	122.68
2	A1	172	OMU	O2-C2-N1	-2.19	119.88	122.79
2	A1	355	OMU	O2-C2-N1	-2.19	119.88	122.79
4	A3	4317	A2M	C6-C5-C4	-2.19	114.24	117.18
4	A3	4138	OMG	N9-C4-N3	2.19	130.33	125.94
2	A1	166	A2M	C6-C5-C4	-2.18	114.25	117.18
4	A3	2658	A2M	C6-C5-C4	-2.18	114.25	117.18
2	A1	34	PSU	C6-N1-C2	-2.18	120.45	122.68
2	A1	513	A2M	C6-C5-C4	-2.18	114.25	117.18
2	A1	645	OMG	C8-N7-C5	2.18	108.19	104.24
4	A3	2244	A2M	C6-C5-C4	-2.18	114.25	117.18
4	A3	1489	A2M	O3'-C3'-C2'	2.18	117.35	111.17
4	A3	3456	A2M	C6-C5-C4	-2.18	114.26	117.18
2	A1	577	A2M	C6-C5-C4	-2.18	114.26	117.18
2	A1	27	A2M	C6-C5-C4	-2.18	114.26	117.18
4	A3	4267	PSU	C6-N1-C2	-2.18	120.46	122.68
4	A3	4317	A2M	C2'-C1'-N9	2.18	117.19	113.53
2	A1	1032	A2M	C6-C5-C4	-2.17	114.26	117.18
4	A3	3583	PSU	C6-N1-C2	-2.17	120.46	122.68
2	A1	816	PSU	C6-N1-C2	-2.17	120.46	122.68
4	A3	4203	PSU	C6-N1-C2	-2.17	120.46	122.68
2	A1	602	OMG	C8-N7-C5	2.17	108.17	104.24
4	A3	3502	PSU	C6-N1-C2	-2.17	120.47	122.68
4	A3	1731	PSU	O2-C2-N1	-2.17	120.40	122.79
4	A3	4042	PSU	C6-N1-C2	-2.17	120.47	122.68
4	A3	3466	PSU	O4'-C1'-C2'	2.16	108.19	105.14
2	A1	1057	PSU	C6-N1-C2	-2.16	120.47	122.68
4	A3	2244	A2M	O4'-C1'-C2'	2.16	110.36	106.57
4	A3	3631	OMG	C4-C5-N7	-2.16	107.30	110.72
2	A1	1239	PSU	C6-N1-C2	-2.16	120.48	122.68
4	A3	4045	PSU	C6-N1-C2	-2.16	120.48	122.68
2	A1	437	OMG	C2'-C1'-N9	-2.15	110.04	114.22
4	A3	1270	A2M	C4-N9-C1'	-2.15	121.46	126.59
4	A3	2194	OMC	C1'-N1-C6	-2.15	116.15	120.84
4	A3	4107	PSU	O2-C2-N1	-2.15	120.42	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	1810	A2M	C4'-O4'-C1'	-2.15	104.73	109.47
4	A3	4382	PSU	O4'-C1'-C2'	2.15	108.17	105.14
4	A3	4269	A2M	C6-C5-C4	-2.15	114.30	117.18
4	A3	1537	PSU	O4-C4-N3	-2.15	116.00	120.12
2	A1	628	OMU	O2-C2-N1	-2.14	119.94	122.79
4	A3	3585	PSU	C6-N1-C2	-2.14	120.49	122.68
2	A1	437	OMG	C8-N7-C5	2.14	108.11	104.24
4	A3	1632	PSU	C6-N1-C2	-2.14	120.50	122.68
29	K1	4	OMC	C2'-C1'-N1	-2.14	110.07	114.22
4	A3	3557	A2M	O4'-C1'-C2'	2.13	110.31	106.57
10	C3	55	PSU	C6-N1-C2	-2.13	120.50	122.68
2	A1	1032	A2M	O4'-C1'-C2'	2.13	110.30	106.57
4	A3	3557	A2M	C6-C5-C4	-2.13	114.32	117.18
4	A3	1270	A2M	C1'-N9-C8	2.13	131.94	127.14
4	A3	4188	PSU	C6-N1-C2	-2.13	120.51	122.68
2	A1	159	A2M	C2-N1-C6	-2.13	115.12	118.77
4	A3	4711	PSU	C6-N1-C2	-2.13	120.51	122.68
4	A3	3476	OMG	C8-N7-C5	2.12	108.08	104.24
4	A3	4138	OMG	C8-N7-C5	2.12	108.08	104.24
10	C3	75	OMG	C8-N7-C5	2.12	108.08	104.24
2	A1	210	PSU	C6-N1-C2	-2.12	120.51	122.68
2	A1	1348	PSU	C6-N1-C2	-2.12	120.52	122.68
2	A1	1046	PSU	C6-N1-C2	-2.12	120.52	122.68
2	A1	485	A2M	C6-C5-C4	-2.11	114.34	117.18
2	A1	469	A2M	O4'-C1'-C2'	2.11	110.28	106.57
2	A1	1249	B8N	O4-C4-N3	-2.11	116.39	119.98
4	A3	2704	OMC	O2-C2-N3	-2.11	118.89	122.33
4	A3	1270	A2M	O3'-C3'-C4'	-2.11	104.94	111.05
2	A1	469	A2M	C6-C5-C4	-2.11	114.34	117.18
2	A1	602	OMG	N2-C2-N1	2.11	121.21	116.71
4	A3	4240	OMG	C8-N7-C5	2.11	108.06	104.24
2	A1	1329	OMG	C8-N7-C5	2.11	108.06	104.24
4	A3	4052	OMU	O2-C2-N1	-2.11	119.98	122.79
4	A3	4282	OMC	O2-C2-N3	-2.11	118.91	122.33
4	A3	1489	A2M	O3'-C3'-C4'	-2.10	104.97	111.05
2	A1	823	PSU	O4'-C1'-C2'	2.10	108.11	105.14
2	A1	591	A2M	C6-C5-C4	-2.10	114.36	117.18
4	A3	3462	PSU	C6-N1-C2	-2.10	120.54	122.68
4	A3	4107	PSU	C6-N1-C2	-2.10	120.54	122.68
2	A1	1327	OMU	O2-C2-N1	-2.09	120.01	122.79
4	A3	398	A2M	C6-C5-C4	-2.09	114.37	117.18
2	A1	1384	A2M	O4'-C1'-C2'	2.09	110.23	106.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A1	1082	PSU	C6-N1-C2	-2.09	120.55	122.68
4	A3	400	A2M	O4'-C1'-C2'	2.09	110.23	106.57
4	A3	4149	PSU	C6-N1-C2	-2.09	120.55	122.68
2	A1	218	PSU	C6-N1-C2	-2.09	120.55	122.68
4	A3	1489	A2M	C2'-C1'-N9	2.08	117.04	113.53
2	A1	166	A2M	C4'-O4'-C1'	-2.08	104.88	109.47
29	K1	58	1MA	C6-C5-C4	2.08	122.87	118.42
4	A3	4244	OMU	O2-C2-N1	-2.08	120.02	122.79
4	A3	3942	OMG	C8-N7-C5	2.08	108.00	104.24
4	A3	2265	OMC	O2-C2-N3	-2.08	118.96	122.33
4	A3	400	A2M	C2-N1-C6	-2.07	115.21	118.77
2	A1	669	A2M	O3'-C3'-C4'	-2.07	105.06	111.05
4	A3	4383	OMG	C4-C5-N7	-2.07	107.45	110.72
4	A3	3973	OMU	O2-C2-N1	-2.07	120.04	122.79
2	A1	1384	A2M	C4'-O4'-C1'	-2.07	104.91	109.47
10	C3	69	PSU	O4'-C1'-C2'	2.07	108.06	105.14
4	A3	4317	A2M	O3'-C3'-C4'	-2.07	105.07	111.05
4	A3	1731	PSU	C6-N1-C2	-2.07	120.57	122.68
2	A1	577	A2M	O4'-C1'-C2'	2.06	110.19	106.57
4	A3	3599	A2M	C2-N1-C6	-2.06	115.22	118.77
2	A1	1679	A2M	C6-C5-C4	-2.06	114.41	117.18
4	A3	400	A2M	C2'-C1'-N9	2.06	117.00	113.53
4	A3	2351	PSU	C6-N1-C2	-2.06	120.57	122.68
4	A3	3540	OMC	O2-C2-N3	-2.06	118.98	122.33
2	A1	645	OMG	C4-C5-N7	-2.06	107.46	110.72
4	A3	2630	A2M	C2-N1-C6	-2.06	115.23	118.77
2	A1	1448	OMG	C8-N7-C5	2.06	107.97	104.24
4	A3	2630	A2M	O3'-C3'-C4'	-2.06	105.10	111.05
4	A3	1260	OMG	N2-C2-N1	2.06	121.09	116.71
4	A3	3524	OMG	C8-N7-C5	2.06	107.96	104.24
4	A3	4202	OMC	C1'-N1-C2	2.06	123.01	118.42
4	A3	4116	OMG	C8-N7-C5	2.05	107.96	104.24
4	A3	1810	A2M	O4'-C1'-C2'	2.05	110.17	106.57
29	K1	4	OMC	O4'-C4'-C3'	-2.05	101.05	105.11
4	A3	398	A2M	C2-N1-C6	-2.05	115.25	118.77
4	A3	1479	A2M	C3'-C2'-C1'	-2.05	99.04	102.89
4	A3	400	A2M	C6-C5-C4	-2.05	114.43	117.18
4	A3	1270	A2M	C6-C5-C4	-2.05	114.43	117.18
4	A3	4138	OMG	C4-C5-N7	-2.05	107.48	110.72
4	A3	2680	OMU	O2-C2-N1	-2.05	120.07	122.79
2	A1	1338	4AC	C1'-N1-C2	2.04	122.98	118.42
4	A3	3657	OMU	O2-C2-N1	-2.04	120.07	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A1	437	OMG	N2-C2-N1	2.04	121.06	116.71
2	A1	1843	4AC	O7-C7-CM7	-2.04	118.27	122.06
4	A3	4364	OMG	C2'-C1'-N9	-2.04	110.26	114.22
4	A3	4245	OMG	N1-C2-N3	-2.04	119.52	123.32
4	A3	4188	PSU	O4'-C1'-C2'	2.04	108.02	105.14
4	A3	1489	A2M	O4'-C1'-C2'	2.04	110.14	106.57
4	A3	3524	OMG	N1-C2-N3	-2.04	119.53	123.32
4	A3	3476	OMG	N2-C2-N1	2.03	121.04	116.71
4	A3	1270	A2M	O4'-C4'-C3'	2.03	109.13	105.11
2	A1	99	A2M	C2-N1-C6	-2.03	115.29	118.77
2	A1	868	OMG	C8-N7-C5	2.03	107.91	104.24
2	A1	159	A2M	C6-C5-C4	-2.02	114.46	117.18
4	A3	4166	PSU	C6-N1-C2	-2.02	120.62	122.68
10	C3	75	OMG	C4-C5-N7	-2.02	107.53	110.72
2	A1	1329	OMG	N2-C2-N1	2.02	121.00	116.71
4	A3	3652	PSU	C6-N1-C2	-2.01	120.62	122.68
2	A1	109	PSU	O4'-C1'-C2'	2.01	107.98	105.14
2	A1	510	OMG	C8-N7-C5	2.01	107.88	104.24
2	A1	602	OMG	C4-C5-N7	-2.01	107.54	110.72
4	A3	1489	A2M	C6-C5-C4	-2.01	114.48	117.18
2	A1	669	A2M	C2-N1-C6	-2.01	115.32	118.77
2	A1	1679	A2M	C2-N1-C6	-2.01	115.32	118.77
2	A1	469	A2M	C2-N1-C6	-2.01	115.32	118.77
2	A1	121	OMU	O2-C2-N1	-2.00	120.12	122.79
4	A3	4149	PSU	O4'-C1'-C2'	2.00	107.97	105.14
4	A3	2630	A2M	O4'-C4'-C3'	2.00	109.08	105.11

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A3	398	A2M	C1'-C2'-O2'-CM'
4	A3	2207	OMG	C1'-C2'-O2'-CM2
4	A3	2658	A2M	C1'-C2'-O2'-CM'
4	A3	3433	OMC	C2'-C1'-N1-C6
4	A3	3450	A2M	C1'-C2'-O2'-CM'
4	A3	3599	A2M	C3'-C4'-C5'-O5'
4	A3	4166	PSU	C2'-C1'-C5-C4
4	A3	4166	PSU	C2'-C1'-C5-C6
4	A3	4336	A2M	C4'-C5'-O5'-P
4	A3	4382	PSU	C3'-C4'-C5'-O5'
4	A3	4383	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
56	X2	5	MLZ	N-CA-CB-CG
56	X2	5	MLZ	C-CA-CB-CG
68	e1	67	NMM	O-C-CA-CB
2	A1	27	A2M	C1'-C2'-O2'-CM'
2	A1	116	OMU	C1'-C2'-O2'-CM2
2	A1	121	OMU	C1'-C2'-O2'-CM2
2	A1	159	A2M	C1'-C2'-O2'-CM'
2	A1	645	OMG	O4'-C4'-C5'-O5'
2	A1	645	OMG	C3'-C4'-C5'-O5'
2	A1	669	A2M	C1'-C2'-O2'-CM'
2	A1	684	OMG	O4'-C4'-C5'-O5'
2	A1	684	OMG	C3'-C4'-C5'-O5'
2	A1	868	OMG	O4'-C4'-C5'-O5'
2	A1	1249	B8N	C31-C32-C33-N34
2	A1	1384	A2M	C1'-C2'-O2'-CM'
2	A1	1443	OMU	C1'-C2'-O2'-CM2
2	A1	1448	OMG	C3'-C4'-C5'-O5'
2	A1	1679	A2M	C1'-C2'-O2'-CM'
29	K1	4	OMC	C1'-C2'-O2'-CM2
29	K1	32	OMU	C1'-C2'-O2'-CM2
29	K1	39	OMU	C1'-C2'-O2'-CM2
4	A3	3433	OMC	C2'-C1'-N1-C2
4	A3	1270	A2M	C3'-C4'-C5'-O5'
4	A3	1632	PSU	C3'-C4'-C5'-O5'
4	A3	3676	OMG	O4'-C4'-C5'-O5'
4	A3	4382	PSU	O4'-C4'-C5'-O5'
2	A1	868	OMG	C3'-C4'-C5'-O5'
29	K1	13	PSU	O4'-C4'-C5'-O5'
4	A3	1632	PSU	O4'-C4'-C5'-O5'
4	A3	1731	PSU	O4'-C4'-C5'-O5'
4	A3	3599	A2M	O4'-C4'-C5'-O5'
4	A3	3676	OMG	C3'-C4'-C5'-O5'
4	A3	4364	OMG	O4'-C4'-C5'-O5'
29	K1	13	PSU	C3'-C4'-C5'-O5'
2	A1	429	OMU	C2'-C1'-N1-C6
4	A3	4166	PSU	C3'-C4'-C5'-O5'
56	X2	5	MLZ	CD-CE-NZ-CM
4	A3	4193	5MC	C2'-C1'-N1-C6
4	A3	3494	PSU	C3'-C4'-C5'-O5'
4	A3	4364	OMG	C3'-C4'-C5'-O5'
2	A1	513	A2M	C3'-C4'-C5'-O5'
2	A1	1448	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A1	1640	G7M	C3'-C4'-C5'-O5'
79	j2	53	MLZ	CG-CD-CE-NZ
4	A3	2265	OMC	O4'-C4'-C5'-O5'
4	A3	3494	PSU	O4'-C4'-C5'-O5'
4	A3	4166	PSU	O4'-C4'-C5'-O5'
2	A1	1640	G7M	O4'-C4'-C5'-O5'
56	X2	5	MLZ	CA-CB-CG-CD
4	A3	1731	PSU	C3'-C4'-C5'-O5'
4	A3	2265	OMC	C3'-C4'-C5'-O5'
4	A3	3583	PSU	C3'-C4'-C5'-O5'
2	A1	469	A2M	C3'-C4'-C5'-O5'
4	A3	2630	A2M	C2'-C1'-N9-C8
4	A3	1270	A2M	O4'-C4'-C5'-O5'
4	A3	1720	PSU	C3'-C4'-C5'-O5'
4	A3	3517	A2M	O4'-C4'-C5'-O5'
2	A1	513	A2M	O4'-C4'-C5'-O5'
2	A1	669	A2M	O4'-C4'-C5'-O5'
4	A3	3631	OMG	O4'-C4'-C5'-O5'
2	A1	437	OMG	O4'-C4'-C5'-O5'
4	A3	2267	OMG	C1'-C2'-O2'-CM2
4	A3	4193	5MC	O4'-C1'-N1-C6
2	A1	429	OMU	O4'-C1'-N1-C6
2	A1	429	OMU	C2'-C1'-N1-C2
76	i1	62	HY3	O-C-CA-C3
4	A3	1489	A2M	C4'-C5'-O5'-P
2	A1	645	OMG	C4'-C5'-O5'-P
2	A1	469	A2M	O4'-C4'-C5'-O5'
2	A1	1245	PSU	O4'-C4'-C5'-O5'
2	A1	1249	B8N	C31-C32-C33-C34
4	A3	3433	OMC	O4'-C1'-N1-C2
4	A3	4244	OMU	C3'-C2'-O2'-CM2
2	A1	1338	4AC	N3-C4-N4-C7
4	A3	4246	PSU	C4'-C5'-O5'-P
2	A1	577	A2M	C4'-C5'-O5'-P
2	A1	1392	OMC	C3'-C4'-C5'-O5'
29	K1	49	5MC	O4'-C4'-C5'-O5'
4	A3	4193	5MC	C2'-C1'-N1-C2
4	A3	3433	OMC	O4'-C1'-N1-C6
4	A3	1270	A2M	C4'-C5'-O5'-P
4	A3	3550	UY1	C4'-C5'-O5'-P
2	A1	210	PSU	C3'-C4'-C5'-O5'
4	A3	4193	5MC	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
2	A1	429	OMU	O4'-C1'-N1-C2
4	A3	3576	PSU	C4'-C5'-O5'-P
2	A1	1491	OMG	C4'-C5'-O5'-P
2	A1	1852	MA6	C4'-C5'-O5'-P
29	K1	9	1MG	C4'-C5'-O5'-P
54	W2	39	V5N	O2-CB-CG-CD2
29	K1	49	5MC	C3'-C4'-C5'-O5'
2	A1	463	OMC	C3'-C2'-O2'-CM2
2	A1	577	A2M	C3'-C4'-C5'-O5'
54	W2	39	V5N	O2-CB-CG-ND1
4	A3	2630	A2M	C2'-C1'-N9-C4
4	A3	2194	OMC	C2'-C1'-N1-C6
4	A3	1479	A2M	O4'-C1'-N9-C8
4	A3	3550	UY1	O4'-C1'-C5-C4
4	A3	3517	A2M	C3'-C2'-O2'-CM'
4	A3	3601	OMC	C3'-C2'-O2'-CM2
4	A3	4116	OMG	C3'-C2'-O2'-CM2
2	A1	174	OMC	C3'-C2'-O2'-CM2
4	A3	4107	PSU	O4'-C4'-C5'-O5'
4	A3	1489	A2M	O4'-C4'-C5'-O5'
4	A3	3359	OMG	O4'-C4'-C5'-O5'
2	A1	510	OMG	O4'-C4'-C5'-O5'
2	A1	591	A2M	O4'-C1'-N9-C8
4	A3	4217	PSU	C3'-C4'-C5'-O5'
2	A1	669	A2M	C3'-C4'-C5'-O5'
2	A1	1392	OMC	O4'-C4'-C5'-O5'
4	A3	3601	OMC	C1'-C2'-O2'-CM2
4	A3	4269	A2M	C1'-C2'-O2'-CM'
2	A1	174	OMC	C1'-C2'-O2'-CM2
2	A1	628	OMU	C3'-C2'-O2'-CM2
4	A3	2630	A2M	O4'-C1'-N9-C8
4	A3	3466	PSU	O4'-C4'-C5'-O5'
4	A3	3583	PSU	O4'-C4'-C5'-O5'
2	A1	577	A2M	O4'-C4'-C5'-O5'
4	A3	1632	PSU	O4'-C1'-C5-C6
4	A3	4382	PSU	O4'-C1'-C5-C6
4	A3	3550	UY1	O4'-C1'-C5-C6
4	A3	2194	OMC	C2'-C1'-N1-C2
4	A3	1720	PSU	O4'-C4'-C5'-O5'
4	A3	2194	OMC	O4'-C4'-C5'-O5'
4	A3	3517	A2M	C3'-C4'-C5'-O5'
4	A3	3631	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A1	1245	PSU	C3'-C4'-C5'-O5'
4	A3	3619	OMC	C4'-C5'-O5'-P
2	A1	210	PSU	O4'-C4'-C5'-O5'
2	A1	437	OMG	C3'-C4'-C5'-O5'
2	A1	669	A2M	O4'-C1'-N9-C8
13	D3	216	V5N	O-C-CA-CB
10	C3	75	OMG	C4'-C5'-O5'-P
29	K1	14	1MA	C4'-C5'-O5'-P
2	A1	1249	B8N	N34-C33-C34-O36

There are no ring outliers.

61 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A1	485	A2M	1	0
2	A1	1640	G7M	1	0
2	A1	1392	OMC	1	0
2	A1	669	A2M	1	0
2	A1	1338	4AC	2	0
4	A3	4203	PSU	1	0
2	A1	1833	6MZ	1	0
4	A3	1638	PSU	1	0
2	A1	682	PSU	1	0
2	A1	1289	OMU	1	0
4	A3	4364	OMG	1	0
4	A3	2267	OMG	1	0
10	C3	75	OMG	1	0
2	A1	469	A2M	1	0
2	A1	27	A2M	2	0
2	A1	1384	A2M	1	0
2	A1	121	OMU	1	0
4	A3	1810	A2M	1	0
4	A3	2658	A2M	2	0
2	A1	159	A2M	2	0
2	A1	1233	PSU	2	0
2	A1	650	PSU	1	0
4	A3	1580	OMG	1	0
2	A1	99	A2M	3	0
2	A1	1446	PSU	1	0
29	K1	16	H2U	2	0
4	A3	3450	A2M	3	0
4	A3	3456	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A3	4099	PSU	1	0
4	A3	3540	OMC	1	0
4	A3	1489	A2M	2	0
4	A3	4383	OMG	2	0
4	A3	4276	UR3	1	0
29	K1	32	OMU	1	0
4	A3	4193	5MC	1	0
29	K1	39	OMU	1	0
4	A3	4138	OMG	2	0
4	A3	3599	A2M	4	0
4	A3	2194	OMC	1	0
4	A3	4269	A2M	2	0
2	A1	463	OMC	1	0
4	A3	1479	A2M	2	0
4	A3	400	A2M	1	0
2	A1	1032	A2M	1	0
4	A3	3490	PSU	1	0
4	A3	2206	A2M	2	0
2	A1	1843	4AC	1	0
4	A3	1284	OMC	1	0
29	K1	4	OMC	1	0
2	A1	1679	A2M	1	0
4	A3	2207	OMG	1	0
4	A3	4177	PSU	1	0
4	A3	4366	OMU	1	0
4	A3	2258	OMU	1	0
4	A3	3657	OMU	1	0
2	A1	610	PSU	1	0
2	A1	577	A2M	2	0
4	A3	1491	PSU	1	0
2	A1	429	OMU	1	0
2	A1	116	OMU	1	0
4	A3	3676	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 417 ligands modelled in this entry, 412 are monoatomic - leaving 5 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	$\# Z > 2$
94	SF4	q2	601	88	0,12,12	-	-	-		
92	SPD	A3	5161	-	9,9,9	0.32	0	8,8,8	0.83	0
92	SPD	A3	5160	-	9,9,9	0.34	0	8,8,8	0.80	0
93	GTP	B3	201	7	30,34,34	1.53	5 (16%)	46,54,54	1.43	6 (13%)
94	SF4	q2	602	88	0,12,12	-	-	-		

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
94	SF4	q2	601	88	-	-	0/6/5/5
92	SPD	A3	5161	-	-	4/7/7/7	-
92	SPD	A3	5160	-	-	2/7/7/7	-
93	GTP	B3	201	7	-	2/22/38/38	0/3/3/3
94	SF4	q2	602	88	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
93	B3	201	GTP	PA-O5'	5.63	1.82	1.59
93	B3	201	GTP	O5'-C5'	-2.55	1.35	1.44
93	B3	201	GTP	C4-N3	2.21	1.39	1.34
93	B3	201	GTP	C8-N9	2.08	1.42	1.37
93	B3	201	GTP	C2-N2	2.04	1.39	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	B3	201	GTP	O5'-PA-O1A	-3.78	94.30	109.07
93	B3	201	GTP	C3'-C2'-C1'	-2.46	96.75	101.43
93	B3	201	GTP	C2-N1-C6	-2.45	120.63	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	B3	201	GTP	O6-C6-N1	-2.44	115.44	120.12
93	B3	201	GTP	N1-C2-N3	2.32	127.66	123.32
93	B3	201	GTP	O2A-PA-O5'	-2.29	97.12	107.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

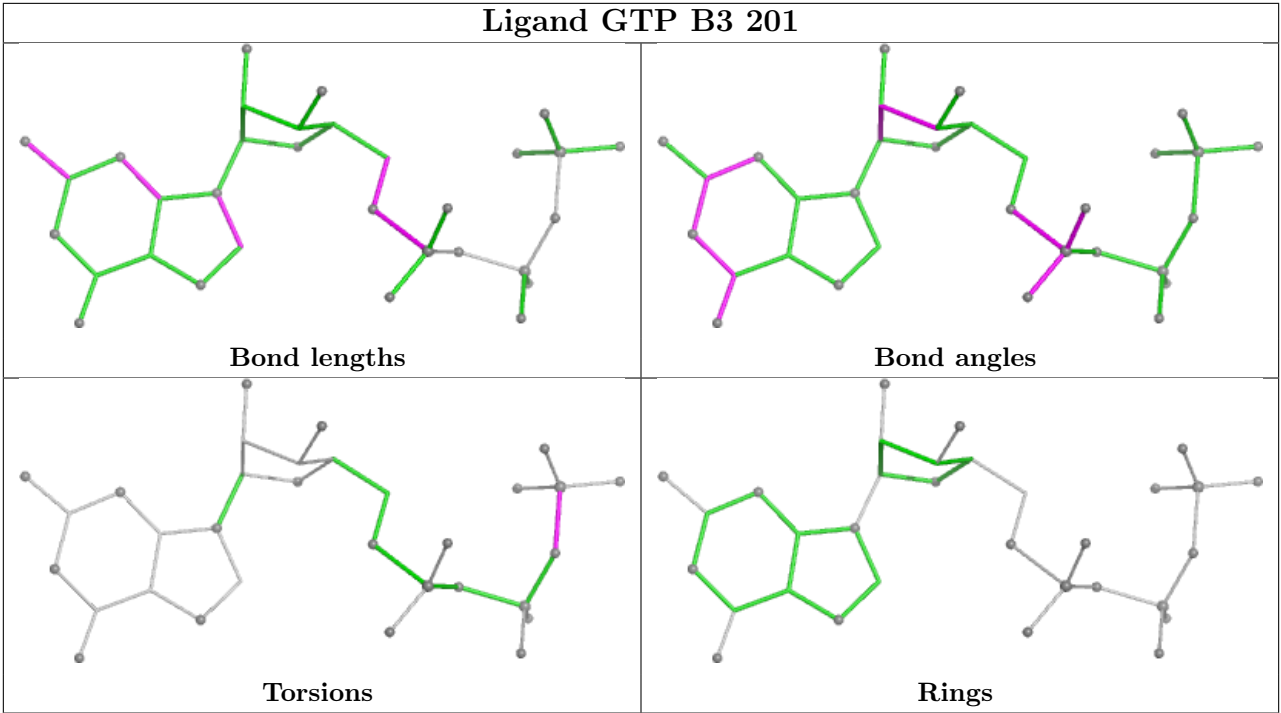
Mol	Chain	Res	Type	Atoms
93	B3	201	GTP	PB-O3B-PG-O3G
92	A3	5160	SPD	N6-C7-C8-C9
92	A3	5161	SPD	N6-C7-C8-C9
92	A3	5161	SPD	C7-C8-C9-N10
92	A3	5160	SPD	C3-C4-C5-N6
92	A3	5161	SPD	C2-C3-C4-C5
92	A3	5161	SPD	N1-C2-C3-C4
93	B3	201	GTP	PB-O3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	A3	5161	SPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
29	K1	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K1	16:H2U	O3'	18:G	P	1.95
1	K1	46:A	O3'	48:C	P	1.95

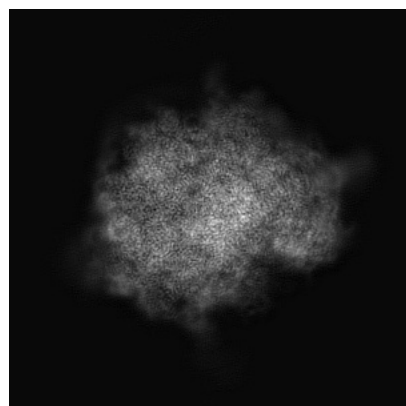
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53976. These allow visual inspection of the internal detail of the map and identification of artifacts.

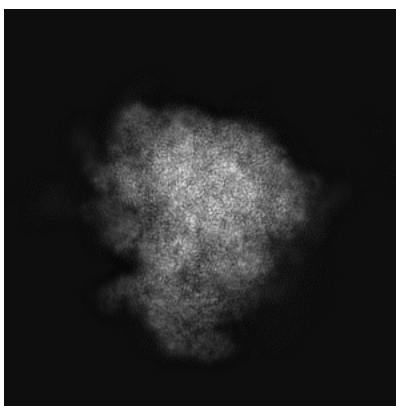
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

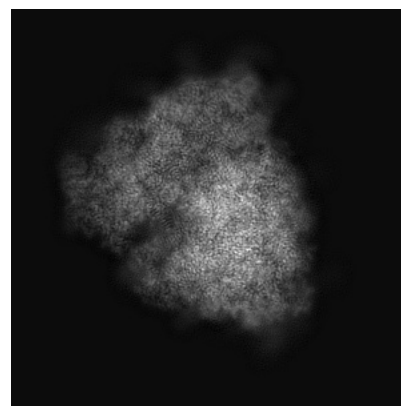
6.1.1 Primary map



X

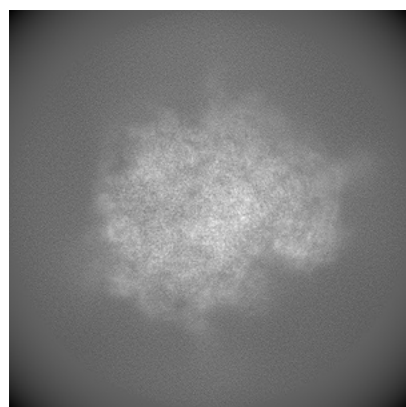


Y

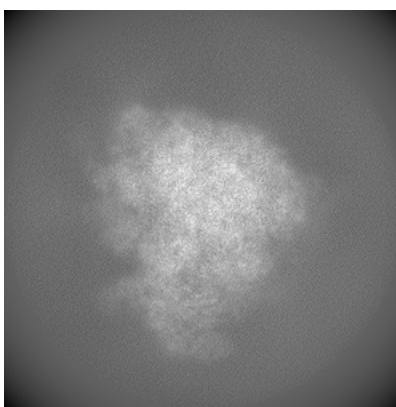


Z

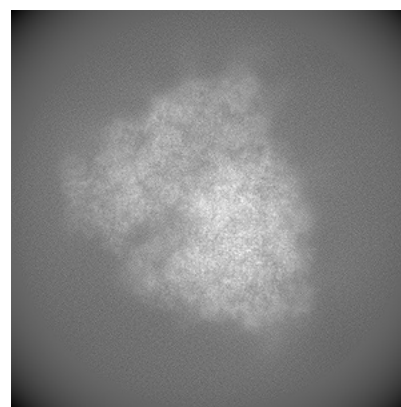
6.1.2 Raw map



X



Y

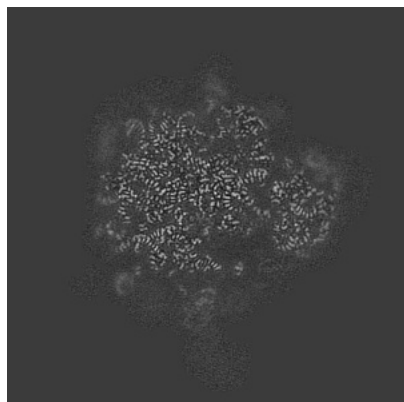


Z

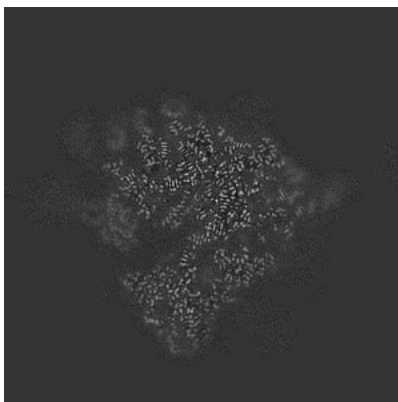
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

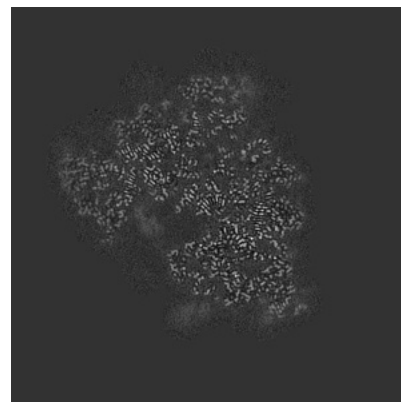
6.2.1 Primary map



X Index: 300

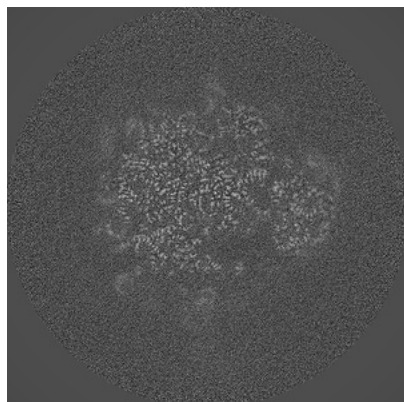


Y Index: 300

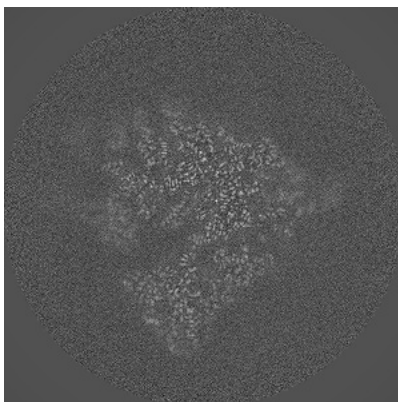


Z Index: 300

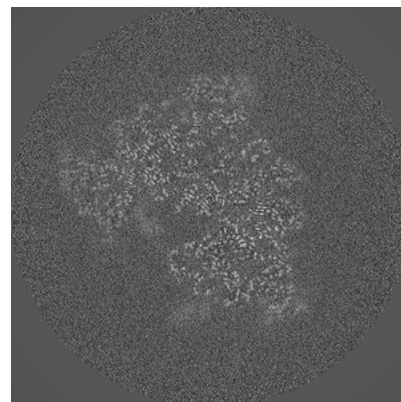
6.2.2 Raw map



X Index: 300



Y Index: 300

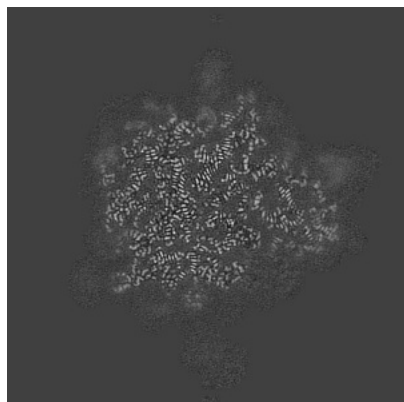


Z Index: 300

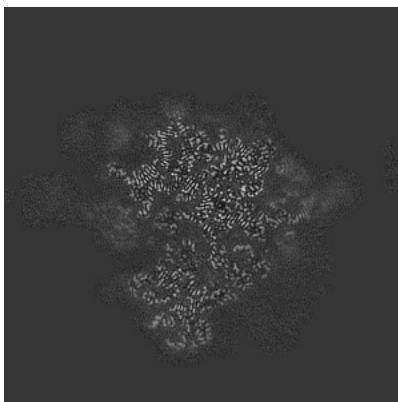
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

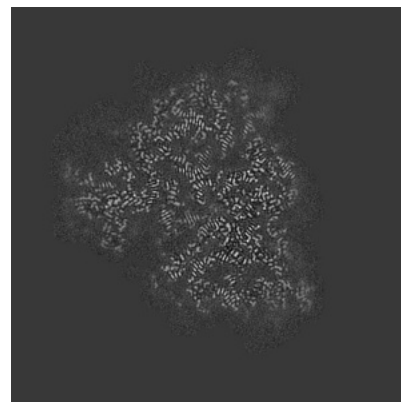
6.3.1 Primary map



X Index: 322

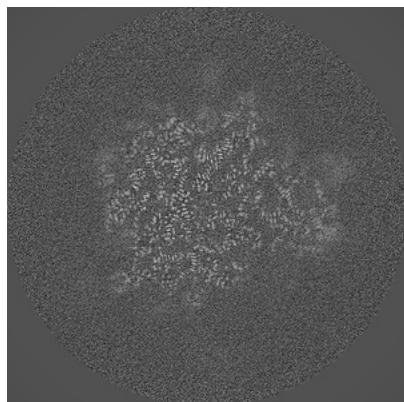


Y Index: 309

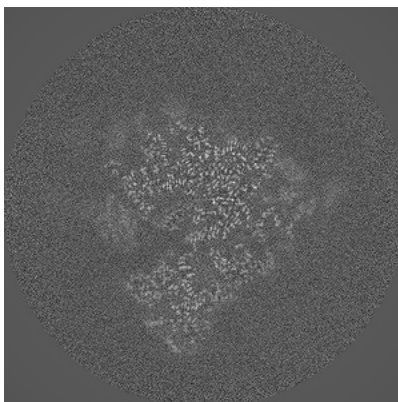


Z Index: 281

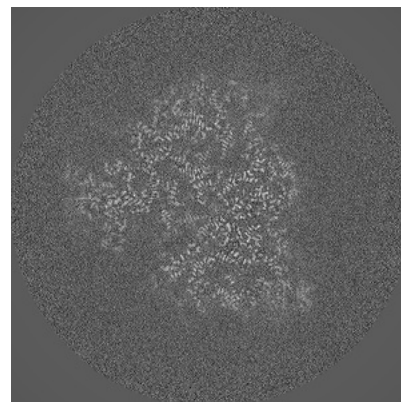
6.3.2 Raw map



X Index: 323



Y Index: 303

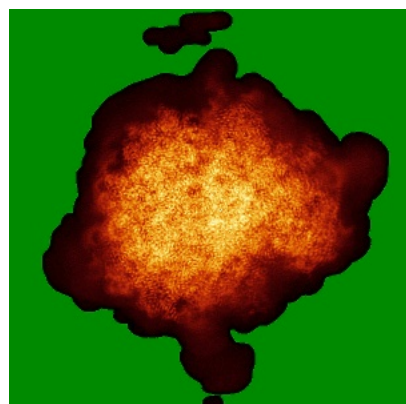


Z Index: 281

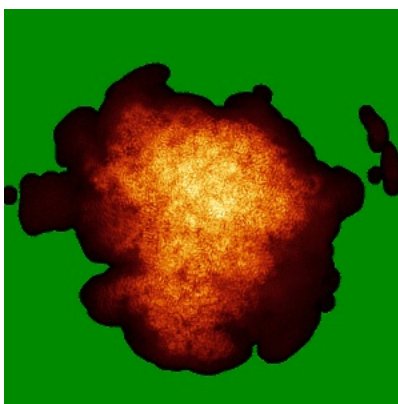
The images above show the largest variance slices of the map in three orthogonal directions.

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

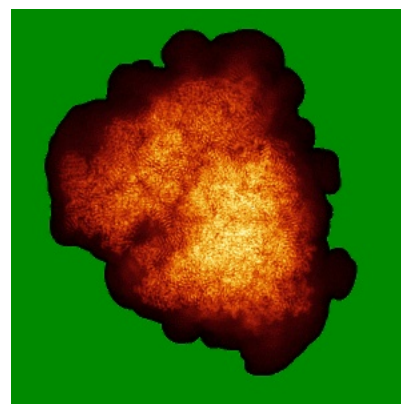
6.4.1 Primary map



X

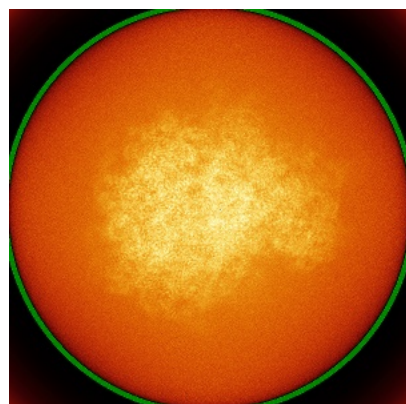


Y

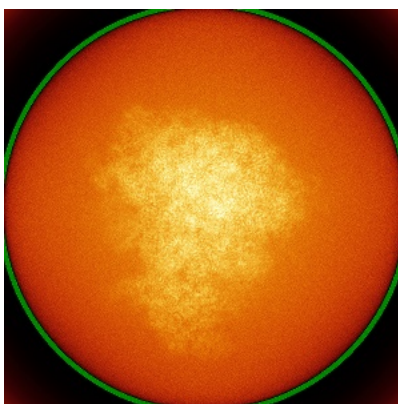


Z

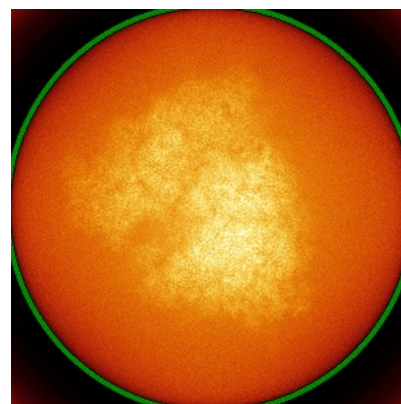
6.4.2 Raw map



X



Y

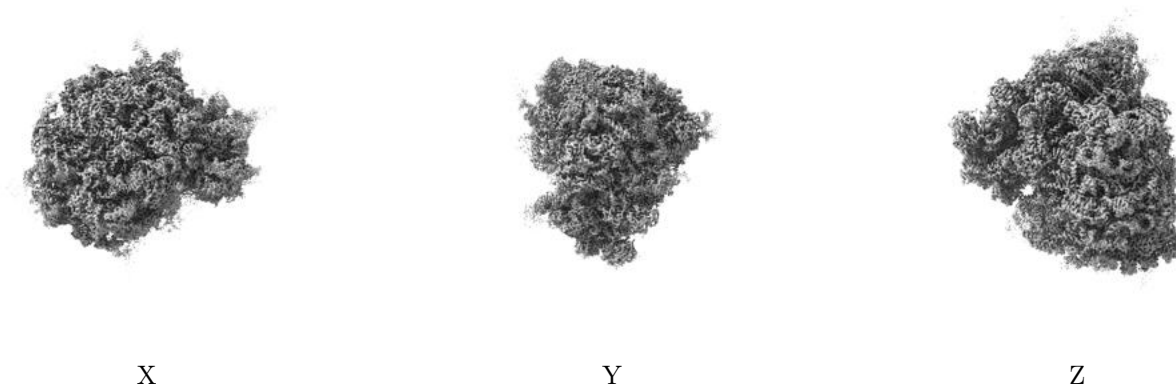


Z

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.

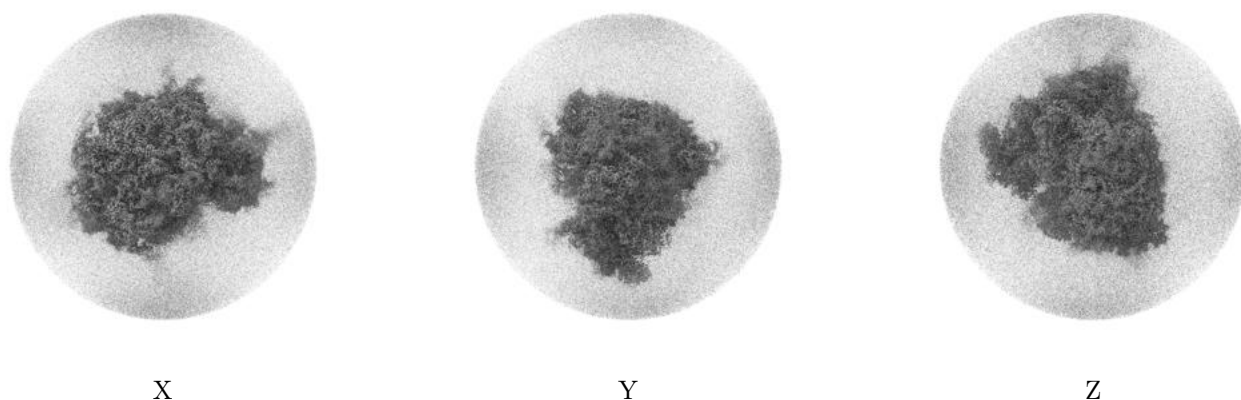
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

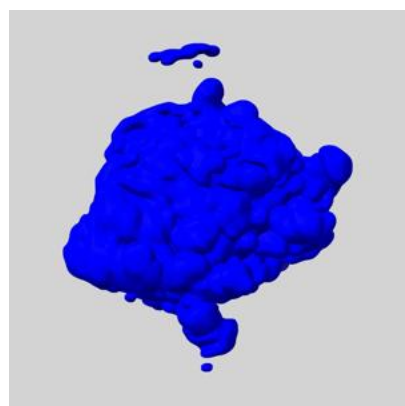
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

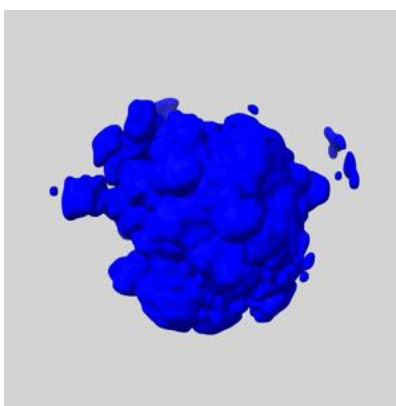
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

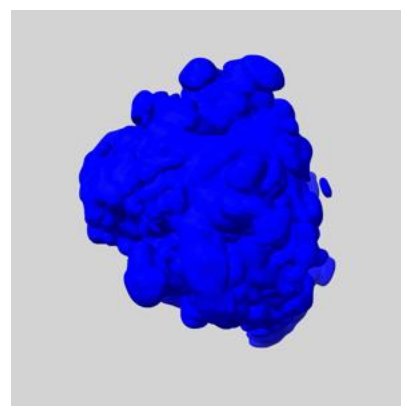
6.6.1 emd_53976_msk_1.map [i](#)



X



Y

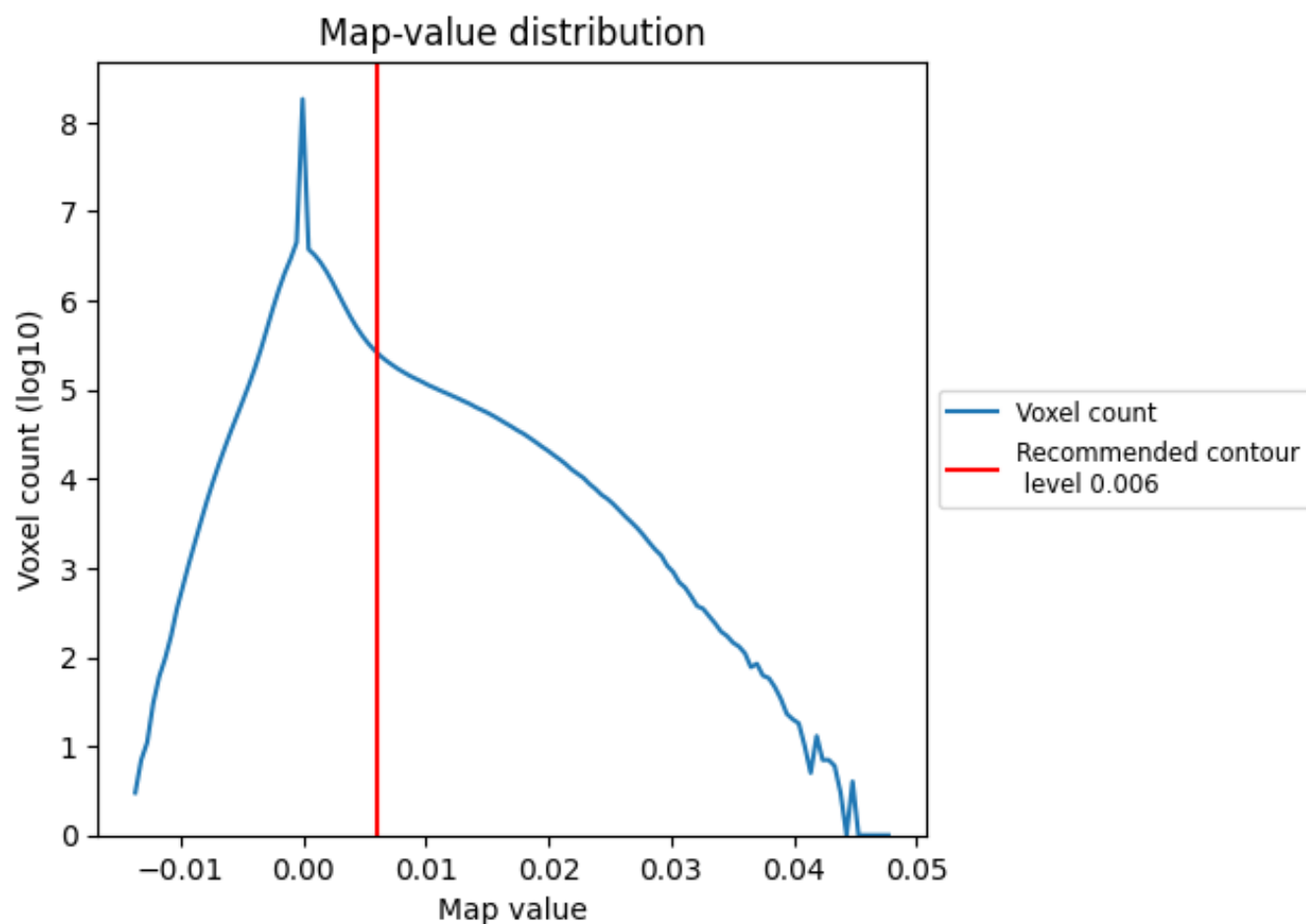


Z

7 Map analysis [i](#)

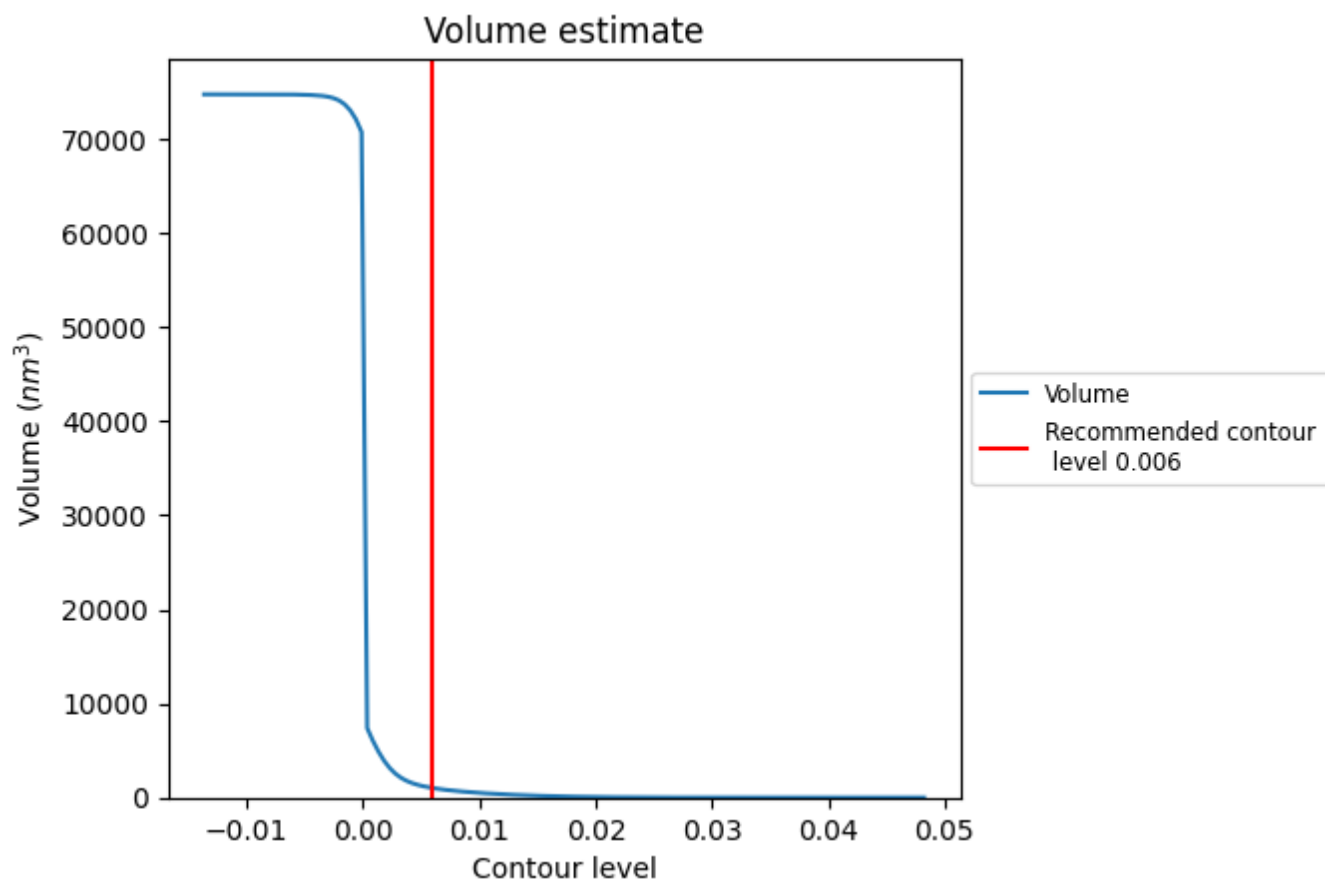
This section contains the results of statistical analysis of the map.

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.

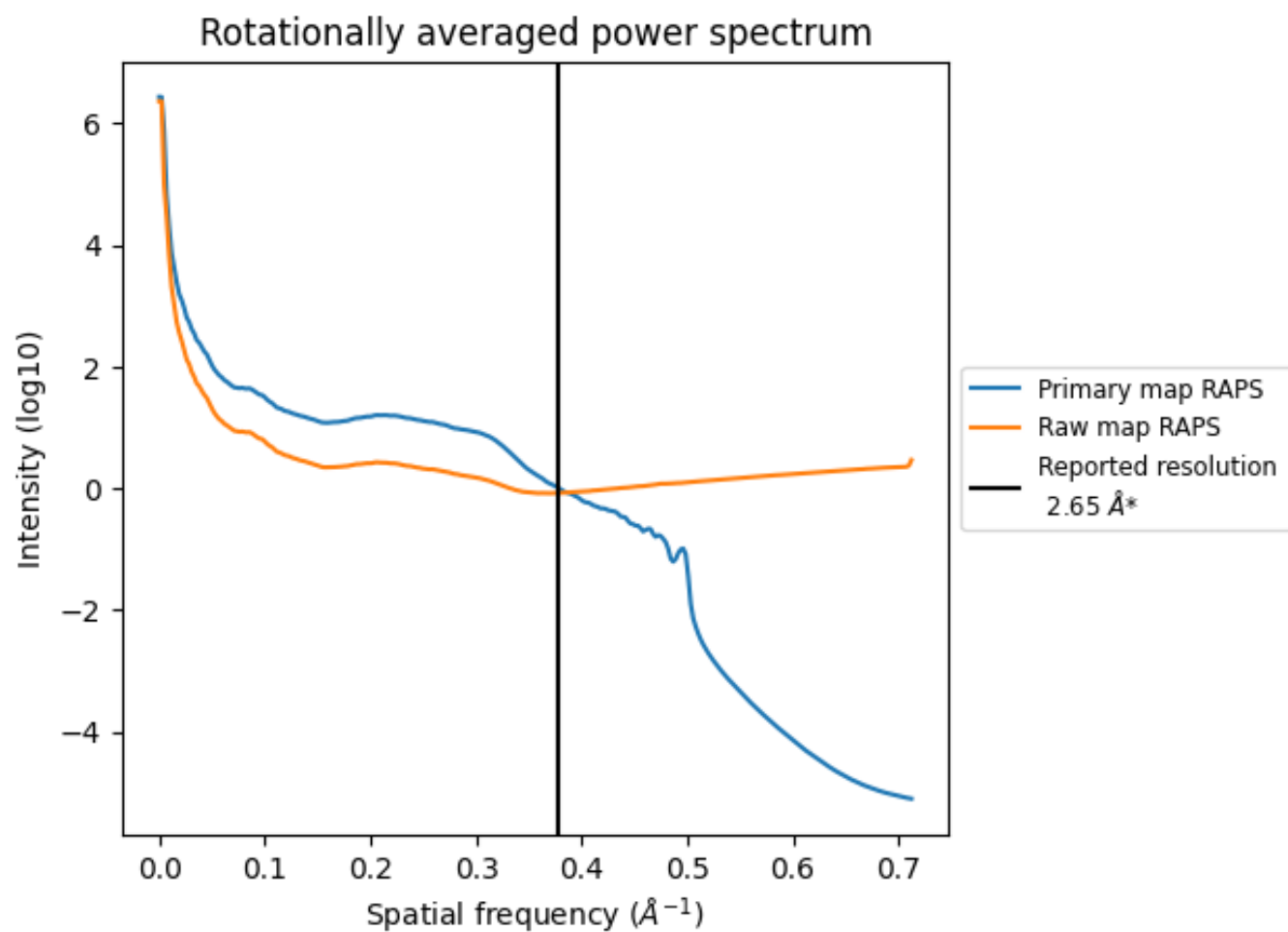
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1010 nm^3 ; this corresponds to an approximate mass of 913 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 ⓘ

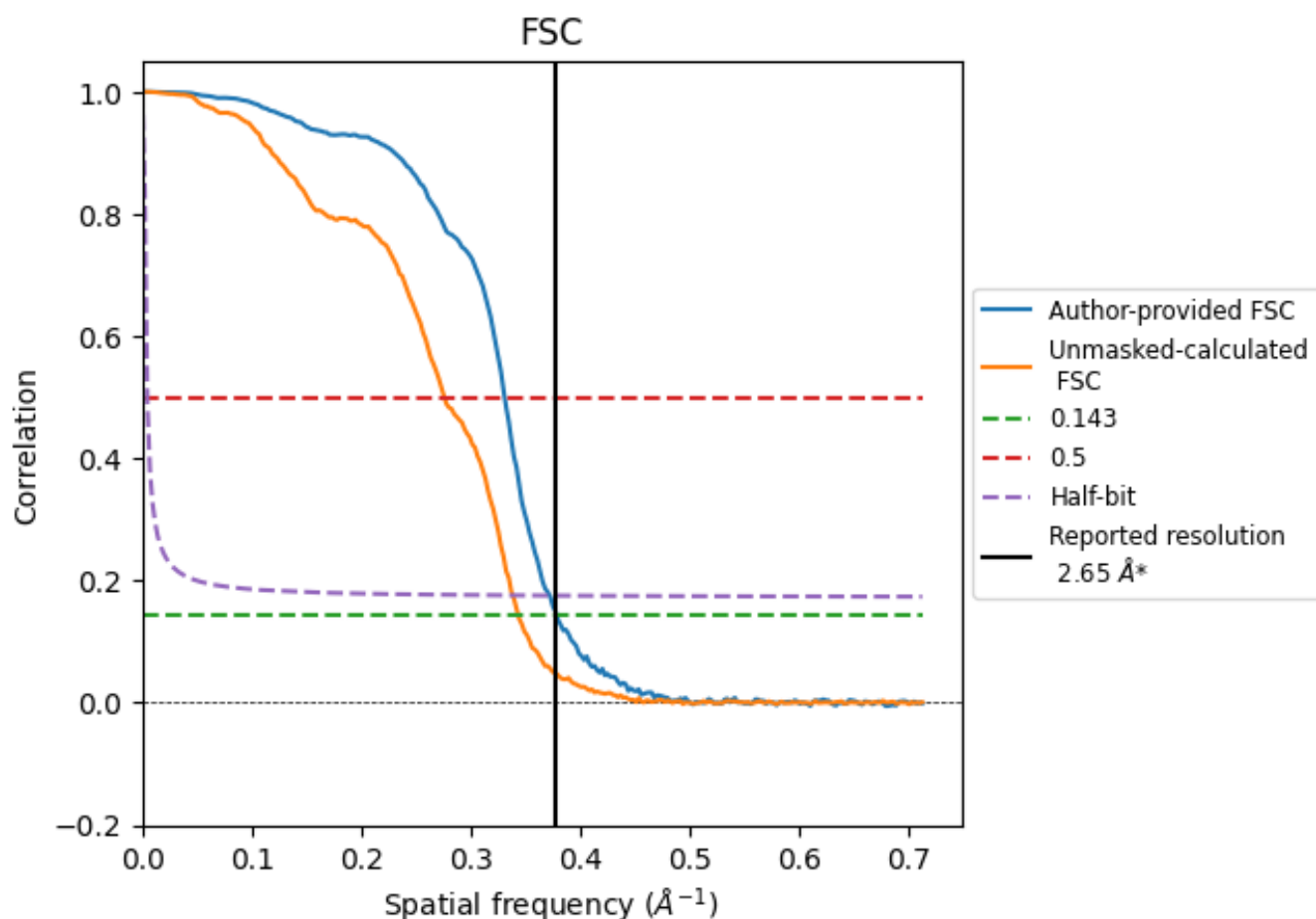


*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.377 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

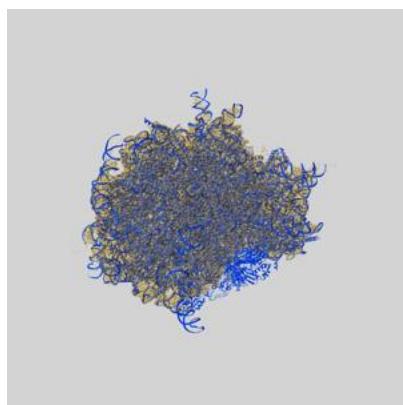
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.64	3.02	2.69
Unmasked-calculated*	2.91	3.62	2.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

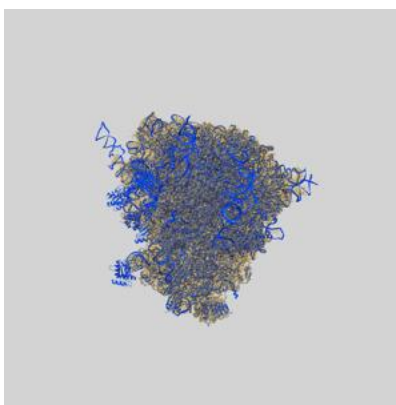
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53976 and PDB model 9RHU. Per-residue inclusion information can be found in section [3](#) on page [26](#).

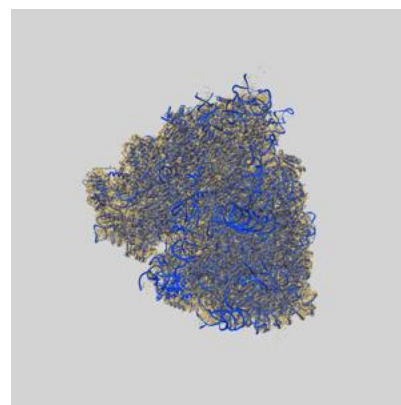
9.1 Map-model overlay [i](#)



X



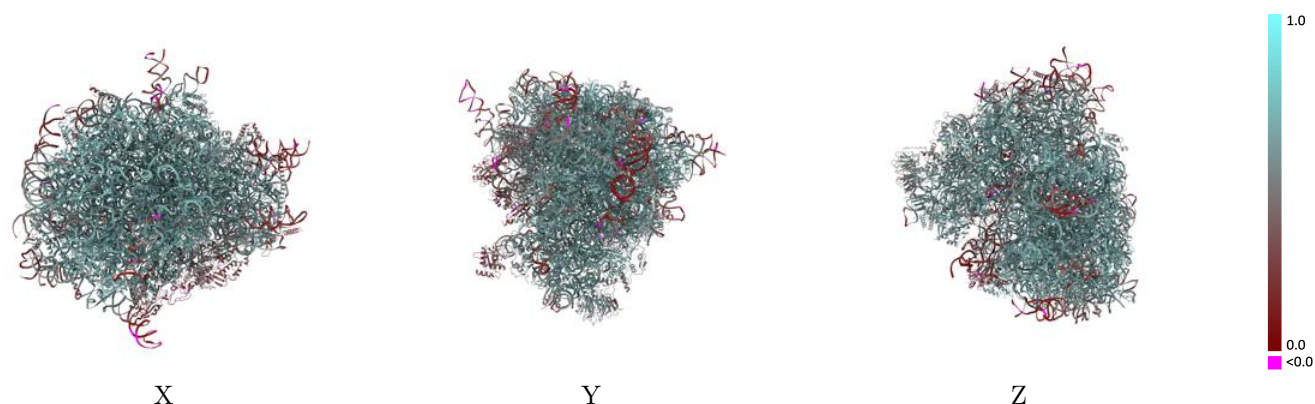
Y



Z

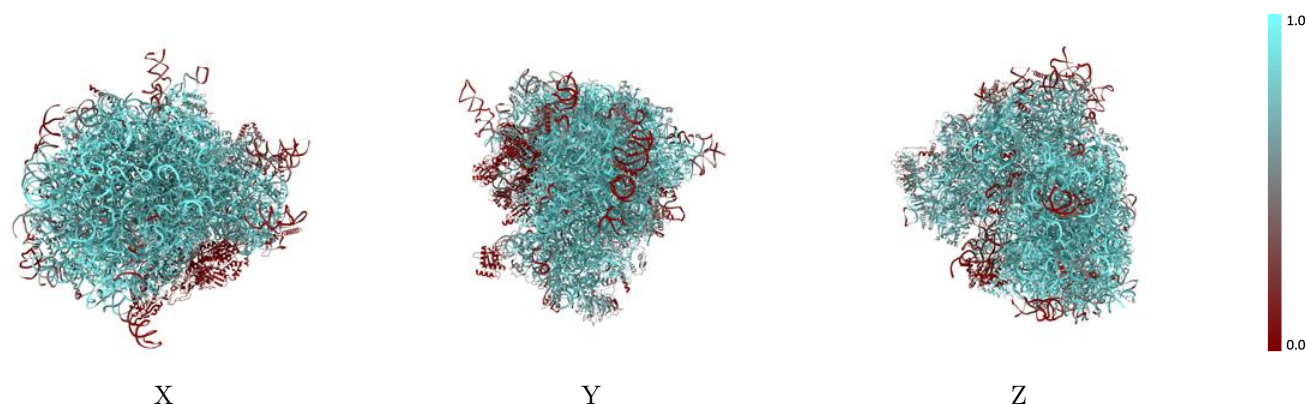
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



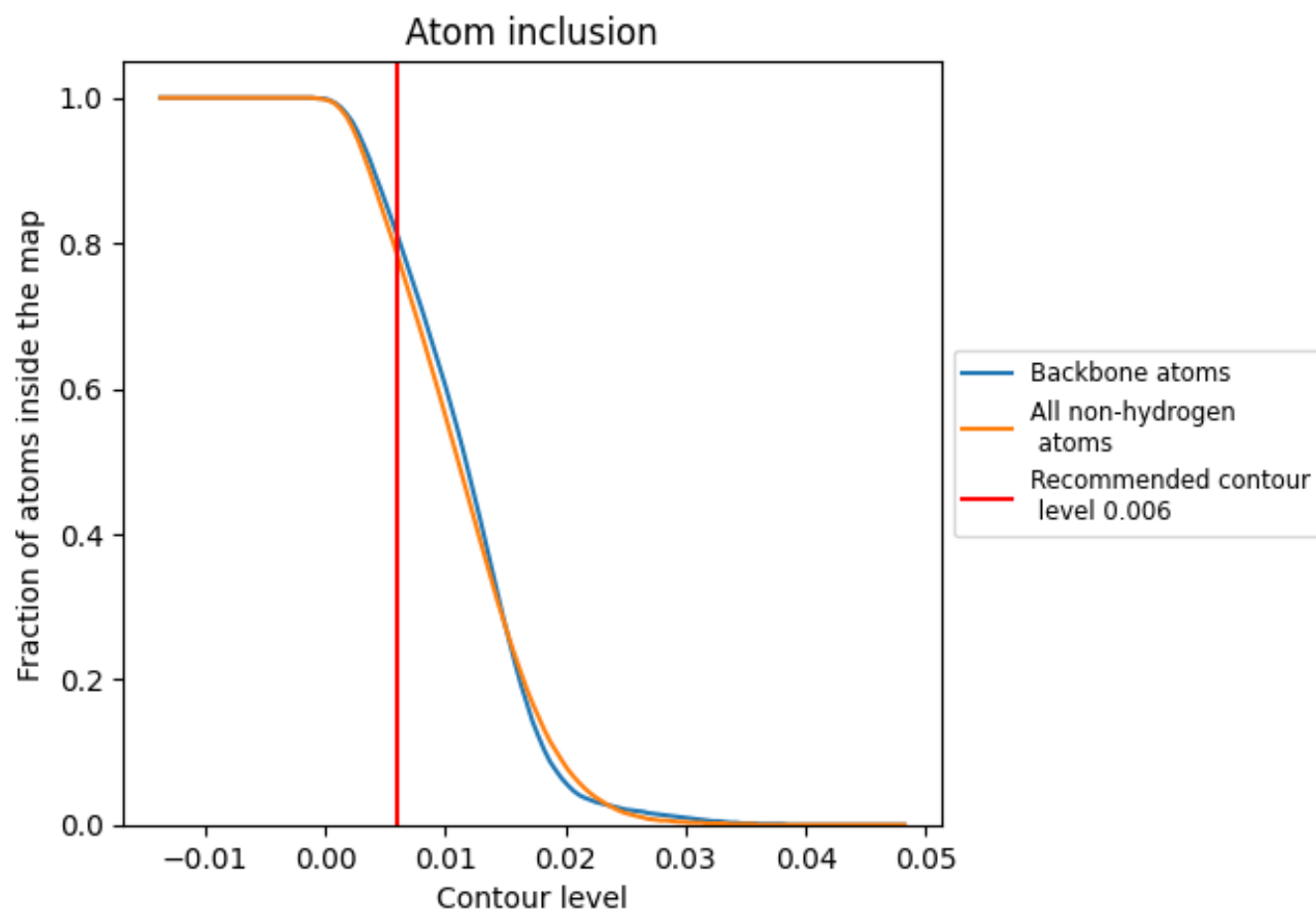
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 78% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.5850
A1	 0.8370	 0.5770
A2	 0.7420	 0.5900
A3	 0.8460	 0.5900
B1	 0.6980	 0.5850
B2	 0.9230	 0.6750
B3	 0.9770	 0.6570
C1	 0.7070	 0.5880
C2	 0.7550	 0.5970
C3	 0.9100	 0.6260
D1	 0.0850	 0.3660
D2	 0.8290	 0.6310
D3	 0.9240	 0.6770
E1	 0.6290	 0.5670
E2	 0.8510	 0.6420
E3	 0.8940	 0.6600
F1	 0.8240	 0.6230
F2	 0.8030	 0.6210
F3	 0.9160	 0.6610
G1	 0.5450	 0.5060
G2	 0.4430	 0.4950
G3	 0.8560	 0.6320
H1	 0.8740	 0.6320
H2	 0.8480	 0.6340
I1	 0.7370	 0.5550
I2	 0.8780	 0.6400
J1	 0.3300	 0.3500
J2	 0.9700	 0.6840
K1	 0.9240	 0.6170
K2	 0.9190	 0.6680
L1	 0.7640	 0.5960
L2	 0.8800	 0.6600
M1	 0.7620	 0.6100
M2	 0.9340	 0.6750
MB	 0.8590	 0.6410



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Chain	Atom inclusion	Q-score
N1	 0.8240	 0.6240
N2	 0.8190	 0.6210
O1	 0.6550	 0.5650
O2	 0.9230	 0.6670
P1	 0.8290	 0.6100
P2	 0.8560	 0.6430
Q1	 0.7740	 0.6040
Q2	 0.6730	 0.5580
R1	 0.5380	 0.4720
R2	 0.8580	 0.6570
S1	 0.4980	 0.5040
S2	 0.5020	 0.4870
T1	 0.7840	 0.6050
T2	 0.8530	 0.6330
U1	 0.7770	 0.5950
U2	 0.8630	 0.6300
V1	 0.6430	 0.5490
V2	 0.8520	 0.6390
W1	 0.7850	 0.6070
W2	 0.9420	 0.6770
X1	 0.0240	 0.2890
X2	 0.6900	 0.5760
Y1	 0.8370	 0.6300
Y2	 0.7590	 0.5850
Z1	 0.8230	 0.6250
Z2	 0.8450	 0.6380
a1	 0.6610	 0.5690
a2	 0.9130	 0.6720
b1	 0.7910	 0.6070
b2	 0.9470	 0.6800
c1	 0.6220	 0.5450
d1	 0.7500	 0.5950
d2	 0.8410	 0.6350
e1	 0.7860	 0.6030
e2	 0.8130	 0.6170
f1	 0.6090	 0.5330
f2	 0.9500	 0.6760
g1	 0.7420	 0.6040
g2	 0.6590	 0.5720
h1	 0.8870	 0.6450
h2	 0.9020	 0.6450
i1	 0.8670	 0.6440

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Chain	Atom inclusion	Q-score
i2	 0.8740	 0.6440
j1	 0.7010	 0.5710
j2	 0.8680	 0.6630
k1	 0.6880	 0.5850
k2	 0.8720	 0.6560
l1	 0.8760	 0.6510
l2	 0.9110	 0.6560
m2	 0.0220	 0.2620
n2	 0.0820	 0.3120
o2	 0.0180	 0.2240
p2	 0.5290	 0.5010
q2	 0.0150	 0.4050