



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:04 AM UTC

PDB ID : 8A3W / pdb_00008a3w
EMDB ID : EMD-15124
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :
WILD TYPE
Authors : Rajan, K.S.; Yonath, A.; Bashan, A.
Deposited on : 2022-06-09
Resolution : 2.89 Å (reported)
Based on initial models : 6AZ1, 6AZ3, 5T2A

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

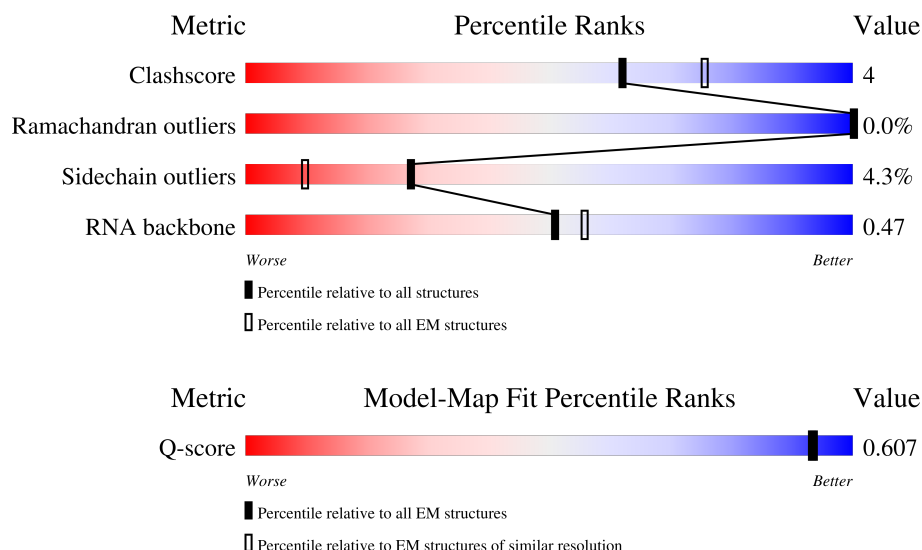
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.89 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.



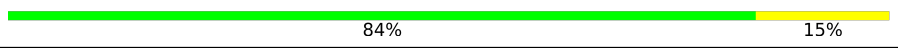
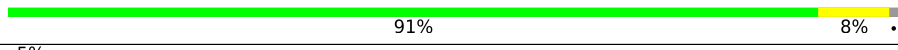
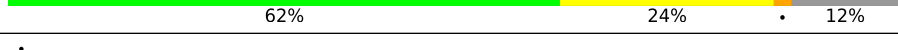
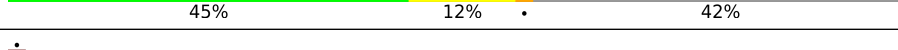
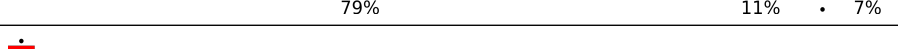
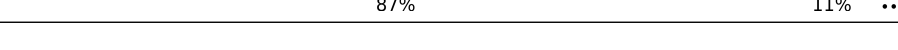
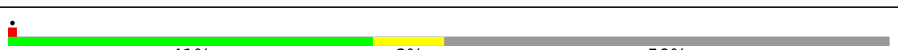
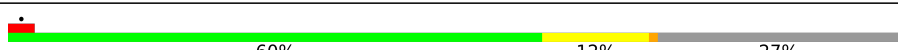
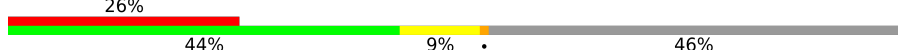
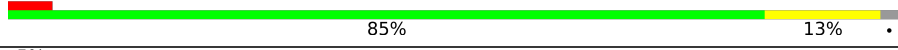
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12148 (2.39 - 3.39)

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	SD	190	
2	SE	273	
3	SF	265	

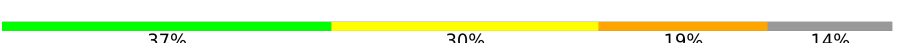
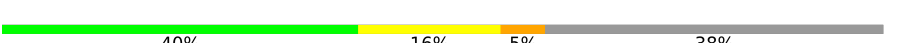
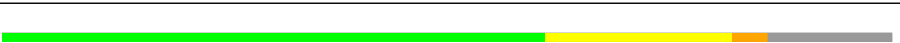
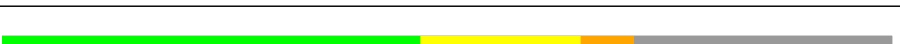
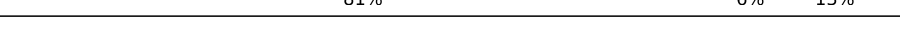
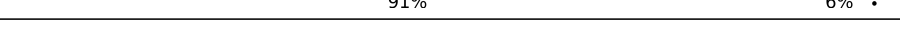
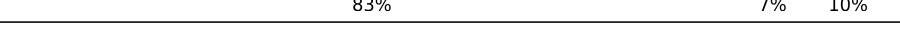
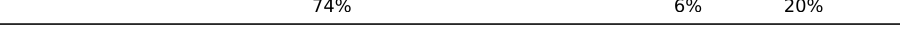
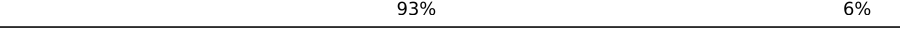
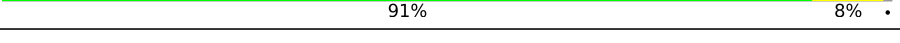
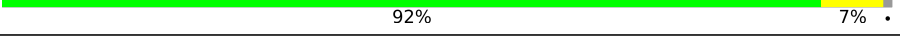
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Mol	Chain	Length	Quality of chain
4	SG	249	
5	SH	190	
6	SI	200	
7	SJ	130	
8	SK	220	
9	SL	149	
10	SM	116	
11	SN	168	
12	SO	144	
13	SP	143	
14	SR	153	
15	SS	57	
16	ST	151	
17	SU	173	
18	SV	143	
19	SW	152	
20	SX	161	
21	SY	164	
22	SZ	137	
23	Sa	120	
24	Sb	112	
25	Sc	86	
26	Sd	87	
27	Se	66	
28	Sg	312	

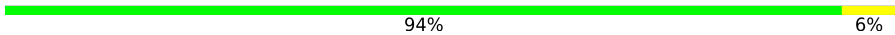
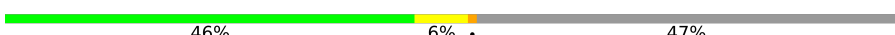
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Mol	Chain	Length	Quality of chain
29	S1	2204	
30	SA	264	
31	SB	246	
32	SC	219	
33	Sh	235	
34	S4	20	
35	8	123	
36	6	73	
37	2	1522	
38	7	171	
39	5	135	
40	4	183	
41	3	216	
42	1	1782	
43	B	419	
44	C	373	
45	A	260	
46	c	252	
47	O	305	
48	M	204	
49	H	222	
50	G	264	
51	P	198	
52	R	179	
53	I	220	

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Mol	Chain	Length	Quality of chain
54	Q	254	
55	T	166	
56	S	159	
57	L	145	
58	F	195	
59	E	190	
60	Y	134	
61	f	133	
62	g	144	
63	a	127	
64	J	139	
65	W	143	
66	V	145	
67	h	168	
68	Z	147	
69	K	175	
70	j	83	
71	i	105	
72	U	129	
73	p	106	
74	o	92	
75	D	188	
76	d	104	
77	X	124	
78	b	70	

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Mol	Chain	Length	Quality of chain
79	k	83	72%13%14%
80	l	51	86%12%
81	n	34	44%74%26%
82	e	188	73%7%20%

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 183881 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 Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	SD	163	Total	C	N	O	S	1	0
			1347	852	266	221	8		

- Molecule 2 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SE	260	Total	C	N	O	S	2	0
			2060	1307	397	347	9		

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SF	205	Total	C	N	O	S	0	0
			1555	1000	279	267	9		

- Molecule 4 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SG	233	Total	C	N	O	S	1	0
			1810	1132	370	305	3		

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SH	183	Total	C	N	O	S	0	0
			1404	876	263	258	7		

- Molecule 6 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SI	199	Total	C	N	O	S	0	0
			1583	1010	301	265	7		

- Molecule 7 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SJ	129	Total	C	N	O	S	0	0
			1017	644	188	177	8		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SK	184	Total	C	N	O	S	0	0
			1453	912	307	232	2		

- Molecule 9 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SL	142	Total	C	N	O	S	0	0
			1112	715	205	189	3		

- Molecule 10 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SM	102	Total	C	N	O	S	2	0
			807	503	150	152	2		

- Molecule 11 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SN	98	Total	C	N	O	S	0	0
			791	507	139	138	7		

- Molecule 12 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SO	134	Total	C	N	O	S	0	0
			975	602	192	174	7		

- Molecule 13 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SP	142	Total	C	N	O	S	3	0
			1119	706	223	187	3		

- Molecule 14 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SR	135	Total	C	N	O	S	1	0
			1077	681	212	180	4		

- Molecule 15 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SS	54	Total	C	N	O	S	0	0
			417	257	84	71	5		

- Molecule 16 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	ST	140	Total	C	N	O	S	0	0
			1140	720	227	185	8		

- Molecule 17 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SU	154	Total	C	N	O	S	0	0
			1218	771	241	201	5		

- Molecule 18 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SV	71	Total	C	N	O	S	0	0
			577	368	110	97	2		

- Molecule 19 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SW	111	Total	C	N	O	S	0	0
			866	553	164	145	4		

- Molecule 20 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SX	140	Total	C	N	O	S	0	0
			1092	694	211	183	4		

- Molecule 21 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SY	88	Total	C	N	O	S	0	0
			622	382	116	121	3		

- Molecule 22 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SZ	122	Total	C	N	O	S	0	0
			972	623	187	160	2		

- Molecule 23 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sa	70	Total	C	N	O	S	0	0
			549	351	97	98	3		

- Molecule 24 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Sb	84	Total	C	N	O	S	0	0
			661	410	138	106	7		

- Molecule 25 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Sc	84	Total	C	N	O	S	0	0
			624	390	118	112	4		

- Molecule 26 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Sd	54	Total	C	N	O	S	0	0
			390	240	80	66	4		

- Molecule 27 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Se	46	Total	C	N	O	S	0	0
			350	221	71	57	1		

- Molecule 28 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sg	290	Total	C	N	O	S	1	0
			2173	1369	381	411	12		

- Molecule 29 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S1	1663	Total	C	N	O	P	0	0
			35569	15906	6433	11567	1663		

- Molecule 30 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SA	204	Total	C	N	O	S	1	0
			1653	1043	314	287	9		

- Molecule 31 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SB	210	Total	C	N	O	S	0	0
			1595	1015	281	287	12		

- Molecule 32 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SC	202	Total	C	N	O	S	1	0
			1525	974	272	266	13		

- Molecule 33 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sh	95	Total	C	N	O	S	0	0
			668	413	128	125	2		

- Molecule 34 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S4	17	Total	C	N	O	P	0	0
			359	161	66	116	16		

- Molecule 35 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	119	Total	C	N	O	P	0	0
			2531	1132	452	828	119		

- Molecule 36 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	6	63	Total	C	N	O	P	0	0
			1329	595	238	433	63		

- Molecule 37 is a RNA chain called LSub_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	2	947	Total	C	N	O	P	0	0
			20228	9057	3635	6589	947		

- Molecule 38 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	7	163	Total	C	N	O	P	0	0
			3463	1551	613	1137	162		

- Molecule 39 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5	98	Total	C	N	O	P	0	0
			2096	934	381	683	98		

- Molecule 40 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4	158	Total	C	N	O	P	0	0
			3378	1507	611	1102	158		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	4	G	A	conflict	GB 321438308

- Molecule 41 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3	153	Total	C	N	O	P	0	0
			3252	1454	570	1075	153		

- Molecule 42 is a RNA chain called LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1	1467	Total	C	N	O	P	1	0
			31495	14076	5781	10171	1467		

- Molecule 43 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	B	395	Total	C	N	O	S	4	0
			2955	1874	575	494	12		

- Molecule 44 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	C	325	Total	C	N	O	S	0	0
			2343	1481	447	401	14		

- Molecule 45 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	A	254	Total	C	N	O	S	1	0
			1852	1153	375	314	10		

- Molecule 46 is a protein called uL30_chain_c.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	c	227	Total	C	N	O	S	0	0
			1779	1134	340	294	11		

- Molecule 47 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	O	243	Total	C	N	O	S	1	0
			1764	1130	333	298	3		

- Molecule 48 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	M	203	Total	C	N	O	S	0	0
			1692	1068	360	256	8		

- Molecule 49 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	H	220	Total	C	N	O	S	0	0
			1690	1071	340	272	7		

- Molecule 50 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	G	212	Total	C	N	O	S	0	0
			1635	1036	324	268	7		

- Molecule 51 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	P	196	Total	C	N	O	S	0	0
			1513	952	303	252	6		

- Molecule 52 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	R	178	Total	C	N	O	S	0	0
			1399	894	267	233	5		

- Molecule 53 is a protein called eL13_chain_I.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	I	169	Total	C	N	O	S	0	0
			1299	822	262	208	7		

- Molecule 54 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Q	168	Total	C	N	O	S	0	0
			1290	802	276	206	6		

- Molecule 55 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	T	152	Total	C	N	O	S	0	0
			1217	761	241	204	11		

- Molecule 56 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	S	151	Total	C	N	O	S	0	0
			1164	738	228	195	3		

- Molecule 57 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	L	144	Total	C	N	O	S	0	0
			1114	703	226	179	6		

- Molecule 58 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	F	142	Total	C	N	O	S	0	0
			1032	658	191	181	2		

- Molecule 59 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	E	148	Total	C	N	O	S	0	0
			1032	659	191	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Y	132	Total	C	N	O	S	0	0
			1008	649	198	159	2		

- Molecule 61 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	f	123	Total	C	N	O	S	0	0
			993	624	197	168	4		

- Molecule 62 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	g	124	Total	C	N	O	S	0	0
			989	618	207	159	5		

- Molecule 63 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	a	123	Total	C	N	O	S	0	0
			955	597	199	157	2		

- Molecule 64 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	J	129	Total	C	N	O	S	0	0
			933	590	174	163	6		

- Molecule 65 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	W	117	Total	C	N	O	S	0	0
			928	580	193	151	4		

- Molecule 66 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	V	118	Total	C	N	O	S	0	0
			917	582	174	159	2		

- Molecule 67 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	h	112	Total	C	N	O	S	0	0
			889	548	195	142	4		

- Molecule 68 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Z	120	Total	C	N	O	S	0	0
			892	548	182	157	5		

- Molecule 69 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	K	119	Total	C	N	O	S	0	0
			883	557	176	146	4		

- Molecule 70 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j	80	Total	C	N	O	S	0	0
			659	401	152	100	6		

- Molecule 71 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	i	86	Total	C	N	O	S	0	0
			660	421	133	104	2		

- Molecule 72 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	U	114	Total	C	N	O	S	0	0
			795	508	147	138	2		

- Molecule 73 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	p	83	Total	C	N	O	S	0	0
			640	410	126	102	2		

- Molecule 74 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	o	88	Total	C	N	O	S	0	0
			659	410	135	108	6		

- Molecule 75 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	D	100	Total	C	N	O	S	0	0
			649	406	129	109	5		

- Molecule 76 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	d	88	Total	C	N	O	S	0	0
			607	379	109	114	5		

- Molecule 77 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	X	64	Total	C	N	O	S	0	0
			548	359	105	80	4		

- Molecule 78 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	b	66	Total	C	N	O		0	0
			520	318	120	82			

- Molecule 79 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	k	71	Total	C	N	O	S	0	0
			508	323	96	86	3		

- Molecule 80 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	l	50	Total	C	N	O	S	0	0
			440	285	91	63	1		

- Molecule 81 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	n	25	Total	C	N	O		0	0
			159	97	36	26			

- Molecule 82 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	e	151	Total	C	N	O	S	0	0
			1103	698	210	193	2		

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
83	SD	1	Total 1	Mg 1	0
83	S1	30	Total 30	Mg 30	0
83	2	25	Total 25	Mg 25	0
83	7	2	Total 2	Mg 2	0
83	5	1	Total 1	Mg 1	0
83	3	1	Total 1	Mg 1	0
83	1	52	Total 52	Mg 52	0
83	C	1	Total 1	Mg 1	0
83	T	1	Total 1	Mg 1	0

- Molecule 84 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
84	SO	1	Total 1	Na 1	0
84	S1	23	Total 23	Na 23	0
84	2	9	Total 9	Na 9	0
84	4	1	Total 1	Na 1	0
84	1	22	Total 22	Na 22	0
84	J	1	Total 1	Na 1	0

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	SS	1	Total 1	Zn 1	0
85	Sb	1	Total 1	Zn 1	0
85	j	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
85	o	1	Total 1	Zn 1	0

- Molecule 86 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
86	Sb	1	Total 1	K 1	0
86	S1	4	Total 4	K 4	0
86	8	1	Total 1	K 1	0
86	2	3	Total 3	K 3	0
86	4	1	Total 1	K 1	0
86	1	3	Total 3	K 3	0

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
87	SH	1	Total 1	O 1	0
87	SN	2	Total 2	O 2	0
87	SR	1	Total 1	O 1	0
87	ST	1	Total 1	O 1	0
87	SX	1	Total 1	O 1	0
87	S1	36	Total 36	O 36	0
87	8	5	Total 5	O 5	0
87	6	1	Total 1	O 1	0
87	2	148	Total 148	O 148	0
87	7	40	Total 40	O 40	0

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Mol	Chain	Residues	Atoms		AltConf
87	5	19	Total 19	O 19	0
87	4	29	Total 29	O 29	0
87	3	17	Total 17	O 17	0
87	1	283	Total 283	O 283	0
87	B	9	Total 9	O 9	0
87	C	11	Total 11	O 11	0
87	A	10	Total 10	O 10	0
87	c	3	Total 3	O 3	0
87	M	9	Total 9	O 9	0
87	H	3	Total 3	O 3	0
87	G	3	Total 3	O 3	0
87	P	8	Total 8	O 8	0
87	R	1	Total 1	O 1	0
87	I	4	Total 4	O 4	0
87	Q	4	Total 4	O 4	0
87	T	7	Total 7	O 7	0
87	S	1	Total 1	O 1	0
87	L	3	Total 3	O 3	0
87	f	2	Total 2	O 2	0
87	g	1	Total 1	O 1	0
87	a	1	Total 1	O 1	0

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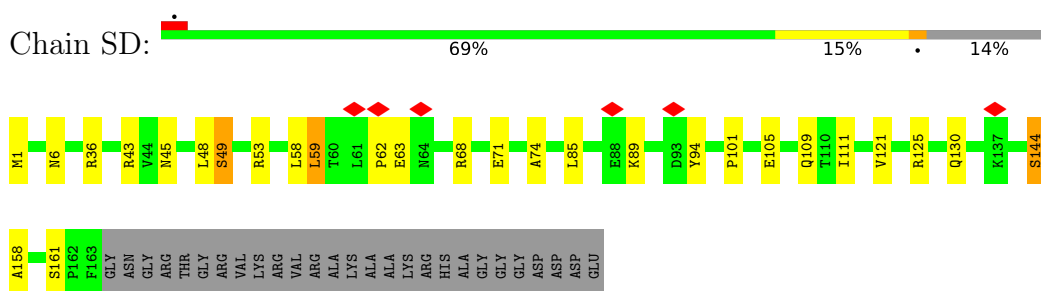
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Mol	Chain	Residues	Atoms		AltConf
87	J	1	Total 1	O 1	0
87	W	1	Total 1	O 1	0
87	V	2	Total 2	O 2	0
87	h	3	Total 3	O 3	0
87	j	7	Total 7	O 7	0
87	d	1	Total 1	O 1	0
87	X	1	Total 1	O 1	0
87	l	4	Total 4	O 4	0
87	e	3	Total 3	O 3	0

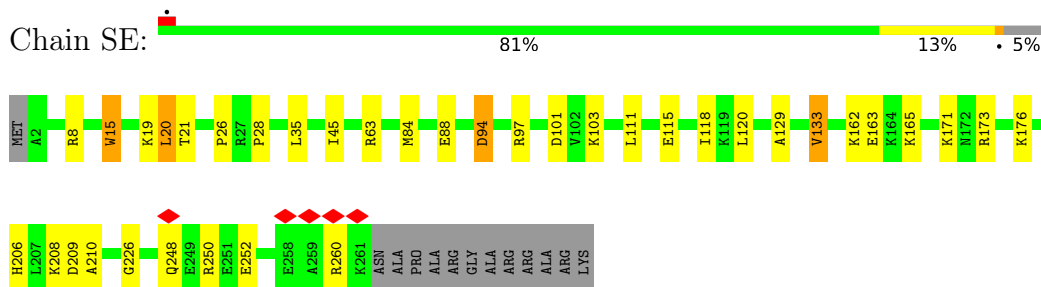
3 Residue-property plots

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.

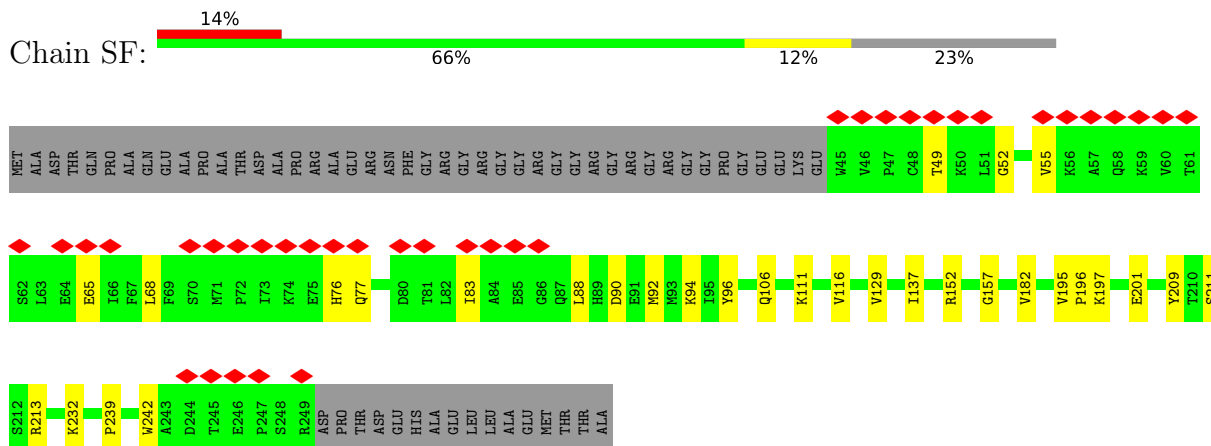
- Molecule 1: Putative 40S ribosomal protein S9



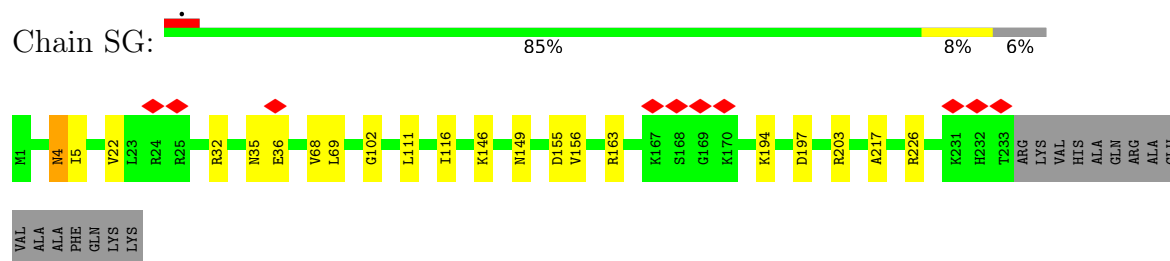
- Molecule 2: 40S ribosomal protein S4



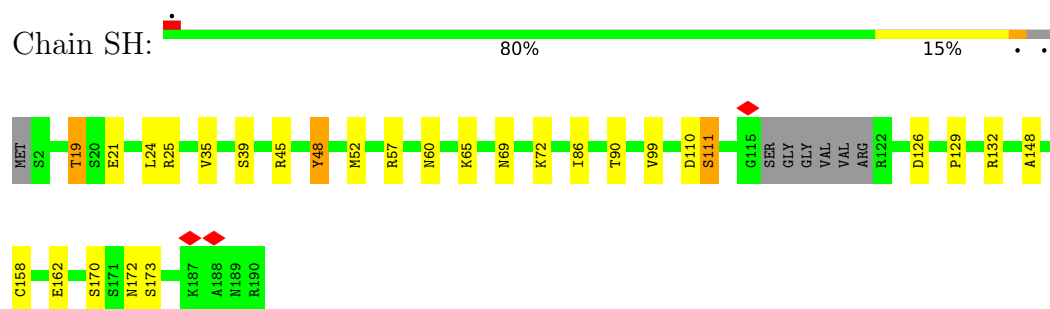
- Molecule 3: 40S ribosomal protein S2



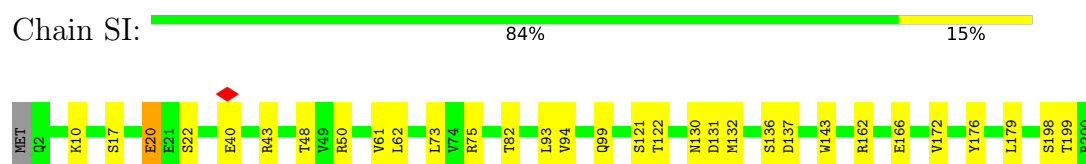
- Molecule 4: 40S ribosomal protein S6



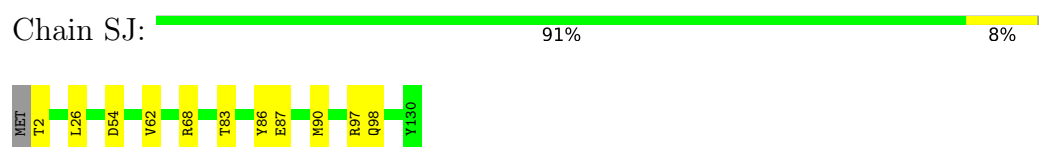
- Molecule 5: 40S ribosomal protein S5



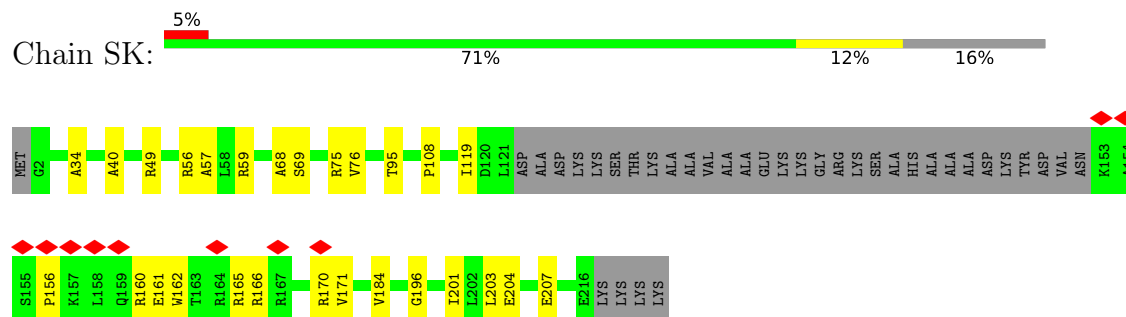
- Molecule 6: 40S ribosomal protein S7



- Molecule 7: Putative 40S ribosomal protein S15A

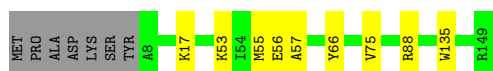


- Molecule 8: 40S ribosomal protein S8



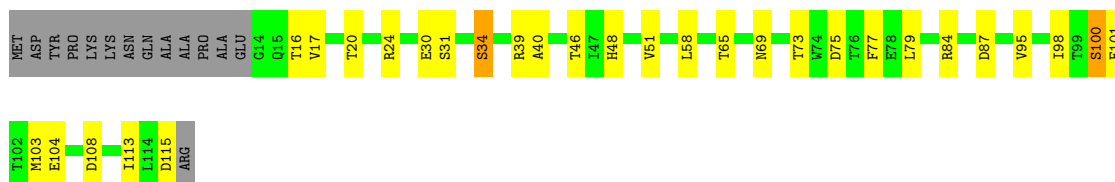
- Molecule 9: Putative 40S ribosomal protein S16





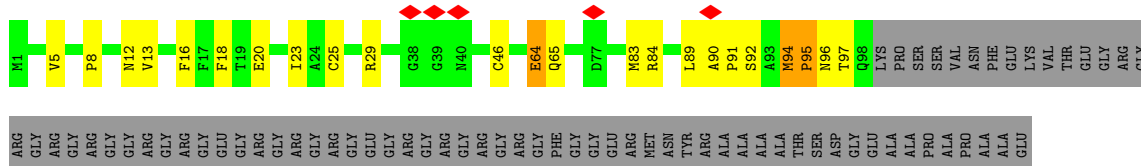
- Molecule 10: Putative ribosomal protein S20

Chain SM: 62% 24% 12%



- Molecule 11: Putative 40S ribosomal protein S10

Chain SN: 45% 12% 42%



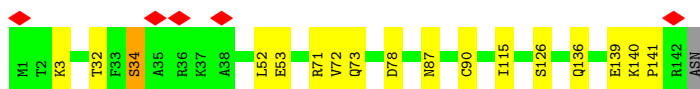
- Molecule 12: 40S ribosomal protein S14

Chain SO: 79% 11% 7%



- Molecule 13: Putative 40S ribosomal protein S23

Chain SP: 87% 11% 2%



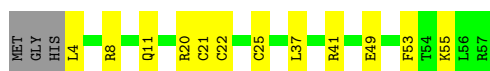
- Molecule 14: Putative 40S ribosomal protein S18

Chain SR: 73% 15% 12%



- Molecule 15: Putative ribosomal protein S29

Chain SS: 74% 21% 5%



- Molecule 16: Putative 40S ribosomal protein S13

Chain ST: 81% 12% 7%



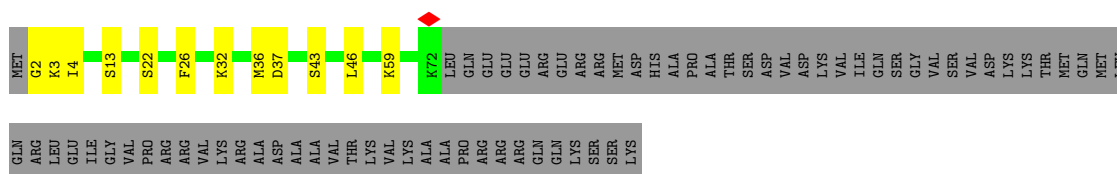
- Molecule 17: Putative 40S ribosomal protein S11

Chain SU: 6% 83% 6% 11%



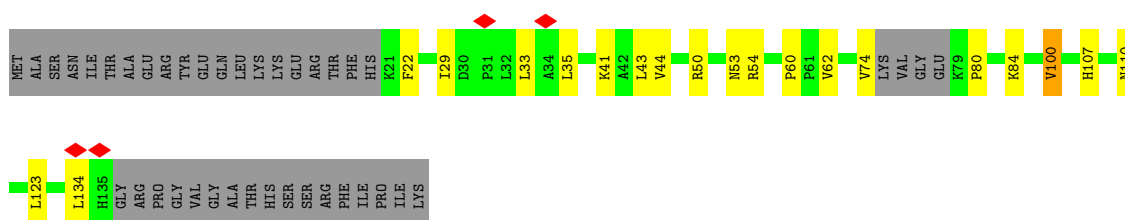
- Molecule 18: Putative 40S ribosomal protein S17

Chain SV: 41% 8% 50%



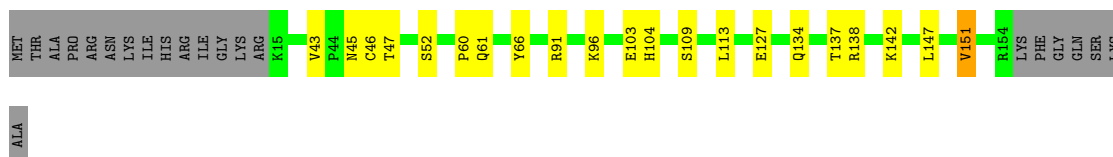
- Molecule 19: Putative 40S ribosomal protein S15

Chain SW: 60% 12% 27%

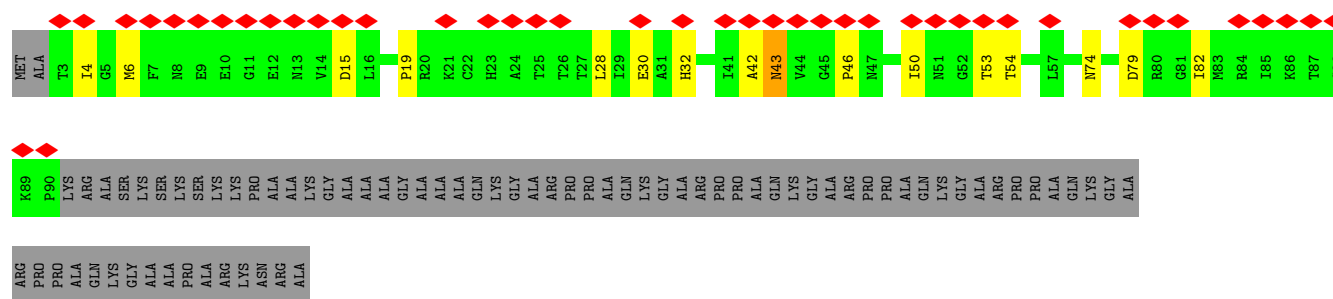


- Molecule 20: 40S ribosomal protein S19-like protein

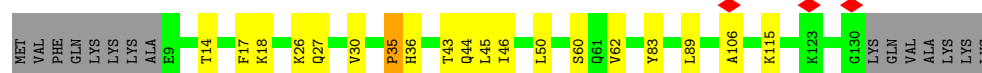
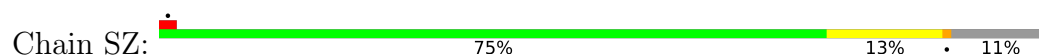
Chain SX: 74% 12% 13%



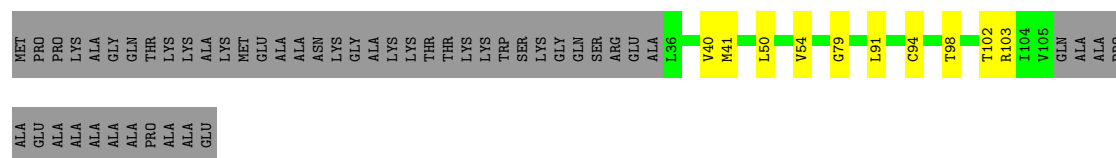
- Molecule 21: Putative 40S ribosomal protein S21



- Molecule 22: 40S ribosomal protein S24



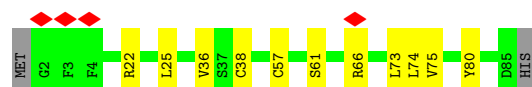
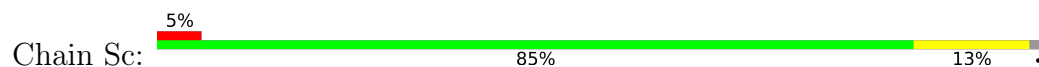
- Molecule 23: 40S ribosomal protein S25



- Molecule 24: 40S ribosomal protein S26

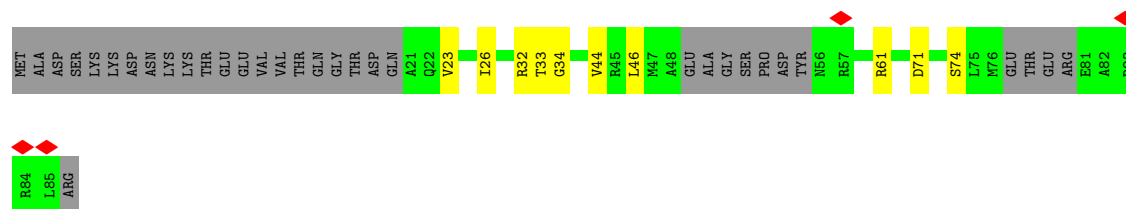


- Molecule 25: Putative 40S ribosomal protein S27-1

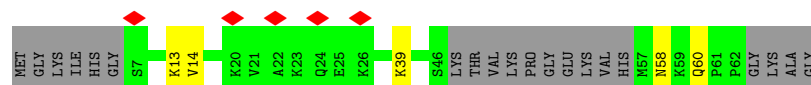


- Molecule 26: Putative 40S ribosomal protein S33

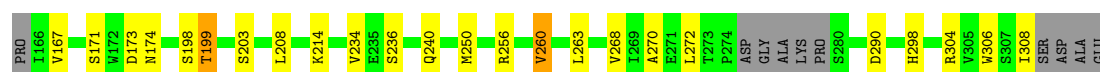
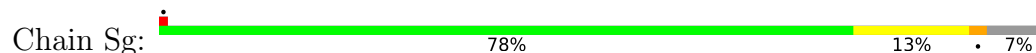




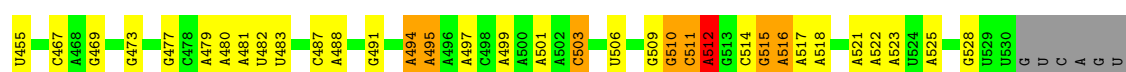
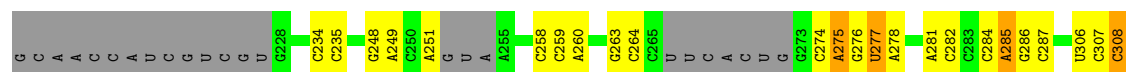
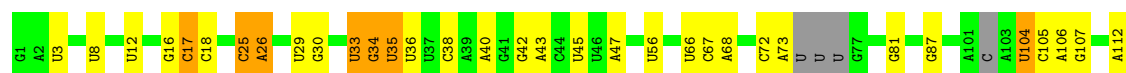
- Molecule 27: 40S ribosomal protein S30



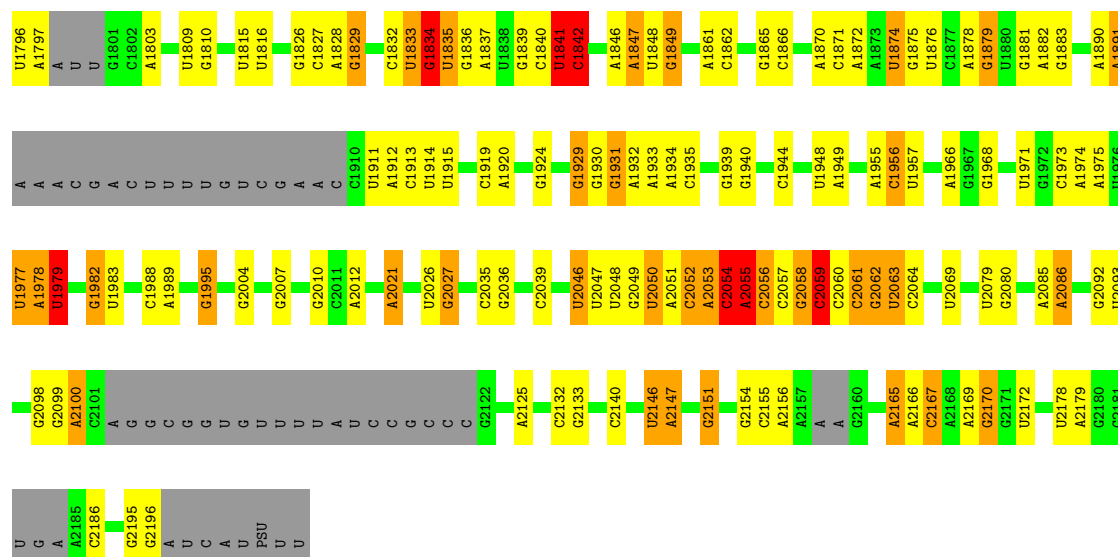
- Molecule 28: Small ribosomal subunit protein RACK1



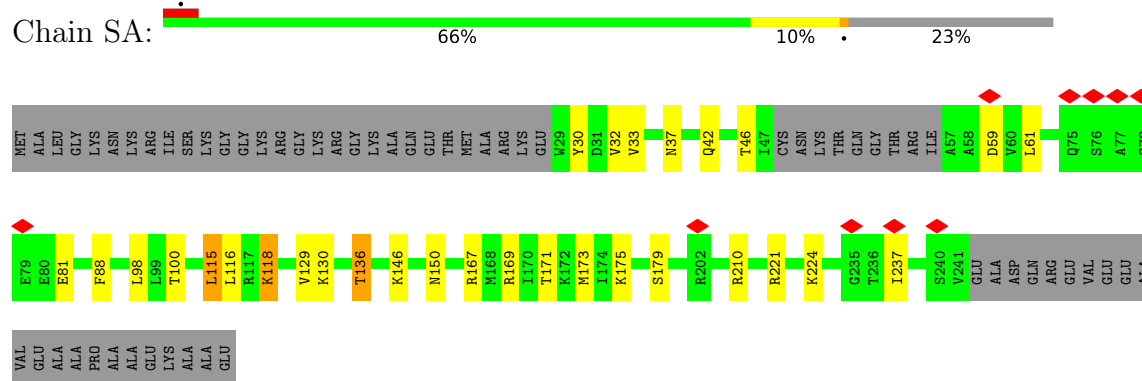
- Molecule 29: SSU_rRNA_chain_S1



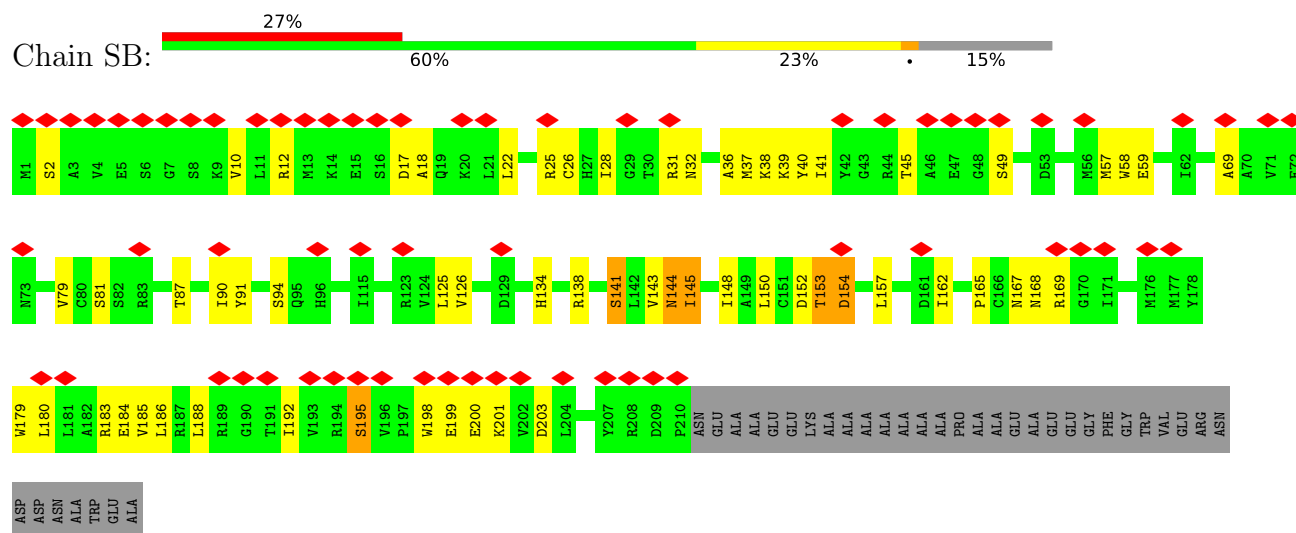




• Molecule 30: 40S ribosomal protein S3a



• Molecule 31: 40S ribosomal protein SA

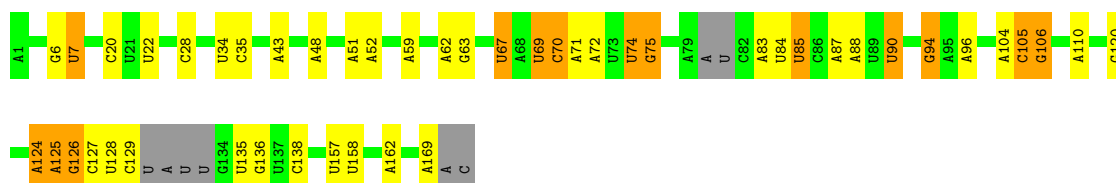


• Molecule 32: Putative 40S ribosomal protein S3

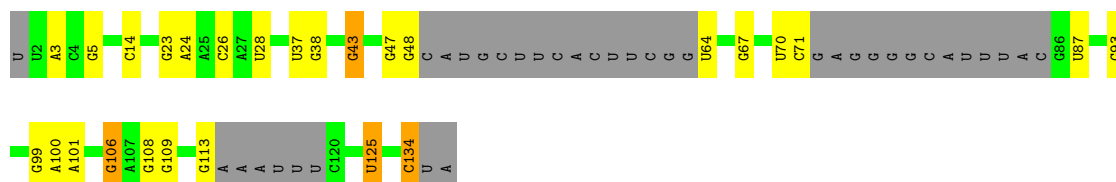




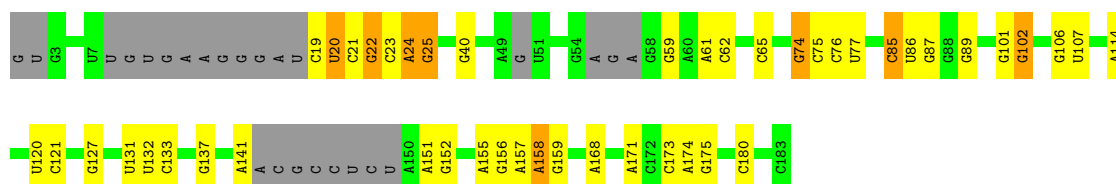
- Molecule 38: 5.8S rRNA chain 7



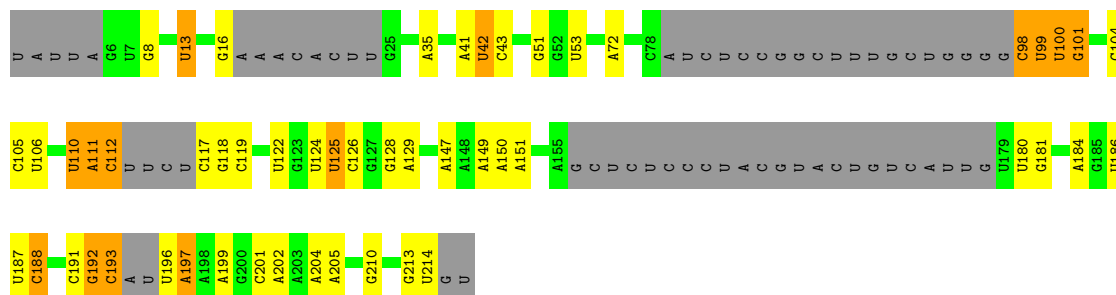
- Molecule 39: SR4 chain 5



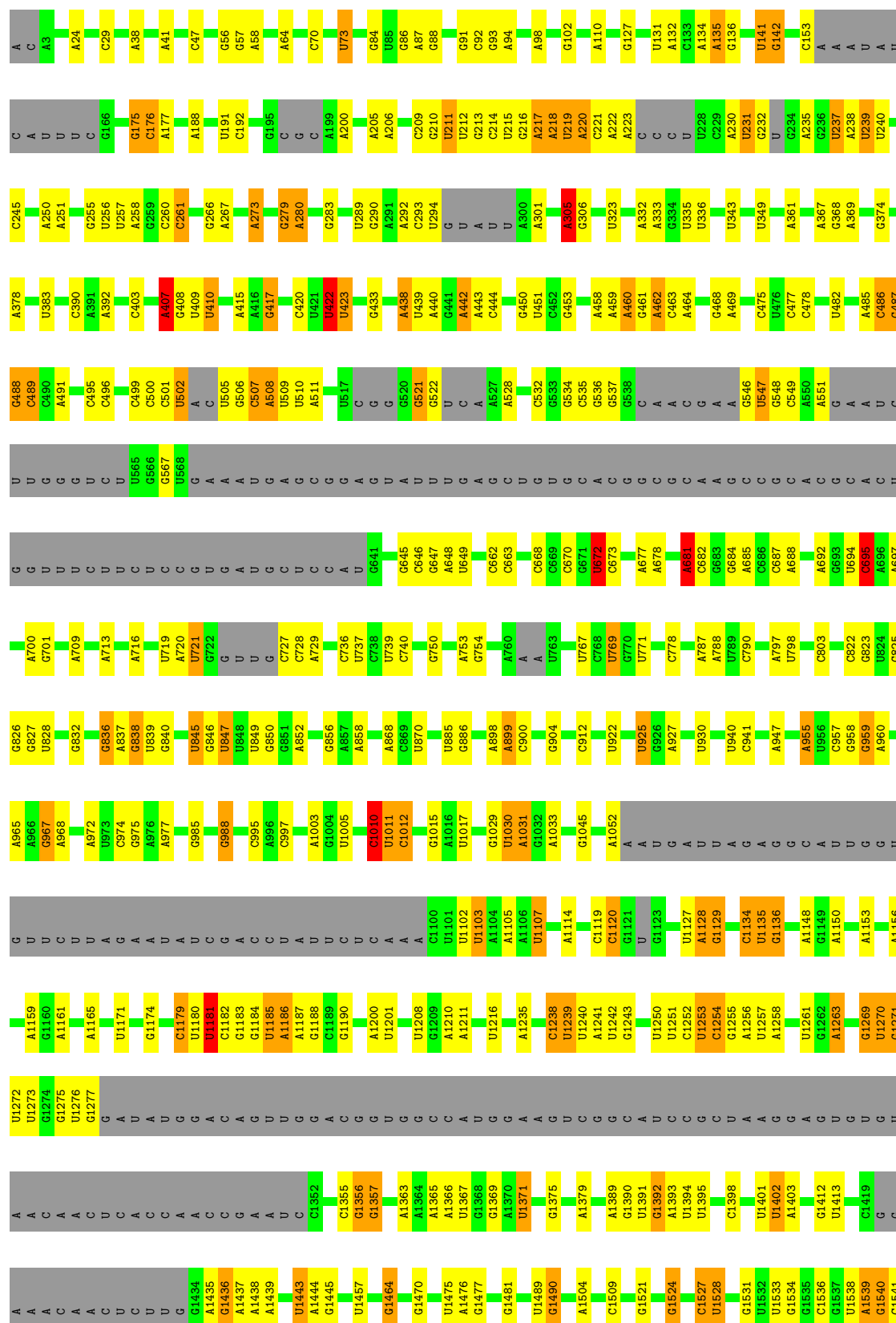
- Molecule 40: SR2_chain_4

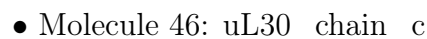


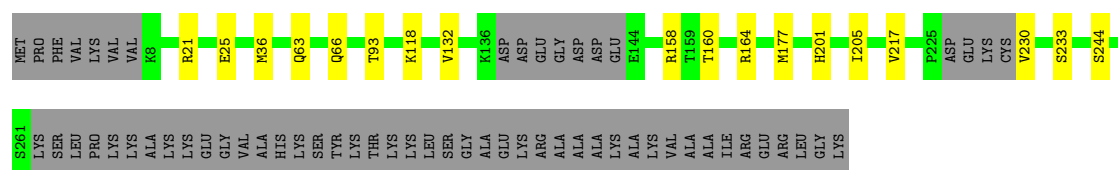
- Molecule 41: SR1_chain_3



- Molecule 42: LSUa rRNA chain 1

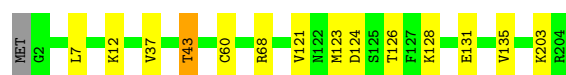
Chain 1: 





- Molecule 48: Ribosomal protein L15

Chain M: 93% 6%



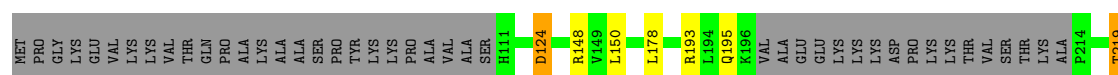
- Molecule 49: Putative 60S ribosomal protein L13a

Chain H: 91% 8%



- Molecule 50: 60S ribosomal protein L7a

Chain G: 73% 6% 20%



- Molecule 51: 60S ribosomal protein L18

Chain P: 92% 7%



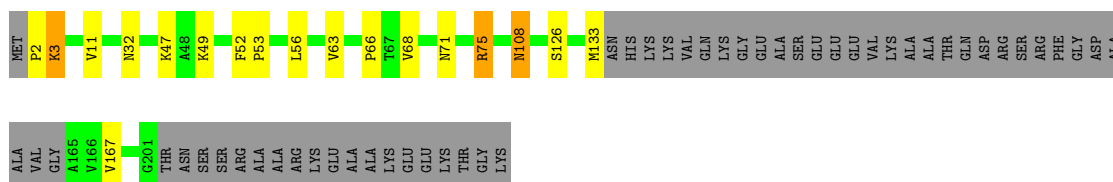
- Molecule 52: 60S ribosomal protein L18a

Chain R: 86% 13%

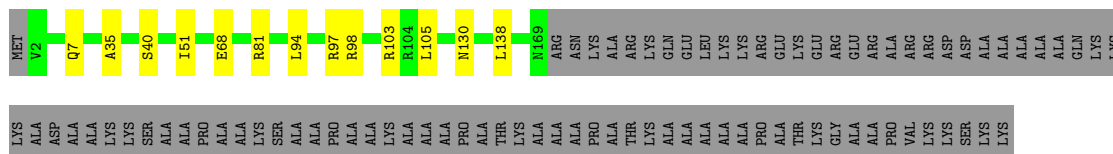


- Molecule 53: eL13_chain_I

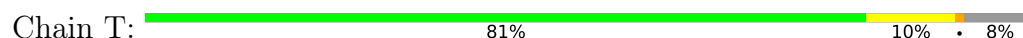
Chain I: 69% 7% 23%



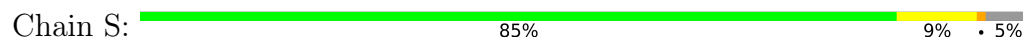
- Molecule 54: Putative 60S ribosomal protein L19



- Molecule 55: Putative 60S ribosomal protein L17



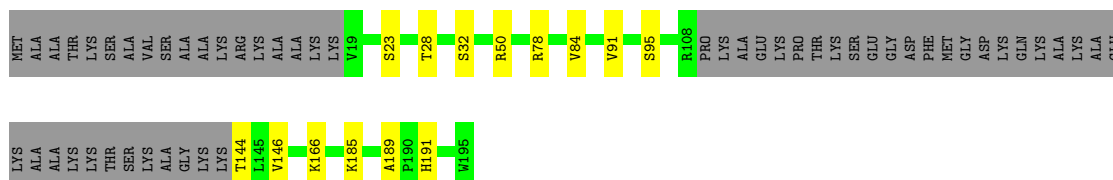
- Molecule 56: Putative 60S ribosomal protein L21



- Molecule 57: Putative 60S ribosomal protein L27A/L29

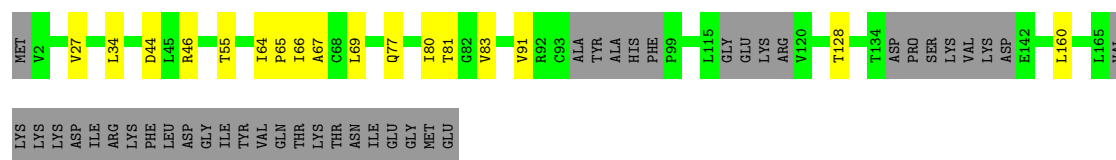


- Molecule 58: Putative 60S ribosomal protein L6



- Molecule 59: Putative 60S ribosomal protein L9

Chain E:  69% 9% 22%



- Molecule 60: 60S ribosomal protein L27

Chain Y:  87% 11%



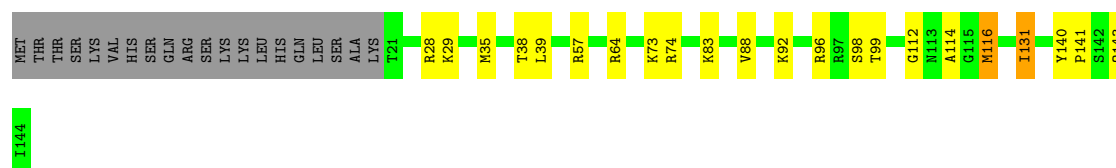
- Molecule 61: 60S ribosomal protein L32

Chain f:  87% 5% 8%



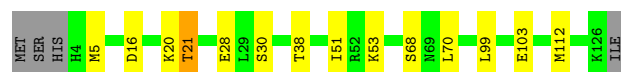
- Molecule 62: Putative ribosomal protein l35a

Chain g:  71% 14% 14%



- Molecule 63: Putative 60S ribosomal protein L35

Chain a:  86% 10%



- Molecule 64: Putative 60S ribosomal protein L23

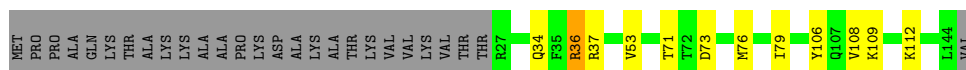
Chain J:  86% 7% 7%



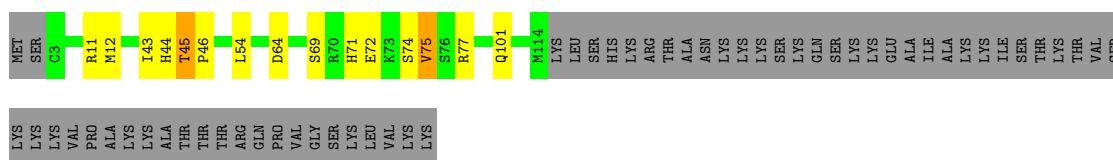
- Molecule 65: Putative 60S ribosomal protein L26

Chain W:  72% 10% 18%

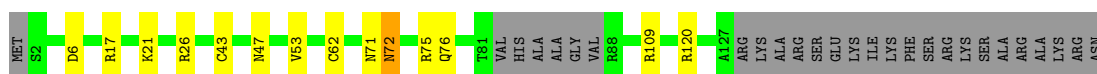
- Molecule 66: Putative 60S ribosomal protein L23a



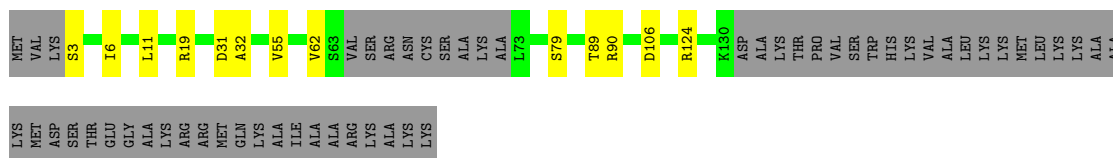
- Molecule 67: Putative 60S ribosomal protein L34



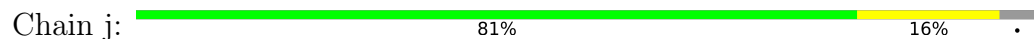
- Molecule 68: Putative 60S ribosomal protein L28



- Molecule 69: Putative 40S ribosomal protein L14



- Molecule 70: Ribosomal protein L37

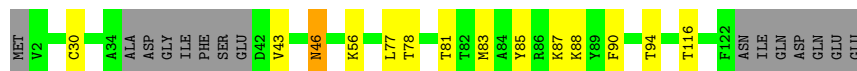


- Molecule 71: Putative 60S Ribosomal protein L36



- Molecule 72: Putative 60S ribosomal protein L22

Chain U:  78% 10% 12%



- Molecule 73: Putative 60S ribosomal protein L44

Chain p:  66% 12% 22%

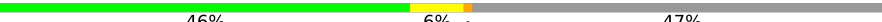


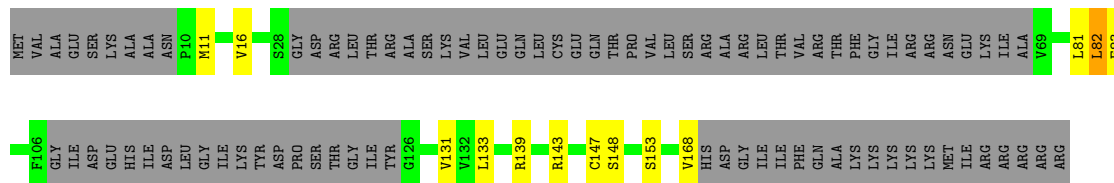
- Molecule 74: 60S ribosomal protein L37a

Chain o:  78% 16% 6%



- Molecule 75: 60S ribosomal protein L11

Chain D:  46% 6% 47%



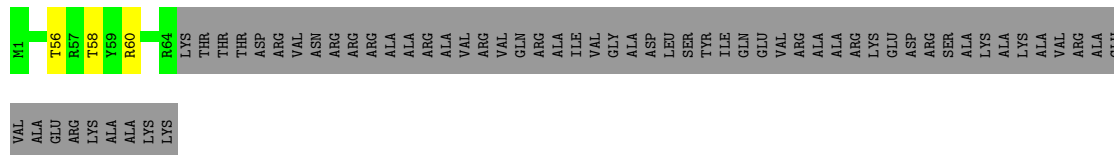
- Molecule 76: 60S ribosomal protein L30

Chain d:  69% 14% 15%



- Molecule 77: Putative ribosomal protein L24

Chain X:  49% 48%



- Molecule 78: 60S ribosomal protein L29

Chain b:  84% 10% 6%



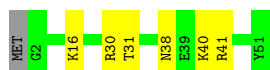
- Molecule 79: Putative ribosomal protein L38

Chain k:  72% 13% 14%



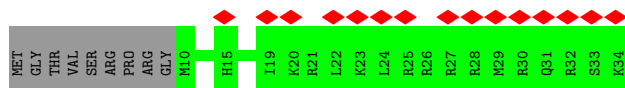
- Molecule 80: Putative 60S ribosomal protein L39

Chain l:  86% 12% .



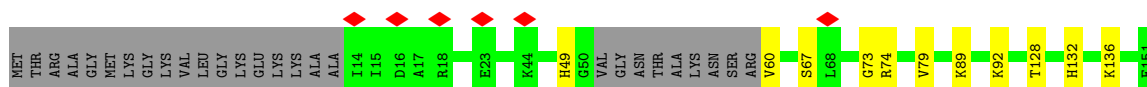
- Molecule 81: 60S ribosomal protein L41

Chain n:  44% 74% 26%



- Molecule 82: Putative 60S ribosomal subunit protein L31

Chain e:  73% 7% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	742580	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.292	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, OMU, ZN, G7M, PSU, 5MC, C4J, K, OMG, NA, MG, A2M

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	SD	0.14	0/1374	0.28	0/1850
2	SE	0.16	0/2104	0.30	0/2834
3	SF	0.14	0/1589	0.25	0/2152
4	SG	0.12	0/1836	0.22	0/2462
5	SH	0.29	0/1426	0.30	0/1919
6	SI	0.13	0/1613	0.24	0/2179
7	SJ	0.17	0/1034	0.23	0/1386
8	SK	0.17	0/1475	0.26	0/1978
9	SL	0.25	0/1132	0.28	0/1522
10	SM	0.21	0/817	0.30	0/1109
11	SN	0.54	2/813 (0.2%)	0.90	4/1103 (0.4%)
12	SO	0.31	0/989	0.41	0/1333
13	SP	0.15	0/1148	0.26	0/1538
14	SR	0.28	0/1099	0.33	0/1477
15	SS	0.22	0/422	0.32	0/565
16	ST	0.19	0/1163	0.28	0/1560
17	SU	0.17	0/1245	0.24	0/1677
18	SV	0.23	0/584	0.28	0/777
19	SW	0.23	0/885	0.29	0/1197
20	SX	0.26	0/1121	0.30	0/1512
21	SY	0.60	2/631 (0.3%)	0.81	3/863 (0.3%)
22	SZ	0.32	1/991 (0.1%)	0.53	3/1324 (0.2%)
23	Sa	0.26	0/554	0.34	0/745
24	Sb	0.36	0/676	0.53	0/906
25	Sc	0.14	0/637	0.26	0/862
26	Sd	0.25	0/388	0.27	0/517
27	Se	0.11	0/355	0.22	0/474
28	Sg	0.22	0/2225	0.33	0/3035
29	S1	0.29	0/38833	0.46	82/60463 (0.1%)
30	SA	0.24	0/1677	0.33	0/2260
31	SB	0.10	0/1629	0.27	0/2215
32	SC	0.18	0/1551	0.31	0/2080

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sh	0.13	0/676	0.34	0/920
34	S4	0.24	0/399	0.33	0/618
35	8	0.29	0/2829	0.32	0/4405
36	6	0.36	0/1484	0.44	0/2306
37	2	0.50	1/21251 (0.0%)	0.49	25/33095 (0.1%)
38	7	0.51	0/3723	0.45	4/5795 (0.1%)
39	5	0.46	0/2340	0.42	0/3640
40	4	0.45	0/3746	0.38	0/5829
41	3	0.41	0/3605	0.39	0/5602
42	1	0.52	0/34332	0.47	31/53510 (0.1%)
43	B	0.40	0/3026	0.41	0/4105
44	C	0.40	0/2391	0.38	0/3249
45	A	0.40	0/1893	0.40	0/2556
46	c	0.38	0/1812	0.37	0/2440
47	O	0.24	0/1798	0.31	0/2435
48	M	0.46	0/1732	0.41	0/2316
49	H	0.37	0/1724	0.39	0/2330
50	G	0.35	0/1660	0.39	0/2241
51	P	0.41	0/1537	0.40	0/2057
52	R	0.34	0/1433	0.35	0/1943
53	I	0.37	0/1328	0.41	0/1792
54	Q	0.34	0/1307	0.35	0/1751
55	T	0.46	0/1241	0.46	0/1665
56	S	0.32	0/1190	0.31	0/1609
57	L	0.42	0/1141	0.42	0/1525
58	F	0.31	0/1051	0.34	0/1434
59	E	0.15	0/1042	0.29	0/1418
60	Y	0.30	0/1029	0.32	0/1389
61	f	0.48	0/1013	0.46	0/1358
62	g	0.44	0/1010	0.46	0/1360
63	a	0.33	0/965	0.31	0/1295
64	J	0.36	0/950	0.36	0/1291
65	W	0.35	0/941	0.47	2/1257 (0.2%)
66	V	0.40	0/932	0.40	0/1259
67	h	0.37	0/903	0.39	0/1207
68	Z	0.32	0/905	0.39	0/1221
69	K	0.25	0/897	0.29	0/1220
70	j	0.49	0/673	0.44	0/899
71	i	0.27	0/668	0.32	0/889
72	U	0.22	0/803	0.36	0/1082
73	p	0.34	0/649	0.37	0/864
74	o	0.36	0/670	0.47	0/897
75	D	0.15	0/658	0.27	0/889

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	d	0.26	0/617	0.28	0/848
77	X	0.36	0/569	0.36	0/767
78	b	0.34	0/531	0.35	0/712
79	k	0.24	0/515	0.26	0/699
80	l	0.47	0/453	0.41	0/606
81	n	0.12	0/159	0.20	0/215
82	e	0.36	0/1117	0.39	1/1505 (0.1%)
All	All	0.39	6/193334 (0.0%)	0.43	155/284189 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	SY	46	PRO	CG-CD	-13.62	1.04	1.50
11	SN	95	PRO	CG-CD	-12.32	1.08	1.50
22	SZ	35	PRO	CG-CD	-7.16	1.26	1.50
11	SN	95	PRO	N-CD	5.72	1.55	1.47
21	SY	46	PRO	N-CD	5.52	1.55	1.47
37	2	73	OMU	O3'-P	5.09	1.61	1.56

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1264	PSU	O3'-P-O5'	18.48	131.71	104.00
11	SN	95	PRO	N-CD-CG	-18.11	76.04	103.20
21	SY	46	PRO	N-CD-CG	-17.03	77.65	103.20
11	SN	95	PRO	CA-N-CD	-13.86	92.60	112.00
11	SN	95	PRO	CA-CB-CG	-12.10	81.50	104.50
22	SZ	35	PRO	CA-N-CD	-12.10	95.06	112.00
29	S1	512	A2M	P-O3'-C3'	-10.15	107.51	119.70
37	2	1264	PSU	OP2-P-O3'	-9.89	78.34	108.00
21	SY	46	PRO	CA-N-CD	-9.47	98.74	112.00
21	SY	46	PRO	CA-CB-CG	-9.39	86.66	104.50
11	SN	95	PRO	CB-CG-CD	9.11	135.26	106.10
42	1	1185	U	P-O3'-C3'	-8.97	106.75	120.20
37	2	1265	U	O5'-P-OP2	-8.88	81.36	108.00
29	S1	1834	G	P-O3'-C3'	-8.79	107.02	120.20
29	S1	2062	G	P-O3'-C3'	-8.74	107.09	120.20
22	SZ	35	PRO	N-CD-CG	-8.60	90.30	103.20
29	S1	607	PSU	P-O3'-C3'	-8.55	107.38	120.20
29	S1	2058	G	P-O3'-C3'	-8.52	107.42	120.20
37	2	472	PSU	P-O3'-C3'	-8.42	107.56	120.20
29	S1	2059	C	P-O3'-C3'	-8.42	107.57	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1403	PSU	P-O3'-C3'	-8.41	107.59	120.20
37	2	71	OMG	P-O3'-C3'	-8.25	107.82	120.20
29	S1	2050	U	P-O3'-C3'	-8.16	107.97	120.20
29	S1	2048	PSU	P-O3'-C3'	-8.15	107.97	120.20
29	S1	1247	U	P-O3'-C3'	-8.02	108.17	120.20
29	S1	1246	PSU	P-O3'-C3'	-8.00	108.19	120.20
42	1	1184	G	P-O3'-C3'	-8.00	108.20	120.20
29	S1	2055	A	P-O3'-C3'	-7.97	108.24	120.20
29	S1	1264	C	P-O3'-C3'	-7.97	108.25	120.20
42	1	1661	U	P-O3'-C3'	-7.96	108.26	120.20
42	1	1730	A	P-O3'-C3'	-7.94	108.30	120.20
29	S1	1642	C	P-O3'-C3'	-7.92	108.32	120.20
29	S1	35	U	P-O3'-C3'	-7.90	108.35	120.20
29	S1	673	G	P-O3'-C3'	-7.89	108.36	120.20
29	S1	33	PSU	P-O3'-C3'	-7.85	108.43	120.20
29	S1	656	G	P-O3'-C3'	-7.84	108.45	120.20
29	S1	2166	A	P-O3'-C3'	-7.79	108.52	120.20
37	2	591	A2M	P-O3'-C3'	-7.79	110.35	119.70
29	S1	1533	PSU	P-O3'-C3'	-7.78	108.53	120.20
29	S1	1839	G	P-O3'-C3'	-7.77	108.54	120.20
29	S1	2046	PSU	P-O3'-C3'	-7.77	108.55	120.20
29	S1	653	A	P-O3'-C3'	-7.76	108.56	120.20
42	1	239	PSU	P-O3'-C3'	-7.76	108.55	120.20
29	S1	1147	A	P-O3'-C3'	-7.75	108.57	120.20
42	1	1664	PSU	P-O3'-C3'	-7.71	108.64	120.20
42	1	1531	G	P-O3'-C3'	-7.70	108.66	120.20
29	S1	2063	U	P-O3'-C3'	-7.69	108.67	120.20
29	S1	1531	G	P-O3'-C3'	-7.67	108.70	120.20
29	S1	575	C	P-O3'-C3'	-7.64	108.74	120.20
29	S1	1841	PSU	P-O3'-C3'	-7.63	108.76	120.20
37	2	1144	PSU	P-O3'-C3'	-7.62	108.77	120.20
29	S1	515	G	P-O3'-C3'	-7.61	108.78	120.20
29	S1	609	PSU	P-O3'-C3'	-7.56	108.85	120.20
42	1	1017	PSU	P-O3'-C3'	-7.56	108.86	120.20
38	7	69	PSU	P-O3'-C3'	-7.55	108.88	120.20
37	2	1060	PSU	P-O3'-C3'	-7.54	108.89	120.20
29	S1	1156	PSU	P-O3'-C3'	-7.54	108.89	120.20
42	1	1533	PSU	P-O3'-C3'	-7.49	108.97	120.20
29	S1	1154	A	P-O3'-C3'	-7.47	108.99	120.20
37	2	597	PSU	P-O3'-C3'	-7.47	108.99	120.20
29	S1	1539	PSU	P-O3'-C3'	-7.46	109.01	120.20
29	S1	572	A	P-O3'-C3'	-7.43	109.05	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	1179	C	P-O3'-C3'	-7.42	109.06	120.20
29	S1	573	C	P-O3'-C3'	-7.40	109.10	120.20
29	S1	1619	G	P-O3'-C3'	-7.33	109.21	120.20
29	S1	2146	U	P-O3'-C3'	-7.32	109.22	120.20
37	2	1058	PSU	P-O3'-C3'	-7.32	109.22	120.20
38	7	70	C	P-O3'-C3'	-7.29	109.26	120.20
29	S1	1842	C	P-O3'-C3'	-7.25	109.32	120.20
29	S1	1641	U	P-O3'-C3'	-7.25	109.33	120.20
29	S1	1192	PSU	P-O3'-C3'	-7.22	109.37	120.20
29	S1	2147	A	P-O3'-C3'	-7.20	109.40	120.20
37	2	1303	PSU	P-O3'-C3'	-7.16	109.45	120.20
37	2	1401	C	P-O3'-C3'	-7.12	109.52	120.20
29	S1	1146	G	P-O3'-C3'	-7.11	109.53	120.20
29	S1	560	G	P-O3'-C3'	-7.10	109.56	120.20
42	1	1528	PSU	P-O3'-C3'	-7.04	109.65	120.20
37	2	78	PSU	P-O3'-C3'	-7.02	109.67	120.20
29	S1	2057	C	P-O3'-C3'	-7.01	109.68	120.20
38	7	67	U	P-O3'-C3'	-7.00	109.70	120.20
37	2	1179	A	P-O3'-C3'	-6.97	109.75	120.20
29	S1	1623	OMG	P-O3'-C3'	-6.93	109.80	120.20
37	2	1301	G	P-O3'-C3'	-6.92	109.82	120.20
42	1	451	U	P-O3'-C3'	-6.89	109.87	120.20
29	S1	576	A	P-O3'-C3'	-6.88	109.89	120.20
29	S1	1148	G	P-O3'-C3'	-6.84	109.94	120.20
29	S1	1643	G	P-O3'-C3'	-6.84	109.94	120.20
42	1	1534	G	P-O3'-C3'	-6.84	109.95	120.20
29	S1	1263	C	P-O3'-C3'	-6.80	110.00	120.20
29	S1	1244	G	P-O3'-C3'	-6.78	110.03	120.20
29	S1	1273	A	P-O3'-C3'	-6.75	110.07	120.20
29	S1	2054	C	P-O3'-C3'	-6.75	110.08	120.20
29	S1	1832	C	P-O3'-C3'	-6.74	110.09	120.20
29	S1	654	A	P-O3'-C3'	-6.73	110.11	120.20
42	1	1732	G	P-O3'-C3'	-6.73	110.11	120.20
29	S1	672	G	P-O3'-C3'	-6.70	110.16	120.20
42	1	1181	PSU	P-O3'-C3'	-6.65	110.23	120.20
29	S1	1261	G	P-O3'-C3'	-6.64	110.24	120.20
29	S1	510	G	P-O3'-C3'	-6.62	110.27	120.20
29	S1	1271	C	P-O3'-C3'	-6.61	110.29	120.20
29	S1	651	U	P-O3'-C3'	-6.59	110.31	120.20
29	S1	2167	C	P-O3'-C3'	-6.59	110.32	120.20
29	S1	1176	A	P-O3'-C3'	-6.57	110.34	120.20
38	7	72	A	P-O3'-C3'	-6.57	110.34	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	1186	A	P-O3'-C3'	-6.57	110.35	120.20
29	S1	1157	C	P-O3'-C3'	-6.54	110.39	120.20
37	2	75	C	P-O3'-C3'	-6.46	110.51	120.20
37	2	76	A	P-O3'-C3'	-6.44	110.54	120.20
42	1	450	G	P-O3'-C3'	-6.42	110.57	120.20
29	S1	516	A	P-O3'-C3'	-6.39	110.62	120.20
29	S1	2051	A	P-O3'-C3'	-6.29	110.76	120.20
29	S1	2165	A	P-O3'-C3'	-6.26	110.81	120.20
42	1	685	A	P-O3'-C3'	-6.25	110.83	120.20
42	1	1541	C	P-O3'-C3'	-6.24	110.84	120.20
29	S1	1262	U	P-O3'-C3'	-6.22	110.88	120.20
42	1	237	U	P-O3'-C3'	-6.18	110.94	120.20
29	S1	1274	A	P-O3'-C3'	-6.11	111.04	120.20
29	S1	1620	G	P-O3'-C3'	-6.10	111.05	120.20
29	S1	1620	G	OP2-P-O3'	6.06	126.19	108.00
42	1	670	C	P-O3'-C3'	-6.04	111.14	120.20
29	S1	2052	C	P-O3'-C3'	-6.04	111.14	120.20
29	S1	1272	A	P-O3'-C3'	-6.02	111.16	120.20
37	2	595	U	P-O3'-C3'	-6.01	111.19	120.20
65	W	73	LEU	N-CA-C	-5.91	106.41	113.97
42	1	672	PSU	P-O3'-C3'	-5.88	111.38	120.20
42	1	1731	G	P-O3'-C3'	-5.83	111.46	120.20
29	S1	1177	A	P-O3'-C3'	-5.81	111.48	120.20
29	S1	1174	C	P-O3'-C3'	-5.81	111.49	120.20
37	2	470	A	P-O3'-C3'	-5.80	111.50	120.20
29	S1	1835	U	P-O3'-C3'	-5.78	111.53	120.20
42	1	420	C	P-O3'-C3'	-5.78	111.54	120.20
29	S1	1655	U	P-O3'-C3'	-5.76	111.56	120.20
29	S1	1657	PSU	P-O3'-C3'	-5.76	111.56	120.20
37	2	605	C	P-O3'-C3'	-5.76	111.57	120.20
42	1	1670	A	P-O3'-C3'	-5.71	111.63	120.20
37	2	593	PSU	P-O3'-C3'	-5.71	111.63	120.20
42	1	1015	G	P-O3'-C3'	-5.68	111.69	120.20
29	S1	34	G	P-O3'-C3'	-5.60	111.80	120.20
42	1	1542	A	P-O3'-C3'	-5.56	111.86	120.20
37	2	1145	A	P-O3'-C3'	-5.52	111.92	120.20
37	2	1142	A	P-O3'-C3'	-5.52	111.92	120.20
29	S1	1640	G	P-O3'-C3'	-5.45	112.02	120.20
29	S1	514	C	P-O3'-C3'	-5.44	112.04	120.20
82	e	73	GLY	N-CA-C	5.35	117.33	110.96
29	S1	1537	U	P-O3'-C3'	-5.29	112.26	120.20
29	S1	2061	5MC	P-O3'-C3'	-5.29	112.26	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	W	74	LYS	N-CA-C	-5.24	105.74	113.61
42	1	1669	A	P-O3'-C3'	-5.23	112.35	120.20
37	2	1404	G	P-O3'-C3'	-5.21	112.38	120.20
22	SZ	35	PRO	CA-CB-CG	-5.11	94.78	104.50
29	S1	1178	C	P-O3'-C3'	-5.06	112.61	120.20
42	1	1586	G	C4'-C3'-O3'	5.06	116.99	109.40
42	1	684	G	P-O3'-C3'	-5.04	112.64	120.20
29	S1	1151	G	P-O3'-C3'	-5.04	112.64	120.20
42	1	1183	G	P-O3'-C3'	-5.01	112.69	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	SD	1347	0	1385	19	0
2	SE	2060	0	2166	27	0
3	SF	1555	0	1614	19	0
4	SG	1810	0	1893	14	0
5	SH	1404	0	1407	16	0
6	SI	1583	0	1620	18	0
7	SJ	1017	0	1046	7	0
8	SK	1453	0	1531	15	0
9	SL	1112	0	1170	4	0
10	SM	807	0	840	17	0
11	SN	791	0	762	15	0
12	SO	975	0	979	19	0
13	SP	1119	0	1168	9	0
14	SR	1077	0	1115	15	0
15	SS	417	0	398	8	0
16	ST	1140	0	1209	15	0
17	SU	1218	0	1231	6	0
18	SV	577	0	626	7	0
19	SW	866	0	858	11	0
20	SX	1092	0	1095	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	SY	622	0	588	8	0
22	SZ	972	0	1022	12	0
23	Sa	549	0	595	6	0
24	Sb	661	0	675	11	0
25	Sc	624	0	592	11	0
26	Sd	390	0	413	6	0
27	Se	350	0	369	3	0
28	Sg	2173	0	2023	25	0
29	S1	35569	0	17959	313	0
30	SA	1653	0	1727	22	0
31	SB	1595	0	1560	38	0
32	SC	1525	0	1557	19	0
33	Sh	668	0	624	15	0
34	S4	359	0	189	7	0
35	8	2531	0	1283	13	0
36	6	1329	0	678	17	0
37	2	20228	0	10271	132	0
38	7	3463	0	1758	14	0
39	5	2096	0	1065	10	0
40	4	3378	0	1714	26	0
41	3	3252	0	1650	32	0
42	1	31495	0	15888	188	0
43	B	2955	0	2926	20	0
44	C	2343	0	2272	11	0
45	A	1852	0	1830	13	0
46	c	1779	0	1822	9	0
47	O	1764	0	1693	8	0
48	M	1692	0	1759	6	0
49	H	1690	0	1732	12	0
50	G	1635	0	1702	10	0
51	P	1513	0	1610	6	0
52	R	1399	0	1393	17	0
53	I	1299	0	1317	12	0
54	Q	1290	0	1288	6	0
55	T	1217	0	1251	11	0
56	S	1164	0	1172	5	0
57	L	1114	0	1143	2	0
58	F	1032	0	1031	7	0
59	E	1032	0	966	8	0
60	Y	1008	0	1012	5	0
61	f	993	0	1025	3	0
62	g	989	0	1028	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	a	955	0	983	9	0
64	J	933	0	937	6	0
65	W	928	0	997	10	0
66	V	917	0	953	7	0
67	h	889	0	912	13	0
68	Z	892	0	885	9	0
69	K	883	0	855	7	0
70	j	659	0	667	7	0
71	i	660	0	714	7	0
72	U	795	0	734	8	0
73	p	640	0	657	6	0
74	o	659	0	656	10	0
75	D	649	0	516	7	0
76	d	607	0	549	8	0
77	X	548	0	553	1	0
78	b	520	0	531	4	0
79	k	508	0	493	6	0
80	l	440	0	461	4	0
81	n	159	0	122	0	0
82	e	1103	0	1097	8	0
83	1	52	0	0	0	0
83	2	25	0	0	0	0
83	3	1	0	0	0	0
83	5	1	0	0	0	0
83	7	2	0	0	0	0
83	C	1	0	0	0	0
83	S1	30	0	0	0	0
83	SD	1	0	0	0	0
83	T	1	0	0	0	0
84	1	22	0	0	0	0
84	2	9	0	0	0	0
84	4	1	0	0	0	0
84	J	1	0	0	0	0
84	S1	23	0	0	0	0
84	SO	1	0	0	0	0
85	SS	1	0	0	0	0
85	Sb	1	0	0	0	0
85	j	1	0	0	0	0
85	o	1	0	0	0	0
86	1	3	0	0	0	0
86	2	3	0	0	0	0
86	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	8	1	0	0	0	0
86	S1	4	0	0	0	0
86	Sb	1	0	0	0	0
87	1	283	0	0	2	0
87	2	148	0	0	0	0
87	3	17	0	0	0	0
87	4	29	0	0	2	0
87	5	19	0	0	0	0
87	6	1	0	0	0	0
87	7	40	0	0	1	0
87	8	5	0	0	0	0
87	A	10	0	0	0	0
87	B	9	0	0	0	0
87	C	11	0	0	0	0
87	G	3	0	0	0	0
87	H	3	0	0	0	0
87	I	4	0	0	0	0
87	J	1	0	0	2	0
87	L	3	0	0	0	0
87	M	9	0	0	0	0
87	P	8	0	0	0	0
87	Q	4	0	0	0	0
87	R	1	0	0	0	0
87	S	1	0	0	0	0
87	S1	36	0	0	1	0
87	SH	1	0	0	0	0
87	SN	2	0	0	2	0
87	SR	1	0	0	0	0
87	ST	1	0	0	0	0
87	SX	1	0	0	0	0
87	T	7	0	0	0	0
87	V	2	0	0	0	0
87	W	1	0	0	0	0
87	X	1	0	0	0	0
87	a	1	0	0	0	0
87	c	3	0	0	0	0
87	d	1	0	0	1	0
87	e	3	0	0	1	0
87	f	2	0	0	0	0
87	g	1	0	0	0	0
87	h	3	0	0	0	0
87	j	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	1	4	0	0	0	0
All	All	183881	0	132557	1323	0

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

All (1323) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3:41:A:H62	41:3:188:C:N4	1.27	1.32
41:3:41:A:N6	41:3:188:C:H42	1.32	1.26
22:SZ:35:PRO:HD2	22:SZ:36:HIS:H	1.27	0.98
37:2:814:A:H62	37:2:964:G:H1	1.03	0.97
37:2:514:U:H3	37:2:518:G:H1	0.99	0.94
42:1:509:U:H3	42:1:546:G:H1	1.11	0.94
42:1:1565:A:N3	82:e:74:ARG:NH1	2.18	0.92
29:S1:953:U:H3	29:S1:982:G:H22	1.19	0.90
12:SO:55:VAL:HG11	12:SO:60:ASP:HB2	1.51	0.89
42:1:509:U:O2	42:1:546:G:N2	2.06	0.89
40:4:133:C:N3	40:4:157:A:N1	2.21	0.88
31:SB:31:ARG:H	31:SB:31:ARG:HE	1.23	0.87
29:S1:354:C:H5	29:S1:400:G:H1	1.24	0.86
41:3:42:U:N3	41:3:187:U:O4	2.07	0.85
41:3:16:G:N7	67:h:71:HIS:NE2	2.27	0.83
52:R:50:LYS:NZ	56:S:147:ALA:O	2.12	0.82
35:8:53:A:H5'	47:O:233:SER:HB2	1.62	0.81
62:g:73:LYS:HA	62:g:141:PRO:HG2	1.63	0.80
29:S1:955:A:H2	29:S1:980:G:H1	1.26	0.79
42:1:1676:G:O6	42:1:1723:A:N6	2.15	0.79
29:S1:1912:A:H2	29:S1:1929:G:H1	1.31	0.78
42:1:335:U:H4'	42:1:336:U:H5''	1.64	0.78
41:3:119:C:N4	41:3:125:U:O4	2.15	0.77
22:SZ:35:PRO:HD2	22:SZ:36:HIS:N	1.92	0.77
40:4:133:C:O2	40:4:157:A:N6	2.15	0.76
42:1:487:G:O6	42:1:646:C:N4	2.17	0.76
42:1:1271:G:H22	42:1:1356:G:H1	1.33	0.76
29:S1:528:G:H1	29:S1:553:U:H3	1.34	0.76
28:Sg:39:ILE:HD11	28:Sg:57:PRO:HB3	1.67	0.76
42:1:700:A:N1	42:1:845:OMU:H5	2.00	0.76
37:2:984:G:H1	37:2:1000:U:H3	1.34	0.75
37:2:815:G:H22	37:2:965:C:H42	1.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:F:50:ARG:NH1	69:K:106:ASP:OD2	2.19	0.75
36:6:10:C:H5	36:6:70:G:H1	1.33	0.74
29:S1:1911:U:H5	29:S1:1930:G:H1	1.34	0.74
37:2:569:G:O2'	37:2:571:G:OP2	2.06	0.74
42:1:260:C:O2'	42:1:261:C:OP1	2.06	0.74
29:S1:1706:A:H62	29:S1:1766:G:H22	1.33	0.74
7:SJ:2:THR:N	29:S1:1281:C:HO2'	1.85	0.73
37:2:425:C:H5	45:A:173:GLY:H	1.36	0.73
55:T:20:SER:O	55:T:145:HIS:ND1	2.21	0.73
11:SN:46:CYS:SG	87:SN:201:HOH:O	2.47	0.72
29:S1:511:C:O2'	29:S1:512:A2M:H8	1.88	0.72
39:5:26:C:N3	39:5:125:U:O2'	2.22	0.72
41:3:192:G:O6	67:h:44:HIS:NE2	2.19	0.72
29:S1:955:A:N1	29:S1:980:G:O6	2.23	0.72
39:5:64:U:H3	39:5:93:G:H1	1.35	0.72
64:J:111:MET:SD	87:J:301:HOH:O	2.47	0.71
2:SE:63:ARG:NH1	29:S1:497:A:OP2	2.24	0.71
29:S1:87:G:N2	29:S1:495:A:OP1	2.24	0.71
42:1:1254:C:OP1	42:1:1255:G:N2	2.23	0.71
8:SK:75:ARG:NH1	29:S1:309:G:O6	2.24	0.70
42:1:507:C:O2'	42:1:508:A:O5'	2.08	0.70
29:S1:275:A:H3'	29:S1:276:G:H21	1.54	0.70
10:SM:77:PHE:HB3	15:SS:53:PHE:HB3	1.73	0.70
24:Sb:47:LEU:HD12	24:Sb:68:MET:HE1	1.71	0.70
29:S1:558:U:H2'	29:S1:559:G:C8	2.27	0.70
4:SG:4:ASN:HD22	4:SG:111:LEU:HD11	1.56	0.70
42:1:1391:U:OP1	69:K:19:ARG:NH2	2.24	0.70
16:ST:67:THR:O	16:ST:69:ARG:NH1	2.25	0.70
11:SN:84:ARG:NH1	11:SN:91:PRO:O	2.25	0.69
2:SE:196:GLU:OE2	2:SE:206:HIS:NE2	2.23	0.69
32:SC:30:GLU:OE2	32:SC:30:GLU:N	2.25	0.69
42:1:957:C:O2'	42:1:960:A:N3	2.26	0.69
37:2:815:G:N2	37:2:965:C:H42	1.91	0.69
5:SH:45:ARG:HG3	5:SH:48:TYR:HB2	1.73	0.69
14:SR:89:ARG:NH1	29:S1:1968:G:OP1	2.25	0.69
35:8:76:U:H3	35:8:107:C:H42	1.40	0.69
37:2:1459:U:O2'	37:2:1464:A:N7	2.26	0.69
37:2:75:C:O2'	37:2:76:A:OP1	2.11	0.69
42:1:769:U:OP2	51:P:101:ARG:NH2	2.27	0.68
8:SK:34:ALA:HB2	8:SK:56:ARG:HD2	1.74	0.68
29:S1:1288:G:OP1	31:SB:38:LYS:NZ	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Z:71:ASN:O	68:Z:72:ASN:ND2	2.25	0.68
29:S1:1890:A:N6	29:S1:1891:A:N3	2.42	0.68
42:1:852:A:OP1	57:L:27:LYS:NZ	2.26	0.68
42:1:219:U:H2'	42:1:220:A:H8	1.58	0.68
50:G:219:THR:HG21	50:G:275:ILE:HD13	1.76	0.68
37:2:602:A:OP1	55:T:140:MET:N	2.22	0.67
12:SO:54:LYS:NZ	12:SO:73:ASP:OD2	2.27	0.67
30:SA:81:GLU:OE2	30:SA:81:GLU:N	2.26	0.67
29:S1:964:U:H5'	29:S1:965:G:H5''	1.77	0.67
42:1:188:A:H5''	65:W:121:ARG:HH11	1.60	0.67
33:Sh:217:GLU:OE1	33:Sh:217:GLU:N	2.23	0.67
31:SB:81:SER:HB3	31:SB:90:ILE:HD13	1.77	0.67
35:8:48:U:OP2	75:D:139:ARG:NH2	2.27	0.67
39:5:3:A:H62	39:5:134:C:H5	1.43	0.67
68:Z:43:CYS:O	68:Z:47:ASN:ND2	2.28	0.66
11:SN:25:CYS:SG	87:SN:201:HOH:O	2.53	0.66
20:SX:60:PRO:O	29:S1:1878:A:O2'	2.12	0.66
49:H:95:SER:OG	49:H:124:GLU:OE2	2.14	0.66
21:SY:19:PRO:HG2	21:SY:28:LEU:HD22	1.76	0.66
29:S1:2063:U:H2'	29:S1:2064:C:C6	2.29	0.66
6:SI:75:ARG:NH1	6:SI:131:ASP:OD1	2.25	0.66
41:3:41:A:N6	41:3:188:C:N4	2.09	0.66
42:1:645:G:O2'	62:g:88:VAL:O	2.14	0.66
29:S1:1288:G:H1	29:S1:1426:U:H3	1.44	0.66
54:Q:94:LEU:HD23	54:Q:97:ARG:HH21	1.60	0.66
76:d:90:CYS:SG	87:d:201:HOH:O	2.52	0.66
8:SK:57:ALA:HB2	8:SK:196:GLY:HA2	1.78	0.66
29:S1:1644:G:H2'	29:S1:1645:U:C6	2.31	0.66
52:R:153:LEU:HB3	52:R:156:ARG:HD2	1.77	0.66
3:SF:111:LYS:HG3	3:SF:129:VAL:HG22	1.78	0.65
5:SH:126:ASP:OD1	26:Sd:61:ARG:NH2	2.29	0.65
29:S1:814:G:N2	29:S1:819:G:O2'	2.29	0.65
39:5:24:A:H5''	43:B:179:LYS:HG3	1.78	0.65
52:R:119:ARG:HG3	52:R:119:ARG:HH11	1.61	0.65
5:SH:170:SER:OG	5:SH:172:ASN:OD1	2.15	0.65
29:S1:783:A:H2	29:S1:837:G:H1	1.42	0.65
59:E:66:ILE:HA	59:E:69:LEU:HD12	1.79	0.65
42:1:1005:U:OP2	78:b:6:ASN:ND2	2.29	0.65
31:SB:2:SER:O	31:SB:12:ARG:NH1	2.29	0.64
42:1:210:G:H4'	42:1:211:U:H5''	1.79	0.64
72:U:83:MET:HA	72:U:83:MET:HE3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SF:92:MET:HE3	3:SF:137:ILE:HG23	1.79	0.64
54:Q:98:ARG:NH2	54:Q:130:ASN:OD1	2.31	0.64
37:2:134:C:H5	37:2:344:G:H1	1.46	0.64
31:SB:38:LYS:HA	31:SB:41:ILE:HD12	1.77	0.64
42:1:1186:A:H2'	42:1:1187:A:C8	2.33	0.64
60:Y:88:ASP:O	60:Y:119:ARG:NH2	2.31	0.64
3:SF:90:ASP:HB3	3:SF:116:VAL:HG12	1.79	0.64
2:SE:103:LYS:NZ	29:S1:889:A:OP1	2.31	0.64
41:3:8:G:O6	41:3:13:OMU:H5	1.97	0.64
18:SV:22:SER:O	28:Sg:214:LYS:NZ	2.31	0.64
42:1:507:C:O2'	42:1:508:A:H8	1.80	0.64
37:2:516:A:H2'	37:2:517:A:C8	2.33	0.63
1:SD:144:SER:OG	29:S1:522:A:OP1	2.14	0.63
29:S1:1890:A:C6	29:S1:1891:A:H1'	2.33	0.63
52:R:173:THR:HG22	52:R:175:ARG:H	1.62	0.63
5:SH:19:THR:O	5:SH:25:ARG:NH2	2.28	0.63
5:SH:154:SER:OG	5:SH:157:GLU:OE2	2.15	0.63
32:SC:40:VAL:HG22	32:SC:45:THR:HG23	1.80	0.63
72:U:46:ASN:OD1	72:U:46:ASN:N	2.30	0.63
29:S1:1630:G:OP1	32:SC:184:LYS:NZ	2.32	0.63
37:2:814:A:N6	37:2:964:G:H1	1.87	0.63
79:k:52:LYS:O	79:k:56:ILE:HG13	1.97	0.63
2:SE:260:ARG:NH2	29:S1:885:C:O2	2.31	0.63
16:ST:13:SER:OG	25:Sc:22:ARG:NH1	2.32	0.63
42:1:988:G:N2	42:1:1012:C:OP1	2.32	0.62
29:S1:762:A:O2'	29:S1:770:A:N6	2.33	0.62
42:1:1588:G:O2'	42:1:1590:G:OP2	2.17	0.62
42:1:219:U:O2'	42:1:220:A:OP1	2.18	0.62
31:SB:31:ARG:H	31:SB:31:ARG:NE	1.96	0.62
31:SB:183:ARG:HA	31:SB:198:TRP:HZ3	1.65	0.62
6:SI:40:GLU:HB3	6:SI:73:LEU:HD11	1.82	0.62
29:S1:783:A:C2	29:S1:837:G:N1	2.61	0.62
33:Sh:210:GLU:OE1	33:Sh:210:GLU:N	2.32	0.62
36:6:32:U:O2'	59:E:46:ARG:NE	2.30	0.62
12:SO:45:THR:HG21	29:S1:1142:G:H21	1.65	0.62
40:4:85:C:H4'	82:e:92:LYS:HE2	1.82	0.62
29:S1:971:U:H2'	29:S1:972:A:C8	2.35	0.61
30:SA:130:LYS:HG3	30:SA:136:THR:HG22	1.82	0.61
16:ST:87:ASP:N	16:ST:87:ASP:OD1	2.33	0.61
25:Sc:66:ARG:HB3	25:Sc:73:LEU:HB3	1.82	0.61
47:O:21:ARG:O	47:O:25:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SL:56:GLU:OE1	9:SL:88:ARG:NH2	2.33	0.61
42:1:305:A2M:H2	42:1:333:A:H62	1.65	0.61
41:3:53:U:O4	72:U:88:LYS:NZ	2.34	0.61
8:SK:119:ILE:HD11	8:SK:166:ARG:HE	1.65	0.61
14:SR:134:GLY:HA3	29:S1:1978:A:H5''	1.82	0.61
33:Sh:217:GLU:HA	33:Sh:220:ASN:HB2	1.81	0.61
37:2:75:C:HO2'	37:2:76:A:P	2.23	0.61
41:3:41:A:H62	41:3:188:C:H42	0.66	0.61
42:1:1271:G:N2	42:1:1356:G:H1	1.98	0.61
29:S1:628:A:H61	32:SC:178:ALA:HB1	1.64	0.61
37:2:68:A:O2'	37:2:69:A:O5'	2.19	0.61
42:1:485:A:H2	42:1:647:G:H22	1.49	0.61
31:SB:150:LEU:O	31:SB:168:ASN:ND2	2.33	0.61
29:S1:2053:A:H4'	29:S1:2054:C:O5'	2.01	0.60
29:S1:363:G:H4'	29:S1:367:A:C8	2.36	0.60
29:S1:1117:A:H2'	29:S1:1118:G:C8	2.35	0.60
33:Sh:205:SER:HB2	33:Sh:207:ARG:HD3	1.83	0.60
34:S4:66:U:H2'	34:S4:67:C:C6	2.36	0.60
42:1:218:A:H2'	42:1:218:A:OP1	2.01	0.60
42:1:727:C:O2'	42:1:728:C:H2'	2.01	0.60
62:g:64:ARG:NH1	62:g:112:GLY:O	2.32	0.60
42:1:216:G:H2'	42:1:217:A:H4'	1.84	0.60
42:1:521:G:H2'	42:1:522:G:C8	2.36	0.60
16:ST:40:SER:HA	16:ST:43:LYS:HG3	1.83	0.60
29:S1:1150:U:H1'	29:S1:1153:A:N7	2.17	0.60
29:S1:2052:C:H1'	29:S1:2056:C:H5	1.67	0.60
31:SB:186:LEU:HD12	31:SB:198:TRP:HH2	1.66	0.60
46:c:116:LEU:HD21	46:c:133:MET:HE1	1.82	0.60
17:SU:73:CYS:HG	17:SU:127:SER:HG	1.47	0.60
29:S1:511:C:HO2'	29:S1:512:A2M:H8	1.64	0.60
3:SF:49:THR:HG23	3:SF:52:GLY:H	1.67	0.59
29:S1:1156:PSU:H2'	29:S1:1157:C:C6	2.37	0.59
29:S1:1605:U:HO2'	29:S1:1606:C:H6	1.49	0.59
42:1:403:C:OP2	70:j:56:ARG:NH2	2.36	0.59
37:2:558:A:OP1	37:2:560:OMU:H5	2.02	0.59
29:S1:1659:U:O4	29:S1:1670:G:N1	2.34	0.59
82:e:60:VAL:N	87:e:201:HOH:O	2.35	0.59
12:SO:77:ARG:HB3	12:SO:77:ARG:NH1	2.18	0.59
30:SA:59:ASP:OD1	30:SA:59:ASP:N	2.36	0.59
37:2:514:U:O2	37:2:518:G:O6	2.21	0.59
42:1:70:C:O2'	53:I:71:ASN:OD1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SM:17:VAL:HG21	10:SM:95:VAL:HG21	1.85	0.59
29:S1:148:G:H2'	29:S1:149:G:C8	2.38	0.59
29:S1:691:G:H1	29:S1:754:G:H22	1.49	0.59
43:B:216:GLN:NE2	43:B:288:TYR:O	2.35	0.59
2:SE:97:ARG:NH2	2:SE:118:ILE:O	2.32	0.59
16:ST:104:ARG:HB2	16:ST:104:ARG:NH1	2.17	0.59
51:P:40:THR:HG22	51:P:42:SER:H	1.66	0.59
28:Sg:53:ASP:OD1	28:Sg:53:ASP:N	2.35	0.58
29:S1:783:A:H2	29:S1:837:G:H22	1.51	0.58
29:S1:2060:C:H2'	29:S1:2061:5MC:HM53	1.85	0.58
37:2:790:U:H3	37:2:805:G:H1	1.51	0.58
42:1:188:A:N3	42:1:245:C:O2'	2.36	0.58
46:c:70:LYS:O	46:c:74:THR:HG23	2.03	0.58
22:SZ:14:THR:O	29:S1:879:A:N6	2.36	0.58
42:1:1239:U:OP1	49:H:141:ARG:NH1	2.37	0.58
42:1:1489:U:H2'	42:1:1490:G:C8	2.38	0.58
62:g:74:ARG:HD3	62:g:141:PRO:HB3	1.85	0.58
49:H:217:LYS:HA	49:H:222:ALA:HB2	1.84	0.58
21:SY:50:ILE:H	21:SY:50:ILE:HD12	1.67	0.58
42:1:1561:A:N6	42:1:1569:U:H3	2.00	0.58
42:1:1571:C:H5	55:T:85:ARG:HH21	1.49	0.58
3:SF:152:ARG:HH12	21:SY:6:MET:HE2	1.67	0.58
7:SJ:87:GLU:OE1	7:SJ:97:ARG:NH1	2.37	0.58
37:2:459:A:H2'	37:2:460:A:C8	2.38	0.58
2:SE:260:ARG:HH21	29:S1:885:C:H1'	1.68	0.58
29:S1:2085:A:HO2'	29:S1:2086:A:H8	1.50	0.58
37:2:83:G:O2'	37:2:580:U:O4	2.18	0.58
42:1:487:G:H2'	42:1:489:C:C6	2.39	0.58
6:SI:50:ARG:NH1	29:S1:760:G:OP1	2.36	0.58
29:S1:1287:U:H2'	29:S1:1288:G:C8	2.39	0.58
31:SB:148:ILE:HG13	31:SB:162:ILE:HB	1.85	0.58
42:1:501:C:O2'	42:1:502:U:O5'	2.22	0.58
42:1:505:U:H2'	42:1:506:G:H8	1.67	0.58
45:A:80:GLU:HG3	74:o:66:GLY:HA2	1.85	0.58
3:SF:242:TRP:CD2	7:SJ:68:ARG:HD3	2.38	0.58
37:2:1021:A:O2'	37:2:1022:U:H5'	2.04	0.58
43:B:224:SER:HB3	43:B:343:MET:HG2	1.85	0.58
48:M:68:ARG:NH1	48:M:124:ASP:O	2.33	0.58
29:S1:1977:U:H4'	29:S1:1978:A:H4'	1.84	0.57
63:a:16:ASP:O	63:a:20:LYS:HG2	2.04	0.57
42:1:1003:A:OP1	78:b:18:ARG:NH2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1:219:U:H2'	42:1:220:A:C8	2.39	0.57
25:Sc:66:ARG:HH11	25:Sc:66:ARG:HB2	1.69	0.57
4:SG:226:ARG:NH1	29:S1:823:G:OP1	2.38	0.57
2:SE:94:ASP:OD1	2:SE:94:ASP:N	2.35	0.57
30:SA:88:PHE:HB3	30:SA:100:THR:HB	1.86	0.57
34:S4:2:C:H2'	34:S4:3:G:C8	2.40	0.57
63:a:38:THR:HG22	66:V:71:THR:HG21	1.86	0.57
2:SE:209:ASP:OD1	2:SE:210:ALA:N	2.35	0.57
26:Sd:33:THR:OG1	26:Sd:34:GLY:N	2.38	0.57
29:S1:2052:C:H1'	29:S1:2056:C:C5	2.40	0.57
37:2:755:U:O2'	37:2:756:C:O5'	2.14	0.57
14:SR:3:LEU:HD11	23:Sa:79:GLY:HA2	1.87	0.57
28:Sg:298:HIS:CE1	28:Sg:304:ARG:HD2	2.40	0.56
29:S1:1132:G:H2'	29:S1:1133:U:C6	2.40	0.56
33:Sh:208:SER:H	33:Sh:211:LYS:HE2	1.69	0.56
52:R:40:LYS:NZ	52:R:63:CYS:SG	2.78	0.56
76:d:42:LYS:NZ	76:d:95:THR:O	2.37	0.56
29:S1:1178:C:H5'	30:SA:118:LYS:HG2	1.86	0.56
29:S1:1203:U:OP1	29:S1:1421:C:O2'	2.22	0.56
29:S1:1765:C:H2'	29:S1:1766:G:C8	2.41	0.56
29:S1:1795:G:H22	29:S1:1803:A:H2	1.52	0.56
29:S1:2046:PSU:H2'	29:S1:2047:U:C6	2.40	0.56
41:3:112:C:H1'	41:3:117:C:C6	2.39	0.56
42:1:1356:G:HO2'	42:1:1357:G:P	2.28	0.56
68:Z:21:LYS:HG3	68:Z:26:ARG:HG2	1.86	0.56
29:S1:1701:A:H2'	29:S1:1702:A:H8	1.70	0.56
37:2:1263:C:H42	37:2:1302:A:H61	1.53	0.56
53:I:47:LYS:HD3	53:I:56:LEU:HD11	1.86	0.56
71:i:64:LEU:HD13	71:i:94:GLU:HG3	1.88	0.56
23:Sa:91:LEU:HD21	23:Sa:94:CYS:HB3	1.87	0.56
25:Sc:36:VAL:HG12	25:Sc:38:CYS:H	1.70	0.56
42:1:475:C:OP1	62:g:83:LYS:NZ	2.39	0.56
12:SO:77:ARG:HB3	12:SO:77:ARG:HH11	1.71	0.56
28:Sg:171:SER:OG	28:Sg:173:ASP:OD1	2.24	0.56
31:SB:36:ALA:O	31:SB:39:LYS:NZ	2.38	0.56
29:S1:274:C:O2'	29:S1:965:G:OP2	2.21	0.56
29:S1:285:A:H2'	29:S1:817:A:H2	1.70	0.56
37:2:630:G:C2	42:1:462:A:H2'	2.41	0.56
42:1:1263:A:O2'	42:1:1363:A:N6	2.38	0.56
37:2:422:U:OP1	45:A:54:ARG:NH2	2.37	0.55
57:L:72:THR:HG22	57:L:108:LYS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SF:90:ASP:N	3:SF:90:ASP:OD1	2.39	0.55
4:SG:5:ILE:HD11	4:SG:116:ILE:HG12	1.87	0.55
29:S1:792:G:O6	29:S1:833:G:O6	2.24	0.55
37:2:451:U:H3	37:2:483:C:H42	1.55	0.55
29:S1:328:C:HO2'	29:S1:329:C:H6	1.53	0.55
30:SA:30:TYR:HB2	30:SA:46:THR:HG22	1.89	0.55
48:M:121:VAL:HG21	48:M:131:GLU:HG3	1.88	0.55
1:SD:158:ALA:O	1:SD:161:SER:OG	2.25	0.55
29:S1:1413:C:H2'	29:S1:1414:A:C8	2.42	0.55
31:SB:45:THR:OG1	31:SB:49:SER:OG	2.24	0.55
48:M:123:MET:HG3	48:M:128:LYS:HG3	1.88	0.55
37:2:809:C:H3'	37:2:810:G:H21	1.71	0.55
37:2:1463:A:OP2	49:H:185:ARG:NH2	2.35	0.55
29:S1:1620:G:H1'	29:S1:1849:G:H5''	1.89	0.55
19:SW:50:ARG:NH2	29:S1:1971:U:OP2	2.40	0.55
29:S1:1511:C:N4	29:S1:1637:A:H5'	2.22	0.55
40:4:132:U:H2'	40:4:133:C:H6	1.71	0.55
38:7:138:C:N3	87:7:301:HOH:O	2.33	0.55
42:1:482:U:H4'	42:1:487:G:H4'	1.89	0.55
76:d:48:ASN:OD1	76:d:49:ASN:N	2.40	0.55
1:SD:45:ASN:O	1:SD:49:SER:OG	2.24	0.55
25:Sc:66:ARG:HB2	25:Sc:66:ARG:NH1	2.22	0.55
40:4:20:U:H2'	40:4:21:C:C6	2.42	0.55
29:S1:1642:C:H2'	29:S1:1643:G:N3	2.22	0.54
37:2:469:G:H2'	37:2:470:A:C8	2.42	0.54
8:SK:68:ALA:HB2	8:SK:201:ILE:HD11	1.88	0.54
20:SX:134:GLN:NE2	29:S1:1915:U:OP1	2.41	0.54
29:S1:838:U:H2'	29:S1:839:G:C8	2.42	0.54
29:S1:1682:G:N2	32:SC:205:ASP:OD1	2.30	0.54
37:2:496:G:H1	37:2:512:PSU:HN3	1.55	0.54
42:1:188:A:H5''	65:W:121:ARG:NH1	2.23	0.54
29:S1:1179:U:H5''	30:SA:118:LYS:HZ1	1.72	0.54
42:1:305:A2M:C2	42:1:333:A:H62	2.21	0.54
42:1:1356:G:O2'	42:1:1357:G:OP1	2.18	0.54
11:SN:84:ARG:HD3	11:SN:90:ALA:HA	1.89	0.54
29:S1:2098:G:H21	29:S1:2125:A:H62	1.55	0.54
42:1:70:C:H1'	53:I:66:PRO:O	2.07	0.54
42:1:1270:U:H2'	42:1:1271:G:C8	2.43	0.54
42:1:1659:OMU:H6	42:1:1659:OMU:O5'	2.07	0.54
62:g:140:TYR:O	62:g:143:GLN:N	2.40	0.54
29:S1:1181:C:HO2'	29:S1:1425:U:HO2'	1.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:S1:1649:G:N2	29:S1:1652:A:OP2	2.37	0.54
37:2:655:OMG:HM21	37:2:657:U:H5''	1.89	0.54
42:1:336:U:N3	42:1:336:U:O2	2.40	0.54
45:A:13:GLY:O	45:A:17:GLN:NE2	2.40	0.54
79:k:26:LYS:NZ	79:k:28:ASN:OD1	2.40	0.54
1:SD:59:LEU:O	1:SD:68:ARG:NH1	2.41	0.54
29:S1:811:C:H2'	29:S1:812:A:H8	1.73	0.54
40:4:89:G:N7	87:4:302:HOH:O	2.33	0.54
10:SM:40:ALA:HA	10:SM:98:ILE:HD12	1.90	0.54
29:S1:1890:A:C5	29:S1:1891:A:H1'	2.43	0.54
33:Sh:195:PHE:HB2	33:Sh:200:LEU:HD12	1.90	0.54
37:2:1198:G:H1	37:2:1225:A:H61	1.56	0.54
42:1:453:G:OP1	55:T:62:ARG:NH1	2.41	0.54
42:1:959[B]:OMG:H8	42:1:959[B]:OMG:H3'	1.73	0.54
43:B:216:GLN:O	43:B:287:ILE:HG12	2.08	0.54
62:g:74:ARG:N	62:g:141:PRO:HG3	2.22	0.54
31:SB:201:LYS:HD3	31:SB:203:ASP:HB2	1.90	0.54
29:S1:1706:A:N6	29:S1:1766:G:H1	2.06	0.54
37:2:776:C:H3'	37:2:777:A:H5''	1.90	0.54
44:C:93:ASN:OD1	44:C:93:ASN:N	2.40	0.54
59:E:34:LEU:HD12	59:E:83:VAL:HG13	1.90	0.54
29:S1:364:G:O2'	29:S1:366:G:N7	2.33	0.53
36:6:64:U:OP2	58:F:78:ARG:NH2	2.28	0.53
42:1:535:C:H2'	42:1:536:G:H8	1.71	0.53
42:1:499:C:H2'	42:1:500:C:H6	1.72	0.53
22:SZ:106:ALA:O	29:S1:503:C:N4	2.32	0.53
24:Sb:42:VAL:HG23	24:Sb:73:MET:HG3	1.89	0.53
29:S1:1121:C:H2'	29:S1:1122:G:C8	2.43	0.53
29:S1:1155:U:H1'	29:S1:1244:G:H1'	1.91	0.53
12:SO:57:ALA:HB1	12:SO:59:ARG:HH11	1.74	0.53
29:S1:67:C:H5	29:S1:81:G:H21	1.57	0.53
29:S1:106:A:H2'	29:S1:107:G:C8	2.44	0.53
42:1:407:A2M:HM'2	42:1:408:G:H5''	1.91	0.53
52:R:18:SER:OG	52:R:19:GLU:N	2.42	0.53
67:h:74:SER:OG	67:h:75:VAL:N	2.42	0.53
29:S1:306:U:H2'	29:S1:307:C:O4'	2.08	0.53
29:S1:1701:A:H2'	29:S1:1702:A:C8	2.43	0.53
32:SC:93:ARG:NH1	32:SC:93:ARG:HB2	2.24	0.53
36:6:47:G:OP1	69:K:124:ARG:NH2	2.42	0.53
59:E:44:ASP:OD2	59:E:46:ARG:NH1	2.41	0.53
1:SD:49:SER:O	1:SD:53:ARG:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SE:111:LEU:HD22	2:SE:115:GLU:HG3	1.91	0.53
4:SG:197:ASP:OD1	4:SG:197:ASP:N	2.39	0.53
10:SM:30:GLU:OE2	10:SM:84:ARG:NH2	2.35	0.53
35:8:16:C:OP2	35:8:71:C:O2'	2.26	0.53
53:I:49:LYS:HB2	53:I:49:LYS:NZ	2.23	0.53
29:S1:1246:PSU:H2'	29:S1:1247:U:C6	2.44	0.53
29:S1:1614:U:H2'	29:S1:1615:G:C8	2.44	0.53
31:SB:138:ARG:O	31:SB:141:SER:OG	2.26	0.53
37:2:467:G:N7	71:i:70:LYS:NZ	2.55	0.53
37:2:999:U:O2'	37:2:1000:U:O5'	2.22	0.53
4:SG:155:ASP:OD1	4:SG:156:VAL:N	2.42	0.53
19:SW:60:PRO:O	29:S1:1595:G:N2	2.23	0.53
29:S1:1157:C:H2'	29:S1:1158:U:C6	2.44	0.53
29:S1:2058:G:C2	29:S1:2059:C:H1'	2.44	0.53
39:5:106:G:H8	82:e:89:LYS:HA	1.74	0.53
29:S1:779:A:H2'	29:S1:780:A:C8	2.44	0.52
29:S1:2085:A:O2'	29:S1:2086:A:H8	1.92	0.52
37:2:998:G:H1'	37:2:999:U:H5'	1.91	0.52
42:1:93:G:H2'	42:1:94:A:C8	2.43	0.52
46:c:175:ASP:OD1	46:c:178:MET:HG3	2.09	0.52
55:T:88:VAL:O	55:T:92:MET:HG3	2.08	0.52
13:SP:3:LYS:NZ	29:S1:661:OMU:OP2	2.42	0.52
28:Sg:33:SER:OG	28:Sg:34:ARG:N	2.41	0.52
28:Sg:154:SER:OG	28:Sg:198:SER:O	2.26	0.52
29:S1:1833:U:H4'	29:S1:1834:G:OP1	2.09	0.52
31:SB:58:TRP:HZ3	31:SB:180:LEU:HD12	1.74	0.52
40:4:24:A:H5''	49:H:7:LYS:HB2	1.90	0.52
77:X:56:THR:O	77:X:60:ARG:HG2	2.09	0.52
13:SP:52:LEU:HD11	13:SP:73:GLN:HB2	1.92	0.52
29:S1:1841:PSU:H2'	29:S1:1842:C:C6	2.43	0.52
31:SB:144:ASN:OD1	31:SB:144:ASN:N	2.43	0.52
32:SC:157:ILE:HD13	32:SC:163:HIS:HB2	1.91	0.52
42:1:73:U:H5'	53:I:63:VAL:HB	1.90	0.52
44:C:252:GLN:O	44:C:256:GLU:HG3	2.09	0.52
29:S1:258:C:H42	29:S1:969:A:H61	1.57	0.52
29:S1:327:U:H2'	29:S1:328:C:C6	2.44	0.52
29:S1:1193:U:H2'	29:S1:1194:C:C6	2.44	0.52
41:3:53:U:OP1	72:U:87:LYS:NZ	2.42	0.52
42:1:1477:G:O2'	61:f:100:THR:HG22	2.09	0.52
62:g:57:ARG:HB2	62:g:116:MET:HE2	1.91	0.52
63:a:99:LEU:HD22	63:a:103:GLU:HB3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:134:C:HO2'	37:2:135:A:H8	1.57	0.52
59:E:77:GLN:O	59:E:80:ILE:HG13	2.09	0.52
42:1:1403:A:OP1	51:P:2:GLY:N	2.43	0.52
29:S1:952:U:H2'	29:S1:953:U:C6	2.45	0.52
37:2:1265:U:H1'	37:2:1301:G:N2	2.25	0.52
38:7:128:U:H2'	38:7:129:C:C6	2.44	0.52
29:S1:838:U:H2'	29:S1:839:G:H8	1.75	0.52
66:V:71:THR:HA	66:V:76:MET:HE2	1.92	0.52
13:SP:139:GLU:OE2	13:SP:139:GLU:HA	2.10	0.52
29:S1:1523:A:H2'	29:S1:1524:G:C8	2.45	0.52
32:SC:131:LYS:HB2	32:SC:190:PRO:HB3	1.92	0.52
42:1:885:U:H2'	42:1:886:G:O4'	2.11	0.52
42:1:1565:A:C2	82:e:74:ARG:NH1	2.78	0.52
43:B:80:GLU:OE1	43:B:321:TYR:OH	2.24	0.52
47:O:201:HIS:O	47:O:205:ILE:HG13	2.10	0.52
13:SP:140:LYS:HD2	13:SP:141:PRO:HD2	1.91	0.51
22:SZ:17:PHE:HZ	22:SZ:26:LYS:HD2	1.75	0.51
2:SE:19:LYS:HG3	2:SE:20:LEU:HD12	1.92	0.51
29:S1:17:C:O2'	29:S1:1489:A:N1	2.38	0.51
29:S1:904:G:OP2	29:S1:904:G:N2	2.29	0.51
29:S1:1881:G:H2'	29:S1:1882:A:C8	2.45	0.51
37:2:970:A:OP2	37:2:971:A:N6	2.43	0.51
4:SG:146:LYS:NZ	29:S1:148:G:OP1	2.39	0.51
41:3:191:C:H3'	41:3:192:G:H5''	1.92	0.51
42:1:1436:G:O5'	68:Z:109:ARG:NH2	2.43	0.51
6:SI:179:LEU:O	29:S1:758:G:O2'	2.29	0.51
29:S1:813:U:H3	29:S1:821:A:H61	1.59	0.51
42:1:221:C:H2'	42:1:222:A:C8	2.46	0.51
37:2:1020:C:H2'	37:2:1021:A:O4'	2.11	0.51
69:K:89:THR:OG1	69:K:90:ARG:N	2.44	0.51
52:R:156:ARG:NH2	69:K:55:VAL:O	2.44	0.51
13:SP:73:GLN:NE2	13:SP:78:ASP:OD1	2.44	0.51
24:Sb:38:VAL:HG13	24:Sb:40:ARG:NE	2.26	0.51
29:S1:259:C:H2'	29:S1:260:A:C8	2.46	0.51
29:S1:1248:A:H2'	29:S1:1249:G:C8	2.46	0.51
37:2:4:C:H2'	37:2:5:A:C8	2.46	0.51
42:1:438:A:H4'	42:1:439:U:H3'	1.92	0.51
73:p:65:THR:HG22	73:p:89:LYS:HG2	1.93	0.51
1:SD:89:LYS:HE2	1:SD:94:TYR:HB3	1.93	0.51
21:SY:15:ASP:OD1	21:SY:15:ASP:N	2.40	0.51
21:SY:74:ASN:ND2	31:SB:40:TYR:OH	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:S1:875:A:H62	29:S1:887:U:H5	1.58	0.51
10:SM:75:ASP:HB2	15:SS:55:LYS:HD2	1.93	0.51
22:SZ:43:THR:HA	22:SZ:46:ILE:HD12	1.92	0.51
31:SB:134:HIS:HB2	31:SB:138:ARG:HH21	1.74	0.51
37:2:1117:G:H5'	37:2:1118:A:OP2	2.11	0.51
42:1:1271:G:N2	42:1:1356:G:H22	2.09	0.51
54:Q:7:GLN:NE2	54:Q:35:ALA:O	2.34	0.51
10:SM:48:HIS:HB2	10:SM:87:ASP:HB2	1.91	0.50
20:SX:91:ARG:HH21	29:S1:1940:G:H22	1.59	0.50
37:2:478:A:H2'	37:2:479:C:O2	2.11	0.50
23:Sa:102:THR:OG1	23:Sa:103:ARG:N	2.44	0.50
29:S1:1530:G:H5'	29:S1:1542:C:H41	1.76	0.50
39:5:106:G:C8	82:e:89:LYS:HA	2.46	0.50
41:3:98:C:H2'	41:3:99:U:H6	1.76	0.50
42:1:408:G:O2'	42:1:410:U:OP1	2.29	0.50
29:S1:559:G:H1	29:S1:592:C:H5	1.59	0.50
72:U:77:LEU:HD12	72:U:78:THR:N	2.26	0.50
8:SK:69:SER:OG	8:SK:204:GLU:OE1	2.26	0.50
8:SK:160:ARG:HA	8:SK:160:ARG:NE	2.26	0.50
12:SO:55:VAL:CG1	12:SO:60:ASP:HB2	2.33	0.50
33:Sh:212:LEU:HA	33:Sh:215:ARG:HD3	1.94	0.50
37:2:75:C:O2'	37:2:76:A:P	2.70	0.50
40:4:133:C:H42	40:4:157:A:H2	1.58	0.50
42:1:1238:C:H42	52:R:179:ALA:HB1	1.76	0.50
42:1:1443:U:O2'	42:1:1444:A:H3'	2.11	0.50
40:4:174:A:C6	49:H:4:PRO:HD3	2.46	0.50
29:S1:813:U:H2'	29:S1:814:G:C8	2.46	0.50
42:1:720:A:C8	42:1:721:U:H2'	2.47	0.50
10:SM:100:SER:O	10:SM:100:SER:OG	2.26	0.50
29:S1:955:A:N1	29:S1:980:G:C6	2.80	0.50
29:S1:1521:G:N1	29:S1:1995:G7M:OP2	2.42	0.50
40:4:132:U:H2'	40:4:133:C:C6	2.47	0.50
29:S1:782:C:N4	29:S1:839:G:O6	2.44	0.50
29:S1:2069:U:H3	29:S1:2154:G:H1	1.59	0.50
31:SB:198:TRP:CG	31:SB:200:GLU:HG2	2.47	0.50
37:2:984:G:H22	37:2:1000:U:H3	1.57	0.50
74:o:52:VAL:O	74:o:68:ALA:HA	2.11	0.50
2:SE:171:LYS:HE2	2:SE:173:ARG:HH12	1.77	0.50
5:SH:21:GLU:HG2	5:SH:24:LEU:HD13	1.94	0.50
10:SM:65:THR:O	15:SS:41:ARG:NH2	2.44	0.50
34:S4:76:A:O2'	37:2:1191:C:H5	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:514:U:H2'	37:2:515:U:H2'	1.93	0.50
37:2:603:A:H2'	37:2:604:A2M:H8	1.94	0.50
40:4:158:A:H3'	40:4:159:G:H8	1.77	0.50
42:1:508:A:N1	42:1:547:U:H5	2.09	0.50
42:1:1127:U:O2'	78:b:43:ASN:OD1	2.21	0.50
43:B:135:GLN:O	43:B:139:THR:HG23	2.12	0.50
45:A:36:GLU:OE2	45:A:163:ARG:NH1	2.45	0.50
15:SS:8:ARG:NH1	15:SS:11:GLN:OE1	2.45	0.49
25:Sc:74:LEU:HB3	25:Sc:80:TYR:CZ	2.47	0.49
29:S1:35:U:H2'	29:S1:36:U:C6	2.47	0.49
29:S1:656:G:H5'	29:S1:662:G:N2	2.27	0.49
14:SR:6:ILE:HD13	23:Sa:41:MET:HB2	1.94	0.49
29:S1:755:C:H2'	29:S1:757:C:H5''	1.95	0.49
18:SV:46:LEU:HD23	32:SC:207:ILE:HD11	1.94	0.49
19:SW:54:ARG:NH1	29:S1:1974:A:OP2	2.45	0.49
25:Sc:61:SER:O	25:Sc:61:SER:OG	2.24	0.49
74:o:32:SER:OG	74:o:69:TYR:O	2.26	0.49
4:SG:32:ARG:NH1	4:SG:35:ASN:OD1	2.46	0.49
4:SG:163:ARG:HH11	29:S1:66:U:H6	1.59	0.49
29:S1:2061:5MC:H2'	29:S1:2062:G:C8	2.47	0.49
37:2:134:C:O2'	37:2:135:A:H8	1.94	0.49
37:2:553:G:O2'	37:2:556:U:OP2	2.30	0.49
39:5:47:G:H2'	39:5:48:G:N3	2.26	0.49
42:1:1443:U:H5'	42:1:1464:G:H21	1.77	0.49
12:SO:60:ASP:O	12:SO:63:SER:OG	2.31	0.49
15:SS:49:GLU:OE2	15:SS:49:GLU:N	2.46	0.49
1:SD:130:GLN:NE2	29:S1:558:U:O2'	2.37	0.49
16:ST:14:SER:HB2	29:S1:1206:C:H5''	1.94	0.49
29:S1:1138:G:H2'	29:S1:1139:G:C8	2.48	0.49
29:S1:975:G:H3'	29:S1:976:A:H8	1.77	0.49
42:1:499:C:N4	42:1:500:C:H41	2.11	0.49
63:a:70:LEU:HD13	66:V:53:VAL:HG12	1.95	0.49
67:h:43:ILE:HG22	67:h:54:LEU:HD12	1.94	0.49
71:i:56:LEU:HD13	71:i:79:ARG:HG3	1.95	0.49
76:d:20:MET:HE1	76:d:83:CYS:SG	2.52	0.49
1:SD:43:ARG:NH1	29:S1:521:A:OP1	2.37	0.49
29:S1:1413:C:H2'	29:S1:1414:A:H8	1.77	0.49
31:SB:31:ARG:HE	31:SB:31:ARG:N	2.03	0.49
32:SC:131:LYS:NZ	32:SC:155:TYR:HB2	2.27	0.49
61:f:114:MET:O	68:Z:120:ARG:NH1	2.45	0.49
65:W:80:ASP:OD1	65:W:81:LYS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SP:32:THR:HG22	13:SP:34:SER:H	1.78	0.49
42:1:422:PSU:H2'	42:1:423:U:C6	2.48	0.49
55:T:137:THR:HG23	55:T:138:PRO:HD2	1.93	0.49
19:SW:84:LYS:HB2	29:S1:1593:G:H5'	1.95	0.49
29:S1:510:G:C2'	29:S1:511:C:H5'	2.42	0.49
29:S1:1875:G:H2'	29:S1:1876:U:C6	2.48	0.49
29:S1:1891:A:N6	87:S1:2408:HOH:O	2.46	0.49
31:SB:69:ALA:HB2	31:SB:185:VAL:HG23	1.95	0.49
42:1:499:C:H2'	42:1:500:C:C6	2.48	0.49
9:SL:135:TRP:CH2	10:SM:73:THR:HG23	2.48	0.48
15:SS:22:CYS:SG	15:SS:25:CYS:N	2.72	0.48
22:SZ:35:PRO:CD	22:SZ:36:HIS:N	2.71	0.48
40:4:133:C:N3	40:4:157:A:C6	2.81	0.48
42:1:487:G:H2'	42:1:489:C:C5	2.47	0.48
42:1:1739:A:H4'	67:h:12:MET:HE3	1.95	0.48
3:SF:65:GLU:OE1	3:SF:65:GLU:N	2.45	0.48
6:SI:132:MET:HE1	6:SI:176:TYR:HB2	1.95	0.48
14:SR:88:GLN:HA	14:SR:96:THR:HG23	1.95	0.48
29:S1:2178:U:H2'	29:S1:2179:A:C8	2.48	0.48
31:SB:184:GLU:O	31:SB:188:LEU:HD12	2.13	0.48
29:S1:276:G:H2'	29:S1:277:U:O4'	2.14	0.48
37:2:68:A:HO2'	37:2:69:A:P	2.36	0.48
55:T:36:ILE:HD12	55:T:114:ILE:HD13	1.96	0.48
27:Se:13:LYS:NZ	29:S1:612:U:O2'	2.43	0.48
29:S1:1197:C:H2'	29:S1:1198:A:C8	2.47	0.48
35:8:114:G:H2'	35:8:115:C:C6	2.49	0.48
37:2:1024:U:H2'	37:2:1025:G:C8	2.47	0.48
42:1:836:G:OP1	51:P:149:ARG:NH1	2.46	0.48
2:SE:250:ARG:NH2	29:S1:864:G:OP1	2.44	0.48
28:Sg:250:MET:HE2	28:Sg:263:LEU:HD21	1.96	0.48
29:S1:1678:A:H4'	32:SC:155:TYR:HD1	1.79	0.48
36:6:9:U:H3	37:2:1443:A:H62	1.60	0.48
37:2:590:U:H2'	37:2:591:A2M:H8	1.95	0.48
37:2:969:A:O2'	37:2:970:A:O4'	2.30	0.48
42:1:898:A:H2'	42:1:899:A:C8	2.48	0.48
28:Sg:272:LEU:HD11	28:Sg:306:TRP:CG	2.48	0.48
29:S1:1224:A:N7	29:S1:1271:C:H5	2.11	0.48
74:o:8:MET:HE1	74:o:15:GLY:O	2.13	0.48
79:k:5:ILE:HD11	79:k:43:TYR:HB3	1.95	0.48
29:S1:978:C:H2'	29:S1:979:U:H6	1.79	0.48
41:3:204:A:H2'	41:3:205:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:E:27:VAL:HG11	59:E:80:ILE:HG22	1.95	0.48
63:a:38:THR:O	63:a:38:THR:OG1	2.29	0.48
66:V:73:ASP:OD1	66:V:73:ASP:N	2.45	0.48
72:U:43:VAL:HA	72:U:46:ASN:ND2	2.27	0.48
5:SH:129:PRO:HA	5:SH:132:ARG:HG3	1.96	0.48
5:SH:162:GLU:OE2	5:SH:173:SER:OG	2.31	0.48
8:SK:156:PRO:HB3	8:SK:160:ARG:HH22	1.78	0.48
17:SU:77:SER:OG	17:SU:78:ASN:N	2.42	0.48
29:S1:1170:A:H2'	29:S1:1171:A:C8	2.48	0.48
31:SB:26:CYS:HB3	31:SB:57:MET:HE1	1.95	0.48
42:1:188:A:OP1	65:W:121:ARG:NH1	2.47	0.48
73:p:47:GLN:OE1	73:p:54:THR:OG1	2.17	0.48
2:SE:28:PRO:HG2	2:SE:35:LEU:HG	1.95	0.48
6:SI:162:ARG:NH1	6:SI:166:GLU:OE1	2.46	0.48
32:SC:140:LYS:H	32:SC:146:ALA:HA	1.78	0.48
34:S4:2:C:H2'	34:S4:3:G:H8	1.78	0.48
37:2:1264:PSU:H2'	37:2:1265:U:C6	2.48	0.48
1:SD:62:PRO:O	1:SD:63:GLU:HG2	2.14	0.48
6:SI:82:THR:HG23	6:SI:94:VAL:HG23	1.95	0.48
8:SK:76:VAL:HG12	8:SK:108:PRO:HG2	1.96	0.48
15:SS:20:ARG:CZ	15:SS:21:CYS:H	2.27	0.48
29:S1:25:C:H5''	29:S1:26:A:H5'	1.96	0.48
37:2:402:U:OP2	45:A:241:ARG:NH2	2.46	0.48
37:2:1173:G:N2	37:2:1176:A:OP2	2.39	0.48
42:1:135:A:N1	63:a:112:MET:HE1	2.28	0.48
42:1:1657:G:H2'	42:1:1658:U:C6	2.49	0.48
2:SE:15:TRP:CD1	2:SE:15:TRP:N	2.82	0.47
13:SP:3:LYS:NZ	29:S1:663:C:OP2	2.31	0.47
29:S1:895:A:H3'	29:S1:896:A:H8	1.78	0.47
36:6:51:A:H4'	36:6:52:G:O5'	2.14	0.47
37:2:795:U:H2'	37:2:799:G:C2	2.49	0.47
37:2:795:U:H2'	37:2:799:G:N2	2.29	0.47
37:2:1034:G:OP1	45:A:233:GLN:NE2	2.42	0.47
41:3:105:C:H2'	41:3:106:U:C6	2.49	0.47
52:R:70:LYS:O	52:R:74:ARG:NH2	2.47	0.47
64:J:134:HIS:ND1	87:J:301:HOH:O	2.33	0.47
14:SR:97:GLU:OE2	14:SR:107:ARG:NH2	2.47	0.47
40:4:19:C:O2'	40:4:20:U:H5'	2.14	0.47
42:1:662:C:H2'	42:1:663:C:C6	2.48	0.47
18:SV:32:LYS:O	18:SV:36:MET:HG3	2.13	0.47
29:S1:56:U:OP1	29:S1:446:A:N6	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:603:A:H5'	55:T:137:THR:HG23	1.96	0.47
37:2:646:G:O2'	37:2:647:A:OP1	2.30	0.47
37:2:970:A:H5''	37:2:971:A:C5	2.49	0.47
38:7:125:A:H3'	38:7:126:G:H8	1.79	0.47
53:I:2:PRO:O	53:I:3:LYS:C	2.57	0.47
38:7:6:G:H2'	38:7:7:OMU:H6	1.95	0.47
10:SM:24:ARG:HD2	10:SM:79:LEU:HD11	1.97	0.47
28:Sg:135:ASN:HD21	28:Sg:139:GLU:HG3	1.80	0.47
29:S1:1568:C:O2	29:S1:1847:A:N6	2.47	0.47
42:1:487:G:H3'	42:1:488:G:C5'	2.44	0.47
42:1:495:C:OP1	58:F:28:THR:HG21	2.14	0.47
45:A:46:LYS:HA	45:A:46:LYS:HD2	1.77	0.47
76:d:50:CYS:O	76:d:55:ARG:NH2	2.46	0.47
7:SJ:86:TYR:O	7:SJ:90:MET:HG3	2.15	0.47
29:S1:494:A:O2'	29:S1:495:A:OP1	2.29	0.47
29:S1:779:A:H2'	29:S1:780:A:H8	1.78	0.47
29:S1:1510:C:H2'	29:S1:1510:C:O2	2.14	0.47
35:8:55:G:H21	75:D:11:MET:HE3	1.80	0.47
42:1:219:U:HO2'	42:1:220:A:P	2.35	0.47
42:1:462:A:N6	87:1:1918:HOH:O	2.48	0.47
50:G:298:ASN:OD1	50:G:301:ARG:NH2	2.46	0.47
2:SE:162:LYS:HE2	2:SE:162:LYS:HB2	1.66	0.47
3:SF:157:GLY:H	7:SJ:98:GLN:NE2	2.13	0.47
3:SF:213:ARG:HH11	3:SF:213:ARG:HG2	1.79	0.47
18:SV:43:SER:OG	18:SV:46:LEU:HB2	2.15	0.47
22:SZ:115:LYS:HE3	29:S1:506:U:OP1	2.15	0.47
24:Sb:44:ARG:NH2	24:Sb:71:LEU:HB2	2.30	0.47
37:2:809:C:H3'	37:2:810:G:N2	2.29	0.47
42:1:175:G:C2'	42:1:176:C:H5'	2.44	0.47
42:1:1238:C:H5'	62:g:114:ALA:HB2	1.95	0.47
43:B:56:ILE:HD13	43:B:363:LEU:HD22	1.97	0.47
51:P:62:ILE:HG12	51:P:63:SER:H	1.80	0.47
60:Y:16:GLY:O	67:h:77:ARG:HG3	2.15	0.47
66:V:106:TYR:O	66:V:108:VAL:N	2.46	0.47
70:j:67:LEU:HA	70:j:70:VAL:HG12	1.97	0.47
36:6:55:U:H4'	36:6:56:A:OP1	2.15	0.47
37:2:1404:G:H2'	37:2:1405:A:C8	2.50	0.47
37:2:1456:C:O2'	37:2:1457:C:OP1	2.27	0.47
42:1:739:U:H2'	42:1:740:C:C6	2.49	0.47
42:1:1664:PSU:H6	42:1:1664:PSU:H5'	1.80	0.47
43:B:247:THR:HB	43:B:251:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Z:71:ASN:C	68:Z:72:ASN:HD22	2.18	0.47
6:SI:10:LYS:HD3	29:S1:986:C:OP2	2.15	0.47
11:SN:29:ARG:NH2	29:S1:1569:G:C8	2.83	0.47
20:SX:43:VAL:HG12	20:SX:66:TYR:CD2	2.50	0.47
27:Se:60:GLN:HB2	29:S1:607:PSU:H5''	1.97	0.47
29:S1:883:G:H2'	29:S1:884:A:C8	2.50	0.47
31:SB:198:TRP:HD1	31:SB:199:GLU:N	2.12	0.47
37:2:71:OMG:H1'	37:2:71:OMG:HM23	1.65	0.47
37:2:591:A2M:HM'3	37:2:591:A2M:H1'	1.53	0.47
37:2:1263:C:H2'	37:2:1264:PSU:C6	2.50	0.47
37:2:1309:G:H5''	37:2:1310:A:H5''	1.97	0.47
37:2:1404:G:H5'	45:A:220:GLY:HA3	1.97	0.47
44:C:140:GLY:HA2	68:Z:17:ARG:HD2	1.95	0.47
75:D:81:LEU:C	75:D:83:GLU:H	2.22	0.47
20:SX:138:ARG:O	20:SX:142:LYS:HG3	2.15	0.47
24:Sb:44:ARG:CZ	24:Sb:44:ARG:HB2	2.44	0.47
29:S1:853:A:H2	29:S1:898:G:H22	1.63	0.47
42:1:462:A:H3'	42:1:462:A:N3	2.30	0.47
79:k:33:LYS:HG2	79:k:46:VAL:HG22	1.97	0.47
37:2:29:C:OP1	37:2:32:C:N4	2.46	0.46
37:2:340:A:H4'	37:2:341:A:O5'	2.15	0.46
37:2:511:C:H2'	37:2:512:PSU:O4'	2.16	0.46
41:3:110:U:O2'	41:3:128:G:O6	2.20	0.46
41:3:122:U:OP2	54:Q:103:ARG:NH1	2.47	0.46
50:G:124:ASP:N	50:G:124:ASP:OD1	2.47	0.46
10:SM:31:SER:OG	10:SM:104:GLU:OE2	2.27	0.46
19:SW:35:LEU:HD12	19:SW:35:LEU:HA	1.77	0.46
28:Sg:272:LEU:HD11	28:Sg:306:TRP:CD2	2.50	0.46
29:S1:1156:PSU:H2'	29:S1:1157:C:H6	1.79	0.46
29:S1:1186:A:H2'	29:S1:1187:A:C8	2.50	0.46
29:S1:1870:A:H2'	29:S1:1871:C:C6	2.51	0.46
37:2:472:PSU:H2'	37:2:473:C:C6	2.50	0.46
37:2:979:A:O2'	37:2:980:A:H8	1.97	0.46
42:1:959[B]:OMG:C3'	42:1:959[B]:OMG:C8	2.98	0.46
82:e:128:THR:O	82:e:132:HIS:HB3	2.15	0.46
12:SO:127:PRO:HB3	29:S1:1134:A:H5''	1.97	0.46
29:S1:259:C:H2'	29:S1:260:A:H8	1.79	0.46
30:SA:224:LYS:HE3	30:SA:224:LYS:HB3	1.77	0.46
32:SC:133:CYS:SG	32:SC:134:GLU:N	2.87	0.46
37:2:73:OMU:HM23	37:2:73:OMU:H1'	1.58	0.46
37:2:383:U:H5	37:2:388:A:N7	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:22:G:H2'	40:4:23:C:C6	2.51	0.46
42:1:787:A:H2'	42:1:788:A:C8	2.51	0.46
49:H:90:HIS:O	49:H:92:ARG:NH1	2.47	0.46
5:SH:65:LYS:HA	5:SH:65:LYS:HD3	1.76	0.46
6:SI:61:VAL:HG12	6:SI:93:LEU:HB2	1.98	0.46
6:SI:122:THR:HG23	29:S1:688:G:OP2	2.15	0.46
8:SK:49:ARG:NH2	29:S1:442:A:OP1	2.48	0.46
28:Sg:116:SER:OG	28:Sg:118:ASP:OD1	2.26	0.46
29:S1:608:C:H2'	29:S1:609:PSU:C6	2.51	0.46
29:S1:883:G:H2'	29:S1:884:A:H8	1.81	0.46
29:S1:911:A:H2'	29:S1:912:A:C8	2.50	0.46
29:S1:1702:A:H2'	29:S1:1703:U:C6	2.50	0.46
47:O:36:MET:HE3	47:O:36:MET:HB2	1.81	0.46
50:G:193:ARG:C	50:G:195:GLN:H	2.24	0.46
2:SE:26:PRO:HD3	29:S1:491:G:OP1	2.14	0.46
9:SL:53:LYS:HD2	9:SL:53:LYS:HA	1.72	0.46
20:SX:96:LYS:NZ	29:S1:1982:G:OP1	2.47	0.46
29:S1:1367:U:H1'	30:SA:150:ASN:HD21	1.80	0.46
33:Sh:134:ASN:OD1	33:Sh:134:ASN:N	2.49	0.46
37:2:984:G:H2'	37:2:985:A:C8	2.50	0.46
40:4:19:C:H2'	40:4:20:U:C6	2.51	0.46
42:1:904:G:N7	74:o:2:ALA:N	2.64	0.46
42:1:1664:PSU:H5'	42:1:1664:PSU:C6	2.51	0.46
52:R:153:LEU:HD13	69:K:6:ILE:HG13	1.97	0.46
72:U:90:PHE:O	72:U:94:THR:OG1	2.29	0.46
6:SI:62:LEU:N	6:SI:93:LEU:O	2.43	0.46
16:ST:100:LYS:HE3	16:ST:100:LYS:HB2	1.81	0.46
22:SZ:18:LYS:HE3	22:SZ:27:GLN:HE21	1.80	0.46
28:Sg:290:ASP:OD1	28:Sg:290:ASP:N	2.43	0.46
32:SC:23:PHE:O	32:SC:27:GLU:HG2	2.16	0.46
33:Sh:216:GLN:O	33:Sh:220:ASN:N	2.48	0.46
35:8:67:C:H2'	35:8:68:A:H5'	1.97	0.46
42:1:273:A:C6	70:j:79:LYS:HA	2.50	0.46
42:1:1240:U:H2'	42:1:1241:A:C8	2.50	0.46
42:1:1271:G:H2'	42:1:1272:U:H5''	1.98	0.46
74:o:8:MET:HE2	74:o:12:GLY:HA2	1.97	0.46
37:2:1456:C:HO2'	37:2:1457:C:P	2.37	0.46
4:SG:32:ARG:NH2	29:S1:2100:A:O3'	2.48	0.46
11:SN:90:ALA:N	11:SN:91:PRO:HD3	2.31	0.46
21:SY:42:ALA:HA	21:SY:54:THR:HG22	1.98	0.46
29:S1:559:G:H22	29:S1:592:C:H5	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:7:94:G:H1'	70:j:81:PRO:HD3	1.98	0.46
43:B:244:PRO:O	43:B:251:LEU:HD22	2.16	0.46
50:G:250:TRP:CD1	50:G:250:TRP:H	2.34	0.46
58:F:185:LYS:HE3	58:F:185:LYS:HB2	1.52	0.46
5:SH:60:ASN:OD1	5:SH:72:LYS:NZ	2.47	0.46
20:SX:127:GLU:HB3	20:SX:137:THR:HG22	1.96	0.46
29:S1:640:A:H2'	29:S1:641:A:C8	2.50	0.46
37:2:969:A:H2'	37:2:970:A:C5	2.51	0.46
42:1:505:U:H2'	42:1:506:G:C8	2.50	0.46
42:1:1128:A:H1'	42:1:1129:G:H5'	1.98	0.46
42:1:1135:U:H2'	42:1:1135:U:O2	2.15	0.46
42:1:1392:G:H2'	42:1:1392:G:N3	2.31	0.46
3:SF:182:VAL:HB	3:SF:209:TYR:HB2	1.96	0.46
18:SV:37:ASP:OD1	18:SV:37:ASP:N	2.49	0.46
29:S1:691:G:H22	29:S1:754:G:N2	2.13	0.46
30:SA:115:LEU:H	30:SA:115:LEU:HG	1.52	0.46
32:SC:84:GLN:HA	32:SC:84:GLN:OE1	2.16	0.46
35:8:50:G:OP1	47:O:164:ARG:HG3	2.16	0.46
37:2:1383:G:H5'	37:2:1385:G:N7	2.31	0.46
2:SE:193:VAL:HG21	2:SE:208:LYS:HG3	1.98	0.45
12:SO:59:ARG:HG2	29:S1:1152:A:H5''	1.96	0.45
12:SO:128:ILE:O	29:S1:1133:U:O2'	2.34	0.45
17:SU:39:LYS:NZ	29:S1:248:G:N7	2.53	0.45
29:S1:569:U:H1'	29:S1:572:A:N7	2.31	0.45
29:S1:909:C:C2	29:S1:910:A:C8	3.04	0.45
31:SB:167:ASN:OD1	31:SB:169:ARG:NH1	2.49	0.45
35:8:47:U:OP1	75:D:139:ARG:HG3	2.17	0.45
40:4:133:C:C4	40:4:157:A:N1	2.83	0.45
42:1:700:A:C2	42:1:845:OMU:H5	2.51	0.45
64:J:125:ALA:HB1	64:J:132:SER:HB3	1.98	0.45
4:SG:68:VAL:HG23	4:SG:102:GLY:HA2	1.99	0.45
29:S1:307:C:H2'	29:S1:308:C:C6	2.51	0.45
29:S1:752:C:H2'	29:S1:753:A:C8	2.51	0.45
64:J:106:ASN:N	64:J:110:GLU:O	2.49	0.45
14:SR:131:ARG:HB3	14:SR:135:GLN:OE1	2.16	0.45
28:Sg:203:SER:HB2	28:Sg:208:LEU:HB2	1.98	0.45
29:S1:677:G:H21	29:S1:1218:A:H62	1.64	0.45
29:S1:836:C:H2'	29:S1:837:G:C8	2.52	0.45
37:2:1116:A:N3	37:2:1116:A:H2'	2.30	0.45
42:1:486:C:H6	42:1:487:G:N2	2.14	0.45
42:1:546:G:O2'	42:1:547:U:O2	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1:1269:G:HO2'	42:1:1270:U:P	2.38	0.45
26:Sd:32:ARG:NH1	29:S1:2036:G:H4'	2.30	0.45
28:Sg:260:VAL:HG13	28:Sg:270:ALA:HB3	1.98	0.45
29:S1:510:G:H2'	29:S1:511:C:H5'	1.98	0.45
29:S1:2060:C:H6	29:S1:2060:C:O5'	1.99	0.45
30:SA:136:THR:HG23	30:SA:221:ARG:HB3	1.98	0.45
36:6:49:C:N4	62:g:29:LYS:O	2.49	0.45
37:2:1398:C:H2'	37:2:1399:G:C8	2.52	0.45
46:c:75:LEU:HD23	46:c:75:LEU:HA	1.75	0.45
50:G:259:LYS:HA	50:G:259:LYS:HD2	1.75	0.45
63:a:28:GLU:HG2	63:a:51:ILE:HD13	1.97	0.45
12:SO:57:ALA:HB3	12:SO:60:ASP:OD2	2.17	0.45
12:SO:73:ASP:N	12:SO:73:ASP:OD1	2.48	0.45
14:SR:35:LYS:HE2	14:SR:35:LYS:HB3	1.82	0.45
25:Sc:57:CYS:O	25:Sc:61:SER:HB2	2.17	0.45
37:2:780:G:H1	37:2:811:U:H3	1.64	0.45
37:2:1089:A:H2'	37:2:1090:G:C8	2.51	0.45
43:B:302:THR:OG1	43:B:308:THR:O	2.28	0.45
43:B:391:LYS:O	43:B:395:ILE:HG23	2.17	0.45
73:p:88:THR:OG1	73:p:89:LYS:N	2.50	0.45
26:Sd:46:LEU:HD23	26:Sd:46:LEU:HA	1.84	0.45
29:S1:651:U:H2'	29:S1:652:U:C6	2.52	0.45
29:S1:2055:A:H5'	29:S1:2058:G:H4'	1.98	0.45
37:2:667:OMU:HM23	37:2:667:OMU:H1'	1.58	0.45
37:2:970:A:H4'	37:2:972:C:OP1	2.16	0.45
38:7:74:PSU:O2	65:W:71:TYR:HA	2.17	0.45
42:1:305:A2M:H2	42:1:333:A:N6	2.31	0.45
42:1:694:U:H2'	42:1:695:OMC:C6	2.52	0.45
26:Sd:26:ILE:HD12	26:Sd:71:ASP:HB2	1.98	0.45
29:S1:40:A:H62	29:S1:515:G:H21	1.64	0.45
29:S1:594:A:H61	29:S1:643:A:H5''	1.82	0.45
29:S1:783:A:H2	29:S1:837:G:N2	2.13	0.45
29:S1:2061:5MC:H2'	29:S1:2062:G:H8	1.82	0.45
37:2:406:G:H2'	37:2:407:C:C6	2.52	0.45
41:3:98:C:O2'	41:3:99:U:O5'	2.32	0.45
42:1:1271:G:H22	42:1:1356:G:N2	2.15	0.45
60:Y:126:MET:O	60:Y:130:GLN:HG2	2.17	0.45
16:ST:104:ARG:HB2	16:ST:104:ARG:HH11	1.82	0.45
28:Sg:109:ASP:OD2	28:Sg:127:ARG:NH1	2.42	0.45
29:S1:976:A:C4	29:S1:977:G:C8	3.05	0.45
30:SA:169:ARG:O	30:SA:173:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SB:91:TYR:O	31:SB:94:SER:OG	2.31	0.45
37:2:1323:C:O2'	42:1:1365:A:H1'	2.17	0.45
12:SO:144:LEU:HD23	12:SO:144:LEU:HA	1.79	0.45
28:Sg:199:THR:HG21	28:Sg:240:GLN:HA	1.98	0.45
29:S1:1171:A:H2'	29:S1:1172:G:C8	2.52	0.45
42:1:1629:G:O6	67:h:11:ARG:NH2	2.50	0.45
19:SW:43:LEU:HD23	19:SW:43:LEU:HA	1.84	0.45
28:Sg:236:SER:HB2	28:Sg:256:ARG:HH11	1.82	0.45
29:S1:1146:G:N3	29:S1:1162:A:C2	2.85	0.45
29:S1:1415:C:O2'	30:SA:150:ASN:OD1	2.32	0.45
31:SB:152:ASP:OD1	31:SB:153:THR:N	2.49	0.45
35:8:55:G:H21	75:D:11:MET:CE	2.30	0.45
37:2:653:C:H2'	37:2:654:U:H6	1.82	0.45
37:2:1136:U:H2'	37:2:1137:G:C8	2.52	0.45
40:4:155:A:H2'	40:4:156:G:O4'	2.17	0.45
42:1:279:G:H2'	42:1:280:A:C6	2.52	0.45
42:1:509:U:P	46:c:77:ARG:HH21	2.40	0.45
42:1:846:G:H2'	42:1:847:OMU:H6	1.99	0.45
42:1:1271:G:H1	42:1:1356:G:H1	1.63	0.45
42:1:1763:A:OP2	79:k:65:LYS:NZ	2.39	0.45
67:h:64:ASP:OD1	67:h:64:ASP:N	2.49	0.45
67:h:69:SER:OG	67:h:72:GLU:OE1	2.31	0.45
73:p:37:ALA:O	73:p:41:ARG:HG3	2.17	0.45
80:l:38:ASN:C	80:l:40:LYS:H	2.25	0.45
1:SD:71:GLU:HA	1:SD:74:ALA:HB3	1.99	0.44
1:SD:85:LEU:HD12	1:SD:85:LEU:HA	1.85	0.44
1:SD:109:GLN:NE2	1:SD:125:ARG:HB2	2.32	0.44
4:SG:194:LYS:NZ	29:S1:315:A:OP1	2.41	0.44
6:SI:137:ASP:N	6:SI:137:ASP:OD1	2.50	0.44
29:S1:1278:U:H5	29:S1:1445:A:N7	2.15	0.44
34:S4:67:C:H2'	34:S4:68:C:C6	2.53	0.44
37:2:41:A:C4	42:1:1587:A:OP2	2.70	0.44
60:Y:52:LYS:O	60:Y:65:ARG:NH2	2.36	0.44
65:W:80:ASP:OD1	65:W:81:LYS:HG2	2.17	0.44
20:SX:45:ASN:N	29:S1:1920:A:N7	2.55	0.44
29:S1:285:A:H8	29:S1:816:C:N3	2.15	0.44
29:S1:1264:C:H2'	29:S1:1265:A:C8	2.53	0.44
29:S1:2061:5MC:H6	29:S1:2061:5MC:O5'	2.01	0.44
30:SA:32:VAL:O	30:SA:42:GLN:HA	2.18	0.44
55:T:36:ILE:HA	55:T:39:MET:SD	2.57	0.44
56:S:152:ASP:OD1	56:S:152:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:h:75:VAL:HG13	67:h:77:ARG:H	1.82	0.44
2:SE:163:GLU:OE2	2:SE:165:LYS:HG3	2.18	0.44
2:SE:176:LYS:HG3	2:SE:226:GLY:O	2.18	0.44
37:2:1096:U:H2'	37:2:1097:G:C8	2.52	0.44
39:5:37:U:H5''	43:B:315:MET:HE2	2.00	0.44
42:1:507:C:HO2'	42:1:508:A:P	2.38	0.44
42:1:1010:OMC:HM22	42:1:1010:OMC:H1'	1.65	0.44
1:SD:151:SER:O	1:SD:151:SER:OG	2.33	0.44
2:SE:84:MET:HE3	2:SE:84:MET:HB3	1.82	0.44
2:SE:101:ASP:OD2	2:SE:101:ASP:C	2.60	0.44
3:SF:76:HIS:NE2	3:SF:77:GLN:OE1	2.51	0.44
5:SH:69:ASN:ND2	29:S1:2007:G:O2'	2.42	0.44
5:SH:86:ILE:O	5:SH:90:THR:OG1	2.34	0.44
15:SS:37:LEU:HD23	15:SS:37:LEU:HA	1.82	0.44
18:SV:2:GLY:HA2	29:S1:1815:U:H4'	1.99	0.44
28:Sg:125:ALA:HB2	28:Sg:131:ILE:HG12	1.99	0.44
29:S1:1415:C:H2'	29:S1:1416:G:H8	1.81	0.44
29:S1:2178:U:H2'	29:S1:2179:A:H8	1.82	0.44
37:2:342:U:H2'	37:2:343:U:H6	1.82	0.44
37:2:802:U:H3'	37:2:803:A:H2	1.82	0.44
37:2:1323:C:O2'	37:2:1324:U:H5'	2.17	0.44
41:3:16:G:N7	67:h:71:HIS:CE1	2.86	0.44
42:1:218:A:H1'	42:1:219:U:H1'	1.99	0.44
42:1:486:C:C6	42:1:487:G:N2	2.83	0.44
42:1:506:G:O2'	42:1:507:C:H5'	2.17	0.44
69:K:31:ASP:CG	69:K:32:ALA:N	2.76	0.44
74:o:41:PHE:CZ	74:o:62:LYS:HD2	2.53	0.44
14:SR:6:ILE:CD1	23:Sa:41:MET:HB2	2.48	0.44
29:S1:983:C:H2'	29:S1:984:G:C8	2.52	0.44
29:S1:1623:OMG:HM22	29:S1:1623:OMG:H1'	1.56	0.44
29:S1:1979:OMU:HM23	29:S1:1979:OMU:H1'	1.62	0.44
36:6:68:A:N3	36:6:68:A:H2'	2.32	0.44
37:2:1254:G:O4'	37:2:1308:5MC:HM53	2.16	0.44
37:2:1303:PSU:O2'	37:2:1304:C:H5'	2.18	0.44
42:1:719:U:O2'	42:1:720:A:H5''	2.17	0.44
42:1:967:G:H5'	42:1:968:A:OP1	2.18	0.44
43:B:50:LYS:HA	43:B:79:LEU:HD23	1.98	0.44
68:Z:75:ARG:HG3	68:Z:76:GLN:HG3	1.99	0.44
70:j:39:TYR:CD1	70:j:40:PRO:HA	2.53	0.44
3:SF:213:ARG:HG2	3:SF:213:ARG:NH1	2.31	0.44
5:SH:110:ASP:OD1	5:SH:111:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SL:57:ALA:O	9:SL:66:TYR:OH	2.33	0.44
29:S1:957:G:H3'	29:S1:958:G:C8	2.52	0.44
29:S1:1706:A:H62	29:S1:1766:G:N2	2.09	0.44
34:S4:67:C:H2'	34:S4:68:C:H6	1.83	0.44
37:2:1457:C:H2'	37:2:1458:G:C8	2.52	0.44
82:e:49:HIS:HA	82:e:60:VAL:HA	2.00	0.44
20:SX:147:LEU:O	20:SX:151:VAL:HG12	2.17	0.44
23:Sa:50:LEU:HD12	23:Sa:54:VAL:HG21	1.99	0.44
29:S1:1637:A:H8	29:S1:1638:U:N3	2.15	0.44
31:SB:179:TRP:NE1	31:SB:200:GLU:OE2	2.51	0.44
37:2:964:G:H4'	37:2:965:C:H5'	2.00	0.44
40:4:101:G:H2'	40:4:102:G:O4'	2.18	0.44
41:3:147:A:H4'	79:k:4:GLU:HG3	2.00	0.44
42:1:837:A:H4'	42:1:838:G:O5'	2.18	0.44
53:I:133:MET:HE2	53:I:133:MET:HB3	1.71	0.44
62:g:74:ARG:HB2	62:g:141:PRO:HG3	1.99	0.44
63:a:5:MET:HE2	63:a:21:THR:HG21	1.99	0.44
11:SN:8:PRO:O	11:SN:12:ASN:ND2	2.45	0.44
11:SN:89:LEU:CB	11:SN:91:PRO:HD3	2.48	0.44
19:SW:22:PHE:HE1	19:SW:29:ILE:HB	1.83	0.44
29:S1:587:A:H2'	29:S1:588:G:C8	2.52	0.44
29:S1:1560:A:H5'	29:S1:1561:C:OP2	2.18	0.44
39:5:3:A:N3	40:4:180:C:O2'	2.50	0.44
47:O:118:LYS:HB2	47:O:118:LYS:HE2	1.72	0.44
62:g:39:LEU:HD23	62:g:131:ILE:HA	2.00	0.44
1:SD:89:LYS:HD2	1:SD:94:TYR:CG	2.53	0.44
3:SF:195:VAL:HB	3:SF:196:PRO:HD3	2.00	0.44
24:Sb:40:ARG:HD2	24:Sb:77:PHE:CE2	2.53	0.44
29:S1:374:U:H2'	29:S1:375:G:C8	2.53	0.44
29:S1:1911:U:H2'	29:S1:1912:A:O4'	2.16	0.44
29:S1:1956:C:O2	29:S1:1956:C:H2'	2.18	0.44
29:S1:2092:G:H2'	29:S1:2093:U:C6	2.52	0.44
30:SA:146:LYS:HB3	30:SA:210:ARG:HB2	2.00	0.44
31:SB:198:TRP:CD2	31:SB:200:GLU:HG2	2.52	0.44
39:5:43:G:C8	39:5:100:A:H8	2.36	0.44
42:1:239:PSU:H2'	42:1:240:U:C6	2.53	0.44
42:1:790:C:H41	44:C:305:LEU:N	2.16	0.44
42:1:1563:U:H2'	42:1:1564:C:O4'	2.18	0.44
52:R:153:LEU:HD23	52:R:156:ARG:NH1	2.33	0.44
73:p:6:LYS:HE2	73:p:94:ASN:HA	1.98	0.44
11:SN:18:PHE:CE1	11:SN:91:PRO:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SO:118:LYS:HA	12:SO:118:LYS:HD2	1.79	0.43
16:ST:42:ARG:HG3	16:ST:42:ARG:HH11	1.83	0.43
29:S1:1523:A:H2'	29:S1:1524:G:H8	1.83	0.43
29:S1:1621:U:C6	29:S1:1621:U:H5''	2.52	0.43
29:S1:1912:A:H2	29:S1:1929:G:N1	2.06	0.43
31:SB:25:ARG:HD2	31:SB:28:ILE:HG13	2.00	0.43
37:2:665:A:H2'	37:2:666:C:C6	2.53	0.43
37:2:1058:PSU:H2'	37:2:1059:G:C8	2.53	0.43
42:1:508:A:N1	42:1:547:U:C5	2.86	0.43
56:S:100:ARG:NH1	56:S:103:GLU:OE2	2.47	0.43
67:h:45:THR:HG23	67:h:46:PRO:HD2	2.00	0.43
17:SU:73:CYS:SG	17:SU:127:SER:OG	2.64	0.43
28:Sg:4:GLU:OE2	28:Sg:4:GLU:HA	2.18	0.43
29:S1:285:A:H3'	29:S1:285:A:N3	2.33	0.43
29:S1:1826:G:O2'	29:S1:1827:C:H5'	2.18	0.43
29:S1:2046:PSU:H2'	29:S1:2047:U:H6	1.81	0.43
29:S1:2155:C:H2'	29:S1:2156:A:H8	1.83	0.43
35:8:49:U:H2'	35:8:50:G:H8	1.82	0.43
37:2:464:G:H2'	37:2:465:A:C8	2.52	0.43
37:2:528:U:OP1	37:2:1411:G:O2'	2.31	0.43
37:2:1154:C:O2'	37:2:1155:A:H2'	2.18	0.43
37:2:1368:A:HO2'	64:J:40:SER:HG	1.64	0.43
38:7:69:PSU:H2'	38:7:70:C:C6	2.53	0.43
42:1:1134:C:O2'	42:1:1135:U:O4'	2.36	0.43
71:i:47:ILE:O	71:i:51:VAL:HG22	2.18	0.43
19:SW:80:PRO:HD2	19:SW:100:VAL:HG23	2.00	0.43
20:SX:103:GLU:O	20:SX:104:HIS:ND1	2.51	0.43
29:S1:1114:G:H1	29:S1:1207:U:H3	1.65	0.43
29:S1:1155:U:H6	29:S1:1155:U:H5''	1.84	0.43
29:S1:1702:A:H2'	29:S1:1703:U:H6	1.83	0.43
31:SB:186:LEU:HD12	31:SB:198:TRP:CH2	2.50	0.43
36:6:24:C:H2'	36:6:25:U:H5''	2.00	0.43
37:2:1042:G:H2'	37:2:1043:C:H6	1.84	0.43
40:4:25:G:OP2	49:H:6:ARG:N	2.51	0.43
41:3:191:C:H3'	41:3:192:G:C5'	2.48	0.43
58:F:166:LYS:HB2	58:F:166:LYS:HE3	1.67	0.43
11:SN:64:GLU:HG3	11:SN:65:GLN:N	2.32	0.43
31:SB:152:ASP:CG	31:SB:153:THR:H	2.26	0.43
36:6:7:A:H1'	62:g:99:THR:OG1	2.18	0.43
38:7:28:C:H5'	53:I:32:ASN:HB3	2.00	0.43
65:W:52:GLU:HB2	65:W:105:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SD:36:ARG:HE	1:SD:36:ARG:HB3	1.52	0.43
11:SN:18:PHE:HE1	11:SN:91:PRO:HG2	1.83	0.43
11:SN:92:SER:O	11:SN:97:THR:HG23	2.18	0.43
12:SO:92:ALA:H	12:SO:126:THR:HB	1.83	0.43
29:S1:1248:A:C4	29:S1:1249:G:N7	2.87	0.43
29:S1:1276:G:O2'	29:S1:1278:U:O2	2.36	0.43
40:4:175:G:N7	87:4:303:HOH:O	2.36	0.43
2:SE:84:MET:HE2	2:SE:120:LEU:HB2	2.00	0.43
4:SG:203:ARG:NH2	29:S1:185:A:OP1	2.52	0.43
11:SN:94:MET:H	11:SN:95:PRO:CD	2.31	0.43
16:ST:115:LEU:O	16:ST:119:GLU:HG3	2.17	0.43
29:S1:1560:A:H1'	29:S1:1621:U:H2'	2.00	0.43
29:S1:1763:U:H2'	29:S1:1764:U:O2	2.18	0.43
31:SB:32:ASN:HB2	31:SB:154:ASP:OD1	2.19	0.43
32:SC:122:ILE:HG12	32:SC:133:CYS:SG	2.59	0.43
33:Sh:143:ILE:HD11	33:Sh:173:ALA:HB2	2.00	0.43
37:2:660:G:OP1	42:1:959[A]:OMG:N1	2.35	0.43
37:2:814:A:N6	37:2:964:G:C6	2.86	0.43
37:2:1189:A:H2'	37:2:1190:U:O2	2.18	0.43
42:1:141:U:H1'	42:1:142:G:H5''	2.00	0.43
42:1:925:U:OP1	43:B:246:LYS:HG3	2.19	0.43
43:B:192:SER:O	43:B:196:LYS:HG3	2.18	0.43
61:f:41:SER:O	61:f:45:ARG:HG3	2.18	0.43
14:SR:114:ARG:HE	14:SR:114:ARG:HB3	1.64	0.43
28:Sg:38:ALA:HB3	28:Sg:61:LEU:HD12	2.01	0.43
29:S1:661:OMU:HM23	29:S1:661:OMU:H1'	1.78	0.43
29:S1:2079:U:H2'	29:S1:2080:G:H8	1.83	0.43
30:SA:32:VAL:HG22	30:SA:98:LEU:HD12	1.99	0.43
31:SB:195:SER:O	31:SB:195:SER:OG	2.34	0.43
41:3:100:U:HO2'	41:3:101:G:H8	1.64	0.43
41:3:112:C:H2'	76:d:86:HIS:CG	2.54	0.43
42:1:305:A2M:HM'3	48:M:12:LYS:HG3	2.00	0.43
42:1:458:A:H2'	42:1:459:A:O4'	2.19	0.43
1:SD:153:ARG:HH12	1:SD:154:HIS:CE1	2.37	0.43
24:Sb:72:TYR:CD1	24:Sb:72:TYR:N	2.87	0.43
28:Sg:46:ASP:OD1	28:Sg:46:ASP:N	2.51	0.43
29:S1:1148:G:H2'	29:S1:1149:G:C8	2.53	0.43
29:S1:1193:U:H2'	29:S1:1194:C:H6	1.84	0.43
29:S1:2146:U:H2'	29:S1:2147:A:H8	1.84	0.43
29:S1:2167:C:H3'	29:S1:2170:G:N7	2.33	0.43
40:4:151:A:H2'	40:4:152:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1:790:C:H41	44:C:305:LEU:H	1.66	0.43
42:1:959[B]:OMG:H8	42:1:959[B]:OMG:C3'	2.31	0.43
44:C:113:LYS:HD3	48:M:203:LYS:O	2.18	0.43
52:R:27:TYR:CZ	52:R:51:ASN:ND2	2.86	0.43
52:R:119:ARG:HG3	52:R:119:ARG:NH1	2.29	0.43
71:i:5:THR:O	71:i:22:ARG:NH1	2.51	0.43
80:l:16:LYS:HD3	80:l:16:LYS:HA	1.85	0.43
29:S1:1572:C:H2'	29:S1:1573:A:H8	1.83	0.43
38:7:124:A:N1	66:V:109:LYS:HD2	2.34	0.43
60:Y:67:GLN:HA	60:Y:117:GLN:NE2	2.34	0.43
1:SD:101:PRO:O	1:SD:105:GLU:HG2	2.19	0.43
8:SK:203:LEU:HD22	8:SK:207:GLU:HG2	2.00	0.43
27:Se:58:ASN:OD1	27:Se:60:GLN:NE2	2.51	0.43
29:S1:307:C:H3'	29:S1:308:C:H2'	2.01	0.43
29:S1:756:C:H5''	29:S1:757:C:H5'	2.00	0.43
29:S1:862:G:O2'	29:S1:863:C:OP2	2.31	0.43
29:S1:1420:U:H2'	29:S1:1421:C:C6	2.54	0.43
29:S1:1459:G:O2'	29:S1:1460:G:H5'	2.18	0.43
30:SA:175:LYS:O	30:SA:179:SER:OG	2.24	0.43
34:S4:66:U:H2'	34:S4:67:C:H6	1.84	0.43
36:6:67:C:H5''	36:6:68:A:OP2	2.19	0.43
37:2:1265:U:H4'	42:1:1185:U:O2	2.19	0.43
42:1:506:G:C2'	42:1:507:C:H5'	2.49	0.43
42:1:681:A2M:H2'	42:1:682:C:C6	2.54	0.43
47:O:158:ARG:HG2	47:O:160:THR:HG23	2.01	0.43
64:J:59:MET:HE3	64:J:59:MET:HB2	1.86	0.43
71:i:79:ARG:HA	71:i:79:ARG:HD3	1.66	0.43
7:SJ:26:LEU:HD12	7:SJ:62:VAL:HG22	2.01	0.42
16:ST:42:ARG:HH12	16:ST:80:LEU:HD21	1.84	0.42
29:S1:29:U:H2'	29:S1:30:G:H8	1.83	0.42
29:S1:600:OMG:HM22	29:S1:601:G:H5'	2.01	0.42
30:SA:37:ASN:OD1	30:SA:37:ASN:N	2.52	0.42
37:2:998:G:O2'	37:2:999:U:C6	2.72	0.42
46:c:106:ASN:HB2	46:c:109:GLN:HG3	2.01	0.42
11:SN:16:PHE:CZ	11:SN:20:GLU:HG3	2.54	0.42
12:SO:27:PHE:HB3	12:SO:34:PHE:HB2	2.00	0.42
29:S1:1966:A:N1	29:S1:1983:U:H5	2.17	0.42
37:2:1046:OMG:HM23	37:2:1046:OMG:H1'	1.68	0.42
43:B:20:LYS:HB2	43:B:20:LYS:HE2	1.80	0.42
43:B:41:PRO:HA	43:B:189:ASN:O	2.19	0.42
44:C:246:ARG:HG3	44:C:247:PHE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:G:246:GLU:N	50:G:246:GLU:OE2	2.53	0.42
52:R:51:ASN:OD1	52:R:51:ASN:N	2.51	0.42
65:W:86:LYS:HB3	65:W:86:LYS:HE3	1.66	0.42
78:b:42:VAL:HG12	78:b:46:ARG:HE	1.84	0.42
5:SH:155:MET:HE3	29:S1:1874:U:C4	2.55	0.42
12:SO:49:VAL:HG13	12:SO:53:MET:HE2	2.01	0.42
29:S1:1583:U:H5'	29:S1:1611:C:H1'	2.01	0.42
36:6:67:C:N4	62:g:96:ARG:O	2.50	0.42
42:1:417:G:O2'	42:1:442:A:N6	2.52	0.42
42:1:459:A:H2'	42:1:460:A:O4'	2.19	0.42
42:1:1030:U:H4'	42:1:1031:A:C8	2.54	0.42
43:B:112:VAL:O	43:B:116[B]:ARG:HG3	2.19	0.42
43:B:204:LEU:HD12	43:B:204:LEU:HA	1.89	0.42
52:R:7:ARG:O	52:R:32:PHE:HA	2.18	0.42
53:I:3:LYS:HB2	53:I:3:LYS:HE2	1.82	0.42
13:SP:87:ASN:HB2	13:SP:90:CYS:SG	2.58	0.42
14:SR:133:ARG:HB2	14:SR:135:GLN:NE2	2.34	0.42
19:SW:123:LEU:HD23	19:SW:123:LEU:HA	1.91	0.42
29:S1:184:C:H5''	29:S1:185:A:H2'	2.02	0.42
29:S1:751:G:N3	29:S1:751:G:H2'	2.35	0.42
29:S1:966:G:H2'	29:S1:967:A:C8	2.54	0.42
29:S1:1809:U:H2'	29:S1:1810:G:O4'	2.20	0.42
29:S1:1931:G:H1'	29:S1:1935:C:C2	2.55	0.42
30:SA:33:VAL:O	30:SA:100:THR:OG1	2.35	0.42
14:SR:86:ASN:OD1	14:SR:87:ARG:N	2.53	0.42
21:SY:30:GLU:HB3	21:SY:32:HIS:CE1	2.55	0.42
25:Sc:25:LEU:HD12	25:Sc:25:LEU:HA	1.89	0.42
31:SB:37:MET:HE1	31:SB:165:PRO:HB3	2.00	0.42
32:SC:168:ASP:OD1	32:SC:169:SER:N	2.52	0.42
42:1:415:A:N3	42:1:417:G:H5''	2.35	0.42
42:1:687:C:H2'	42:1:688:A:C8	2.55	0.42
42:1:1135:U:H4'	42:1:1136:G:O5'	2.18	0.42
42:1:1252:C:H2'	42:1:1253:U:H5'	2.01	0.42
55:T:5:SER:H	55:T:147:GLN:HE22	1.68	0.42
56:S:148:ARG:HA	56:S:148:ARG:HD2	1.82	0.42
74:o:67:GLY:HA3	74:o:70:THR:O	2.18	0.42
14:SR:27:VAL:HG23	14:SR:55:ARG:O	2.19	0.42
16:ST:99:ARG:NH1	16:ST:99:ARG:HG2	2.35	0.42
28:Sg:272:LEU:HD11	28:Sg:306:TRP:CD1	2.54	0.42
29:S1:608:C:H2'	29:S1:609:PSU:H6	1.84	0.42
29:S1:783:A:H2	29:S1:837:G:N1	2.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SB:18:ALA:O	31:SB:22:LEU:HD12	2.19	0.42
37:2:352:A:OP2	54:Q:81:ARG:NH2	2.52	0.42
37:2:1096:U:H2'	37:2:1097:G:H8	1.85	0.42
42:1:501:C:O2'	42:1:502:U:H6	2.01	0.42
45:A:234:LYS:HG2	45:A:238:ILE:HG12	2.01	0.42
70:j:14:ARG:HE	70:j:17:ILE:HG22	1.84	0.42
3:SF:197:LYS:O	3:SF:201:GLU:HG3	2.19	0.42
6:SI:143:TRP:HZ3	7:SJ:54:ASP:HB2	1.84	0.42
29:S1:691:G:H1	29:S1:754:G:N2	2.16	0.42
38:7:90:U:O2'	65:W:22:HIS:ND1	2.39	0.42
42:1:1200:A:H5'	42:1:1457:U:H1'	2.02	0.42
42:1:1565:A:O2'	42:1:1566:A:C8	2.71	0.42
2:SE:8:ARG:NH1	2:SE:21:THR:HB	2.34	0.42
6:SI:162:ARG:O	6:SI:166:GLU:HB2	2.19	0.42
22:SZ:44:GLN:OE1	22:SZ:45:LEU:N	2.53	0.42
29:S1:1192:PSU:H2'	29:S1:1193:U:C6	2.55	0.42
29:S1:1522:G:C2	29:S1:1523:A:C8	3.08	0.42
30:SA:237:ILE:HD12	30:SA:237:ILE:O	2.19	0.42
31:SB:79:VAL:HG22	31:SB:126:VAL:HB	2.02	0.42
38:7:20:C:OP1	44:C:194:LYS:HE2	2.20	0.42
40:4:61:A:H2'	40:4:62:C:H6	1.84	0.42
41:3:98:C:H2'	41:3:99:U:C6	2.55	0.42
55:T:140:MET:HE3	55:T:140:MET:HB3	1.92	0.42
68:Z:6:ASP:OD1	68:Z:6:ASP:N	2.52	0.42
2:SE:248:GLN:O	2:SE:252:GLU:HG3	2.20	0.42
5:SH:148:ALA:HB2	5:SH:158:CYS:SG	2.60	0.42
14:SR:15:ARG:HD2	14:SR:15:ARG:HA	1.89	0.42
29:S1:1367:U:H1'	30:SA:150:ASN:ND2	2.34	0.42
29:S1:2132:C:H2'	29:S1:2133:G:O4'	2.19	0.42
41:3:8:G:C6	41:3:13:OMU:H5	2.54	0.42
42:1:217:A:H4'	42:1:218:A:OP2	2.19	0.42
42:1:487:G:H3'	42:1:488:G:H4'	2.02	0.42
3:SF:239:PRO:HA	3:SF:242:TRP:CD1	2.54	0.42
24:Sb:40:ARG:HD2	24:Sb:77:PHE:HE2	1.84	0.42
29:S1:258:C:H2'	29:S1:259:C:C6	2.54	0.42
29:S1:438:U:H2'	29:S1:439:G:O4'	2.20	0.42
29:S1:651:U:H2'	29:S1:652:U:H6	1.84	0.42
75:D:81:LEU:O	75:D:82:LEU:HG	2.20	0.42
2:SE:163:GLU:OE1	2:SE:165:LYS:NZ	2.46	0.41
8:SK:162:TRP:O	8:SK:166:ARG:HB2	2.20	0.41
10:SM:58:LEU:HB2	10:SM:79:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:S1:16:G:H2'	29:S1:17:C:C6	2.55	0.41
29:S1:811:C:C2	29:S1:812:A:C8	3.08	0.41
29:S1:1879:OMG:HM23	29:S1:1879:OMG:H1'	1.76	0.41
33:Sh:140:VAL:HB	33:Sh:173:ALA:HB3	2.01	0.41
37:2:972:C:H1'	74:o:62:LYS:NZ	2.34	0.41
42:1:218:A:H1'	42:1:219:U:C1'	2.50	0.41
42:1:1180:U:H2'	42:1:1181:PSU:O4'	2.20	0.41
44:C:192:ARG:O	44:C:192:ARG:HG3	2.19	0.41
46:c:116:LEU:O	46:c:117:ARG:HB2	2.19	0.41
46:c:172:LYS:HG3	46:c:173:ILE:N	2.35	0.41
6:SI:17:SER:HB2	6:SI:20:GLU:OE1	2.19	0.41
29:S1:263:G:H2'	29:S1:264:C:C6	2.55	0.41
29:S1:977:G:H2'	29:S1:978:C:H5'	2.01	0.41
29:S1:1367:U:H2'	29:S1:1368:C:C6	2.55	0.41
40:4:75:C:O2'	40:4:76:C:H5'	2.19	0.41
42:1:289:U:H2'	42:1:290:G:C8	2.55	0.41
42:1:736:C:H2'	42:1:737:U:O4'	2.20	0.41
42:1:1119:C:O2'	42:1:1120:C:H5'	2.20	0.41
42:1:1672:U:H5	42:1:1727:A:N7	2.18	0.41
59:E:64:ILE:HB	59:E:65:PRO:HD3	2.02	0.41
3:SF:94:LYS:HE3	3:SF:96:TYR:CD2	2.55	0.41
4:SG:149:ASN:OD1	4:SG:149:ASN:N	2.54	0.41
18:SV:26:PHE:HD2	18:SV:59:LYS:HG2	1.86	0.41
22:SZ:83:TYR:CD2	22:SZ:89:LEU:HD12	2.55	0.41
29:S1:285:A:H61	29:S1:817:A:H4'	1.85	0.41
29:S1:1621:U:H4'	29:S1:1622:G:OP1	2.15	0.41
29:S1:2026:U:H2'	29:S1:2027:G:C8	2.55	0.41
36:6:65:C:H5	42:1:491:A:O2'	2.03	0.41
37:2:1425:A:O2'	43:B:264:ARG:HB2	2.20	0.41
41:3:196:U:H5	41:3:197:A:N3	2.18	0.41
42:1:1562:C:H2'	42:1:1563:U:C6	2.56	0.41
44:C:206:PRO:HB3	44:C:247:PHE:CD2	2.55	0.41
62:g:98:SER:OG	62:g:99:THR:N	2.53	0.41
72:U:56:LYS:O	72:U:85:TYR:OH	2.35	0.41
3:SF:232:LYS:HE3	3:SF:232:LYS:HB2	1.88	0.41
10:SM:39:ARG:NH1	10:SM:101:PHE:HB3	2.34	0.41
20:SX:91:ARG:NH2	29:S1:1940:G:H22	2.18	0.41
37:2:489:A:N7	45:A:245:ARG:HG3	2.34	0.41
37:2:984:G:O2'	37:2:985:A:OP1	2.26	0.41
42:1:968:A:H5''	87:1:1923:HOH:O	2.19	0.41
47:O:177:MET:HE3	47:O:177:MET:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:P:153:ARG:O	51:P:157:ARG:HG3	2.21	0.41
58:F:189:ALA:HB1	58:F:191:HIS:CE1	2.56	0.41
1:SD:58:LEU:HD12	1:SD:58:LEU:HA	1.88	0.41
19:SW:41:LYS:NZ	19:SW:53:ASN:HB3	2.36	0.41
29:S1:436:C:H2'	29:S1:437:C:C6	2.56	0.41
29:S1:1975:A:O2'	29:S1:1979:OMU:OP1	2.37	0.41
29:S1:2049:G:H2'	29:S1:2050:U:C6	2.56	0.41
30:SA:167:ARG:O	30:SA:171:THR:HG22	2.20	0.41
33:Sh:212:LEU:HA	33:Sh:215:ARG:HH11	1.85	0.41
41:3:192:G:H4'	41:3:193:C:OP1	2.21	0.41
42:1:1255:G:H2'	42:1:1256:A:O4'	2.21	0.41
73:p:38:ARG:O	73:p:40:LYS:N	2.52	0.41
2:SE:45:ILE:HD13	2:SE:45:ILE:HA	1.90	0.41
8:SK:40:ALA:O	8:SK:59:ARG:HB2	2.20	0.41
10:SM:108:ASP:OD1	10:SM:108:ASP:C	2.64	0.41
22:SZ:50:LEU:HD23	22:SZ:50:LEU:HA	1.79	0.41
24:Sb:54:ASP:OD1	24:Sb:54:ASP:N	2.54	0.41
28:Sg:263:LEU:HD23	28:Sg:263:LEU:HA	1.73	0.41
29:S1:517:A:H2'	29:S1:518:A:O4'	2.21	0.41
36:6:50:A:H2'	36:6:52:G:C2	2.56	0.41
37:2:426:G:OP1	45:A:174:ARG:NH2	2.54	0.41
37:2:489:A:C8	45:A:245:ARG:HG3	2.55	0.41
37:2:788:C:H42	37:2:807:A:H61	1.68	0.41
40:4:141:A:O2'	59:E:67:ALA:O	2.39	0.41
66:V:36:ARG:HE	66:V:36:ARG:HB3	1.64	0.41
1:SD:89:LYS:HD2	1:SD:94:TYR:CD1	2.55	0.41
4:SG:217:ALA:HB1	29:S1:286:G:H1'	2.03	0.41
6:SI:43:ARG:NH1	29:S1:991:G:O3'	2.54	0.41
8:SK:170:ARG:HB3	17:SU:8:TYR:HB2	2.02	0.41
12:SO:106:GLN:HG2	24:Sb:47:LEU:HD23	2.02	0.41
25:Sc:57:CYS:H	25:Sc:61:SER:HA	1.85	0.41
29:S1:655:U:H4'	29:S1:656:G:O5'	2.20	0.41
32:SC:131:LYS:HZ3	32:SC:155:TYR:HB2	1.86	0.41
33:Sh:133:GLU:HB3	33:Sh:134:ASN:H	1.52	0.41
38:7:71:A:H62	38:7:85:U:H6	1.67	0.41
38:7:105:C:H4'	38:7:106:G:H5''	2.03	0.41
42:1:1675:A:H2'	42:1:1675:A:N3	2.36	0.41
50:G:150:LEU:HD12	50:G:150:LEU:HA	1.89	0.41
50:G:230:LYS:O	50:G:231:LYS:HD3	2.20	0.41
65:W:28:MET:HB3	65:W:98:PRO:HG2	2.02	0.41
5:SH:52:MET:HE3	5:SH:57:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SN:83:MET:HE2	11:SN:83:MET:HB2	1.91	0.41
17:SU:73:CYS:O	17:SU:77:SER:HB3	2.21	0.41
21:SY:43:ASN:HD21	21:SY:53:THR:HG23	1.85	0.41
29:S1:450:A:H2'	29:S1:451:C:H6	1.86	0.41
29:S1:653:A:H2'	29:S1:654:A:O4'	2.20	0.41
29:S1:1513:C:H1'	29:S1:2039:C:H41	1.86	0.41
31:SB:143:VAL:HG23	31:SB:145:ILE:HD13	2.02	0.41
33:Sh:166:ARG:HG2	33:Sh:172:PHE:HB3	2.02	0.41
36:6:52:G:O6	62:g:28:ARG:NH2	2.53	0.41
37:2:603:A:H2'	37:2:604:A2M:C8	2.51	0.41
38:7:127:C:H2'	38:7:128:U:C6	2.56	0.41
41:3:111:A:H4'	41:3:112:C:OP1	2.18	0.41
41:3:112:C:H2'	76:d:86:HIS:ND1	2.35	0.41
42:1:305:A2M:H2'	42:1:305:A2M:H5'	1.91	0.41
42:1:839:U:H2'	42:1:840:G:C8	2.56	0.41
42:1:1102:U:H3'	42:1:1103:U:O2	2.21	0.41
42:1:1538:U:H2'	42:1:1539:A2M:H8	2.03	0.41
42:1:1663:U:H5'	42:1:1663:U:O2	2.21	0.41
49:H:115:LYS:HB3	49:H:115:LYS:HE2	1.80	0.41
49:H:162:LYS:HE2	49:H:162:LYS:HB3	1.85	0.41
80:l:30:ARG:HE	80:l:30:ARG:HB2	1.55	0.41
10:SM:103:MET:H	10:SM:103:MET:HG2	1.68	0.41
14:SR:61:THR:OG1	14:SR:64:GLU:OE1	2.39	0.41
19:SW:107:HIS:HB3	29:S1:1535:A:C2	2.56	0.41
20:SX:46:CYS:SG	29:S1:1920:A:H8	2.44	0.41
28:Sg:128:ASP:OD1	28:Sg:128:ASP:N	2.54	0.41
29:S1:199:C:OP1	33:Sh:152:GLN:NE2	2.54	0.41
29:S1:911:A:H2'	29:S1:912:A:H8	1.84	0.41
29:S1:1913:C:H2'	29:S1:1914:U:C6	2.56	0.41
35:8:8:U:H2'	35:8:9:A:C8	2.56	0.41
35:8:68:A:H3'	35:8:69:G:H8	1.85	0.41
37:2:378:C:O2	37:2:378:C:H2'	2.20	0.41
37:2:604:A2M:H2'	37:2:605:C:O4'	2.21	0.41
37:2:1053:A:H4'	37:2:1054:U:OP1	2.21	0.41
41:3:213:G:H2'	41:3:214:U:O4'	2.21	0.41
42:1:827:G:H2'	42:1:828:U:O4'	2.20	0.41
42:1:1443:U:H6	42:1:1443:U:H2'	1.57	0.41
42:1:1475:U:OP2	44:C:181:ARG:NH1	2.54	0.41
54:Q:105:LEU:HD23	54:Q:138:LEU:HD23	2.03	0.41
58:F:191:HIS:CD2	58:F:191:HIS:H	2.39	0.41
62:g:35:MET:HE3	62:g:35:MET:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:d:46:ILE:HG13	76:d:69:ILE:HD11	2.01	0.41
3:SF:83:ILE:HG21	3:SF:88:LEU:HD13	2.03	0.41
10:SM:69[B]:ASN:HD22	10:SM:69[B]:ASN:HA	1.59	0.41
16:ST:55:ARG:HD3	29:S1:1207:U:H5'	2.03	0.41
16:ST:133:LYS:HD2	29:S1:913:G:N2	2.35	0.41
25:Sc:36:VAL:HG22	25:Sc:80:TYR:CD2	2.56	0.41
29:S1:509:G:H2'	29:S1:510:G:H8	1.86	0.41
29:S1:1105:A:O2'	29:S1:1106:U:H5''	2.21	0.41
41:3:43:C:H42	41:3:186:U:H3	1.68	0.41
49:H:46:LEU:HD23	49:H:46:LEU:HA	1.89	0.41
74:o:16:THR:O	74:o:16:THR:OG1	2.31	0.41
80:l:41:ARG:HA	80:l:41:ARG:HD2	1.80	0.41
2:SE:129:ALA:HB3	2:SE:133:VAL:HG22	2.02	0.40
29:S1:450:A:H2'	29:S1:451:C:C6	2.56	0.40
29:S1:783:A:H2'	29:S1:784:C:H5''	2.03	0.40
29:S1:1248:A:H2'	29:S1:1249:G:H8	1.85	0.40
49:H:159:ASN:OD1	49:H:159:ASN:N	2.54	0.40
52:R:50:LYS:NZ	56:S:148:ARG:HA	2.36	0.40
53:I:108:ASN:HD22	53:I:108:ASN:HA	1.57	0.40
70:j:16:HIS:HA	70:j:27:TYR:O	2.21	0.40
71:i:3:ALA:N	71:i:4:PRO:HD2	2.35	0.40
6:SI:130:ASN:OD1	6:SI:130:ASN:N	2.54	0.40
6:SI:132:MET:HE3	6:SI:172:VAL:HG13	2.03	0.40
13:SP:53:GLU:OE1	13:SP:71[A]:ARG:NH1	2.52	0.40
24:Sb:39:GLY:N	24:Sb:40:ARG:HH21	2.18	0.40
29:S1:885:C:N4	29:S1:887:U:O2	2.54	0.40
29:S1:955:A:C2	29:S1:980:G:N1	2.69	0.40
29:S1:1250:A:O2'	29:S1:1252:A:N7	2.35	0.40
29:S1:1656:G:C8	29:S1:1657:PSU:H2'	2.56	0.40
32:SC:201:GLU:HA	32:SC:202:PRO:HD3	1.92	0.40
37:2:96:U:H2'	37:2:97:A:O4'	2.21	0.40
42:1:102:G:OP1	53:I:75:ARG:NH1	2.54	0.40
42:1:231:U:H2'	42:1:232:G:C8	2.56	0.40
42:1:1238:C:N4	52:R:179:ALA:HB1	2.35	0.40
50:G:148:ARG:HE	50:G:148:ARG:HB3	1.69	0.40
20:SX:142:LYS:HB3	20:SX:142:LYS:HE3	1.82	0.40
26:Sd:32:ARG:NH2	29:S1:2035:C:OP1	2.54	0.40
29:S1:772:A:H2'	29:S1:773:A:O4'	2.22	0.40
29:S1:1882:A:H2'	29:S1:1883:G:O4'	2.21	0.40
37:2:1089:A:H2'	37:2:1090:G:H8	1.86	0.40
48:M:43:THR:OG1	48:M:131:GLU:OE1	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:I:52:PHE:CD1	53:I:53:PRO:HA	2.56	0.40
63:a:53:LYS:HA	63:a:53:LYS:HD3	1.81	0.40
8:SK:161:GLU:O	8:SK:165:ARG:HG2	2.22	0.40
36:6:11:G:H1'	36:6:73:A:N6	2.36	0.40
37:2:570:A2M:H2	42:1:941:C:O2	2.21	0.40
40:4:74:OMG:HM23	40:4:74:OMG:H1'	1.79	0.40
42:1:700:A:H2'	42:1:701:G:C8	2.56	0.40
42:1:955:A2M:H1'	42:1:955:A2M:HM'3	1.86	0.40
67:h:72:GLU:OE1	67:h:72:GLU:N	2.53	0.40
10:SM:30:GLU:O	10:SM:34:SER:OG	2.24	0.40
16:ST:35:LYS:HE2	16:ST:35:LYS:HB2	1.59	0.40
29:S1:285:A:H2'	29:S1:817:A:C2	2.55	0.40
29:S1:910:A:H2'	29:S1:911:A:H8	1.86	0.40
37:2:1352:G:N3	37:2:1372:A2M:H2	2.37	0.40
42:1:56:G:H2'	42:1:57:G:C8	2.57	0.40
42:1:486:C:H6	42:1:487:G:H22	1.67	0.40
42:1:672:PSU:H2'	42:1:673:C:C6	2.57	0.40
42:1:687:C:H2'	42:1:688:A:H8	1.85	0.40
46:c:60:LYS:O	46:c:64:GLU:HG3	2.22	0.40
75:D:139:ARG:O	75:D:143:ARG:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SD	162/190 (85%)	154 (95%)	8 (5%)	0	100	100
2	SE	260/273 (95%)	254 (98%)	6 (2%)	0	100	100
3	SF	203/265 (77%)	198 (98%)	5 (2%)	0	100	100
4	SG	232/249 (93%)	231 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	SH	179/190 (94%)	171 (96%)	8 (4%)	0	100	100
6	SI	197/200 (98%)	191 (97%)	6 (3%)	0	100	100
7	SJ	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
8	SK	180/220 (82%)	178 (99%)	2 (1%)	0	100	100
9	SL	140/149 (94%)	132 (94%)	8 (6%)	0	100	100
10	SM	102/116 (88%)	99 (97%)	3 (3%)	0	100	100
11	SN	96/168 (57%)	88 (92%)	7 (7%)	1 (1%)	12	39
12	SO	132/144 (92%)	126 (96%)	6 (4%)	0	100	100
13	SP	143/143 (100%)	140 (98%)	3 (2%)	0	100	100
14	SR	134/153 (88%)	131 (98%)	3 (2%)	0	100	100
15	SS	52/57 (91%)	50 (96%)	2 (4%)	0	100	100
16	ST	138/151 (91%)	137 (99%)	1 (1%)	0	100	100
17	SU	152/173 (88%)	148 (97%)	4 (3%)	0	100	100
18	SV	69/143 (48%)	67 (97%)	2 (3%)	0	100	100
19	SW	107/152 (70%)	102 (95%)	5 (5%)	0	100	100
20	SX	138/161 (86%)	131 (95%)	7 (5%)	0	100	100
21	SY	86/164 (52%)	84 (98%)	2 (2%)	0	100	100
22	SZ	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
23	Sa	68/120 (57%)	65 (96%)	3 (4%)	0	100	100
24	Sb	82/112 (73%)	77 (94%)	5 (6%)	0	100	100
25	Sc	82/86 (95%)	75 (92%)	7 (8%)	0	100	100
26	Sd	48/87 (55%)	45 (94%)	3 (6%)	0	100	100
27	Se	42/66 (64%)	40 (95%)	2 (5%)	0	100	100
28	Sg	281/312 (90%)	265 (94%)	16 (6%)	0	100	100
30	SA	201/264 (76%)	197 (98%)	4 (2%)	0	100	100
31	SB	208/246 (85%)	204 (98%)	4 (2%)	0	100	100
32	SC	199/219 (91%)	195 (98%)	4 (2%)	0	100	100
33	Sh	93/235 (40%)	84 (90%)	9 (10%)	0	100	100
43	B	397/419 (95%)	381 (96%)	16 (4%)	0	100	100
44	C	321/373 (86%)	308 (96%)	13 (4%)	0	100	100
45	A	253/260 (97%)	245 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	c	225/252 (89%)	215 (96%)	10 (4%)	0	100	100
47	O	238/305 (78%)	225 (94%)	13 (6%)	0	100	100
48	M	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
49	H	218/222 (98%)	215 (99%)	3 (1%)	0	100	100
50	G	208/264 (79%)	199 (96%)	9 (4%)	0	100	100
51	P	194/198 (98%)	187 (96%)	7 (4%)	0	100	100
52	R	176/179 (98%)	173 (98%)	3 (2%)	0	100	100
53	I	165/220 (75%)	157 (95%)	8 (5%)	0	100	100
54	Q	166/254 (65%)	163 (98%)	3 (2%)	0	100	100
55	T	150/166 (90%)	140 (93%)	10 (7%)	0	100	100
56	S	149/159 (94%)	145 (97%)	4 (3%)	0	100	100
57	L	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
58	F	138/195 (71%)	131 (95%)	7 (5%)	0	100	100
59	E	140/190 (74%)	134 (96%)	6 (4%)	0	100	100
60	Y	130/134 (97%)	127 (98%)	3 (2%)	0	100	100
61	f	121/133 (91%)	116 (96%)	5 (4%)	0	100	100
62	g	122/144 (85%)	114 (93%)	8 (7%)	0	100	100
63	a	121/127 (95%)	120 (99%)	1 (1%)	0	100	100
64	J	127/139 (91%)	124 (98%)	3 (2%)	0	100	100
65	W	115/143 (80%)	113 (98%)	2 (2%)	0	100	100
66	V	116/145 (80%)	113 (97%)	3 (3%)	0	100	100
67	h	110/168 (66%)	105 (96%)	5 (4%)	0	100	100
68	Z	116/147 (79%)	114 (98%)	2 (2%)	0	100	100
69	K	115/175 (66%)	113 (98%)	2 (2%)	0	100	100
70	j	78/83 (94%)	75 (96%)	3 (4%)	0	100	100
71	i	82/105 (78%)	81 (99%)	1 (1%)	0	100	100
72	U	110/129 (85%)	106 (96%)	4 (4%)	0	100	100
73	p	79/106 (74%)	74 (94%)	5 (6%)	0	100	100
74	o	86/92 (94%)	78 (91%)	8 (9%)	0	100	100
75	D	94/188 (50%)	91 (97%)	3 (3%)	0	100	100
76	d	86/104 (83%)	85 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	X	62/124 (50%)	60 (97%)	2 (3%)	0	100	100
78	b	64/70 (91%)	64 (100%)	0	0	100	100
79	k	69/83 (83%)	67 (97%)	2 (3%)	0	100	100
80	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
81	n	23/34 (68%)	23 (100%)	0	0	100	100
82	e	145/188 (77%)	134 (92%)	11 (8%)	0	100	100
All	All	10153/12292 (83%)	9786 (96%)	366 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	SN	94	MET

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	SD	142/164 (87%)	134 (94%)	8 (6%)	19	50
2	SE	216/225 (96%)	211 (98%)	5 (2%)	44	76
3	SF	162/208 (78%)	158 (98%)	4 (2%)	42	74
4	SG	181/208 (87%)	177 (98%)	4 (2%)	45	77
5	SH	145/159 (91%)	139 (96%)	6 (4%)	27	61
6	SI	167/186 (90%)	159 (95%)	8 (5%)	23	55
7	SJ	109/111 (98%)	108 (99%)	1 (1%)	70	90
8	SK	141/176 (80%)	138 (98%)	3 (2%)	47	77
9	SL	112/120 (93%)	109 (97%)	3 (3%)	39	73
10	SM	92/104 (88%)	84 (91%)	8 (9%)	9	30
11	SN	82/128 (64%)	77 (94%)	5 (6%)	17	46
12	SO	95/113 (84%)	91 (96%)	4 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	SP	115/117 (98%)	110 (96%)	5 (4%)	26	60
14	SR	111/130 (85%)	106 (96%)	5 (4%)	24	58
15	SS	41/49 (84%)	40 (98%)	1 (2%)	43	75
16	ST	122/132 (92%)	121 (99%)	1 (1%)	73	90
17	SU	126/152 (83%)	122 (97%)	4 (3%)	34	68
18	SV	62/126 (49%)	59 (95%)	3 (5%)	23	55
19	SW	87/130 (67%)	80 (92%)	7 (8%)	11	34
20	SX	109/131 (83%)	103 (94%)	6 (6%)	19	50
21	SY	62/116 (53%)	58 (94%)	4 (6%)	15	44
22	SZ	101/118 (86%)	98 (97%)	3 (3%)	36	70
23	Sa	62/95 (65%)	60 (97%)	2 (3%)	34	68
24	Sb	69/93 (74%)	60 (87%)	9 (13%)	4	13
25	Sc	62/76 (82%)	61 (98%)	1 (2%)	55	83
26	Sd	40/75 (53%)	37 (92%)	3 (8%)	12	37
27	Se	35/54 (65%)	33 (94%)	2 (6%)	18	49
28	Sg	226/265 (85%)	213 (94%)	13 (6%)	18	49
30	SA	178/222 (80%)	172 (97%)	6 (3%)	32	66
31	SB	165/202 (82%)	152 (92%)	13 (8%)	11	34
32	SC	156/184 (85%)	149 (96%)	7 (4%)	24	58
33	Sh	60/177 (34%)	55 (92%)	5 (8%)	10	32
43	B	283/351 (81%)	279 (99%)	4 (1%)	59	85
44	C	222/301 (74%)	209 (94%)	13 (6%)	18	48
45	A	178/204 (87%)	175 (98%)	3 (2%)	53	82
46	c	174/209 (83%)	171 (98%)	3 (2%)	53	82
47	O	150/242 (62%)	143 (95%)	7 (5%)	23	56
48	M	173/180 (96%)	167 (96%)	6 (4%)	32	66
49	H	165/188 (88%)	161 (98%)	4 (2%)	43	75
50	G	162/221 (73%)	154 (95%)	8 (5%)	22	54
51	P	157/164 (96%)	153 (98%)	4 (2%)	42	74
52	R	143/159 (90%)	135 (94%)	8 (6%)	19	50
53	I	130/183 (71%)	123 (95%)	7 (5%)	20	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	Q	117/198 (59%)	114 (97%)	3 (3%)	40	73
55	T	127/143 (89%)	122 (96%)	5 (4%)	28	63
56	S	117/134 (87%)	105 (90%)	12 (10%)	7	23
57	L	110/114 (96%)	105 (96%)	5 (4%)	24	58
58	F	99/153 (65%)	92 (93%)	7 (7%)	13	40
59	E	92/172 (54%)	87 (95%)	5 (5%)	20	51
60	Y	96/116 (83%)	90 (94%)	6 (6%)	16	45
61	f	104/115 (90%)	101 (97%)	3 (3%)	37	71
62	g	100/121 (83%)	96 (96%)	4 (4%)	28	62
63	a	93/118 (79%)	90 (97%)	3 (3%)	34	68
64	J	93/111 (84%)	91 (98%)	2 (2%)	45	77
65	W	98/122 (80%)	96 (98%)	2 (2%)	48	78
66	V	94/124 (76%)	89 (95%)	5 (5%)	20	52
67	h	87/146 (60%)	84 (97%)	3 (3%)	32	66
68	Z	89/118 (75%)	86 (97%)	3 (3%)	32	66
69	K	80/145 (55%)	76 (95%)	4 (5%)	22	53
70	j	66/70 (94%)	64 (97%)	2 (3%)	36	70
71	i	64/88 (73%)	60 (94%)	4 (6%)	16	45
72	U	64/114 (56%)	60 (94%)	4 (6%)	16	45
73	p	61/92 (66%)	59 (97%)	2 (3%)	33	67
74	o	62/74 (84%)	59 (95%)	3 (5%)	23	55
75	D	42/162 (26%)	34 (81%)	8 (19%)	1	5
76	d	58/89 (65%)	53 (91%)	5 (9%)	10	30
77	X	58/104 (56%)	57 (98%)	1 (2%)	53	82
78	b	52/58 (90%)	50 (96%)	2 (4%)	29	64
79	k	47/74 (64%)	46 (98%)	1 (2%)	47	77
80	l	44/47 (94%)	43 (98%)	1 (2%)	44	76
81	n	8/32 (25%)	8 (100%)	0	100	100
82	e	104/158 (66%)	99 (95%)	5 (5%)	23	55
All	All	7896/10260 (77%)	7560 (96%)	336 (4%)	27	60

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	SD	1	MET
1	SD	6	ASN
1	SD	48	LEU
1	SD	49	SER
1	SD	59	LEU
1	SD	111	ILE
1	SD	121	VAL
1	SD	144	SER
2	SE	15	TRP
2	SE	20	LEU
2	SE	88	GLU
2	SE	94	ASP
2	SE	133	VAL
3	SF	55	VAL
3	SF	68	LEU
3	SF	106	GLN
3	SF	211	SER
4	SG	4	ASN
4	SG	22	VAL
4	SG	36	GLU
4	SG	69	LEU
5	SH	19	THR
5	SH	35	VAL
5	SH	39	SER
5	SH	48	TYR
5	SH	99	VAL
5	SH	111	SER
6	SI	20	GLU
6	SI	22	SER
6	SI	48	THR
6	SI	99	GLN
6	SI	121	SER
6	SI	136	SER
6	SI	198	SER
6	SI	199	THR
7	SJ	83	THR
8	SK	95	THR
8	SK	171	VAL
8	SK	184	VAL
9	SL	17	LYS
9	SL	55	MET
9	SL	75	VAL
10	SM	16	THR

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Mol	Chain	Res	Type
10	SM	20	THR
10	SM	34	SER
10	SM	46	THR
10	SM	51	VAL
10	SM	100	SER
10	SM	113	ILE
10	SM	115	ASP
11	SN	5	VAL
11	SN	13	VAL
11	SN	23	ILE
11	SN	64	GLU
11	SN	96	ASN
12	SO	59	ARG
12	SO	60	ASP
12	SO	63	SER
12	SO	126	THR
13	SP	34	SER
13	SP	72	VAL
13	SP	115	ILE
13	SP	126	SER
13	SP	136	GLN
14	SR	5	LEU
14	SR	60	LEU
14	SR	61	THR
14	SR	63	GLU
14	SR	93	THR
15	SS	4	LEU
16	ST	37	VAL
17	SU	55	LEU
17	SU	80	VAL
17	SU	92	SER
17	SU	102	ARG
18	SV	3	LYS
18	SV	4	ILE
18	SV	13	SER
19	SW	33	LEU
19	SW	44	VAL
19	SW	62	VAL
19	SW	74	VAL
19	SW	100	VAL
19	SW	110	ASN
19	SW	134	LEU

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Mol	Chain	Res	Type
20	SX	47	THR
20	SX	52	SER
20	SX	61	GLN
20	SX	109	SER
20	SX	113	LEU
20	SX	151	VAL
21	SY	4	ILE
21	SY	43	ASN
21	SY	79	ASP
21	SY	82	ILE
22	SZ	30	VAL
22	SZ	60	SER
22	SZ	62	VAL
23	Sa	40	VAL
23	Sa	98	THR
24	Sb	38	VAL
24	Sb	40	ARG
24	Sb	44	ARG
24	Sb	54	ASP
24	Sb	71	LEU
24	Sb	72	TYR
24	Sb	73	MET
24	Sb	75	GLN
24	Sb	79	ILE
25	Sc	75	VAL
26	Sd	23	VAL
26	Sd	44	VAL
26	Sd	74	SER
27	Se	14	VAL
27	Se	39	LYS
28	Sg	39	ILE
28	Sg	46	ASP
28	Sg	71	VAL
28	Sg	128	ASP
28	Sg	134	TRP
28	Sg	136	VAL
28	Sg	167	VAL
28	Sg	174	ASN
28	Sg	199	THR
28	Sg	234	VAL
28	Sg	260	VAL
28	Sg	268	VAL

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Mol	Chain	Res	Type
28	Sg	308	ILE
30	SA	61	LEU
30	SA	115	LEU
30	SA	116	LEU
30	SA	118	LYS
30	SA	129	VAL
30	SA	136	THR
31	SB	10	VAL
31	SB	17	ASP
31	SB	59	GLU
31	SB	87	THR
31	SB	125	LEU
31	SB	141	SER
31	SB	144	ASN
31	SB	145	ILE
31	SB	153	THR
31	SB	154	ASP
31	SB	157	LEU
31	SB	192	ILE
31	SB	195	SER
32	SC	11	ILE
32	SC	45	THR
32	SC	65	ILE
32	SC	92	VAL
32	SC	156	MET
32	SC	180	CYS
32	SC	208	THR
33	Sh	162	VAL
33	Sh	191	ASN
33	Sh	202	VAL
33	Sh	221	VAL
33	Sh	226	HIS
43	B	287	ILE
43	B	327	ASP
43	B	349	MET
43	B	384	ASN
44	C	20	THR
44	C	62	SER
44	C	93	ASN
44	C	124	VAL
44	C	134	SER
44	C	138	SER

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Mol	Chain	Res	Type
44	C	146	VAL
44	C	153	VAL
44	C	183	ASN
44	C	201	VAL
44	C	253	SER
44	C	276	THR
44	C	291	MET
45	A	18	VAL
45	A	96	LEU
45	A	245	ARG
46	c	35	SER
46	c	72	LEU
46	c	97	THR
47	O	63	GLN
47	O	66	GLN
47	O	93	THR
47	O	132	VAL
47	O	217	VAL
47	O	230	VAL
47	O	244	SER
48	M	7	LEU
48	M	37	VAL
48	M	43	THR
48	M	60	CYS
48	M	126	THR
48	M	135	VAL
49	H	64	THR
49	H	82	THR
49	H	95	SER
49	H	169	SER
50	G	124	ASP
50	G	178	LEU
50	G	219	THR
50	G	230	LYS
50	G	235	MET
50	G	237	VAL
50	G	288	VAL
50	G	316	ARG
51	P	94	LEU
51	P	115	SER
51	P	139	THR
51	P	162	SER

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Mol	Chain	Res	Type
52	R	18	SER
52	R	49	VAL
52	R	75	ASN
52	R	80	ILE
52	R	87	CYS
52	R	114	SER
52	R	136	VAL
52	R	169	VAL
53	I	3	LYS
53	I	11	VAL
53	I	68	VAL
53	I	75	ARG
53	I	108	ASN
53	I	126	SER
53	I	167	VAL
54	Q	40	SER
54	Q	51	ILE
54	Q	68	GLU
55	T	19	VAL
55	T	20	SER
55	T	22	LEU
55	T	125	MET
55	T	148	LEU
56	S	4	SER
56	S	9	SER
56	S	27	VAL
56	S	43	VAL
56	S	46	SER
56	S	52	MET
56	S	55	LYS
56	S	72	VAL
56	S	90	CYS
56	S	134	LEU
56	S	150	VAL
56	S	152	ASP
57	L	6	LYS
57	L	8	CYS
57	L	9	ARG
57	L	30	SER
57	L	95	THR
58	F	23	SER
58	F	32	SER

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Mol	Chain	Res	Type
58	F	84	VAL
58	F	91	VAL
58	F	95	SER
58	F	144	THR
58	F	146	VAL
59	E	55	THR
59	E	81	THR
59	E	91	VAL
59	E	128	THR
59	E	160	LEU
60	Y	5	LEU
60	Y	32	VAL
60	Y	40	ARG
60	Y	68	VAL
60	Y	108	SER
60	Y	132	LEU
61	f	39	GLU
61	f	56	LYS
61	f	62	ARG
62	g	38	THR
62	g	92	LYS
62	g	116	MET
62	g	131	ILE
63	a	21	THR
63	a	30	SER
63	a	68	SER
64	J	103	VAL
64	J	120	VAL
65	W	61	LYS
65	W	102	GLU
66	V	34	GLN
66	V	36	ARG
66	V	37	ARG
66	V	79	ILE
66	V	112	LYS
67	h	45	THR
67	h	75	VAL
67	h	101	GLN
68	Z	53	VAL
68	Z	62	CYS
68	Z	72	ASN
69	K	3	SER

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Mol	Chain	Res	Type
69	K	11	LEU
69	K	62	VAL
69	K	79	SER
70	j	43	SER
70	j	69	VAL
71	i	5	THR
71	i	21	THR
71	i	53	LEU
71	i	84	THR
72	U	30	CYS
72	U	46	ASN
72	U	81	THR
72	U	116	THR
73	p	2	VAL
73	p	77	CYS
74	o	41	PHE
74	o	57	CYS
74	o	58	ASP
75	D	16	VAL
75	D	82	LEU
75	D	131	VAL
75	D	133	LEU
75	D	147	CYS
75	D	148	SER
75	D	153	SER
75	D	168	VAL
76	d	26	VAL
76	d	65	SER
76	d	89	THR
76	d	95	THR
76	d	97	VAL
77	X	58	THR
78	b	4	SER
78	b	37	TRP
79	k	66	LYS
80	l	31	THR
82	e	67	SER
82	e	79	VAL
82	e	136	LYS
82	e	172	SER
82	e	180	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83)

such sidechains are listed below:

Mol	Chain	Res	Type
1	SD	45	ASN
1	SD	64	ASN
2	SE	64	GLN
2	SE	110	ASN
2	SE	230	ASN
2	SE	248	GLN
4	SG	4	ASN
4	SG	232	HIS
6	SI	116	GLN
7	SJ	70	ASN
7	SJ	120	ASN
9	SL	76	HIS
9	SL	103	HIS
12	SO	106	GLN
13	SP	92	HIS
16	ST	77	HIS
16	ST	78	ASN
17	SU	19	HIS
17	SU	24	GLN
17	SU	113	GLN
17	SU	142	GLN
20	SX	61	GLN
20	SX	94	ASN
22	SZ	24	ASN
24	Sb	8	HIS
26	Sd	62	ASN
28	Sg	98	GLN
28	Sg	100	GLN
28	Sg	240	GLN
30	SA	101	GLN
30	SA	151	GLN
43	B	11	HIS
44	C	40	HIS
44	C	115	ASN
44	C	158	GLN
44	C	221	ASN
44	C	318	ASN
45	A	86	GLN
46	c	84	ASN
46	c	109	GLN
46	c	123	ASN
46	c	176	ASN

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Mol	Chain	Res	Type
46	c	197	GLN
47	O	17	GLN
48	M	95	ASN
49	H	187	HIS
49	H	211	HIS
50	G	161	ASN
50	G	232	GLN
52	R	107	GLN
52	R	116	HIS
52	R	121	HIS
52	R	127	ASN
53	I	10	HIS
53	I	36	GLN
53	I	62	GLN
53	I	91	ASN
54	Q	141	HIS
54	Q	143	HIS
55	T	78	GLN
55	T	97	ASN
55	T	147	GLN
57	L	62	HIS
57	L	102	GLN
58	F	191	HIS
59	E	77	GLN
60	Y	28	ASN
60	Y	117	GLN
61	f	21	HIS
62	g	113	ASN
63	a	93	HIS
65	W	16	HIS
65	W	41	ASN
66	V	39	HIS
66	V	82	ASN
67	h	101	GLN
69	K	51	ASN
70	j	77	HIS
74	o	37	HIS
75	D	97	ASN
76	d	31	GLN
80	l	38	ASN
82	e	27	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	S1	1627/2204 (73%)	312 (19%)	19 (1%)
34	S4	15/20 (75%)	6 (40%)	0
35	8	118/123 (95%)	18 (15%)	0
36	6	61/73 (83%)	30 (49%)	2 (3%)
37	2	933/1522 (61%)	186 (19%)	12 (1%)
38	7	160/171 (93%)	32 (20%)	1 (0%)
39	5	94/135 (69%)	18 (19%)	0
40	4	153/183 (83%)	23 (15%)	1 (0%)
41	3	148/216 (68%)	29 (19%)	6 (4%)
42	1	1445/1782 (81%)	308 (21%)	20 (1%)
All	All	4754/6429 (73%)	962 (20%)	61 (1%)

All (962) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	S1	3	U
29	S1	17	C
29	S1	25	C
29	S1	26	A
29	S1	33	PSU
29	S1	34	G
29	S1	42	G
29	S1	43	A
29	S1	45	U
29	S1	47	A
29	S1	68	A
29	S1	73	A
29	S1	104	PSU
29	S1	105	C
29	S1	112	A
29	S1	117	G
29	S1	128	C
29	S1	143	A
29	S1	145	A
29	S1	146	U
29	S1	151	U
29	S1	152	A
29	S1	158	G
29	S1	162	A
29	S1	165	G
29	S1	172	U

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Mol	Chain	Res	Type
29	S1	173	A
29	S1	176	A
29	S1	184	C
29	S1	197	U
29	S1	235	C
29	S1	249	A
29	S1	251	A
29	S1	275	A
29	S1	278	A
29	S1	281	A
29	S1	282	C
29	S1	284	C
29	S1	285	A
29	S1	287	C
29	S1	308	C
29	S1	309	G
29	S1	310	U
29	S1	313	G
29	S1	315	A
29	S1	316	A
29	S1	320	G
29	S1	323	U
29	S1	329	C
29	S1	330	G
29	S1	349	C
29	S1	356	A
29	S1	358	C
29	S1	360	G
29	S1	364	G
29	S1	365	U
29	S1	381	G
29	S1	382	A
29	S1	404	C
29	S1	443	A
29	S1	444	A
29	S1	445	U
29	S1	447	G
29	S1	467	C
29	S1	469	G
29	S1	473	G
29	S1	477	G
29	S1	479	A

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Mol	Chain	Res	Type
29	S1	480	A
29	S1	481	A
29	S1	482	U
29	S1	483	U
29	S1	487	C
29	S1	488	A
29	S1	495	A
29	S1	499	A
29	S1	501	A
29	S1	503	C
29	S1	511	C
29	S1	512	A2M
29	S1	516	A
29	S1	523	A
29	S1	525	A
29	S1	553	U
29	S1	554	U
29	S1	560	G
29	S1	575	C
29	S1	587	A
29	S1	600	OMG
29	S1	606	G
29	S1	607	PSU
29	S1	608	C
29	S1	610	G
29	S1	614	C
29	S1	617	G
29	S1	628	A
29	S1	629	A
29	S1	631	U
29	S1	643	A
29	S1	656	G
29	S1	657	C
29	S1	660	U
29	S1	664	U
29	S1	668	A2M
29	S1	669	A
29	S1	671	G
29	S1	672	G
29	S1	688	G
29	S1	689	U
29	S1	751	G

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Mol	Chain	Res	Type
29	S1	771	G
29	S1	773	A
29	S1	784	C
29	S1	786	G
29	S1	787	G
29	S1	788	A
29	S1	789	G
29	S1	792	G
29	S1	793	G
29	S1	811	C
29	S1	814	G
29	S1	815	U
29	S1	817	A
29	S1	819	G
29	S1	820	C
29	S1	821	A
29	S1	842	U
29	S1	844	U
29	S1	845	U
29	S1	856	A
29	S1	863	C
29	S1	866	G
29	S1	867	A
29	S1	875	A
29	S1	876	G
29	S1	883	G
29	S1	884	A
29	S1	886	U
29	S1	887	U
29	S1	912	A
29	S1	915	A
29	S1	916	G
29	S1	917	C
29	S1	953	U
29	S1	955	A
29	S1	956	A
29	S1	957	G
29	S1	958	G
29	S1	978	C
29	S1	990	U
29	S1	991	G
29	S1	1103	G

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Mol	Chain	Res	Type
29	S1	1105	A
29	S1	1109	A
29	S1	1110	G
29	S1	1111	G
29	S1	1119	U
29	S1	1123	G
29	S1	1129	A
29	S1	1139	G
29	S1	1145	A
29	S1	1146	G
29	S1	1150	U
29	S1	1155	U
29	S1	1156	PSU
29	S1	1157	C
29	S1	1160	A
29	S1	1161	G
29	S1	1162	A
29	S1	1176	A
29	S1	1178	C
29	S1	1180	A
29	S1	1181	C
29	S1	1182	A
29	S1	1199	A
29	S1	1207	U
29	S1	1213	A
29	S1	1235	A
29	S1	1239	A
29	S1	1240	A
29	S1	1244	G
29	S1	1251	A
29	S1	1262	U
29	S1	1263	C
29	S1	1273	A
29	S1	1274	A
29	S1	1275	C
29	S1	1289	A
29	S1	1290	A
29	S1	1423	G
29	S1	1442	U
29	S1	1443	U
29	S1	1444	G
29	S1	1449	U

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Mol	Chain	Res	Type
29	S1	1452	A
29	S1	1458	A
29	S1	1466	G
29	S1	1490	A
29	S1	1502	G
29	S1	1503	A
29	S1	1504	A
29	S1	1510	C
29	S1	1537	U
29	S1	1542	C
29	S1	1543	C4J
29	S1	1544	5MC
29	S1	1546	A
29	S1	1548	A
29	S1	1550	OMG
29	S1	1551	G
29	S1	1552	G
29	S1	1554	A
29	S1	1565	A
29	S1	1569	G
29	S1	1570	G
29	S1	1573	A
29	S1	1582	A
29	S1	1592	U
29	S1	1593	G
29	S1	1595	G
29	S1	1597	G
29	S1	1598	U
29	S1	1602	U
29	S1	1603	U
29	S1	1606	C
29	S1	1608	A
29	S1	1611	C
29	S1	1613	C
29	S1	1621	U
29	S1	1622	G
29	S1	1624	U
29	S1	1638	U
29	S1	1653	U
29	S1	1658	U
29	S1	1659	U
29	S1	1660	G

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Mol	Chain	Res	Type
29	S1	1661	G
29	S1	1666	U
29	S1	1667	U
29	S1	1668	C
29	S1	1673	A
29	S1	1677	G
29	S1	1699	A
29	S1	1706	A
29	S1	1773	U
29	S1	1774	U
29	S1	1789	U
29	S1	1790	C
29	S1	1796	U
29	S1	1797	A
29	S1	1816	U
29	S1	1828	A
29	S1	1829	OMG
29	S1	1833	U
29	S1	1834	G
29	S1	1835	U
29	S1	1836	G
29	S1	1837	A
29	S1	1840	C
29	S1	1841	PSU
29	S1	1842	C
29	S1	1846	A
29	S1	1847	A
29	S1	1848	U
29	S1	1849	G
29	S1	1861	A
29	S1	1862	C
29	S1	1872	A
29	S1	1874	U
29	S1	1891	A
29	S1	1919	C
29	S1	1924	G
29	S1	1929	G
29	S1	1931	G
29	S1	1932	A
29	S1	1933	A
29	S1	1934	A
29	S1	1939	G

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Mol	Chain	Res	Type
29	S1	1944	C
29	S1	1948	U
29	S1	1949	A
29	S1	1955	A
29	S1	1956	C
29	S1	1957	U
29	S1	1973	C
29	S1	1977	U
29	S1	1978	A
29	S1	1979	OMU
29	S1	1982	G
29	S1	1988	C
29	S1	1989	A
29	S1	2004	G
29	S1	2010	G
29	S1	2012	A
29	S1	2021	A2M
29	S1	2027	G
29	S1	2053	A
29	S1	2054	C
29	S1	2055	A
29	S1	2056	C
29	S1	2059	C
29	S1	2086	A
29	S1	2099	G
29	S1	2100	A
29	S1	2151	OMG
29	S1	2165	A
29	S1	2169	A
29	S1	2170	G
29	S1	2172	U
29	S1	2186	C
29	S1	2195	G
29	S1	2196	G
34	S4	3	G
34	S4	4	C
34	S4	5	G
34	S4	70	C
34	S4	73	A
34	S4	76	A
35	8	11	G
35	8	31	A

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Mol	Chain	Res	Type
35	8	32	C
35	8	37	U
35	8	38	C
35	8	46	A
35	8	53	A
35	8	54	A
35	8	56	U
35	8	67	C
35	8	68	A
35	8	69	G
35	8	70	G
35	8	94	A
35	8	95	U
35	8	104	A
35	8	114	G
35	8	123	C
36	6	5	C
36	6	7	A
36	6	11	G
36	6	12	C
36	6	13	C
36	6	14	A
36	6	15	C
36	6	24	C
36	6	25	U
36	6	26	G
36	6	30	C
36	6	31	U
36	6	32	U
36	6	33	G
36	6	51	A
36	6	52	G
36	6	53	U
36	6	54	A
36	6	55	U
36	6	56	A
36	6	57	U
36	6	58	U
36	6	60	A
36	6	64	U
36	6	65	C
36	6	67	C

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Mol	Chain	Res	Type
36	6	68	A
36	6	69	A
36	6	72	C
36	6	73	A
37	2	6	A
37	2	22	A
37	2	25	A
37	2	29	C
37	2	50	A
37	2	54	U
37	2	61	C
37	2	63	U
37	2	64	A
37	2	68	A
37	2	69	A
37	2	72	G
37	2	75	C
37	2	76	A
37	2	78	PSU
37	2	90	G
37	2	91	C
37	2	135	A
37	2	136	A
37	2	341	A
37	2	344	G
37	2	349	C
37	2	368	G
37	2	377	A
37	2	380	G
37	2	386	U
37	2	388	A
37	2	390	A
37	2	404	A
37	2	437	PSU
37	2	438	C
37	2	443	OMC
37	2	444	A
37	2	450	C
37	2	510	PSU
37	2	512	PSU
37	2	513	C
37	2	514	U

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Mol	Chain	Res	Type
37	2	516	A
37	2	518	G
37	2	519	G
37	2	526	A
37	2	527	A2M
37	2	528	U
37	2	529	G
37	2	530	C
37	2	534	OMG
37	2	544	U
37	2	551	G
37	2	552	C
37	2	553	G
37	2	554	C
37	2	556	U
37	2	559	A
37	2	561	G
37	2	565	U
37	2	570	A2M
37	2	571	G
37	2	580	U
37	2	582	U
37	2	596	C
37	2	601	G
37	2	602	A
37	2	619	A
37	2	620	C
37	2	621	G
37	2	639	G
37	2	643	A
37	2	647	A
37	2	648	A
37	2	649	G
37	2	650	A
37	2	657	U
37	2	664	G
37	2	681	G
37	2	755	U
37	2	756	C
37	2	760	U
37	2	761	A
37	2	768	G

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Mol	Chain	Res	Type
37	2	769	A
37	2	777	A
37	2	778	A
37	2	779	U
37	2	783	U
37	2	784	U
37	2	786	A
37	2	787	G
37	2	795	U
37	2	800	G
37	2	801	C
37	2	812	C
37	2	813	U
37	2	964	G
37	2	965	C
37	2	966	U
37	2	967	G
37	2	969	A
37	2	970	A
37	2	971	A
37	2	972	C
37	2	973	U
37	2	979	A
37	2	984	G
37	2	985	A
37	2	999	U
37	2	1000	U
37	2	1011	G
37	2	1012	U
37	2	1019	A
37	2	1020	C
37	2	1022	U
37	2	1033	G
37	2	1034	G
37	2	1041	G
37	2	1045	G
37	2	1046	OMG
37	2	1053	A
37	2	1054	U
37	2	1055	A
37	2	1060	PSU
37	2	1063	C

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Mol	Chain	Res	Type
37	2	1064	A
37	2	1075	G
37	2	1078	OMG
37	2	1079	U
37	2	1083	A
37	2	1093	C
37	2	1116	A
37	2	1118	A
37	2	1120	C
37	2	1121	A
37	2	1123	A
37	2	1131	A
37	2	1141	G
37	2	1142	A
37	2	1143	U
37	2	1145	A
37	2	1146	A
37	2	1147	C
37	2	1155	A
37	2	1156	G
37	2	1157	U
37	2	1165	G
37	2	1180	A
37	2	1181	G
37	2	1185	A2M
37	2	1189	A
37	2	1215	A
37	2	1216	A
37	2	1237	A
37	2	1238	G
37	2	1239	A
37	2	1240	A
37	2	1241	U
37	2	1248	OMC
37	2	1252	G
37	2	1255	A
37	2	1265	U
37	2	1302	A
37	2	1305	C
37	2	1309	G
37	2	1314	C
37	2	1325	A

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Mol	Chain	Res	Type
37	2	1355	G
37	2	1356	G
37	2	1373	C
37	2	1374	A
37	2	1379	A
37	2	1380	C
37	2	1381	G
37	2	1385	G
37	2	1409	A
37	2	1416	U
37	2	1421	C
37	2	1428	U
37	2	1430	G
37	2	1436	A
37	2	1438	U
37	2	1441	C
37	2	1443	A
37	2	1456	C
37	2	1457	C
37	2	1459	U
37	2	1464	A
37	2	1466	C
38	7	22	U
38	7	34	U
38	7	35	C
38	7	48	A
38	7	51	A
38	7	52	A
38	7	59	A
38	7	62	A
38	7	63	G
38	7	67	U
38	7	75	OMG
38	7	83	A
38	7	84	U
38	7	85	U
38	7	87	A
38	7	88	A
38	7	90	U
38	7	94	G
38	7	96	A
38	7	104	A

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Mol	Chain	Res	Type
38	7	105	C
38	7	106	G
38	7	110	A
38	7	120	G
38	7	124	A
38	7	125	A
38	7	126	G
38	7	135	U
38	7	136	G
38	7	157	U
38	7	158	U
38	7	169	A
39	5	5	G
39	5	14	C
39	5	23	G
39	5	28	U
39	5	38	G
39	5	43	G
39	5	67	G
39	5	70	U
39	5	71	C
39	5	87	U
39	5	99	G
39	5	101	A
39	5	106	G
39	5	108	G
39	5	109	G
39	5	113	G
39	5	125	U
39	5	134	C
40	4	20	U
40	4	22	G
40	4	24	A
40	4	25	G
40	4	40	G
40	4	59	G
40	4	65	C
40	4	77	U
40	4	85	C
40	4	86	U
40	4	87	G
40	4	102	G

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Mol	Chain	Res	Type
40	4	107	U
40	4	114	A
40	4	120	U
40	4	121	C
40	4	127	G
40	4	131	U
40	4	137	G
40	4	158	A
40	4	168	A
40	4	171	A
40	4	173	C
41	3	35	A
41	3	42	U
41	3	51	G
41	3	72	A
41	3	99	U
41	3	100	U
41	3	101	G
41	3	104	C
41	3	110	U
41	3	112	C
41	3	118	G
41	3	124	U
41	3	125	U
41	3	126	C
41	3	129	A
41	3	149	A
41	3	150	A
41	3	151	A
41	3	180	U
41	3	181	G
41	3	184	A
41	3	188	C
41	3	192	G
41	3	193	C
41	3	197	A
41	3	199	A
41	3	201	C
41	3	202	A
41	3	210	G
42	1	24	A
42	1	29	C

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Mol	Chain	Res	Type
42	1	38	A
42	1	41	A
42	1	47	C
42	1	58	A
42	1	64	A
42	1	73	U
42	1	84	G
42	1	86	G
42	1	87	A
42	1	88	G
42	1	91	G
42	1	92	C
42	1	98	A
42	1	110	A
42	1	127	G
42	1	131	U
42	1	132	A
42	1	134	A
42	1	135	A
42	1	136	G
42	1	141	U
42	1	142	G
42	1	153	C
42	1	175	G
42	1	176	C
42	1	177	A
42	1	191	U
42	1	192	C
42	1	200	A
42	1	205	A
42	1	206	A
42	1	209	C
42	1	211	U
42	1	212	U
42	1	213	G
42	1	214	C
42	1	215	U
42	1	217	A
42	1	218	A
42	1	219	U
42	1	220	A
42	1	223	A

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Mol	Chain	Res	Type
42	1	230	A
42	1	231	U
42	1	237	U
42	1	238	A
42	1	250	A
42	1	251	A
42	1	255	G
42	1	256	U
42	1	257	U
42	1	258	A
42	1	261	C
42	1	266	G
42	1	267	A
42	1	273	A
42	1	279	G
42	1	280	A
42	1	283	G
42	1	292	A
42	1	293	C
42	1	294	U
42	1	301	A
42	1	305	A2M
42	1	306	G
42	1	323	U
42	1	332	A
42	1	343	U
42	1	349	U
42	1	361	A
42	1	367	A
42	1	368	G
42	1	369	A
42	1	374	G
42	1	378	A
42	1	383	U
42	1	390	C
42	1	392	A
42	1	407	A2M
42	1	409	U
42	1	410	U
42	1	417	G
42	1	422	PSU
42	1	423	U

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Mol	Chain	Res	Type
42	1	433	G
42	1	438	A
42	1	440	A
42	1	442	A
42	1	444	C
42	1	460	A
42	1	461	G
42	1	462	A
42	1	463	C
42	1	464	A
42	1	469	A
42	1	477	C
42	1	478	C
42	1	486	C
42	1	487	G
42	1	488	G
42	1	489	C
42	1	496	C
42	1	502	U
42	1	507	C
42	1	508	A
42	1	510	U
42	1	511	A
42	1	521	G
42	1	528	A
42	1	532	C
42	1	534	G
42	1	537	G
42	1	547	U
42	1	548	G
42	1	549	C
42	1	551	A
42	1	567	G
42	1	649	U
42	1	668	C
42	1	672	PSU
42	1	677	A
42	1	681	A2M
42	1	692	A
42	1	695	OMC
42	1	709	A
42	1	713	A

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Mol	Chain	Res	Type
42	1	716	A
42	1	721	U
42	1	729	A
42	1	750	G
42	1	753	A
42	1	754	G
42	1	767	U
42	1	769	U
42	1	771	U
42	1	778	C
42	1	797	A
42	1	798	U
42	1	803	C
42	1	822	C
42	1	823	G
42	1	825	G
42	1	826	G
42	1	832	G
42	1	836	G
42	1	838	G
42	1	849	U
42	1	850	G
42	1	868	A
42	1	899	A
42	1	900	C
42	1	912	C
42	1	922	U
42	1	925	U
42	1	930	U
42	1	947	A
42	1	958	G
42	1	965	A
42	1	967	G
42	1	972	A
42	1	974	C
42	1	975	G
42	1	977	A
42	1	985	G
42	1	988	G
42	1	995	C
42	1	997	C
42	1	1010	OMC

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Mol	Chain	Res	Type
42	1	1011	PSU
42	1	1012	C
42	1	1029	G
42	1	1030	U
42	1	1031	A
42	1	1033	A
42	1	1045	G
42	1	1052	A
42	1	1103	U
42	1	1105	A
42	1	1107	OMU
42	1	1114	A
42	1	1120	C
42	1	1128	A
42	1	1129	G
42	1	1135	U
42	1	1136	G
42	1	1148	A
42	1	1150	A
42	1	1153	A
42	1	1156	A
42	1	1159	A
42	1	1161	A
42	1	1165	A
42	1	1174	G
42	1	1179	C
42	1	1181	PSU
42	1	1182	C
42	1	1188	G
42	1	1201	U
42	1	1208	U
42	1	1210	A
42	1	1211	A
42	1	1216	U
42	1	1235	A
42	1	1238	C
42	1	1239	U
42	1	1242	U
42	1	1243	G
42	1	1250	U
42	1	1251	U
42	1	1253	U

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Mol	Chain	Res	Type
42	1	1254	C
42	1	1257	U
42	1	1258	A
42	1	1261	U
42	1	1263	A
42	1	1269	G
42	1	1270	U
42	1	1271	G
42	1	1273	U
42	1	1275	G
42	1	1277	G
42	1	1355	C
42	1	1357	G
42	1	1366	A
42	1	1367	U
42	1	1369	G
42	1	1371	OMU
42	1	1375	G
42	1	1379	A
42	1	1389	A
42	1	1390	G
42	1	1392	G
42	1	1394	U
42	1	1395	U
42	1	1398	C
42	1	1401	U
42	1	1402	PSU
42	1	1412	G
42	1	1413	U
42	1	1435	A
42	1	1436	G
42	1	1437	A
42	1	1438	A
42	1	1439	A
42	1	1443	U
42	1	1445	G
42	1	1464	G
42	1	1470	G
42	1	1476	A
42	1	1481	G
42	1	1490	G
42	1	1504	A

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Mol	Chain	Res	Type
42	1	1509	C
42	1	1521	G
42	1	1524	OMG
42	1	1527	OMC
42	1	1528	PSU
42	1	1536	C
42	1	1540	OMG
42	1	1545	G
42	1	1557	A
42	1	1560	U
42	1	1561	A
42	1	1562	C
42	1	1565	A
42	1	1566	A
42	1	1586	G
42	1	1587	A
42	1	1589	C
42	1	1590	G
42	1	1605	G
42	1	1612	G
42	1	1613	C
42	1	1625	A
42	1	1631	U
42	1	1645	C
42	1	1654	A
42	1	1655	U
42	1	1661	U
42	1	1662	G
42	1	1663	U
42	1	1664	PSU
42	1	1665	A
42	1	1666	G
42	1	1667	G
42	1	1668	A
42	1	1670	A
42	1	1672	U
42	1	1673	G
42	1	1674	A
42	1	1675	A
42	1	1676	G
42	1	1677	G
42	1	1727	A

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Mol	Chain	Res	Type
42	1	1730	A
42	1	1738	C
42	1	1739	A
42	1	1744	A
42	1	1747	U
42	1	1751	A
42	1	1753	U
42	1	1761	A
42	1	1762	A
42	1	1763	A
42	1	1766	G
42	1	1776	G

All (61) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	S1	33	PSU
29	S1	72	C
29	S1	234	C
29	S1	277	U
29	S1	309	G
29	S1	494	A
29	S1	607	PSU
29	S1	656	G
29	S1	916	G
29	S1	1108	A
29	S1	1145	A
29	S1	1156	PSU
29	S1	1621	U
29	S1	1667	U
29	S1	1672	C
29	S1	1833	U
29	S1	1841	PSU
29	S1	2053	A
29	S1	2054	C
36	6	51	A
36	6	72	C
37	2	68	A
37	2	340	A
37	2	443	OMC
37	2	646	G
37	2	648	A

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Mol	Chain	Res	Type
37	2	755	U
37	2	984	G
37	2	1052	C
37	2	1053	A
37	2	1092	U
37	2	1239	A
37	2	1456	C
38	7	157	U
40	4	106	G
41	3	98	C
41	3	111	A
41	3	150	A
41	3	180	U
41	3	192	G
41	3	201	C
42	1	141	U
42	1	191	U
42	1	214	C
42	1	217	A
42	1	219	U
42	1	422	PSU
42	1	443	A
42	1	468	G
42	1	510	U
42	1	648	A
42	1	947	A
42	1	1011	PSU
42	1	1134	C
42	1	1135	U
42	1	1269	G
42	1	1276	U
42	1	1356	G
42	1	1393	A
42	1	1586	G
42	1	1664	PSU

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

142 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
42	PSU	1	1181	42	18,21,22	1.40	2 (11%)	21,30,33	2.22	5 (23%)
37	A2M	2	604	37,42	22,25,26	3.31	9 (40%)	30,36,39	2.94	12 (40%)
42	PSU	1	1017	83,42	18,21,22	1.50	4 (22%)	21,30,33	2.26	4 (19%)
37	OMG	2	641	37	23,26,27	2.32	8 (34%)	32,38,41	2.49	13 (40%)
37	OMG	2	1078	37	23,26,27	2.30	8 (34%)	32,38,41	2.46	12 (37%)
37	PSU	2	472	37	18,21,22	1.42	3 (16%)	21,30,33	2.23	5 (23%)
29	PSU	S1	1156	29	18,21,22	1.39	3 (16%)	21,30,33	2.24	5 (23%)
29	PSU	S1	12	29	18,21,22	4.56	7 (38%)	21,30,33	1.97	5 (23%)
42	OMG	1	1524	42	23,26,27	2.34	9 (39%)	32,38,41	2.52	11 (34%)
37	PSU	2	510	37	18,21,22	4.76	9 (50%)	21,30,33	1.75	4 (19%)
29	OMC	S1	2140	29	19,22,23	2.96	8 (42%)	25,31,34	0.85	0
42	OMC	1	695	42	19,22,23	2.62	7 (36%)	25,31,34	0.88	1 (4%)
37	A2M	2	1372	37	22,25,26	3.31	10 (45%)	30,36,39	3.21	12 (40%)
37	PSU	2	1354	37	18,21,22	4.36	7 (38%)	21,30,33	2.04	5 (23%)
29	PSU	S1	2046	29	18,21,22	1.46	3 (16%)	21,30,33	2.13	5 (23%)
37	PSU	2	1303	37	18,21,22	1.37	2 (11%)	21,30,33	2.20	5 (23%)
37	OMG	2	1360	37	23,26,27	2.39	8 (34%)	32,38,41	2.53	11 (34%)
42	OMU	1	845	42	19,22,23	2.73	6 (31%)	25,31,34	2.58	9 (36%)
29	OMG	S1	600	29	23,26,27	2.42	9 (39%)	32,38,41	2.65	10 (31%)
42	OMG	1	856	42	23,26,27	2.30	8 (34%)	32,38,41	2.42	13 (40%)
29	PSU	S1	1539	29	18,21,22	1.44	3 (16%)	21,30,33	2.21	5 (23%)
29	PSU	S1	1657	29	18,21,22	1.43	3 (16%)	21,30,33	2.25	4 (19%)
29	OMU	S1	1979	29	19,22,23	2.96	8 (42%)	25,31,34	1.84	5 (20%)
29	OMU	S1	661	29	19,22,23	3.00	8 (42%)	25,31,34	1.83	5 (20%)
29	PSU	S1	1533	29	18,21,22	1.45	3 (16%)	21,30,33	2.16	5 (23%)
37	PSU	2	1413	37	18,21,22	4.23	8 (44%)	21,30,33	2.05	4 (19%)
42	OMG	1	959[A]	42	23,26,27	2.41	9 (39%)	32,38,41	2.68	11 (34%)
37	PSU	2	78	37	18,21,22	1.47	4 (22%)	21,30,33	2.19	5 (23%)
37	OMU	2	667	37	19,22,23	2.76	7 (36%)	25,31,34	2.03	5 (20%)
37	A2M	2	382	37	22,25,26	3.35	10 (45%)	30,36,39	2.98	11 (36%)
29	PSU	S1	1192	29	18,21,22	1.39	3 (16%)	21,30,33	2.29	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	PSU	7	69	38	18,21,22	1.40	3 (16%)	21,30,33	2.32	5 (23%)
42	OMU	1	1659	42	19,22,23	2.77	7 (36%)	25,31,34	1.86	5 (20%)
42	PSU	1	1533	37,42	18,21,22	1.45	3 (16%)	21,30,33	2.32	5 (23%)
42	PSU	1	870	83,42	18,21,22	4.27	8 (44%)	21,30,33	2.01	5 (23%)
29	PSU	S1	104	29	18,21,22	4.61	7 (38%)	21,30,33	1.94	5 (23%)
42	PSU	1	940	42	18,21,22	4.10	8 (44%)	21,30,33	2.18	4 (19%)
37	OMU	2	1359	37	19,22,23	2.85	8 (42%)	25,31,34	1.94	5 (20%)
38	A2M	7	162	38,42	22,25,26	3.27	10 (45%)	30,36,39	3.07	12 (40%)
37	A2M	2	527	37	22,25,26	3.35	10 (45%)	30,36,39	3.34	15 (50%)
38	OMG	7	75	38	23,26,27	1.23	3 (13%)	32,38,41	2.13	7 (21%)
37	A2M	2	1185	37	22,25,26	3.30	9 (40%)	30,36,39	3.00	13 (43%)
40	OMG	4	74	40	23,26,27	2.29	8 (34%)	32,38,41	2.58	13 (40%)
37	A2M	2	628	37	22,25,26	3.34	10 (45%)	30,36,39	3.19	12 (40%)
38	A2M	7	43	38	22,25,26	3.32	10 (45%)	30,36,39	3.12	11 (36%)
29	OMG	S1	2151	29	23,26,27	2.41	9 (39%)	32,38,41	2.63	10 (31%)
37	OMU	2	1077	37	19,22,23	2.88	8 (42%)	25,31,34	1.93	5 (20%)
37	OMG	2	1231	37	23,26,27	2.32	8 (34%)	32,38,41	2.51	13 (40%)
37	PSU	2	593	37	18,21,22	1.50	3 (16%)	21,30,33	2.27	6 (28%)
42	PSU	1	1011	42	18,21,22	4.47	9 (50%)	21,30,33	2.11	6 (28%)
37	A2M	2	95	37	22,25,26	3.30	10 (45%)	30,36,39	2.99	13 (43%)
37	OMG	2	1253	37	23,26,27	2.28	8 (34%)	32,38,41	2.44	9 (28%)
42	A2M	1	235	42	22,25,26	3.31	10 (45%)	30,36,39	3.04	11 (36%)
42	OMG	1	959[B]	42	23,26,27	2.36	9 (39%)	32,38,41	2.21	9 (28%)
29	OMG	S1	1550	29	23,26,27	2.42	9 (39%)	32,38,41	2.55	10 (31%)
29	OMG	S1	1829	84,83,29	23,26,27	2.40	9 (39%)	32,38,41	2.57	10 (31%)
37	PSU	2	1060	37	18,21,22	1.45	3 (16%)	21,30,33	2.25	5 (23%)
37	OMG	2	71	37	23,26,27	1.25	3 (13%)	32,38,41	2.17	8 (25%)
29	OMC	S1	18	29	19,22,23	2.91	8 (42%)	25,31,34	0.76	0
29	PSU	S1	33	29	18,21,22	1.40	3 (16%)	21,30,33	2.14	4 (19%)
42	OMU	1	1107	42	19,22,23	2.87	8 (42%)	25,31,34	1.98	5 (20%)
37	PSU	2	1144	37	18,21,22	1.43	3 (16%)	21,30,33	2.25	5 (23%)
38	PSU	7	74	38	18,21,22	1.43	3 (16%)	21,30,33	2.15	5 (23%)
29	PSU	S1	609	29	18,21,22	1.40	3 (16%)	21,30,33	2.19	5 (23%)
42	A2M	1	407	42	22,25,26	3.36	10 (45%)	30,36,39	3.12	13 (43%)
42	A2M	1	1539	37,83,42	22,25,26	3.33	10 (45%)	30,36,39	3.04	13 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	A2M	2	1384	37	22,25,26	3.32	10 (45%)	30,36,39	3.06	11 (36%)
37	OMU	2	73	37	19,22,23	1.36	3 (15%)	25,31,34	1.95	5 (20%)
42	PSU	1	422	42	18,21,22	1.51	5 (27%)	21,30,33	2.38	5 (23%)
42	OMU	1	847	42	19,22,23	2.78	7 (36%)	25,31,34	1.98	5 (20%)
37	OMC	2	583	37	19,22,23	2.67	7 (36%)	25,31,34	0.76	0
29	OMG	S1	1478	29	23,26,27	2.37	9 (39%)	32,38,41	2.52	10 (31%)
41	OMU	3	13	41	19,22,23	2.87	7 (36%)	25,31,34	2.36	7 (28%)
37	OMG	2	1046	37	23,26,27	2.40	9 (39%)	32,38,41	2.55	11 (34%)
29	OMG	S1	1647	29	23,26,27	2.43	9 (39%)	32,38,41	2.58	10 (31%)
29	OMC	S1	1866	29	19,22,23	2.82	8 (42%)	25,31,34	0.71	0
29	5MC	S1	2061	29	19,22,23	1.46	3 (15%)	26,32,35	1.23	4 (15%)
29	PSU	S1	455	29	18,21,22	4.61	7 (38%)	21,30,33	1.91	5 (23%)
42	PSU	1	672	84,83,42	18,21,22	1.46	3 (16%)	21,30,33	2.28	5 (23%)
42	PSU	1	1528	42	18,21,22	1.46	3 (16%)	21,30,33	2.25	5 (23%)
42	A2M	1	697	42	22,25,26	3.39	10 (45%)	30,36,39	3.06	11 (36%)
37	PSU	2	1194	37	18,21,22	4.37	7 (38%)	21,30,33	1.95	4 (19%)
42	A2M	1	858	42	22,25,26	3.26	10 (45%)	30,36,39	3.17	14 (46%)
42	PSU	1	1171	42	18,21,22	4.34	9 (50%)	21,30,33	2.21	8 (38%)
42	PSU	1	1664	42	18,21,22	1.47	4 (22%)	21,30,33	2.27	4 (19%)
29	C4J	S1	1543	29	25,29,30	2.90	9 (36%)	28,42,45	1.47	3 (10%)
29	A2M	S1	2021	29	22,25,26	3.25	10 (45%)	30,36,39	3.18	13 (43%)
42	PSU	1	239	42	18,21,22	1.41	3 (16%)	21,30,33	2.25	5 (23%)
37	OMC	2	1159	37	19,22,23	2.70	7 (36%)	25,31,34	0.80	0
29	5MC	S1	1544	29	19,22,23	3.78	8 (42%)	26,32,35	0.99	2 (7%)
37	PSU	2	1058	37	18,21,22	1.43	3 (16%)	21,30,33	2.17	5 (23%)
29	OMG	S1	1865	29	23,26,27	2.41	9 (39%)	32,38,41	2.56	12 (37%)
37	OMC	2	1397	37	19,22,23	2.64	7 (36%)	25,31,34	0.81	0
37	PSU	2	1382	37,86	18,21,22	4.35	9 (50%)	21,30,33	1.99	5 (23%)
29	OMG	S1	1879	29	23,26,27	2.38	9 (39%)	32,38,41	2.63	10 (31%)
42	OMC	1	1527	42	19,22,23	0.87	0	25,31,34	0.94	1 (4%)
37	OMU	2	1152	37	19,22,23	2.82	7 (36%)	25,31,34	1.92	5 (20%)
38	OMU	7	7	38,42	19,22,23	2.87	7 (36%)	25,31,34	1.83	5 (20%)
37	OMC	2	1317	37	19,22,23	2.70	7 (36%)	25,31,34	0.80	1 (4%)
37	PSU	2	1264	37	18,21,22	1.49	3 (16%)	21,30,33	2.14	4 (19%)
37	5MC	2	1308	37	19,22,23	4.63	13 (68%)	26,32,35	1.37	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	A2M	1	955	42	22,25,26	3.33	10 (45%)	30,36,39	3.11	13 (43%)
37	OMC	2	443	37,86	19,22,23	2.83	8 (42%)	25,31,34	0.91	0
42	OMG	1	1540	37,42	23,26,27	2.30	8 (34%)	32,38,41	2.38	13 (40%)
42	A2M	1	678	37,42	22,25,26	3.26	10 (45%)	30,36,39	3.03	13 (43%)
29	OMC	S1	38	29	19,22,23	2.95	8 (42%)	25,31,34	0.76	0
37	A2M	2	591	37	22,25,26	1.45	5 (22%)	30,36,39	2.12	10 (33%)
42	OMG	1	1190	42	23,26,27	2.40	9 (39%)	32,38,41	2.52	11 (34%)
37	PSU	2	597	37	18,21,22	1.46	3 (16%)	21,30,33	2.23	5 (23%)
42	OMC	1	1010	42	19,22,23	2.85	8 (42%)	25,31,34	0.88	1 (4%)
42	OMG	1	1626	42	23,26,27	2.26	8 (34%)	32,38,41	2.48	12 (37%)
42	PSU	1	1402	42	18,21,22	4.33	7 (38%)	21,30,33	1.90	5 (23%)
29	OMU	S1	8	29	19,22,23	2.98	8 (42%)	25,31,34	1.86	5 (20%)
29	OMG	S1	1623	29	23,26,27	1.21	3 (13%)	32,38,41	2.09	7 (21%)
29	A2M	S1	668	83,29	22,25,26	3.24	9 (40%)	30,36,39	3.12	11 (36%)
37	OMG	2	534	37	23,26,27	2.34	8 (34%)	32,38,41	2.57	10 (31%)
37	PSU	2	437	37	18,21,22	4.34	8 (44%)	21,30,33	2.05	5 (23%)
29	PSU	S1	1566	29	18,21,22	4.57	8 (44%)	21,30,33	1.82	3 (14%)
37	PSU	2	1361	37	18,21,22	4.49	8 (44%)	21,30,33	1.99	4 (19%)
42	A2M	1	681	42	22,25,26	3.28	10 (45%)	30,36,39	2.97	11 (36%)
29	PSU	S1	607	29	18,21,22	1.36	2 (11%)	21,30,33	2.25	6 (28%)
37	OMU	2	560	84,37	19,22,23	2.83	7 (36%)	25,31,34	1.88	4 (16%)
37	PSU	2	662	84,37	18,21,22	4.22	8 (44%)	21,30,33	1.93	4 (19%)
42	OMU	1	1371	42	19,22,23	2.91	8 (42%)	25,31,34	2.13	7 (28%)
37	PSU	2	512	37	18,21,22	4.64	7 (38%)	21,30,33	1.99	5 (23%)
37	PSU	2	626	37	18,21,22	4.25	8 (44%)	21,30,33	2.02	4 (19%)
42	A2M	1	927	42	22,25,26	3.32	10 (45%)	30,36,39	3.10	12 (40%)
37	A2M	2	572	37	22,25,26	3.33	10 (45%)	30,36,39	3.14	12 (40%)
37	OMG	2	1229	37	23,26,27	2.33	9 (39%)	32,38,41	2.53	13 (40%)
29	A2M	S1	512	84,29	22,25,26	1.49	5 (22%)	30,36,39	2.18	10 (33%)
29	PSU	S1	1246	29	18,21,22	1.41	2 (11%)	21,30,33	2.16	4 (19%)
37	PSU	2	1403	37	18,21,22	1.44	3 (16%)	21,30,33	2.29	5 (23%)
42	A2M	1	305	42	22,25,26	3.34	10 (45%)	30,36,39	3.08	15 (50%)
37	A2M	2	570	37,42	22,25,26	3.34	10 (45%)	30,36,39	3.22	15 (50%)
37	OMG	2	655	37	23,26,27	2.31	8 (34%)	32,38,41	2.50	12 (37%)
29	G7M	S1	1995	29	23,26,27	3.76	11 (47%)	34,39,42	1.74	8 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	OMU	2	1419	37	19,22,23	2.81	7 (36%)	25,31,34	1.91	5 (20%)
29	PSU	S1	2048	29	18,21,22	1.43	3 (16%)	21,30,33	2.27	5 (23%)
29	PSU	S1	1841	29	18,21,22	1.45	3 (16%)	21,30,33	2.22	5 (23%)
37	OMC	2	1248	37	19,22,23	2.73	7 (36%)	25,31,34	1.00	1 (4%)
37	OMC	2	359	37	19,22,23	2.83	8 (42%)	25,31,34	0.71	0
37	PSU	2	1318	37	18,21,22	4.24	8 (44%)	21,30,33	2.02	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	PSU	1	1181	42	-	3/7/25/26	0/2/2/2
37	A2M	2	604	37,42	-	1/9/27/28	0/3/3/3
42	PSU	1	1017	83,42	-	0/7/25/26	0/2/2/2
37	OMG	2	641	37	-	0/9/27/28	0/3/3/3
37	OMG	2	1078	37	-	0/9/27/28	0/3/3/3
37	PSU	2	472	37	-	0/7/25/26	0/2/2/2
29	PSU	S1	1156	29	-	0/7/25/26	0/2/2/2
29	PSU	S1	12	29	-	0/7/25/26	0/2/2/2
42	OMG	1	1524	42	-	1/9/27/28	0/3/3/3
37	PSU	2	510	37	-	5/7/25/26	0/2/2/2
29	OMC	S1	2140	29	-	2/9/27/28	0/2/2/2
42	OMC	1	695	42	-	2/9/27/28	0/2/2/2
37	A2M	2	1372	37	-	0/9/27/28	0/3/3/3
37	PSU	2	1354	37	-	0/7/25/26	0/2/2/2
29	PSU	S1	2046	29	-	2/7/25/26	0/2/2/2
37	PSU	2	1303	37	-	0/7/25/26	0/2/2/2
37	OMG	2	1360	37	-	0/9/27/28	0/3/3/3
42	OMU	1	845	42	-	2/9/27/28	0/2/2/2
29	OMG	S1	600	29	-	2/9/27/28	0/3/3/3
42	OMG	1	856	42	-	0/9/27/28	0/3/3/3
29	PSU	S1	1539	29	-	0/7/25/26	0/2/2/2
29	PSU	S1	1657	29	-	2/7/25/26	0/2/2/2
29	OMU	S1	1979	29	-	1/9/27/28	0/2/2/2
29	OMU	S1	661	29	-	0/9/27/28	0/2/2/2
29	PSU	S1	1533	29	-	0/7/25/26	0/2/2/2
37	PSU	2	1413	37	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	OMG	1	959[A]	42	-	2/9/27/28	0/3/3/3
37	PSU	2	78	37	-	2/7/25/26	0/2/2/2
37	OMU	2	667	37	-	1/9/27/28	0/2/2/2
37	A2M	2	382	37	-	0/9/27/28	0/3/3/3
29	PSU	S1	1192	29	-	0/7/25/26	0/2/2/2
38	PSU	7	69	38	-	0/7/25/26	0/2/2/2
42	OMU	1	1659	42	-	0/9/27/28	0/2/2/2
42	PSU	1	1533	37,42	-	1/7/25/26	0/2/2/2
42	PSU	1	870	83,42	-	1/7/25/26	0/2/2/2
29	PSU	S1	104	29	-	2/7/25/26	0/2/2/2
42	PSU	1	940	42	-	0/7/25/26	0/2/2/2
37	OMU	2	1359	37	-	0/9/27/28	0/2/2/2
38	A2M	7	162	38,42	-	1/9/27/28	0/3/3/3
37	A2M	2	527	37	-	0/9/27/28	0/3/3/3
38	OMG	7	75	38	-	3/9/27/28	0/3/3/3
37	A2M	2	1185	37	-	2/9/27/28	0/3/3/3
40	OMG	4	74	40	-	0/9/27/28	0/3/3/3
37	A2M	2	628	37	-	0/9/27/28	0/3/3/3
38	A2M	7	43	38	-	0/9/27/28	0/3/3/3
29	OMG	S1	2151	29	-	2/9/27/28	0/3/3/3
37	OMU	2	1077	37	-	1/9/27/28	0/2/2/2
37	OMG	2	1231	37	-	0/9/27/28	0/3/3/3
37	PSU	2	593	37	-	0/7/25/26	0/2/2/2
42	PSU	1	1011	42	-	2/7/25/26	0/2/2/2
37	A2M	2	95	37	-	0/9/27/28	0/3/3/3
37	OMG	2	1253	37	-	0/9/27/28	0/3/3/3
42	A2M	1	235	42	-	1/9/27/28	0/3/3/3
42	OMG	1	959[B]	42	-	0/9/27/28	0/3/3/3
29	OMG	S1	1550	29	-	2/9/27/28	0/3/3/3
29	OMG	S1	1829	84,83,29	-	1/9/27/28	0/3/3/3
37	PSU	2	1060	37	-	2/7/25/26	0/2/2/2
37	OMG	2	71	37	-	2/9/27/28	0/3/3/3
29	OMC	S1	18	29	-	1/9/27/28	0/2/2/2
29	PSU	S1	33	29	-	4/7/25/26	0/2/2/2
42	OMU	1	1107	42	-	2/9/27/28	0/2/2/2
37	PSU	2	1144	37	-	1/7/25/26	0/2/2/2
38	PSU	7	74	38	-	2/7/25/26	0/2/2/2
29	PSU	S1	609	29	-	0/7/25/26	0/2/2/2
42	A2M	1	407	42	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	A2M	1	1539	37,83,42	-	1/9/27/28	0/3/3/3
37	A2M	2	1384	37	-	0/9/27/28	0/3/3/3
37	OMU	2	73	37	-	1/9/27/28	0/2/2/2
42	PSU	1	422	42	-	2/7/25/26	0/2/2/2
42	OMU	1	847	42	-	0/9/27/28	0/2/2/2
37	OMC	2	583	37	-	1/9/27/28	0/2/2/2
29	OMG	S1	1478	29	-	0/9/27/28	0/3/3/3
41	OMU	3	13	41	-	3/9/27/28	0/2/2/2
37	OMG	2	1046	37	-	3/9/27/28	0/3/3/3
29	OMG	S1	1647	29	-	0/9/27/28	0/3/3/3
29	OMC	S1	1866	29	-	0/9/27/28	0/2/2/2
29	5MC	S1	2061	29	-	0/7/25/26	0/2/2/2
29	PSU	S1	455	29	-	3/7/25/26	0/2/2/2
42	PSU	1	672	84,83,42	-	2/7/25/26	0/2/2/2
42	PSU	1	1528	42	-	2/7/25/26	0/2/2/2
42	A2M	1	697	42	-	0/9/27/28	0/3/3/3
37	PSU	2	1194	37	-	0/7/25/26	0/2/2/2
42	A2M	1	858	42	-	0/9/27/28	0/3/3/3
42	PSU	1	1171	42	-	2/7/25/26	0/2/2/2
42	PSU	1	1664	42	-	2/7/25/26	0/2/2/2
29	C4J	S1	1543	29	-	8/16/34/35	0/2/2/2
29	A2M	S1	2021	29	-	2/9/27/28	0/3/3/3
42	PSU	1	239	42	-	0/7/25/26	0/2/2/2
37	OMC	2	1159	37	-	0/9/27/28	0/2/2/2
29	5MC	S1	1544	29	-	2/7/25/26	0/2/2/2
37	PSU	2	1058	37	-	1/7/25/26	0/2/2/2
29	OMG	S1	1865	29	-	1/9/27/28	0/3/3/3
37	OMC	2	1397	37	-	0/9/27/28	0/2/2/2
37	PSU	2	1382	37,86	-	0/7/25/26	0/2/2/2
29	OMG	S1	1879	29	-	0/9/27/28	0/3/3/3
42	OMC	1	1527	42	-	2/9/27/28	0/2/2/2
37	OMU	2	1152	37	-	0/9/27/28	0/2/2/2
38	OMU	7	7	38,42	-	0/9/27/28	0/2/2/2
37	OMC	2	1317	37	-	0/9/27/28	0/2/2/2
37	PSU	2	1264	37	-	0/7/25/26	0/2/2/2
37	5MC	2	1308	37	-	4/7/25/26	0/2/2/2
42	A2M	1	955	42	-	0/9/27/28	0/3/3/3
37	OMC	2	443	37,86	-	5/9/27/28	0/2/2/2
42	OMG	1	1540	37,42	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	A2M	1	678	37,42	-	0/9/27/28	0/3/3/3
29	OMC	S1	38	29	-	0/9/27/28	0/2/2/2
37	A2M	2	591	37	-	1/9/27/28	0/3/3/3
42	OMG	1	1190	42	-	0/9/27/28	0/3/3/3
37	PSU	2	597	37	-	2/7/25/26	0/2/2/2
42	OMC	1	1010	42	-	1/9/27/28	0/2/2/2
42	OMG	1	1626	42	-	1/9/27/28	0/3/3/3
42	PSU	1	1402	42	-	5/7/25/26	0/2/2/2
29	OMU	S1	8	29	-	6/9/27/28	0/2/2/2
29	OMG	S1	1623	29	-	1/9/27/28	0/3/3/3
29	A2M	S1	668	83,29	-	4/9/27/28	0/3/3/3
37	OMG	2	534	37	-	2/9/27/28	0/3/3/3
37	PSU	2	437	37	-	2/7/25/26	0/2/2/2
29	PSU	S1	1566	29	-	2/7/25/26	0/2/2/2
37	PSU	2	1361	37	-	4/7/25/26	0/2/2/2
42	A2M	1	681	42	-	2/9/27/28	0/3/3/3
29	PSU	S1	607	29	-	5/7/25/26	0/2/2/2
37	OMU	2	560	84,37	-	1/9/27/28	0/2/2/2
37	PSU	2	662	84,37	-	0/7/25/26	0/2/2/2
42	OMU	1	1371	42	-	4/9/27/28	0/2/2/2
37	PSU	2	512	37	-	2/7/25/26	0/2/2/2
37	PSU	2	626	37	-	0/7/25/26	0/2/2/2
42	A2M	1	927	42	-	0/9/27/28	0/3/3/3
37	A2M	2	572	37	-	0/9/27/28	0/3/3/3
37	OMG	2	1229	37	-	0/9/27/28	0/3/3/3
29	A2M	S1	512	84,29	-	3/9/27/28	0/3/3/3
29	PSU	S1	1246	29	-	0/7/25/26	0/2/2/2
37	PSU	2	1403	37	-	0/7/25/26	0/2/2/2
42	A2M	1	305	42	-	2/9/27/28	0/3/3/3
37	A2M	2	570	37,42	-	6/9/27/28	0/3/3/3
37	OMG	2	655	37	-	0/9/27/28	0/3/3/3
29	G7M	S1	1995	29	-	2/7/25/26	0/3/3/3
37	OMU	2	1419	37	-	0/9/27/28	0/2/2/2
29	PSU	S1	2048	29	-	0/7/25/26	0/2/2/2
29	PSU	S1	1841	29	-	2/7/25/26	0/2/2/2
37	OMC	2	1248	37	-	1/9/27/28	0/2/2/2
37	OMC	2	359	37	-	0/9/27/28	0/2/2/2
37	PSU	2	1318	37	-	0/7/25/26	0/2/2/2

All (987) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	510	PSU	C6-C5	12.70	1.49	1.35
37	2	512	PSU	C6-C5	12.24	1.48	1.35
29	S1	455	PSU	C6-C5	12.18	1.48	1.35
29	S1	1566	PSU	C6-C5	12.00	1.48	1.35
29	S1	104	PSU	C6-C5	11.98	1.48	1.35
29	S1	12	PSU	C6-C5	11.88	1.48	1.35
37	2	1361	PSU	C6-C5	11.73	1.48	1.35
37	2	1194	PSU	C6-C5	11.61	1.48	1.35
37	2	626	PSU	C6-C5	11.52	1.48	1.35
37	2	1382	PSU	C6-C5	11.49	1.48	1.35
42	1	1171	PSU	C6-C5	11.48	1.48	1.35
37	2	662	PSU	C6-C5	11.48	1.48	1.35
37	2	437	PSU	C6-C5	11.46	1.48	1.35
37	2	1354	PSU	C6-C5	11.45	1.48	1.35
42	1	1402	PSU	C6-C5	11.40	1.47	1.35
37	2	1318	PSU	C6-C5	11.36	1.47	1.35
37	2	1413	PSU	C6-C5	11.27	1.47	1.35
42	1	1011	PSU	C6-C5	11.16	1.47	1.35
42	1	870	PSU	C6-C5	11.05	1.47	1.35
29	S1	1995	G7M	C8-N7	10.91	1.51	1.33
42	1	940	PSU	C6-C5	10.69	1.47	1.35
37	2	512	PSU	C2-N1	10.06	1.49	1.36
37	2	510	PSU	C2-N1	10.05	1.49	1.36
29	S1	1566	PSU	C2-N1	10.01	1.49	1.36
29	S1	104	PSU	C2-N1	9.98	1.49	1.36
42	1	1011	PSU	C2-N1	9.94	1.49	1.36
29	S1	455	PSU	C2-N1	9.92	1.49	1.36
37	2	1361	PSU	C2-N1	9.83	1.49	1.36
29	S1	12	PSU	C2-N1	9.82	1.49	1.36
42	1	1402	PSU	C2-N1	9.73	1.49	1.36
42	1	1171	PSU	C2-N1	9.66	1.49	1.36
29	S1	1543	C4J	C6-C5	9.63	1.48	1.35
42	1	407	A2M	C3'-C4'	-9.39	1.29	1.53
37	2	1382	PSU	C2-N1	9.32	1.48	1.36
37	2	1354	PSU	C2-N1	9.26	1.48	1.36
42	1	697	A2M	C3'-C4'	-9.25	1.29	1.53
42	1	235	A2M	C3'-C4'	-9.25	1.29	1.53
42	1	870	PSU	C2-N1	9.24	1.48	1.36
38	7	43	A2M	C3'-C4'	-9.23	1.29	1.53
37	2	437	PSU	C2-N1	9.20	1.48	1.36
42	1	305	A2M	C3'-C4'	-9.19	1.29	1.53
37	2	628	A2M	C3'-C4'	-9.18	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	604	A2M	C3'-C4'	-9.18	1.29	1.53
42	1	858	A2M	C3'-C4'	-9.16	1.29	1.53
37	2	382	A2M	C3'-C4'	-9.13	1.29	1.53
42	1	955	A2M	C3'-C4'	-9.12	1.29	1.53
37	2	1384	A2M	C3'-C4'	-9.11	1.29	1.53
37	2	95	A2M	C3'-C4'	-9.10	1.29	1.53
42	1	1539	A2M	C3'-C4'	-9.08	1.30	1.53
42	1	927	A2M	C3'-C4'	-9.07	1.30	1.53
37	2	1194	PSU	C2-N1	9.07	1.48	1.36
37	2	572	A2M	C3'-C4'	-9.05	1.30	1.53
29	S1	1544	5MC	C6-C5	9.03	1.49	1.34
37	2	1185	A2M	C3'-C4'	-9.02	1.30	1.53
37	2	1372	A2M	C3'-C4'	-9.00	1.30	1.53
42	1	678	A2M	C3'-C4'	-8.98	1.30	1.53
29	S1	2021	A2M	C3'-C4'	-8.92	1.30	1.53
38	7	162	A2M	C3'-C4'	-8.92	1.30	1.53
29	S1	668	A2M	C3'-C4'	-8.92	1.30	1.53
37	2	1308	5MC	C6-C5	8.87	1.49	1.34
37	2	1308	5MC	C3'-C4'	-8.84	1.30	1.53
37	2	626	PSU	C2-N1	8.83	1.48	1.36
37	2	1318	PSU	C2-N1	8.81	1.48	1.36
42	1	681	A2M	C3'-C4'	-8.78	1.30	1.53
37	2	1413	PSU	C2-N1	8.77	1.48	1.36
37	2	527	A2M	C3'-C4'	-8.72	1.30	1.53
37	2	570	A2M	C3'-C4'	-8.70	1.30	1.53
37	2	662	PSU	C2-N1	8.61	1.47	1.36
42	1	940	PSU	C2-N1	8.60	1.47	1.36
37	2	510	PSU	C2-N3	8.00	1.50	1.37
29	S1	104	PSU	C2-N3	7.84	1.50	1.37
37	2	512	PSU	C2-N3	7.74	1.50	1.37
29	S1	455	PSU	C2-N3	7.73	1.50	1.37
42	1	305	A2M	O4'-C4'	7.70	1.62	1.45
37	2	572	A2M	O4'-C4'	7.65	1.62	1.45
37	2	570	A2M	O4'-C4'	7.64	1.62	1.45
42	1	681	A2M	O4'-C4'	7.60	1.61	1.45
29	S1	12	PSU	C2-N3	7.58	1.50	1.37
29	S1	2021	A2M	O4'-C4'	7.58	1.61	1.45
37	2	1384	A2M	O4'-C4'	7.49	1.61	1.45
37	2	604	A2M	O4'-C4'	7.47	1.61	1.45
38	7	43	A2M	O4'-C4'	7.47	1.61	1.45
29	S1	668	A2M	O4'-C4'	7.46	1.61	1.45
42	1	407	A2M	O4'-C4'	7.46	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	1566	PSU	C2-N3	7.46	1.49	1.37
42	1	955	A2M	O4'-C4'	7.44	1.61	1.45
37	2	1308	5MC	O4'-C4'	7.44	1.61	1.45
42	1	697	A2M	O4'-C4'	7.42	1.61	1.45
37	2	382	A2M	O4'-C4'	7.40	1.61	1.45
37	2	95	A2M	O4'-C4'	7.38	1.61	1.45
37	2	527	A2M	O4'-C4'	7.38	1.61	1.45
37	2	1185	A2M	O4'-C4'	7.37	1.61	1.45
37	2	628	A2M	O4'-C4'	7.35	1.61	1.45
42	1	235	A2M	O4'-C4'	7.35	1.61	1.45
37	2	1372	A2M	O4'-C4'	7.34	1.61	1.45
38	7	162	A2M	O4'-C4'	7.29	1.61	1.45
42	1	1011	PSU	C2-N3	7.24	1.49	1.37
42	1	927	A2M	O4'-C4'	7.23	1.61	1.45
42	1	1371	OMU	C2-N1	7.21	1.49	1.38
41	3	13	OMU	C2-N1	7.21	1.49	1.38
42	1	678	A2M	O4'-C4'	7.18	1.61	1.45
42	1	1539	A2M	O4'-C4'	7.17	1.60	1.45
37	2	1194	PSU	C2-N3	7.11	1.49	1.37
37	2	437	PSU	C2-N3	7.00	1.49	1.37
37	2	1354	PSU	C2-N3	6.99	1.49	1.37
37	2	1361	PSU	C2-N3	6.97	1.48	1.37
42	1	858	A2M	O4'-C4'	6.94	1.60	1.45
29	S1	661	OMU	C2-N1	6.85	1.49	1.38
37	2	1382	PSU	C2-N3	6.85	1.48	1.37
29	S1	8	OMU	C2-N1	6.84	1.49	1.38
37	2	1413	PSU	C2-N3	6.81	1.48	1.37
29	S1	8	OMU	C2-N3	6.75	1.49	1.38
42	1	845	OMU	C2-N1	6.74	1.49	1.38
42	1	870	PSU	C2-N3	6.73	1.48	1.37
37	2	1318	PSU	C2-N3	6.72	1.48	1.37
29	S1	661	OMU	C2-N3	6.71	1.49	1.38
29	S1	1979	OMU	C2-N1	6.69	1.48	1.38
29	S1	1544	5MC	C4-N3	6.69	1.44	1.34
37	2	662	PSU	C2-N3	6.67	1.48	1.37
37	2	560	OMU	C2-N1	6.67	1.48	1.38
37	2	1419	OMU	C2-N1	6.66	1.48	1.38
29	S1	1979	OMU	C2-N3	6.66	1.49	1.38
37	2	1077	OMU	C2-N1	6.62	1.48	1.38
29	S1	1544	5MC	C5-C4	6.59	1.49	1.44
37	2	626	PSU	C2-N3	6.57	1.48	1.37
29	S1	1647	OMG	C4-N3	6.55	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	940	PSU	C2-N3	6.51	1.48	1.37
42	1	1107	OMU	C2-N1	6.50	1.48	1.38
42	1	959[A]	OMG	C4-N3	6.47	1.49	1.34
29	S1	600	OMG	C4-N3	6.47	1.49	1.34
38	7	7	OMU	C2-N3	6.41	1.49	1.38
38	7	7	OMU	C2-N1	6.40	1.48	1.38
37	2	1359	OMU	C2-N1	6.40	1.48	1.38
29	S1	38	OMC	C2-N3	6.37	1.49	1.36
29	S1	1865	OMG	C4-N3	6.36	1.48	1.34
37	2	1046	OMG	C4-N3	6.36	1.48	1.34
42	1	1402	PSU	C2-N3	6.35	1.47	1.37
42	1	1190	OMG	C4-N3	6.35	1.48	1.34
37	2	667	OMU	C2-N1	6.35	1.48	1.38
29	S1	2151	OMG	C4-N3	6.33	1.48	1.34
29	S1	2140	OMC	C2-N3	6.33	1.48	1.36
29	S1	1829	OMG	C4-N3	6.32	1.48	1.34
29	S1	1550	OMG	C4-N3	6.32	1.48	1.34
37	2	1077	OMU	C2-N3	6.30	1.48	1.38
29	S1	1879	OMG	C4-N3	6.29	1.48	1.34
37	2	1152	OMU	C2-N3	6.27	1.48	1.38
42	1	1107	OMU	C2-N3	6.26	1.48	1.38
37	2	1152	OMU	C2-N1	6.26	1.48	1.38
42	1	1659	OMU	C2-N1	6.24	1.48	1.38
42	1	959[B]	OMG	C4-N3	6.24	1.48	1.34
42	1	847	OMU	C2-N1	6.24	1.48	1.38
29	S1	1995	G7M	C2-N3	6.23	1.48	1.33
29	S1	18	OMC	C2-N3	6.23	1.48	1.36
29	S1	1544	5MC	C2-N3	6.22	1.48	1.36
29	S1	1478	OMG	C4-N3	6.21	1.48	1.34
37	2	560	OMU	C2-N3	6.19	1.48	1.38
37	2	1359	OMU	C2-N3	6.18	1.48	1.38
37	2	1360	OMG	C4-N3	6.17	1.48	1.34
29	S1	1543	C4J	C2-N3	6.16	1.49	1.38
42	1	1010	OMC	C2-N3	6.16	1.48	1.36
42	1	1371	OMU	C2-N3	6.15	1.48	1.38
37	2	534	OMG	C4-N3	6.15	1.48	1.34
42	1	1659	OMU	C2-N3	6.13	1.48	1.38
37	2	1419	OMU	C2-N3	6.12	1.48	1.38
41	3	13	OMU	C2-N3	6.09	1.48	1.38
37	2	359	OMC	C2-N3	6.08	1.48	1.36
29	S1	1866	OMC	C2-N3	6.06	1.48	1.36
37	2	1078	OMG	C4-N3	6.04	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	1231	OMG	C4-N3	6.04	1.48	1.34
42	1	847	OMU	C2-N3	6.02	1.48	1.38
37	2	655	OMG	C4-N3	6.01	1.48	1.34
37	2	1229	OMG	C4-N3	6.00	1.48	1.34
42	1	1171	PSU	C2-N3	6.00	1.47	1.37
29	S1	1995	G7M	C8-N9	5.98	1.51	1.35
37	2	1253	OMG	C4-N3	5.94	1.47	1.34
37	2	1308	5MC	C4-N3	5.93	1.43	1.34
42	1	856	OMG	C4-N3	5.93	1.47	1.34
42	1	1626	OMG	C4-N3	5.91	1.47	1.34
42	1	1540	OMG	C4-N3	5.89	1.47	1.34
37	2	667	OMU	C2-N3	5.89	1.48	1.38
37	2	443	OMC	C2-N3	5.88	1.48	1.36
29	S1	38	OMC	C6-C5	5.87	1.48	1.35
29	S1	2140	OMC	C6-C5	5.86	1.48	1.35
40	4	74	OMG	C4-N3	5.86	1.47	1.34
37	2	1248	OMC	C6-C5	5.85	1.48	1.35
29	S1	18	OMC	C6-C5	5.84	1.48	1.35
42	1	1524	OMG	C4-N3	5.84	1.47	1.34
37	2	1159	OMC	C2-N3	5.81	1.47	1.36
37	2	443	OMC	C6-C5	5.80	1.48	1.35
37	2	641	OMG	C4-N3	5.78	1.47	1.34
29	S1	1866	OMC	C6-C5	5.77	1.48	1.35
37	2	1308	5MC	C2-N3	5.75	1.47	1.36
42	1	1010	OMC	C6-C5	5.72	1.48	1.35
37	2	1397	OMC	C2-N3	5.71	1.47	1.36
42	1	845	OMU	C2-N3	5.69	1.47	1.38
37	2	1317	OMC	C2-N3	5.66	1.47	1.36
29	S1	661	OMU	C6-C5	5.65	1.48	1.35
37	2	583	OMC	C2-N3	5.63	1.47	1.36
29	S1	1995	G7M	C5-N7	5.62	1.45	1.39
29	S1	8	OMU	C6-C5	5.60	1.48	1.35
37	2	359	OMC	C6-C5	5.59	1.48	1.35
37	2	527	A2M	O4'-C1'	-5.57	1.29	1.42
29	S1	1979	OMU	C6-C5	5.55	1.47	1.35
37	2	1248	OMC	C2-N3	5.54	1.47	1.36
37	2	510	PSU	C6-N1	5.54	1.45	1.36
37	2	1317	OMC	C6-C5	5.51	1.47	1.35
37	2	1077	OMU	C6-C5	5.49	1.47	1.35
29	S1	1995	G7M	C4-N3	5.49	1.46	1.34
37	2	583	OMC	C6-C5	5.47	1.47	1.35
37	2	1159	OMC	C6-C5	5.44	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	695	OMC	C2-N3	5.40	1.47	1.36
42	1	1107	OMU	C6-C5	5.39	1.47	1.35
38	7	7	OMU	C6-C5	5.36	1.47	1.35
37	2	512	PSU	C6-N1	5.35	1.45	1.36
42	1	1371	OMU	C6-C5	5.32	1.47	1.35
29	S1	104	PSU	C6-N1	5.29	1.45	1.36
37	2	1397	OMC	C6-C5	5.29	1.47	1.35
37	2	1152	OMU	C6-C5	5.29	1.47	1.35
37	2	560	OMU	C6-C5	5.28	1.47	1.35
29	S1	600	OMG	C2-N3	5.28	1.46	1.33
37	2	570	A2M	O4'-C1'	-5.26	1.29	1.42
37	2	1359	OMU	C6-C5	5.26	1.47	1.35
29	S1	1566	PSU	C6-N1	5.26	1.44	1.36
29	S1	455	PSU	C6-N1	5.26	1.44	1.36
42	1	858	A2M	O4'-C1'	-5.25	1.29	1.42
42	1	695	OMC	C6-C5	5.25	1.47	1.35
29	S1	12	PSU	C6-N1	5.22	1.44	1.36
37	2	667	OMU	C6-C5	5.21	1.47	1.35
29	S1	1647	OMG	C2-N3	5.21	1.45	1.33
29	S1	2140	OMC	C4-N3	5.19	1.44	1.34
42	1	847	OMU	C6-C5	5.18	1.47	1.35
42	1	959[A]	OMG	C2-N3	5.17	1.45	1.33
29	S1	1550	OMG	C2-N3	5.15	1.45	1.33
37	2	1361	PSU	C6-N1	5.14	1.44	1.36
29	S1	1829	OMG	C2-N3	5.13	1.45	1.33
42	1	1659	OMU	C6-C5	5.12	1.46	1.35
29	S1	2151	OMG	C2-N3	5.11	1.45	1.33
29	S1	38	OMC	C4-N3	5.09	1.44	1.34
37	2	1372	A2M	O4'-C1'	-5.08	1.30	1.42
37	2	382	A2M	O4'-C1'	-5.08	1.30	1.42
37	2	1419	OMU	C6-C5	5.08	1.46	1.35
42	1	1539	A2M	O4'-C1'	-5.06	1.30	1.42
42	1	927	A2M	O4'-C1'	-5.04	1.30	1.42
37	2	1046	OMG	C2-N3	5.03	1.45	1.33
42	1	235	A2M	O4'-C1'	-5.02	1.30	1.42
42	1	1011	PSU	C6-N1	5.01	1.44	1.36
41	3	13	OMU	C6-C5	5.00	1.46	1.35
29	S1	1879	OMG	C2-N3	5.00	1.45	1.33
37	2	1308	5MC	O4'-C1'	-4.99	1.30	1.42
29	S1	668	A2M	O4'-C1'	-4.97	1.30	1.42
37	2	1194	PSU	C6-N1	4.97	1.44	1.36
29	S1	1478	OMG	C2-N3	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	697	A2M	O4'-C1'	-4.96	1.30	1.42
29	S1	1865	OMG	C2-N3	4.96	1.45	1.33
42	1	1402	PSU	C6-N1	4.96	1.44	1.36
29	S1	18	OMC	C4-N3	4.96	1.44	1.34
37	2	604	A2M	O4'-C1'	-4.95	1.30	1.42
42	1	1190	OMG	C2-N3	4.94	1.45	1.33
42	1	305	A2M	O4'-C1'	-4.94	1.30	1.42
42	1	955	A2M	O4'-C1'	-4.94	1.30	1.42
38	7	162	A2M	O4'-C1'	-4.94	1.30	1.42
38	7	43	A2M	O4'-C1'	-4.94	1.30	1.42
37	2	95	A2M	O4'-C1'	-4.93	1.30	1.42
37	2	1384	A2M	O4'-C1'	-4.93	1.30	1.42
29	S1	2021	A2M	O4'-C1'	-4.92	1.30	1.42
29	S1	2061	5MC	C5-C4	4.90	1.47	1.44
37	2	1185	A2M	O4'-C1'	-4.90	1.30	1.42
37	2	1360	OMG	C2-N3	4.88	1.45	1.33
37	2	572	A2M	O4'-C1'	-4.88	1.30	1.42
42	1	1010	OMC	C4-N3	4.86	1.44	1.34
37	2	1354	PSU	C6-N1	4.84	1.44	1.36
42	1	959[B]	OMG	C2-N3	4.83	1.44	1.33
42	1	681	A2M	O4'-C1'	-4.83	1.30	1.42
29	S1	1550	OMG	C2-N2	4.82	1.45	1.34
42	1	1011	PSU	C1'-C5	-4.82	1.39	1.50
42	1	1171	PSU	C6-N1	4.82	1.44	1.36
37	2	437	PSU	C6-N1	4.81	1.44	1.36
37	2	628	A2M	O4'-C1'	-4.80	1.30	1.42
37	2	1354	PSU	C1'-C5	-4.80	1.39	1.50
42	1	678	A2M	O4'-C1'	-4.79	1.30	1.42
37	2	1382	PSU	C6-N1	4.79	1.44	1.36
29	S1	1866	OMC	C4-N3	4.79	1.44	1.34
37	2	1308	5MC	C5-C4	4.79	1.47	1.44
37	2	359	OMC	C4-N3	4.77	1.44	1.34
42	1	870	PSU	C1'-C5	-4.77	1.39	1.50
29	S1	1829	OMG	C2-N2	4.71	1.45	1.34
42	1	940	PSU	C1'-C5	-4.71	1.39	1.50
29	S1	600	OMG	C2-N2	4.69	1.45	1.34
42	1	1524	OMG	C2-N3	4.69	1.44	1.33
42	1	407	A2M	O4'-C1'	-4.69	1.31	1.42
29	S1	1647	OMG	C2-N2	4.69	1.45	1.34
29	S1	2140	OMC	C4-N4	4.68	1.45	1.33
37	2	626	PSU	C6-N1	4.67	1.43	1.36
29	S1	38	OMC	C4-N4	4.66	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	1229	OMG	C2-N3	4.66	1.44	1.33
37	2	443	OMC	C4-N3	4.63	1.43	1.34
29	S1	1865	OMG	C2-N2	4.63	1.45	1.34
37	2	1318	PSU	C6-N1	4.63	1.43	1.36
37	2	534	OMG	C2-N3	4.63	1.44	1.33
42	1	845	OMU	C6-C5	4.61	1.45	1.35
37	2	1046	OMG	C2-N2	4.61	1.45	1.34
29	S1	12	PSU	C1'-C5	-4.60	1.39	1.50
29	S1	18	OMC	C4-N4	4.59	1.45	1.33
42	1	870	PSU	C6-N1	4.59	1.43	1.36
42	1	1190	OMG	C2-N2	4.58	1.44	1.34
29	S1	1879	OMG	C2-N2	4.57	1.44	1.34
29	S1	1478	OMG	C2-N2	4.56	1.44	1.34
42	1	1171	PSU	C1'-C5	-4.56	1.40	1.50
29	S1	2151	OMG	C2-N2	4.55	1.44	1.34
42	1	959[A]	OMG	C2-N2	4.54	1.44	1.34
37	2	437	PSU	C1'-C5	-4.54	1.40	1.50
37	2	1231	OMG	C2-N3	4.54	1.44	1.33
37	2	359	OMC	C4-N4	4.54	1.44	1.33
37	2	1382	PSU	C1'-C5	-4.53	1.40	1.50
37	2	1360	OMG	C2-N2	4.51	1.44	1.34
37	2	1194	PSU	C1'-C5	-4.49	1.40	1.50
37	2	1413	PSU	C6-N1	4.48	1.43	1.36
42	1	1524	OMG	C2-N2	4.47	1.44	1.34
37	2	655	OMG	C2-N3	4.47	1.44	1.33
37	2	1229	OMG	C2-N2	4.47	1.44	1.34
37	2	662	PSU	C6-N1	4.45	1.43	1.36
37	2	662	PSU	C1'-C5	-4.45	1.40	1.50
37	2	1253	OMG	C2-N3	4.45	1.44	1.33
37	2	1231	OMG	C2-N2	4.44	1.44	1.34
29	S1	512	A2M	C5-C4	4.44	1.47	1.39
29	S1	2140	OMC	C2-N1	4.44	1.49	1.40
37	2	1078	OMG	C2-N2	4.43	1.44	1.34
37	2	1318	PSU	C1'-C5	-4.41	1.40	1.50
37	2	1361	PSU	C1'-C5	-4.41	1.40	1.50
29	S1	1866	OMC	C4-N4	4.41	1.44	1.33
37	2	1078	OMG	C2-N3	4.40	1.43	1.33
37	2	1159	OMC	C4-N3	4.40	1.43	1.34
42	1	959[B]	OMG	C2-N2	4.39	1.44	1.34
37	2	1413	PSU	C1'-C5	-4.39	1.40	1.50
42	1	856	OMG	C2-N2	4.38	1.44	1.34
42	1	1540	OMG	C2-N2	4.37	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	104	PSU	C1'-C5	-4.36	1.40	1.50
29	S1	1544	5MC	C6-N1	4.36	1.45	1.38
29	S1	38	OMC	C2-N1	4.35	1.49	1.40
37	2	443	OMC	C4-N4	4.34	1.44	1.33
37	2	626	PSU	C1'-C5	-4.34	1.40	1.50
37	2	583	OMC	C4-N3	4.34	1.43	1.34
37	2	1317	OMC	C4-N3	4.32	1.43	1.34
29	S1	18	OMC	C2-N1	4.31	1.49	1.40
40	4	74	OMG	C2-N3	4.30	1.43	1.33
29	S1	1544	5MC	C4-N4	4.30	1.45	1.34
42	1	1010	OMC	C4-N4	4.28	1.44	1.33
37	2	1159	OMC	C4-N4	4.27	1.44	1.33
37	2	1253	OMG	C2-N2	4.26	1.44	1.34
29	S1	455	PSU	C1'-C5	-4.25	1.40	1.50
29	S1	668	A2M	C6-N6	4.25	1.45	1.34
37	2	534	OMG	C2-N2	4.25	1.44	1.34
40	4	74	OMG	C2-N2	4.24	1.44	1.34
37	2	1248	OMC	C4-N3	4.24	1.42	1.34
42	1	856	OMG	C2-N3	4.24	1.43	1.33
37	2	1397	OMC	C4-N3	4.23	1.42	1.34
37	2	641	OMG	C2-N2	4.23	1.44	1.34
42	1	940	PSU	C6-N1	4.22	1.43	1.36
42	1	858	A2M	C6-N6	4.22	1.45	1.34
37	2	591	A2M	C5-C4	4.21	1.46	1.39
42	1	235	A2M	C6-N6	4.21	1.45	1.34
37	2	1248	OMC	C4-N4	4.21	1.44	1.33
37	2	583	OMC	C4-N4	4.20	1.44	1.33
29	S1	2021	A2M	C6-N6	4.19	1.44	1.34
37	2	655	OMG	C2-N2	4.19	1.44	1.34
37	2	512	PSU	C1'-C5	-4.19	1.40	1.50
37	2	1372	A2M	C6-N6	4.17	1.44	1.34
42	1	1540	OMG	C2-N3	4.14	1.43	1.33
37	2	1308	5MC	C4-N4	4.14	1.44	1.34
37	2	1397	OMC	C4-N4	4.14	1.43	1.33
42	1	695	OMC	C4-N3	4.14	1.42	1.34
42	1	1402	PSU	C1'-C5	-4.13	1.40	1.50
37	2	641	OMG	C2-N3	4.13	1.43	1.33
37	2	1308	5MC	C6-N1	4.12	1.45	1.38
42	1	1626	OMG	C2-N3	4.12	1.43	1.33
37	2	95	A2M	C6-N6	4.11	1.44	1.34
29	S1	1566	PSU	C1'-C5	-4.11	1.41	1.50
37	2	443	OMC	C2-N1	4.11	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	695	OMC	C4-N4	4.10	1.43	1.33
37	2	604	A2M	C6-N6	4.09	1.44	1.34
42	1	697	A2M	C5-C4	-4.09	1.31	1.39
37	2	527	A2M	C5-C4	-4.08	1.31	1.39
37	2	628	A2M	C5-C4	-4.08	1.31	1.39
37	2	1317	OMC	C4-N4	4.07	1.43	1.33
29	S1	1543	C4J	C6-N1	4.07	1.46	1.36
29	S1	661	OMU	C4-N3	4.06	1.45	1.38
37	2	1185	A2M	C6-N6	4.05	1.44	1.34
37	2	510	PSU	C4-N3	4.04	1.46	1.38
37	2	359	OMC	C2-N1	4.04	1.48	1.40
42	1	678	A2M	C6-N6	4.03	1.44	1.34
37	2	1248	OMC	C2-N1	4.03	1.48	1.40
42	1	1010	OMC	C2-N1	4.01	1.48	1.40
29	S1	1979	OMU	C4-N3	4.01	1.45	1.38
37	2	527	A2M	C6-N6	4.01	1.44	1.34
37	2	570	A2M	C6-N6	4.01	1.44	1.34
42	1	1626	OMG	C2-N2	4.00	1.43	1.34
37	2	1317	OMC	C2-N1	4.00	1.48	1.40
42	1	305	A2M	C6-N6	3.99	1.44	1.34
38	7	162	A2M	C6-N6	3.98	1.44	1.34
29	S1	1544	5MC	C2-N1	3.98	1.48	1.40
37	2	1384	A2M	C6-N6	3.98	1.44	1.34
29	S1	8	OMU	C4-N3	3.98	1.45	1.38
29	S1	104	PSU	C4-N3	3.93	1.46	1.38
42	1	845	OMU	O2-C2	-3.92	1.16	1.23
37	2	628	A2M	C6-N6	3.92	1.44	1.34
42	1	927	A2M	C5-C4	-3.92	1.32	1.39
42	1	681	A2M	C6-N6	3.91	1.44	1.34
42	1	927	A2M	C6-N6	3.91	1.44	1.34
42	1	407	A2M	C5-C4	-3.90	1.32	1.39
37	2	382	A2M	C5-C4	-3.90	1.32	1.39
42	1	955	A2M	C5-C4	-3.89	1.32	1.39
37	2	1159	OMC	C2-N1	3.89	1.48	1.40
42	1	1539	A2M	C5-C4	-3.89	1.32	1.39
29	S1	1866	OMC	C2-N1	3.89	1.48	1.40
37	2	572	A2M	C6-N6	3.88	1.44	1.34
42	1	955	A2M	C6-N6	3.88	1.44	1.34
38	7	43	A2M	C6-N6	3.87	1.44	1.34
37	2	572	A2M	C5-C4	-3.85	1.32	1.39
42	1	697	A2M	C6-N6	3.84	1.44	1.34
42	1	407	A2M	C6-N6	3.84	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	1308	5MC	C2-N1	3.83	1.48	1.40
42	1	1539	A2M	C6-N6	3.83	1.44	1.34
42	1	1171	PSU	O4-C4	-3.82	1.16	1.23
37	2	382	A2M	C6-N6	3.82	1.44	1.34
38	7	43	A2M	C5-C4	-3.82	1.32	1.39
37	2	1384	A2M	C5-C4	-3.81	1.32	1.39
37	2	510	PSU	C1'-C5	-3.81	1.41	1.50
42	1	695	OMC	C2-N1	3.80	1.48	1.40
29	S1	455	PSU	C4-N3	3.78	1.45	1.38
37	2	512	PSU	C4-N3	3.76	1.45	1.38
29	S1	12	PSU	C4-N3	3.75	1.45	1.38
38	7	162	A2M	C5-C4	-3.74	1.32	1.39
41	3	13	OMU	O4-C4	-3.74	1.17	1.24
29	S1	1566	PSU	C4-N3	3.71	1.45	1.38
37	2	1359	OMU	C4-N3	3.70	1.45	1.38
37	2	1372	A2M	C5-C4	-3.70	1.32	1.39
38	7	7	OMU	C4-N3	3.70	1.44	1.38
37	2	583	OMC	C2-N1	3.68	1.47	1.40
37	2	570	A2M	C5-C4	-3.68	1.32	1.39
37	2	570	A2M	C8-N9	-3.65	1.31	1.37
42	1	681	A2M	C5-C4	-3.64	1.32	1.39
42	1	845	OMU	O4-C4	-3.64	1.17	1.24
37	2	1397	OMC	C2-N1	3.64	1.47	1.40
42	1	1107	OMU	C4-N3	3.62	1.44	1.38
42	1	695	OMC	O2-C2	-3.60	1.17	1.23
37	2	1077	OMU	C4-N3	3.60	1.44	1.38
42	1	697	A2M	C8-N9	-3.59	1.31	1.37
37	2	95	A2M	C5-C4	-3.54	1.32	1.39
42	1	678	A2M	C5-C4	-3.52	1.32	1.39
37	2	667	OMU	O4-C4	-3.51	1.17	1.24
42	1	940	PSU	O4-C4	-3.51	1.16	1.23
42	1	1659	OMU	C4-N3	3.49	1.44	1.38
42	1	847	OMU	C4-N3	3.49	1.44	1.38
37	2	1185	A2M	C5-C4	-3.48	1.32	1.39
42	1	1371	OMU	O4-C4	-3.48	1.17	1.24
37	2	1419	OMU	C4-N3	3.47	1.44	1.38
42	1	847	OMU	O4-C4	-3.47	1.17	1.24
42	1	858	A2M	C5-C4	-3.47	1.32	1.39
38	7	7	OMU	O4-C4	-3.47	1.17	1.24
37	2	604	A2M	C5-C4	-3.45	1.32	1.39
42	1	1011	PSU	C4-N3	3.45	1.45	1.38
37	2	1152	OMU	C4-N3	3.45	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	583	OMC	O2-C2	-3.44	1.17	1.23
37	2	1317	OMC	O2-C2	-3.44	1.17	1.23
42	1	235	A2M	C5-C4	-3.44	1.33	1.39
42	1	955	A2M	C8-N9	-3.43	1.31	1.37
29	S1	2021	A2M	C5-C4	-3.43	1.33	1.39
29	S1	1995	G7M	C2-N1	3.43	1.46	1.37
37	2	560	OMU	C4-N3	3.42	1.44	1.38
37	2	1359	OMU	O4-C4	-3.42	1.17	1.24
37	2	1361	PSU	O4-C4	-3.41	1.17	1.23
29	S1	1995	G7M	C6-N1	3.40	1.45	1.38
37	2	382	A2M	C8-N9	-3.39	1.31	1.37
42	1	927	A2M	C8-N9	-3.38	1.31	1.37
42	1	959[B]	OMG	C5-N7	-3.38	1.32	1.39
37	2	95	A2M	C8-N9	-3.38	1.31	1.37
42	1	1659	OMU	O4-C4	-3.38	1.17	1.24
42	1	856	OMG	O6-C6	-3.36	1.17	1.23
42	1	1539	A2M	C5-N7	-3.36	1.33	1.39
42	1	1539	A2M	C8-N9	-3.34	1.31	1.37
37	2	1185	A2M	C8-N9	-3.33	1.31	1.37
37	2	534	OMG	C5-N7	-3.33	1.32	1.39
42	1	1107	OMU	O4-C4	-3.33	1.18	1.24
37	2	1382	PSU	O4-C4	-3.33	1.17	1.23
42	1	407	A2M	C8-N9	-3.32	1.31	1.37
37	2	1248	OMC	O2-C2	-3.32	1.17	1.23
42	1	678	A2M	C8-N9	-3.32	1.31	1.37
37	2	570	A2M	C5-N7	-3.32	1.33	1.39
37	2	1318	PSU	O4-C4	-3.31	1.17	1.23
37	2	1360	OMG	C5-N7	-3.31	1.32	1.39
37	2	1413	PSU	O4-C4	-3.31	1.17	1.23
37	2	662	PSU	O4-C4	-3.30	1.17	1.23
37	2	641	OMG	C5-N7	-3.30	1.32	1.39
29	S1	1156	PSU	C6-C5	3.30	1.38	1.35
42	1	1540	OMG	C4-N9	-3.30	1.29	1.38
37	2	1372	A2M	C8-N9	-3.30	1.31	1.37
37	2	1303	PSU	C6-C5	3.30	1.38	1.35
37	2	1152	OMU	O4-C4	-3.29	1.18	1.24
37	2	1397	OMC	O2-C2	-3.28	1.17	1.23
42	1	870	PSU	O4-C4	-3.28	1.17	1.23
37	2	641	OMG	C4-N9	-3.27	1.29	1.38
37	2	593	PSU	C4-N3	-3.27	1.32	1.38
37	2	527	A2M	C8-N9	-3.27	1.32	1.37
37	2	1361	PSU	C4-N3	3.26	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	1419	OMU	O4-C4	-3.26	1.18	1.24
42	1	1402	PSU	O4-C4	-3.25	1.17	1.23
29	S1	1543	C4J	C4-N3	3.25	1.45	1.40
37	2	1194	PSU	C4-N3	3.25	1.44	1.38
29	S1	1995	G7M	C2-N2	3.25	1.41	1.34
37	2	641	OMG	O6-C6	-3.24	1.17	1.23
29	S1	1995	G7M	C4-N9	3.24	1.46	1.38
42	1	856	OMG	C4-N9	-3.23	1.29	1.38
38	7	43	A2M	C8-N9	-3.22	1.32	1.37
42	1	927	A2M	O2'-C2'	-3.21	1.34	1.42
37	2	527	A2M	C5-N7	-3.21	1.33	1.39
37	2	655	OMG	O6-C6	-3.21	1.17	1.23
42	1	697	A2M	C5-N7	-3.20	1.33	1.39
42	1	1664	PSU	C6-C5	3.20	1.38	1.35
37	2	628	A2M	C8-N9	-3.20	1.32	1.37
37	2	443	OMC	O2-C2	-3.18	1.17	1.23
40	4	74	OMG	C5-N7	-3.18	1.32	1.39
42	1	1371	OMU	C4-N3	3.18	1.44	1.38
29	S1	607	PSU	C6-C5	3.17	1.38	1.35
42	1	1626	OMG	O6-C6	-3.17	1.17	1.23
37	2	560	OMU	O4-C4	-3.17	1.18	1.24
42	1	1524	OMG	C5-N7	-3.17	1.32	1.39
37	2	604	A2M	C8-N9	-3.17	1.32	1.37
29	S1	1995	G7M	O6-C6	-3.16	1.17	1.23
37	2	628	A2M	O2'-C2'	-3.16	1.34	1.42
41	3	13	OMU	O2-C2	-3.15	1.17	1.23
42	1	305	A2M	O2'-C2'	-3.15	1.34	1.42
37	2	95	A2M	C5-N7	-3.15	1.33	1.39
42	1	1659	OMU	O2-C2	-3.15	1.17	1.23
42	1	1017	PSU	C4-N3	-3.15	1.33	1.38
37	2	572	A2M	C8-N9	-3.15	1.32	1.37
37	2	1185	A2M	C5-N7	-3.15	1.33	1.39
42	1	955	A2M	C5-N7	-3.14	1.33	1.39
37	2	437	PSU	O4-C4	-3.14	1.17	1.23
42	1	697	A2M	O2'-C2'	-3.14	1.34	1.42
42	1	1540	OMG	O6-C6	-3.14	1.17	1.23
29	S1	1979	OMU	O4-C4	-3.14	1.18	1.24
42	1	305	A2M	C5-N7	-3.14	1.33	1.39
37	2	73	OMU	C4-N3	-3.14	1.33	1.38
37	2	1354	PSU	C4-N3	3.14	1.44	1.38
37	2	1264	PSU	C6-C5	3.13	1.38	1.35
37	2	1077	OMU	O4-C4	-3.13	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	609	PSU	C6-C5	3.13	1.38	1.35
29	S1	661	OMU	O4-C4	-3.13	1.18	1.24
37	2	1308	5MC	O2-C2	-3.13	1.17	1.23
37	2	1253	OMG	O6-C6	-3.13	1.17	1.23
42	1	1539	A2M	O2'-C2'	-3.13	1.35	1.42
42	1	407	A2M	O2'-C2'	-3.12	1.35	1.42
29	S1	1865	OMG	C5-N7	-3.12	1.32	1.39
37	2	1194	PSU	O4-C4	-3.12	1.17	1.23
37	2	626	PSU	C4-N3	3.12	1.44	1.38
29	S1	38	OMC	C6-N1	3.12	1.45	1.38
29	S1	1543	C4J	C2-N1	3.12	1.48	1.39
42	1	1626	OMG	C4-N9	-3.12	1.30	1.38
29	S1	1539	PSU	C6-C5	3.12	1.38	1.35
37	2	1152	OMU	O2-C2	-3.11	1.17	1.23
37	2	667	OMU	O2-C2	-3.11	1.17	1.23
29	S1	668	A2M	C5-C4	-3.11	1.33	1.39
42	1	681	A2M	C8-N9	-3.10	1.32	1.37
37	2	1185	A2M	O2'-C2'	-3.10	1.35	1.42
37	2	1253	OMG	C5-N7	-3.10	1.32	1.39
42	1	1010	OMC	C6-N1	3.10	1.45	1.38
38	7	162	A2M	C8-N9	-3.10	1.32	1.37
29	S1	8	OMU	O4-C4	-3.09	1.18	1.24
42	1	847	OMU	O2-C2	-3.09	1.17	1.23
42	1	422	PSU	C4-N3	-3.09	1.33	1.38
37	2	359	OMC	O2-C2	-3.09	1.18	1.23
42	1	1010	OMC	O2-C2	-3.09	1.18	1.23
42	1	422	PSU	C6-C5	3.09	1.38	1.35
42	1	927	A2M	C5-N7	-3.09	1.33	1.39
42	1	235	A2M	C8-N9	-3.08	1.32	1.37
37	2	382	A2M	C5-N7	-3.08	1.33	1.39
37	2	655	OMG	C5-N7	-3.08	1.32	1.39
37	2	1354	PSU	O4-C4	-3.08	1.17	1.23
40	4	74	OMG	C4-N9	-3.08	1.30	1.38
29	S1	1995	G7M	C5-C6	3.08	1.51	1.43
37	2	1159	OMC	O2-C2	-3.08	1.18	1.23
37	2	1060	PSU	C4-N3	-3.08	1.33	1.38
37	2	1058	PSU	C6-C5	3.08	1.38	1.35
42	1	678	A2M	C5-N7	-3.08	1.33	1.39
42	1	1533	PSU	C4-N3	-3.07	1.33	1.38
37	2	570	A2M	O3'-C3'	3.07	1.50	1.43
37	2	667	OMU	C4-N3	3.07	1.43	1.38
29	S1	1543	C4J	O4-C4	-3.07	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	2151	OMG	C5-N7	-3.07	1.32	1.39
37	2	597	PSU	C4-N3	-3.07	1.33	1.38
42	1	681	A2M	C5-N7	-3.06	1.33	1.39
29	S1	1533	PSU	C6-C5	3.06	1.38	1.35
37	2	1359	OMU	O2-C2	-3.06	1.17	1.23
42	1	678	A2M	O2'-C2'	-3.05	1.35	1.42
42	1	1181	PSU	C6-C5	3.05	1.38	1.35
29	S1	18	OMC	C6-N1	3.05	1.45	1.38
42	1	672	PSU	C4-N3	-3.05	1.33	1.38
42	1	1528	PSU	C4-N3	-3.04	1.33	1.38
37	2	1403	PSU	C4-N3	-3.04	1.33	1.38
37	2	78	PSU	C4-N3	-3.04	1.33	1.38
29	S1	1192	PSU	C6-C5	3.04	1.38	1.35
40	4	74	OMG	O6-C6	-3.03	1.17	1.23
37	2	1384	A2M	C8-N9	-3.03	1.32	1.37
29	S1	2140	OMC	C6-N1	3.03	1.45	1.38
29	S1	2046	PSU	C6-C5	3.03	1.38	1.35
42	1	235	A2M	C5-N7	-3.03	1.33	1.39
42	1	407	A2M	C5-N7	-3.02	1.33	1.39
37	2	572	A2M	O2'-C2'	-3.02	1.35	1.42
37	2	604	A2M	C5-N7	-3.02	1.33	1.39
37	2	78	PSU	C6-C5	3.02	1.38	1.35
29	S1	33	PSU	C6-C5	3.02	1.38	1.35
37	2	1413	PSU	C4-N3	3.02	1.44	1.38
37	2	382	A2M	O2'-C2'	-3.02	1.35	1.42
37	2	1308	5MC	O2'-C2'	-3.01	1.35	1.43
42	1	1664	PSU	C4-N3	-3.01	1.33	1.38
37	2	1384	A2M	C5-N7	-3.01	1.33	1.39
37	2	626	PSU	O4-C4	-3.01	1.17	1.23
29	S1	1866	OMC	O2-C2	-3.01	1.18	1.23
37	2	1229	OMG	O6-C6	-3.01	1.17	1.23
37	2	1231	OMG	O6-C6	-3.01	1.17	1.23
42	1	235	A2M	O2'-C2'	-3.01	1.35	1.42
37	2	1229	OMG	C5-N7	-3.00	1.33	1.39
42	1	959[A]	OMG	C5-N7	-3.00	1.33	1.39
29	S1	1829	OMG	C5-N7	-3.00	1.33	1.39
42	1	1540	OMG	C5-N7	-3.00	1.33	1.39
37	2	359	OMC	C6-N1	3.00	1.45	1.38
29	S1	2048	PSU	C4-N3	-3.00	1.33	1.38
37	2	1231	OMG	C5-N7	-3.00	1.33	1.39
29	S1	1478	OMG	C5-N7	-3.00	1.33	1.39
38	7	69	PSU	C6-C5	2.99	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	437	PSU	C4-N3	2.99	1.44	1.38
42	1	1626	OMG	C5-N7	-2.99	1.33	1.39
38	7	43	A2M	O2'-C2'	-2.99	1.35	1.42
37	2	534	OMG	O6-C6	-2.99	1.17	1.23
29	S1	2046	PSU	C4-N3	-2.98	1.33	1.38
29	S1	668	A2M	O3'-C3'	2.98	1.50	1.43
38	7	74	PSU	C4-N3	-2.98	1.33	1.38
29	S1	1841	PSU	C4-N3	-2.98	1.33	1.38
37	2	1384	A2M	O2'-C2'	-2.97	1.35	1.42
42	1	1190	OMG	C5-N7	-2.97	1.33	1.39
29	S1	1866	OMC	C6-N1	2.97	1.45	1.38
29	S1	1879	OMG	C5-N7	-2.97	1.33	1.39
37	2	443	OMC	C6-N1	2.96	1.45	1.38
37	2	472	PSU	C4-N3	-2.96	1.33	1.38
38	7	75	OMG	C5-C4	2.96	1.46	1.38
37	2	1419	OMU	O2-C2	-2.96	1.17	1.23
37	2	1144	PSU	C4-N3	-2.96	1.33	1.38
29	S1	1539	PSU	C4-N3	-2.96	1.33	1.38
38	7	69	PSU	C4-N3	-2.95	1.33	1.38
37	2	1264	PSU	C4-N3	-2.95	1.33	1.38
42	1	239	PSU	C4-N3	-2.95	1.33	1.38
42	1	239	PSU	C6-C5	2.95	1.38	1.35
37	2	71	OMG	C6-N1	-2.95	1.33	1.38
42	1	1528	PSU	C6-C5	2.95	1.38	1.35
42	1	681	A2M	O2'-C2'	-2.94	1.35	1.42
37	2	1360	OMG	O6-C6	-2.94	1.18	1.23
29	S1	1623	OMG	C5-C4	2.94	1.46	1.38
29	S1	1246	PSU	C6-C5	2.94	1.38	1.35
42	1	305	A2M	C5-C4	-2.94	1.33	1.39
42	1	955	A2M	O2'-C2'	-2.94	1.35	1.42
38	7	162	A2M	C5-N7	-2.93	1.33	1.39
29	S1	609	PSU	C4-N3	-2.93	1.33	1.38
38	7	43	A2M	C5-N7	-2.93	1.33	1.39
37	2	527	A2M	O3'-C3'	2.93	1.50	1.43
42	1	1190	OMG	O6-C6	-2.92	1.18	1.23
29	S1	1533	PSU	C4-N3	-2.92	1.33	1.38
29	S1	1657	PSU	C4-N3	-2.92	1.33	1.38
37	2	1078	OMG	C5-N7	-2.91	1.33	1.39
37	2	597	PSU	C6-C5	2.91	1.38	1.35
38	7	162	A2M	O2'-C2'	-2.91	1.35	1.42
37	2	604	A2M	O2'-C2'	-2.91	1.35	1.42
42	1	1107	OMU	O2-C2	-2.91	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	1046	OMG	C5-N7	-2.91	1.33	1.39
42	1	1371	OMU	O2-C2	-2.91	1.17	1.23
29	S1	1543	C4J	O4'-C1'	-2.90	1.39	1.43
42	1	1402	PSU	C4-N3	2.90	1.44	1.38
37	2	628	A2M	C5-N7	-2.90	1.33	1.39
29	S1	1192	PSU	C4-N3	-2.89	1.33	1.38
41	3	13	OMU	C4-N3	2.89	1.43	1.38
37	2	1318	PSU	C4-N3	2.89	1.44	1.38
38	7	74	PSU	C6-C5	2.89	1.38	1.35
37	2	572	A2M	C5-N7	-2.89	1.33	1.39
37	2	1231	OMG	C4-N9	-2.89	1.30	1.38
38	7	7	OMU	O2-C2	-2.89	1.18	1.23
37	2	1372	A2M	C5-N7	-2.88	1.33	1.39
37	2	593	PSU	C6-C5	2.88	1.38	1.35
29	S1	1841	PSU	C6-C5	2.88	1.38	1.35
37	2	1144	PSU	C6-C5	2.88	1.38	1.35
37	2	1382	PSU	C4-N3	2.88	1.44	1.38
29	S1	2021	A2M	C8-N9	-2.87	1.32	1.37
37	2	1058	PSU	C4-N3	-2.87	1.33	1.38
37	2	71	OMG	C5-C4	2.87	1.46	1.38
37	2	472	PSU	C6-C5	2.87	1.38	1.35
37	2	1248	OMC	C6-N1	2.86	1.44	1.38
37	2	1308	5MC	O3'-C3'	2.86	1.50	1.43
29	S1	600	OMG	C5-N7	-2.86	1.33	1.39
37	2	1403	PSU	C6-C5	2.86	1.38	1.35
29	S1	1550	OMG	C5-N7	-2.86	1.33	1.39
42	1	858	A2M	O2'-C2'	-2.85	1.35	1.42
37	2	534	OMG	C4-N9	-2.85	1.30	1.38
37	2	1253	OMG	C4-N9	-2.84	1.30	1.38
42	1	1181	PSU	C4-N3	-2.84	1.33	1.38
37	2	655	OMG	C4-N9	-2.84	1.30	1.38
42	1	858	A2M	O3'-C3'	2.84	1.50	1.43
37	2	662	PSU	C4-N3	2.84	1.44	1.38
42	1	858	A2M	C5-N7	-2.84	1.33	1.39
29	S1	18	OMC	O2-C2	-2.83	1.18	1.23
37	2	95	A2M	O2'-C2'	-2.82	1.35	1.42
29	S1	1246	PSU	C4-N3	-2.82	1.33	1.38
37	2	1060	PSU	C6-C5	2.82	1.38	1.35
37	2	382	A2M	C4-N9	-2.82	1.31	1.37
42	1	681	A2M	O3'-C3'	2.82	1.49	1.43
42	1	1017	PSU	C6-C5	2.82	1.38	1.35
37	2	1078	OMG	O6-C6	-2.82	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	1478	OMG	O6-C6	-2.82	1.18	1.23
37	2	1372	A2M	O2'-C2'	-2.81	1.35	1.42
29	S1	1657	PSU	C6-C5	2.81	1.38	1.35
29	S1	2048	PSU	C6-C5	2.81	1.38	1.35
42	1	856	OMG	C5-N7	-2.80	1.33	1.39
29	S1	1647	OMG	C5-N7	-2.80	1.33	1.39
37	2	1229	OMG	C4-N9	-2.80	1.30	1.38
37	2	560	OMU	O2-C2	-2.80	1.18	1.23
29	S1	2151	OMG	O6-C6	-2.79	1.18	1.23
29	S1	33	PSU	C4-N3	-2.79	1.33	1.38
29	S1	38	OMC	O2-C2	-2.79	1.18	1.23
29	S1	1550	OMG	C2-N1	2.79	1.44	1.37
37	2	1046	OMG	C2-N1	2.78	1.44	1.37
42	1	672	PSU	C6-C5	2.78	1.38	1.35
37	2	604	A2M	O3'-C3'	2.78	1.49	1.43
37	2	527	A2M	O2'-C2'	-2.78	1.35	1.42
29	S1	1544	5MC	O2-C2	-2.78	1.18	1.23
37	2	1360	OMG	C4-N9	-2.78	1.31	1.38
42	1	870	PSU	C4-N3	2.77	1.44	1.38
38	7	75	OMG	C6-N1	-2.77	1.33	1.38
29	S1	2021	A2M	O3'-C3'	2.77	1.49	1.43
42	1	1524	OMG	O6-C6	-2.77	1.18	1.23
29	S1	1156	PSU	C4-N3	-2.77	1.33	1.38
29	S1	661	OMU	C6-N1	2.77	1.44	1.38
29	S1	1647	OMG	C2-N1	2.76	1.44	1.37
37	2	1317	OMC	C6-N1	2.76	1.44	1.38
37	2	1159	OMC	C6-N1	2.75	1.44	1.38
29	S1	8	OMU	C6-N1	2.75	1.44	1.38
29	S1	668	A2M	O2'-C2'	-2.75	1.35	1.42
37	2	1303	PSU	C4-N3	-2.75	1.33	1.38
42	1	305	A2M	O3'-C3'	2.75	1.49	1.43
29	S1	1865	OMG	O6-C6	-2.74	1.18	1.23
42	1	959[B]	OMG	O6-C6	-2.74	1.18	1.23
42	1	1524	OMG	C4-N9	-2.74	1.31	1.38
29	S1	1829	OMG	C2-N1	2.74	1.44	1.37
29	S1	455	PSU	O4-C4	-2.74	1.18	1.23
29	S1	1879	OMG	O6-C6	-2.72	1.18	1.23
37	2	73	OMU	C2-N3	-2.72	1.33	1.38
37	2	1077	OMU	O2-C2	-2.72	1.18	1.23
42	1	1533	PSU	C6-C5	2.71	1.38	1.35
29	S1	1865	OMG	C2-N1	2.71	1.44	1.37
29	S1	2140	OMC	O2-C2	-2.71	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	1185	A2M	O3'-C3'	2.71	1.49	1.43
37	2	1397	OMC	C6-N1	2.71	1.44	1.38
29	S1	668	A2M	C8-N9	-2.71	1.32	1.37
29	S1	600	OMG	C2-N1	2.70	1.44	1.37
42	1	955	A2M	O3'-C3'	2.69	1.49	1.43
37	2	1372	A2M	O3'-C3'	2.68	1.49	1.43
42	1	1011	PSU	O4-C4	-2.68	1.18	1.23
37	2	583	OMC	C6-N1	2.68	1.44	1.38
42	1	940	PSU	C4-N3	2.68	1.43	1.38
29	S1	661	OMU	O2-C2	-2.67	1.18	1.23
42	1	1190	OMG	C2-N1	2.67	1.44	1.37
29	S1	607	PSU	C4-N3	-2.67	1.33	1.38
42	1	858	A2M	C8-N9	-2.67	1.33	1.37
37	2	1078	OMG	C4-N9	-2.67	1.31	1.38
29	S1	1865	OMG	C4-N9	-2.66	1.31	1.38
42	1	959[A]	OMG	O6-C6	-2.66	1.18	1.23
37	2	1046	OMG	O6-C6	-2.65	1.18	1.23
29	S1	1550	OMG	O6-C6	-2.65	1.18	1.23
37	2	628	A2M	O3'-C3'	2.65	1.49	1.43
29	S1	1478	OMG	C2-N1	2.64	1.44	1.37
29	S1	1829	OMG	O6-C6	-2.64	1.18	1.23
29	S1	2151	OMG	C2-N1	2.64	1.44	1.37
29	S1	12	PSU	O4-C4	-2.64	1.18	1.23
42	1	695	OMC	C6-N1	2.64	1.44	1.38
29	S1	1566	PSU	O4-C4	-2.63	1.18	1.23
29	S1	1979	OMU	O2-C2	-2.63	1.18	1.23
29	S1	1979	OMU	C6-N1	2.62	1.44	1.38
42	1	959[B]	OMG	C2-N1	2.62	1.44	1.37
29	S1	2021	A2M	C5-N7	-2.62	1.34	1.39
38	7	162	A2M	O3'-C3'	2.62	1.49	1.43
42	1	678	A2M	O3'-C3'	2.62	1.49	1.43
42	1	697	A2M	C4-N9	-2.61	1.32	1.37
37	2	510	PSU	O4-C4	-2.61	1.18	1.23
29	S1	1623	OMG	C6-N1	-2.61	1.34	1.38
37	2	1372	A2M	C4-N9	-2.60	1.32	1.37
37	2	1077	OMU	C6-N1	2.60	1.44	1.38
37	2	1384	A2M	O3'-C3'	2.60	1.49	1.43
37	2	382	A2M	O3'-C3'	2.59	1.49	1.43
42	1	1371	OMU	C6-N1	2.58	1.44	1.38
37	2	572	A2M	O3'-C3'	2.58	1.49	1.43
29	S1	600	OMG	O6-C6	-2.57	1.18	1.23
29	S1	104	PSU	O4-C4	-2.57	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	1647	OMG	O6-C6	-2.57	1.18	1.23
42	1	1539	A2M	O3'-C3'	2.57	1.49	1.43
29	S1	1478	OMG	C4-N9	-2.57	1.31	1.38
29	S1	1543	C4J	O2-C2	-2.57	1.17	1.22
37	2	1359	OMU	C6-N1	2.57	1.44	1.38
42	1	1190	OMG	C4-N9	-2.57	1.31	1.38
42	1	305	A2M	C4-N9	-2.57	1.32	1.37
37	2	512	PSU	O4-C4	-2.56	1.18	1.23
37	2	628	A2M	C4-N9	-2.56	1.32	1.37
42	1	697	A2M	O3'-C3'	2.56	1.49	1.43
37	2	95	A2M	O3'-C3'	2.55	1.49	1.43
37	2	572	A2M	C4-N9	-2.55	1.32	1.37
29	S1	1879	OMG	C4-N9	-2.54	1.31	1.38
37	2	1360	OMG	C2-N1	2.54	1.43	1.37
42	1	407	A2M	C4-N9	-2.53	1.32	1.37
29	S1	1550	OMG	C4-N9	-2.53	1.31	1.38
29	S1	2061	5MC	C6-C5	2.53	1.38	1.34
37	2	591	A2M	C5-N7	-2.53	1.34	1.39
38	7	7	OMU	C6-N1	2.53	1.44	1.38
29	S1	668	A2M	C5-N7	-2.53	1.34	1.39
42	1	959[A]	OMG	C2-N1	2.52	1.43	1.37
29	S1	8	OMU	O2-C2	-2.52	1.18	1.23
42	1	1524	OMG	C2-N1	2.52	1.43	1.37
29	S1	1879	OMG	C2-N1	2.52	1.43	1.37
29	S1	512	A2M	C5-C6	2.51	1.48	1.41
42	1	407	A2M	O3'-C3'	2.51	1.49	1.43
29	S1	2151	OMG	C4-N9	-2.51	1.31	1.38
42	1	1107	OMU	C6-N1	2.51	1.44	1.38
42	1	1539	A2M	C4-N9	-2.49	1.32	1.37
42	1	959[B]	OMG	C4-N9	-2.48	1.31	1.38
37	2	560	OMU	C6-N1	2.47	1.44	1.38
42	1	1011	PSU	O4'-C1'	-2.47	1.40	1.43
38	7	43	A2M	C4-N9	-2.47	1.32	1.37
37	2	591	A2M	C5-C6	2.47	1.47	1.41
37	2	570	A2M	O2'-C2'	-2.46	1.36	1.42
37	2	1229	OMG	C2-N1	2.46	1.43	1.37
37	2	1046	OMG	C5-C6	2.46	1.53	1.44
29	S1	512	A2M	C5-N7	-2.46	1.34	1.39
37	2	593	PSU	C2-N3	-2.45	1.33	1.37
38	7	162	A2M	C4-N9	-2.45	1.32	1.37
37	2	527	A2M	C4-N9	-2.45	1.32	1.37
29	S1	2021	A2M	O2'-C2'	-2.43	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	600	OMG	C5-C6	2.43	1.53	1.44
37	2	1046	OMG	C4-N9	-2.43	1.31	1.38
37	2	641	OMG	C2-N1	2.42	1.43	1.37
42	1	927	A2M	O3'-C3'	2.42	1.49	1.43
37	2	1152	OMU	C6-N1	2.41	1.43	1.38
29	S1	1647	OMG	C6-N1	2.41	1.43	1.38
29	S1	1647	OMG	C5-C6	2.40	1.53	1.44
37	2	1078	OMG	C2-N1	2.40	1.43	1.37
38	7	43	A2M	O3'-C3'	2.40	1.48	1.43
37	2	1419	OMU	C6-N1	2.39	1.43	1.38
42	1	870	PSU	O2-C2	-2.39	1.18	1.23
37	2	95	A2M	C4-N9	-2.39	1.32	1.37
37	2	1384	A2M	C4-N9	-2.39	1.32	1.37
37	2	1078	OMG	C5-C6	2.39	1.53	1.44
42	1	847	OMU	C6-N1	2.38	1.43	1.38
29	S1	2140	OMC	C5-C4	2.37	1.48	1.42
42	1	1171	PSU	C4-N3	2.37	1.43	1.38
42	1	681	A2M	C4-N9	-2.37	1.32	1.37
37	2	1382	PSU	O4'-C1'	-2.37	1.40	1.43
37	2	667	OMU	C6-N1	2.36	1.43	1.38
37	2	655	OMG	C5-C6	2.36	1.53	1.44
42	1	235	A2M	O3'-C3'	2.35	1.48	1.43
42	1	959[A]	OMG	C4-N9	-2.35	1.32	1.38
37	2	1231	OMG	C2-N1	2.35	1.43	1.37
42	1	1171	PSU	O4'-C1'	-2.35	1.40	1.43
29	S1	1829	OMG	C4-N9	-2.35	1.32	1.38
40	4	74	OMG	C2-N1	2.34	1.43	1.37
42	1	927	A2M	C4-N9	-2.33	1.32	1.37
37	2	655	OMG	C2-N1	2.33	1.43	1.37
29	S1	2046	PSU	C2-N3	-2.32	1.33	1.37
42	1	1528	PSU	C2-N3	-2.32	1.33	1.37
29	S1	1647	OMG	C4-N9	-2.32	1.32	1.38
29	S1	1865	OMG	C6-N1	2.32	1.43	1.38
29	S1	38	OMC	C5-C4	2.32	1.48	1.42
29	S1	1829	OMG	C5-C6	2.31	1.53	1.44
37	2	534	OMG	C2-N1	2.31	1.43	1.37
29	S1	1550	OMG	C6-N1	2.31	1.43	1.38
37	2	1413	PSU	O2-C2	-2.31	1.18	1.23
42	1	1190	OMG	C5-C6	2.30	1.53	1.44
37	2	1077	OMU	C5-C4	2.30	1.48	1.43
29	S1	1550	OMG	C5-C6	2.30	1.53	1.44
42	1	1017	PSU	C2-N3	-2.30	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	1879	OMG	C5-C6	2.29	1.53	1.44
29	S1	2151	OMG	C5-C6	2.29	1.53	1.44
42	1	1659	OMU	C6-N1	2.28	1.43	1.38
29	S1	1829	OMG	C6-N1	2.28	1.43	1.38
29	S1	1478	OMG	C5-C6	2.28	1.52	1.44
42	1	672	PSU	C2-N3	-2.27	1.33	1.37
37	2	73	OMU	C5-C4	-2.27	1.38	1.43
29	S1	2061	5MC	C6-N1	-2.27	1.34	1.38
42	1	959[B]	OMG	C5-C6	2.27	1.52	1.44
37	2	78	PSU	C2-N3	-2.27	1.33	1.37
29	S1	600	OMG	C4-N9	-2.27	1.32	1.38
42	1	235	A2M	C4-N9	-2.26	1.33	1.37
37	2	1046	OMG	C6-N1	2.26	1.43	1.38
29	S1	18	OMC	C5-C4	2.25	1.48	1.42
42	1	1524	OMG	C5-C6	2.25	1.52	1.44
37	2	1253	OMG	C2-N1	2.25	1.43	1.37
42	1	959[A]	OMG	C5-C6	2.25	1.52	1.44
29	S1	600	OMG	C6-N1	2.25	1.43	1.38
42	1	422	PSU	C2-N3	-2.24	1.33	1.37
38	7	74	PSU	C2-N3	-2.24	1.33	1.37
37	2	662	PSU	O2-C2	-2.24	1.18	1.23
29	S1	1543	C4J	C31-C3	2.24	1.59	1.52
37	2	597	PSU	C2-N3	-2.24	1.33	1.37
37	2	626	PSU	O2-C2	-2.24	1.18	1.23
42	1	959[A]	OMG	C6-N1	2.23	1.43	1.38
42	1	856	OMG	C5-C6	2.23	1.52	1.44
42	1	1540	OMG	C2-N1	2.22	1.43	1.37
37	2	1060	PSU	C2-N3	-2.22	1.33	1.37
29	S1	8	OMU	C5-C4	2.21	1.48	1.43
37	2	1403	PSU	C2-N3	-2.21	1.33	1.37
29	S1	1657	PSU	C2-N3	-2.21	1.33	1.37
37	2	472	PSU	C2-N3	-2.21	1.33	1.37
42	1	955	A2M	C4-N9	-2.21	1.33	1.37
37	2	71	OMG	C5-N7	-2.20	1.34	1.39
42	1	940	PSU	O2-C2	-2.20	1.18	1.23
42	1	858	A2M	C4-N9	-2.20	1.33	1.37
29	S1	512	A2M	C8-N7	2.19	1.35	1.31
29	S1	661	OMU	C5-C4	2.19	1.48	1.43
29	S1	1478	OMG	C6-N1	2.19	1.42	1.38
42	1	1171	PSU	O2-C2	-2.18	1.18	1.23
41	3	13	OMU	C6-N1	2.18	1.43	1.38
42	1	1626	OMG	C5-C6	2.18	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	305	A2M	C8-N9	-2.18	1.33	1.37
42	1	1524	OMG	C6-N1	2.17	1.42	1.38
38	7	75	OMG	C5-N7	-2.17	1.34	1.39
37	2	1318	PSU	O2-C2	-2.17	1.18	1.23
42	1	856	OMG	C2-N1	2.17	1.42	1.37
42	1	845	OMU	C4-N3	2.17	1.42	1.38
42	1	1533	PSU	C2-N3	-2.17	1.33	1.37
37	2	570	A2M	C4-N9	-2.16	1.33	1.37
29	S1	1879	OMG	C6-N1	2.16	1.42	1.38
42	1	1664	PSU	C2-N3	-2.16	1.33	1.37
42	1	959[B]	OMG	C6-N1	2.15	1.42	1.38
37	2	534	OMG	C5-C6	2.15	1.52	1.44
37	2	1361	PSU	O4'-C1'	-2.15	1.40	1.43
42	1	1626	OMG	C2-N1	2.14	1.42	1.37
29	S1	1841	PSU	C2-N3	-2.14	1.33	1.37
37	2	510	PSU	C4-C5	2.14	1.50	1.44
37	2	1264	PSU	C2-N3	-2.14	1.34	1.37
37	2	1058	PSU	C2-N3	-2.13	1.34	1.37
42	1	1540	OMG	C5-C6	2.13	1.52	1.44
29	S1	1979	OMU	C5-C4	2.13	1.48	1.43
37	2	1144	PSU	C2-N3	-2.12	1.34	1.37
29	S1	609	PSU	C2-N3	-2.12	1.34	1.37
42	1	1190	OMG	C6-N1	2.12	1.42	1.38
29	S1	512	A2M	C4-N9	-2.11	1.33	1.37
37	2	443	OMC	C5-C4	2.11	1.47	1.42
29	S1	1866	OMC	C5-C4	2.11	1.47	1.42
37	2	1253	OMG	C5-C6	2.11	1.52	1.44
38	7	69	PSU	C2-N3	-2.10	1.34	1.37
29	S1	1865	OMG	C5-C6	2.10	1.52	1.44
37	2	1360	OMG	C5-C6	2.10	1.52	1.44
29	S1	2151	OMG	C6-N1	2.10	1.42	1.38
29	S1	1533	PSU	C2-N3	-2.10	1.34	1.37
37	2	510	PSU	O4'-C1'	-2.10	1.40	1.43
42	1	239	PSU	C2-N3	-2.09	1.34	1.37
37	2	1231	OMG	C5-C6	2.09	1.52	1.44
29	S1	2021	A2M	C4-N9	-2.09	1.33	1.37
42	1	678	A2M	C4-N9	-2.08	1.33	1.37
37	2	1229	OMG	C5-C6	2.08	1.52	1.44
42	1	1011	PSU	C4-C5	2.08	1.50	1.44
37	2	359	OMC	C5-C4	2.08	1.47	1.42
29	S1	1539	PSU	C2-N3	-2.08	1.34	1.37
42	1	1664	PSU	C2-N1	-2.07	1.34	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	4	74	OMG	C5-C6	2.07	1.52	1.44
37	2	641	OMG	C5-C6	2.07	1.52	1.44
29	S1	2048	PSU	C2-N3	-2.06	1.34	1.37
29	S1	1623	OMG	C5-N7	-2.05	1.35	1.39
29	S1	1192	PSU	C2-N3	-2.05	1.34	1.37
37	2	1382	PSU	O2-C2	-2.05	1.19	1.23
42	1	1107	OMU	C5-C4	2.04	1.48	1.43
37	2	78	PSU	C2-N1	-2.04	1.34	1.36
29	S1	1566	PSU	C4-C5	2.03	1.50	1.44
29	S1	1156	PSU	C2-N3	-2.03	1.34	1.37
37	2	1359	OMU	C5-C4	2.03	1.48	1.43
37	2	591	A2M	C4-N9	-2.03	1.33	1.37
42	1	1371	OMU	C5-C4	2.03	1.48	1.43
42	1	422	PSU	C2-N1	-2.03	1.34	1.36
29	S1	33	PSU	C2-N3	-2.02	1.34	1.37
37	2	1229	OMG	C6-N1	2.02	1.42	1.38
42	1	422	PSU	C2'-C1'	-2.02	1.51	1.53
37	2	437	PSU	O2-C2	-2.02	1.19	1.23
42	1	1017	PSU	C2'-C1'	-2.00	1.51	1.53
37	2	591	A2M	C8-N7	2.00	1.35	1.31
42	1	1010	OMC	C5-C4	2.00	1.47	1.42

All (986) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	959[A]	OMG	C1'-N9-C8	-8.28	103.20	126.73
29	S1	600	OMG	C1'-N9-C8	-8.13	103.63	126.73
29	S1	2151	OMG	C1'-N9-C8	-8.04	103.88	126.73
29	S1	1879	OMG	C1'-N9-C8	-8.00	104.00	126.73
29	S1	1829	OMG	C1'-N9-C8	-7.95	104.14	126.73
37	2	534	OMG	C1'-N9-C8	-7.81	104.54	126.73
29	S1	1865	OMG	C1'-N9-C8	-7.78	104.62	126.73
40	4	74	OMG	C1'-N9-C8	-7.77	104.64	126.73
29	S1	1550	OMG	C1'-N9-C8	-7.65	105.01	126.73
29	S1	1647	OMG	C1'-N9-C8	-7.62	105.09	126.73
42	1	845	OMU	C4-N3-C2	-7.56	117.22	126.61
37	2	1360	OMG	C1'-N9-C8	-7.52	105.36	126.73
37	2	1046	OMG	C1'-N9-C8	-7.48	105.49	126.73
29	S1	1478	OMG	C1'-N9-C8	-7.44	105.60	126.73
42	1	858	A2M	N6-C6-N1	-7.36	101.98	118.38
37	2	1229	OMG	C1'-N9-C8	-7.22	106.22	126.73
37	2	1231	OMG	C1'-N9-C8	-7.17	106.37	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	1017	PSU	N1-C2-N3	7.16	122.72	115.17
29	S1	1657	PSU	N1-C2-N3	7.16	122.72	115.17
42	1	1190	OMG	C1'-N9-C8	-7.13	106.46	126.73
37	2	628	A2M	N6-C6-N1	-7.11	102.53	118.38
38	7	43	A2M	N6-C6-N1	-7.11	102.54	118.38
42	1	1533	PSU	N1-C2-N3	7.09	122.64	115.17
37	2	1372	A2M	N6-C6-N1	-7.02	102.73	118.38
42	1	422	PSU	N1-C2-N3	7.02	122.57	115.17
37	2	1253	OMG	C1'-N9-C8	-7.01	106.80	126.73
42	1	959[A]	OMG	C1'-N9-C4	7.01	147.20	126.49
29	S1	600	OMG	C1'-N9-C4	6.98	147.11	126.49
42	1	1539	A2M	N6-C6-N1	-6.98	102.83	118.38
42	1	672	PSU	N1-C2-N3	6.98	122.53	115.17
37	2	593	PSU	N1-C2-N3	6.97	122.52	115.17
42	1	1626	OMG	C1'-N9-C8	-6.96	106.96	126.73
37	2	1060	PSU	N1-C2-N3	6.94	122.49	115.17
37	2	597	PSU	N1-C2-N3	6.93	122.48	115.17
37	2	572	A2M	N6-C6-N1	-6.92	102.96	118.38
37	2	1403	PSU	N1-C2-N3	6.91	122.45	115.17
29	S1	1829	OMG	C1'-N9-C4	6.90	146.88	126.49
37	2	655	OMG	C1'-N9-C8	-6.89	107.17	126.73
29	S1	2021	A2M	N6-C6-N1	-6.89	103.04	118.38
42	1	678	A2M	N6-C6-N1	-6.85	103.12	118.38
37	2	78	PSU	N1-C2-N3	6.85	122.39	115.17
29	S1	2048	PSU	N1-C2-N3	6.85	122.39	115.17
37	2	472	PSU	N1-C2-N3	6.84	122.38	115.17
42	1	239	PSU	N1-C2-N3	6.84	122.38	115.17
41	3	13	OMU	C4-N3-C2	-6.83	118.13	126.61
42	1	927	A2M	N6-C6-N1	-6.83	103.16	118.38
38	7	69	PSU	N1-C2-N3	6.81	122.35	115.17
37	2	641	OMG	C1'-N9-C8	-6.80	107.41	126.73
42	1	1540	OMG	C1'-N9-C8	-6.78	107.47	126.73
42	1	1528	PSU	N1-C2-N3	6.78	122.32	115.17
37	2	534	OMG	C1'-N9-C4	6.77	146.47	126.49
29	S1	668	A2M	N6-C6-N1	-6.76	103.32	118.38
37	2	1144	PSU	N1-C2-N3	6.75	122.29	115.17
37	2	1058	PSU	N1-C2-N3	6.75	122.29	115.17
29	S1	1246	PSU	N1-C2-N3	6.74	122.28	115.17
42	1	1181	PSU	N1-C2-N3	6.73	122.27	115.17
29	S1	2151	OMG	C1'-N9-C4	6.73	146.37	126.49
37	2	1264	PSU	N1-C2-N3	6.73	122.26	115.17
42	1	955	A2M	N6-C6-N1	-6.72	103.41	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1879	OMG	C1'-N9-C4	6.70	146.27	126.49
42	1	235	A2M	N6-C6-N1	-6.70	103.47	118.38
42	1	407	A2M	N6-C6-N1	-6.69	103.47	118.38
29	S1	1533	PSU	N1-C2-N3	6.68	122.21	115.17
29	S1	1539	PSU	N1-C2-N3	6.67	122.21	115.17
29	S1	1192	PSU	N1-C2-N3	6.66	122.20	115.17
42	1	697	A2M	N6-C6-N1	-6.65	103.56	118.38
38	7	162	A2M	N6-C6-N1	-6.64	103.59	118.38
29	S1	2046	PSU	N1-C2-N3	6.64	122.17	115.17
42	1	1524	OMG	C1'-N9-C8	-6.63	107.90	126.73
42	1	1664	PSU	N1-C2-N3	6.63	122.16	115.17
37	2	1078	OMG	C1'-N9-C8	-6.62	107.91	126.73
37	2	382	A2M	N6-C6-N1	-6.61	103.64	118.38
42	1	681	A2M	N6-C6-N1	-6.61	103.65	118.38
37	2	95	A2M	N6-C6-N1	-6.59	103.69	118.38
37	2	570	A2M	N6-C6-N1	-6.59	103.70	118.38
29	S1	1841	PSU	N1-C2-N3	6.57	122.09	115.17
38	7	74	PSU	N1-C2-N3	6.54	122.07	115.17
29	S1	607	PSU	N1-C2-N3	6.52	122.05	115.17
37	2	527	A2M	N6-C6-N1	-6.51	103.88	118.38
37	2	1303	PSU	N1-C2-N3	6.51	122.03	115.17
29	S1	1865	OMG	C1'-N9-C4	6.50	145.70	126.49
29	S1	609	PSU	N1-C2-N3	6.48	122.00	115.17
29	S1	1647	OMG	C1'-N9-C4	6.46	145.58	126.49
29	S1	33	PSU	N1-C2-N3	6.46	121.98	115.17
37	2	1372	A2M	C4-N9-C1'	-6.46	111.53	126.63
42	1	305	A2M	N6-C6-N1	-6.45	104.02	118.38
37	2	1360	OMG	C1'-N9-C4	6.44	145.52	126.49
29	S1	1156	PSU	N1-C2-N3	6.44	121.96	115.17
37	2	71	OMG	C5-C4-N3	-6.43	118.16	128.39
37	2	604	A2M	N6-C6-N1	-6.42	104.08	118.38
37	2	1046	OMG	C1'-N9-C4	6.41	145.41	126.49
29	S1	1550	OMG	C1'-N9-C4	6.39	145.35	126.49
29	S1	1478	OMG	C1'-N9-C4	6.34	145.22	126.49
40	4	74	OMG	C1'-N9-C4	6.32	145.17	126.49
37	2	1384	A2M	N6-C6-N1	-6.32	104.30	118.38
38	7	75	OMG	C5-C4-N3	-6.29	118.39	128.39
37	2	667	OMU	C4-N3-C2	-6.27	118.83	126.61
42	1	845	OMU	N3-C2-N1	6.24	123.01	114.89
42	1	856	OMG	C1'-N9-C8	-6.22	109.07	126.73
37	2	1185	A2M	N6-C6-N1	-6.20	104.57	118.38
37	2	628	A2M	C4-N9-C1'	-6.16	112.23	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1359	OMU	C4-N3-C2	-6.15	118.98	126.61
42	1	847	OMU	C4-N3-C2	-6.13	119.00	126.61
42	1	1107	OMU	C4-N3-C2	-6.13	119.01	126.61
37	2	572	A2M	N3-C2-N1	-6.08	119.38	128.58
42	1	1371	OMU	C4-N3-C2	-6.05	119.10	126.61
38	7	162	A2M	N3-C2-N1	-6.04	119.43	128.58
37	2	1372	A2M	N9-C8-N7	-6.04	105.36	113.94
37	2	1077	OMU	C4-N3-C2	-6.03	119.12	126.61
37	2	1253	OMG	C1'-N9-C4	6.01	144.25	126.49
37	2	591	A2M	C5-C4-N3	-6.00	118.45	126.72
37	2	382	A2M	C4-N9-C1'	-6.00	112.60	126.63
42	1	681	A2M	N3-C2-N1	-5.99	119.52	128.58
29	S1	2021	A2M	N9-C8-N7	-5.94	105.51	113.94
37	2	1152	OMU	C4-N3-C2	-5.94	119.24	126.61
42	1	407	A2M	N3-C2-N1	-5.94	119.60	128.58
29	S1	1623	OMG	C5-C4-N3	-5.93	118.94	128.39
42	1	1171	PSU	C4-N3-C2	-5.93	118.21	126.37
29	S1	2021	A2M	C4-N9-C1'	-5.91	112.81	126.63
42	1	1190	OMG	C1'-N9-C4	5.90	143.93	126.49
37	2	1229	OMG	C1'-N9-C4	5.88	143.85	126.49
37	2	655	OMG	C1'-N9-C4	5.87	143.82	126.49
38	7	43	A2M	N3-C2-N1	-5.86	119.71	128.58
37	2	1384	A2M	N3-C2-N1	-5.86	119.71	128.58
37	2	1419	OMU	C4-N3-C2	-5.85	119.34	126.61
37	2	1231	OMG	C1'-N9-C4	5.85	143.78	126.49
37	2	572	A2M	C4-N9-C1'	-5.82	113.02	126.63
42	1	407	A2M	N9-C8-N7	-5.81	105.69	113.94
42	1	697	A2M	N3-C2-N1	-5.79	119.82	128.58
29	S1	8	OMU	C4-N3-C2	-5.77	119.45	126.61
42	1	1626	OMG	C1'-N9-C4	5.76	143.50	126.49
37	2	560	OMU	C4-N3-C2	-5.75	119.47	126.61
37	2	570	A2M	N9-C8-N7	-5.75	105.78	113.94
37	2	527	A2M	N3-C2-N1	-5.73	119.91	128.58
42	1	927	A2M	N3-C2-N1	-5.73	119.91	128.58
37	2	1384	A2M	C4-N9-C1'	-5.73	113.24	126.63
29	S1	668	A2M	C4-N9-C1'	-5.73	113.24	126.63
37	2	527	A2M	N9-C8-N7	-5.73	105.81	113.94
42	1	1524	OMG	C1'-N9-C4	5.72	143.38	126.49
42	1	305	A2M	C5-C6-N6	5.72	137.44	123.29
37	2	628	A2M	N3-C2-N1	-5.71	119.95	128.58
29	S1	1979	OMU	C4-N3-C2	-5.70	119.53	126.61
42	1	858	A2M	C5-C6-N6	5.70	137.40	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	661	OMU	C4-N3-C2	-5.68	119.56	126.61
42	1	1539	A2M	N3-C2-N1	-5.67	120.00	128.58
37	2	641	OMG	C1'-N9-C4	5.67	143.22	126.49
37	2	628	A2M	N9-C8-N7	-5.67	105.90	113.94
29	S1	668	A2M	N9-C8-N7	-5.66	105.90	113.94
42	1	955	A2M	N3-C2-N1	-5.65	120.03	128.58
42	1	858	A2M	N3-C2-N1	-5.65	120.03	128.58
37	2	572	A2M	N9-C8-N7	-5.64	105.93	113.94
42	1	235	A2M	N3-C2-N1	-5.63	120.06	128.58
42	1	927	A2M	N9-C8-N7	-5.63	105.95	113.94
37	2	1078	OMG	C1'-N9-C4	5.62	143.08	126.49
37	2	1185	A2M	N3-C2-N1	-5.62	120.08	128.58
37	2	1372	A2M	N3-C2-N1	-5.62	120.08	128.58
42	1	678	A2M	C5-C4-N3	-5.61	118.99	126.72
37	2	1384	A2M	N9-C8-N7	-5.61	105.98	113.94
42	1	1659	OMU	C4-N3-C2	-5.60	119.66	126.61
38	7	162	A2M	C4-N9-C1'	-5.59	113.56	126.63
42	1	959[B]	OMG	C1'-N9-C4	5.59	142.99	126.49
42	1	697	A2M	N9-C8-N7	-5.58	106.02	113.94
38	7	43	A2M	N9-C8-N7	-5.58	106.03	113.94
37	2	1372	A2M	C5-C6-N6	5.57	137.07	123.29
29	S1	2021	A2M	N3-C2-N1	-5.56	120.17	128.58
37	2	382	A2M	N3-C2-N1	-5.56	120.17	128.58
42	1	697	A2M	C4-N9-C1'	-5.55	113.66	126.63
37	2	570	A2M	N3-C2-N1	-5.55	120.19	128.58
38	7	7	OMU	C4-N3-C2	-5.54	119.73	126.61
42	1	959[B]	OMG	C1'-N9-C8	-5.54	111.00	126.73
38	7	43	A2M	C4-N9-C1'	-5.53	113.69	126.63
37	2	628	A2M	C5-C6-N6	5.53	136.97	123.29
42	1	1539	A2M	C5-C6-N6	5.53	136.97	123.29
38	7	43	A2M	C5-C6-N6	5.52	136.95	123.29
42	1	955	A2M	N9-C8-N7	-5.51	106.11	113.94
42	1	678	A2M	N9-C8-N7	-5.50	106.14	113.94
37	2	1185	A2M	N9-C8-N7	-5.49	106.14	113.94
42	1	955	A2M	C5-C4-N3	-5.48	119.18	126.72
37	2	572	A2M	C5-C6-N6	5.47	136.83	123.29
37	2	527	A2M	C4-N9-C1'	-5.46	113.86	126.63
29	S1	512	A2M	C5-C4-N3	-5.44	119.22	126.72
42	1	940	PSU	C4-N3-C2	-5.44	118.88	126.37
42	1	858	A2M	N9-C8-N7	-5.43	106.23	113.94
42	1	1540	OMG	C1'-N9-C4	5.43	142.52	126.49
42	1	927	A2M	C5-C4-N3	-5.39	119.29	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	2021	A2M	C5-C6-N6	5.39	136.62	123.29
42	1	858	A2M	C4-N9-C1'	-5.38	114.04	126.63
42	1	235	A2M	C4-N9-C1'	-5.38	114.06	126.63
42	1	235	A2M	N9-C8-N7	-5.37	106.32	113.94
37	2	1372	A2M	C4-N9-C8	5.37	111.37	105.74
42	1	1539	A2M	N9-C8-N7	-5.35	106.34	113.94
29	S1	668	A2M	C5-C6-N6	5.35	136.54	123.29
29	S1	668	A2M	N3-C2-N1	-5.34	120.50	128.58
37	2	604	A2M	N9-C8-N7	-5.32	106.39	113.94
42	1	927	A2M	C5-C6-N6	5.31	136.42	123.29
37	2	570	A2M	C5-C6-N6	5.30	136.40	123.29
37	2	604	A2M	N3-C2-N1	-5.29	120.57	128.58
42	1	407	A2M	C4-N9-C1'	-5.29	114.27	126.63
37	2	95	A2M	N9-C8-N7	-5.28	106.44	113.94
42	1	678	A2M	C5-C6-N6	5.27	136.35	123.29
42	1	940	PSU	N1-C2-N3	5.27	120.73	115.17
42	1	407	A2M	C4-N9-C8	5.26	111.26	105.74
38	7	162	A2M	N9-C8-N7	-5.26	106.48	113.94
37	2	1361	PSU	C4-N3-C2	-5.25	119.14	126.37
37	2	382	A2M	N9-C8-N7	-5.23	106.52	113.94
42	1	697	A2M	C5-C6-N6	5.23	136.24	123.29
38	7	162	A2M	C5-C6-N6	5.22	136.20	123.29
37	2	95	A2M	C5-C4-N3	-5.21	119.54	126.72
37	2	95	A2M	C5-C6-N6	5.21	136.19	123.29
42	1	407	A2M	C5-C6-N6	5.20	136.16	123.29
37	2	95	A2M	N3-C2-N1	-5.20	120.71	128.58
42	1	235	A2M	C5-C6-N6	5.20	136.15	123.29
37	2	570	A2M	C4-N9-C8	5.16	111.16	105.74
42	1	1402	PSU	C4-N3-C2	-5.16	119.27	126.37
42	1	678	A2M	N3-C2-N1	-5.16	120.78	128.58
29	S1	2021	A2M	C4-N9-C8	5.16	111.15	105.74
42	1	681	A2M	N9-C8-N7	-5.15	106.62	113.94
42	1	305	A2M	C4-N9-C1'	-5.15	114.58	126.63
38	7	75	OMG	C2-N3-C4	5.15	121.17	112.30
42	1	681	A2M	C5-C6-N6	5.15	136.03	123.29
37	2	71	OMG	C2-N3-C4	5.13	121.14	112.30
42	1	305	A2M	N3-C2-N1	-5.13	120.81	128.58
37	2	604	A2M	C5-C6-N6	5.12	135.97	123.29
42	1	1171	PSU	N1-C2-N3	5.12	120.57	115.17
42	1	1011	PSU	C4-N3-C2	-5.12	119.32	126.37
37	2	604	A2M	C5-C4-N3	-5.12	119.67	126.72
37	2	1382	PSU	C4-N3-C2	-5.11	119.33	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	870	PSU	C4-N3-C2	-5.09	119.36	126.37
37	2	1413	PSU	C4-N3-C2	-5.08	119.37	126.37
37	2	1384	A2M	C4-N9-C8	5.08	111.07	105.74
42	1	697	A2M	C4-N9-C8	5.06	111.06	105.74
37	2	570	A2M	C5-C4-N3	-5.06	119.75	126.72
42	1	681	A2M	C4-N9-C1'	-5.06	114.80	126.63
37	2	73	OMU	C4-N3-C2	-5.05	120.34	126.61
42	1	955	A2M	C5-C6-N6	5.05	135.80	123.29
37	2	1413	PSU	N1-C2-N3	5.03	120.48	115.17
37	2	1185	A2M	C5-C4-N3	-5.02	119.80	126.72
37	2	527	A2M	C5-C6-N6	5.00	135.67	123.29
42	1	955	A2M	C4-N9-C1'	-5.00	114.95	126.63
42	1	1011	PSU	N1-C2-N3	4.98	120.43	115.17
37	2	382	A2M	C5-C6-N6	4.98	135.61	123.29
37	2	1185	A2M	C4-N9-C1'	-4.98	115.00	126.63
37	2	1354	PSU	C4-N3-C2	-4.96	119.53	126.37
37	2	527	A2M	C5-C4-N3	-4.95	119.90	126.72
37	2	437	PSU	C4-N3-C2	-4.95	119.56	126.37
29	S1	1623	OMG	C2-N3-C4	4.94	120.81	112.30
42	1	1539	A2M	C4-N9-C1'	-4.94	115.08	126.63
37	2	572	A2M	C4-N9-C8	4.94	110.92	105.74
37	2	1185	A2M	C5-C6-N6	4.93	135.50	123.29
37	2	527	A2M	C4-N9-C8	4.92	110.91	105.74
37	2	1318	PSU	N1-C2-N3	4.92	120.35	115.17
37	2	626	PSU	N1-C2-N3	4.92	120.35	115.17
38	7	43	A2M	C4-N9-C8	4.91	110.90	105.74
37	2	626	PSU	C4-N3-C2	-4.90	119.62	126.37
42	1	305	A2M	N9-C8-N7	-4.90	106.98	113.94
37	2	1318	PSU	C4-N3-C2	-4.88	119.65	126.37
29	S1	668	A2M	C4-N9-C8	4.88	110.86	105.74
29	S1	668	A2M	C5-C4-N3	-4.87	120.00	126.72
42	1	235	A2M	C5-C4-N3	-4.87	120.01	126.72
37	2	1384	A2M	C5-C6-N6	4.87	135.33	123.29
37	2	1185	A2M	C4-N9-C8	4.86	110.84	105.74
42	1	927	A2M	C4-N9-C8	4.85	110.83	105.74
37	2	437	PSU	N1-C2-N3	4.85	120.28	115.17
37	2	382	A2M	C4-N9-C8	4.84	110.82	105.74
37	2	628	A2M	C5-C4-N3	-4.83	120.06	126.72
29	S1	600	OMG	C5-C4-N3	-4.82	120.71	128.39
37	2	604	A2M	C4-N9-C1'	-4.82	115.36	126.63
29	S1	12	PSU	C4-N3-C2	-4.82	119.74	126.37
42	1	858	A2M	C5-C4-N3	-4.81	120.09	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	955	A2M	C4-N9-C8	4.80	110.78	105.74
42	1	856	OMG	C1'-N9-C4	4.80	140.67	126.49
42	1	678	A2M	C4-N9-C8	4.79	110.77	105.74
29	S1	2021	A2M	C5-C4-N3	-4.79	120.12	126.72
42	1	697	A2M	C5-C4-N3	-4.78	120.13	126.72
37	2	591	A2M	N3-C4-N9	4.78	135.30	127.17
37	2	1384	A2M	C5-C4-N3	-4.77	120.14	126.72
37	2	1144	PSU	C4-N3-C2	-4.77	119.80	126.37
38	7	43	A2M	C5-C4-N3	-4.76	120.16	126.72
37	2	1354	PSU	N1-C2-N3	4.76	120.18	115.17
41	3	13	OMU	N3-C2-N1	4.75	121.07	114.89
37	2	95	A2M	C4-N9-C1'	-4.73	115.57	126.63
37	2	1194	PSU	C4-N3-C2	-4.72	119.87	126.37
37	2	71	OMG	N9-C4-N3	4.72	135.38	125.95
42	1	678	A2M	N3-C4-N9	4.71	135.18	127.17
42	1	1539	A2M	C5-C4-N3	-4.71	120.23	126.72
42	1	959[B]	OMG	C5-C4-N3	-4.70	120.90	128.39
42	1	681	A2M	C5-C4-N3	-4.68	120.27	126.72
37	2	570	A2M	C4-N9-C1'	-4.68	115.70	126.63
37	2	512	PSU	C4-N3-C2	-4.67	119.93	126.37
37	2	95	A2M	C4-N9-C8	4.67	110.64	105.74
42	1	1017	PSU	C4-N3-C2	-4.67	119.94	126.37
37	2	662	PSU	N1-C2-N3	4.66	120.09	115.17
42	1	235	A2M	C4-N9-C8	4.66	110.63	105.74
42	1	955	A2M	N3-C4-N9	4.66	135.09	127.17
37	2	1382	PSU	N1-C2-N3	4.65	120.08	115.17
42	1	870	PSU	N1-C2-N3	4.65	120.07	115.17
37	2	667	OMU	N3-C2-N1	4.64	120.93	114.89
29	S1	104	PSU	C4-N3-C2	-4.64	119.98	126.37
29	S1	2048	PSU	C4-N3-C2	-4.64	119.98	126.37
29	S1	512	A2M	C2'-C1'-N9	-4.63	106.13	113.75
38	7	75	OMG	N9-C4-N3	4.63	135.21	125.95
37	2	512	PSU	N1-C2-N3	4.63	120.05	115.17
42	1	959[A]	OMG	C5-C4-N3	-4.62	121.03	128.39
42	1	422	PSU	C4-N3-C2	-4.61	120.01	126.37
38	7	162	A2M	C5-C4-N3	-4.61	120.36	126.72
37	2	604	A2M	C4-N9-C8	4.61	110.58	105.74
37	2	628	A2M	C4-N9-C8	4.60	110.57	105.74
42	1	1539	A2M	C4-N9-C8	4.60	110.56	105.74
29	S1	1647	OMG	C5-C4-N3	-4.59	121.08	128.39
37	2	662	PSU	C4-N3-C2	-4.59	120.05	126.37
29	S1	1657	PSU	C4-N3-C2	-4.59	120.06	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1194	PSU	N1-C2-N3	4.58	120.00	115.17
29	S1	455	PSU	C4-N3-C2	-4.58	120.06	126.37
37	2	73	OMU	N3-C2-N1	4.57	120.84	114.89
37	2	1361	PSU	N1-C2-N3	4.57	119.99	115.17
37	2	1046	OMG	C5-C4-N3	-4.56	121.13	128.39
42	1	1524	OMG	C2-N3-C4	4.56	120.15	112.30
38	7	69	PSU	C4-N3-C2	-4.55	120.11	126.37
29	S1	1566	PSU	C4-N3-C2	-4.55	120.11	126.37
42	1	858	A2M	C4-N9-C8	4.55	110.51	105.74
37	2	628	A2M	C1'-N9-C8	4.54	137.18	127.09
29	S1	1829	OMG	C5-C4-N3	-4.54	121.16	128.39
37	2	655	OMG	C2-N3-C4	4.54	120.12	112.30
42	1	856	OMG	C2-N3-C4	4.53	120.10	112.30
37	2	1403	PSU	C4-N3-C2	-4.53	120.13	126.37
37	2	1060	PSU	C4-N3-C2	-4.53	120.13	126.37
29	S1	2151	OMG	C5-C4-N3	-4.53	121.18	128.39
37	2	572	A2M	C5-C4-N3	-4.53	120.48	126.72
38	7	162	A2M	C4-N9-C8	4.53	110.49	105.74
42	1	1528	PSU	C4-N3-C2	-4.53	120.14	126.37
37	2	472	PSU	C4-N3-C2	-4.52	120.14	126.37
42	1	681	A2M	C4-N9-C8	4.52	110.49	105.74
42	1	672	PSU	C4-N3-C2	-4.51	120.16	126.37
42	1	927	A2M	C4-N9-C1'	-4.51	116.09	126.63
42	1	1533	PSU	C4-N3-C2	-4.51	120.16	126.37
37	2	597	PSU	C4-N3-C2	-4.50	120.17	126.37
37	2	1372	A2M	C1'-N9-C8	4.50	137.08	127.09
37	2	1229	OMG	C2-N3-C4	4.50	120.04	112.30
37	2	1078	OMG	C2-N3-C4	4.49	120.03	112.30
37	2	593	PSU	C4-N3-C2	-4.49	120.19	126.37
37	2	1152	OMU	N3-C2-N1	4.48	120.73	114.89
37	2	570	A2M	C2'-C1'-N9	-4.48	106.38	113.75
29	S1	1995	G7M	C2-N3-C4	4.48	120.01	112.30
37	2	534	OMG	C5-C4-N3	-4.47	121.28	128.39
42	1	239	PSU	C4-N3-C2	-4.47	120.22	126.37
29	S1	1539	PSU	C4-N3-C2	-4.47	120.22	126.37
37	2	1372	A2M	C5-C4-N3	-4.46	120.57	126.72
42	1	927	A2M	N3-C4-N9	4.46	134.75	127.17
29	S1	12	PSU	N1-C2-N3	4.45	119.86	115.17
37	2	1046	OMG	C2-N3-C4	4.45	119.96	112.30
29	S1	1647	OMG	C2-N3-C4	4.45	119.96	112.30
29	S1	1879	OMG	C5-C4-N3	-4.44	121.32	128.39
42	1	407	A2M	C5-C4-N3	-4.44	120.60	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	1524	OMG	C5-C4-N3	-4.44	121.32	128.39
37	2	1058	PSU	C4-N3-C2	-4.43	120.26	126.37
42	1	1181	PSU	C4-N3-C2	-4.43	120.26	126.37
37	2	570	A2M	N3-C4-N9	4.43	134.69	127.17
29	S1	600	OMG	C2-N3-C4	4.42	119.92	112.30
29	S1	1192	PSU	C4-N3-C2	-4.42	120.28	126.37
37	2	1360	OMG	C5-C4-N3	-4.41	121.37	128.39
29	S1	1478	OMG	C5-C4-N3	-4.41	121.38	128.39
42	1	1107	OMU	N3-C2-N1	4.40	120.62	114.89
29	S1	1246	PSU	C4-N3-C2	-4.40	120.31	126.37
29	S1	1879	OMG	C2-N3-C4	4.39	119.86	112.30
29	S1	104	PSU	N1-C2-N3	4.39	119.80	115.17
37	2	1231	OMG	C2-N3-C4	4.38	119.84	112.30
37	2	78	PSU	C4-N3-C2	-4.38	120.34	126.37
29	S1	455	PSU	N1-C2-N3	4.37	119.78	115.17
37	2	534	OMG	C2-N3-C4	4.37	119.82	112.30
37	2	1360	OMG	C2-N3-C4	4.37	119.82	112.30
29	S1	1623	OMG	N9-C4-N3	4.36	134.67	125.95
42	1	1402	PSU	N1-C2-N3	4.36	119.77	115.17
40	4	74	OMG	C2-N3-C4	4.35	119.80	112.30
42	1	305	A2M	C4-N9-C8	4.35	110.31	105.74
42	1	1626	OMG	C2-N3-C4	4.35	119.79	112.30
42	1	847	OMU	N3-C2-N1	4.35	120.55	114.89
29	S1	1543	C4J	C4-N3-C2	-4.35	120.27	125.62
37	2	655	OMG	C5-C4-N3	-4.35	121.47	128.39
37	2	604	A2M	N3-C4-N9	4.34	134.55	127.17
29	S1	512	A2M	N3-C4-N9	4.34	134.54	127.17
37	2	95	A2M	N3-C4-N9	4.34	134.54	127.17
37	2	1185	A2M	N3-C4-N9	4.33	134.53	127.17
37	2	1253	OMG	C2-N3-C4	4.32	119.75	112.30
42	1	959[A]	OMG	C2-N3-C4	4.32	119.74	112.30
29	S1	1995	G7M	C5-C4-N3	-4.32	119.99	128.15
37	2	641	OMG	C2-N3-C4	4.32	119.73	112.30
37	2	382	A2M	C5-C4-N3	-4.31	120.78	126.72
38	7	74	PSU	C4-N3-C2	-4.31	120.44	126.37
29	S1	1550	OMG	C5-C4-N3	-4.30	121.55	128.39
42	1	1190	OMG	C2-N3-C4	4.29	119.69	112.30
42	1	1190	OMG	C5-C4-N3	-4.28	121.57	128.39
29	S1	1533	PSU	C4-N3-C2	-4.28	120.47	126.37
29	S1	1657	PSU	O2-C2-N1	-4.26	118.39	122.79
29	S1	1566	PSU	N1-C2-N3	4.26	119.66	115.17
42	1	1664	PSU	C4-N3-C2	-4.26	120.50	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1419	OMU	N3-C2-N1	4.25	120.42	114.89
37	2	382	A2M	C1'-N9-C8	4.25	136.53	127.09
42	1	1371	OMU	C5-C4-N3	4.24	120.74	114.80
29	S1	1550	OMG	C2-N3-C4	4.24	119.60	112.30
42	1	959[B]	OMG	C2-N3-C4	4.24	119.60	112.30
29	S1	1829	OMG	C2-N3-C4	4.23	119.58	112.30
29	S1	1478	OMG	C2-N3-C4	4.23	119.58	112.30
29	S1	1865	OMG	C5-C4-N3	-4.22	121.68	128.39
42	1	1540	OMG	C2-N3-C4	4.22	119.56	112.30
37	2	1077	OMU	N3-C2-N1	4.22	120.38	114.89
29	S1	2151	OMG	C2-N3-C4	4.21	119.55	112.30
37	2	510	PSU	C4-N3-C2	-4.20	120.59	126.37
29	S1	1865	OMG	C2-N3-C4	4.20	119.53	112.30
37	2	1384	A2M	N3-C4-N9	4.20	134.31	127.17
41	3	13	OMU	C5-C4-N3	4.19	120.67	114.80
37	2	1359	OMU	C5-C4-N3	4.19	120.67	114.80
42	1	1371	OMU	N3-C2-N1	4.19	120.34	114.89
37	2	1303	PSU	C4-N3-C2	-4.18	120.61	126.37
37	2	560	OMU	N3-C2-N1	4.17	120.32	114.89
37	2	1359	OMU	N3-C2-N1	4.17	120.31	114.89
29	S1	1841	PSU	C4-N3-C2	-4.15	120.65	126.37
37	2	1231	OMG	C5-C4-N3	-4.15	121.78	128.39
37	2	1078	OMG	C5-C4-N3	-4.15	121.78	128.39
37	2	1264	PSU	C4-N3-C2	-4.15	120.65	126.37
29	S1	2046	PSU	C4-N3-C2	-4.15	120.65	126.37
37	2	1253	OMG	C5-C4-N3	-4.14	121.79	128.39
37	2	527	A2M	N3-C4-N9	4.13	134.19	127.17
29	S1	8	OMU	N3-C2-N1	4.11	120.25	114.89
37	2	1229	OMG	C5-C4-N3	-4.11	121.85	128.39
42	1	697	A2M	N3-C4-N9	4.11	134.16	127.17
42	1	305	A2M	O4'-C1'-C2'	-4.11	99.52	106.59
41	3	13	OMU	C1'-N1-C2	4.10	124.95	117.59
29	S1	607	PSU	C4-N3-C2	-4.10	120.73	126.37
37	2	73	OMU	C5-C4-N3	4.10	120.54	114.80
29	S1	33	PSU	C4-N3-C2	-4.08	120.75	126.37
42	1	845	OMU	C1'-N1-C2	4.05	124.87	117.59
29	S1	609	PSU	C4-N3-C2	-4.05	120.80	126.37
29	S1	1156	PSU	C4-N3-C2	-4.04	120.80	126.37
37	2	572	A2M	C1'-N9-C8	4.03	136.05	127.09
40	4	74	OMG	C5-C4-N3	-4.03	121.97	128.39
29	S1	2021	A2M	C1'-N9-C8	4.02	136.02	127.09
42	1	235	A2M	N3-C4-N9	4.02	134.01	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	667	OMU	C5-C4-N3	4.02	120.43	114.80
42	1	847	OMU	C5-C4-N3	4.00	120.40	114.80
42	1	678	A2M	C4-N9-C1'	-4.00	117.28	126.63
42	1	672	PSU	O2-C2-N1	-4.00	118.67	122.79
42	1	422	PSU	O2-C2-N1	-3.99	118.67	122.79
29	S1	1156	PSU	C3'-C2'-C1'	3.98	106.39	101.69
42	1	1533	PSU	O2-C2-N1	-3.98	118.68	122.79
37	2	527	A2M	O4'-C1'-C2'	-3.98	99.73	106.59
29	S1	2048	PSU	O2-C2-N1	-3.97	118.69	122.79
29	S1	661	OMU	N3-C2-N1	3.97	120.06	114.89
29	S1	668	A2M	C1'-N9-C8	3.97	135.90	127.09
42	1	1626	OMG	C5-C4-N3	-3.95	122.10	128.39
42	1	305	A2M	O4'-C1'-N9	3.95	115.67	108.09
29	S1	668	A2M	N3-C4-N9	3.94	133.87	127.17
42	1	681	A2M	N3-C4-N9	3.94	133.87	127.17
42	1	1539	A2M	N3-C4-N9	3.94	133.87	127.17
42	1	858	A2M	N3-C4-N9	3.92	133.83	127.17
37	2	1077	OMU	C5-C4-N3	3.91	120.28	114.80
37	2	510	PSU	N1-C2-N3	3.91	119.30	115.17
38	7	43	A2M	N3-C4-N9	3.91	133.82	127.17
37	2	1229	OMG	N9-C8-N7	-3.91	106.15	113.40
42	1	1017	PSU	O2-C2-N1	-3.90	118.76	122.79
37	2	1144	PSU	O2-C2-N1	-3.90	118.77	122.79
37	2	1318	PSU	C6-N1-C2	-3.90	119.07	122.69
37	2	641	OMG	C5-C4-N3	-3.90	122.19	128.39
42	1	1107	OMU	C5-C4-N3	3.90	120.26	114.80
37	2	527	A2M	C4'-O4'-C1'	-3.89	100.87	109.47
38	7	162	A2M	C1'-N9-C8	3.89	135.72	127.09
37	2	1308	5MC	C5-C6-N1	-3.89	119.09	123.31
37	2	71	OMG	C2'-C1'-N9	-3.88	106.87	114.24
42	1	1659	OMU	N3-C2-N1	3.87	119.94	114.89
29	S1	2021	A2M	N3-C4-N9	3.87	133.75	127.17
37	2	1384	A2M	C1'-N9-C8	3.87	135.68	127.09
37	2	662	PSU	C6-N1-C2	-3.86	119.11	122.69
38	7	7	OMU	N3-C2-N1	3.85	119.90	114.89
29	S1	1979	OMU	N3-C2-N1	3.84	119.90	114.89
40	4	74	OMG	N9-C8-N7	-3.83	106.29	113.40
42	1	1659	OMU	C5-C4-N3	3.83	120.17	114.80
42	1	856	OMG	N9-C8-N7	-3.83	106.30	113.40
42	1	1181	PSU	O2-C2-N1	-3.83	118.84	122.79
38	7	7	OMU	C5-C4-N3	3.83	120.16	114.80
37	2	1231	OMG	N9-C8-N7	-3.83	106.31	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	1528	PSU	O2-C2-N1	-3.82	118.85	122.79
42	1	1540	OMG	N9-C8-N7	-3.80	106.35	113.40
42	1	407	A2M	N3-C4-N9	3.80	133.63	127.17
29	S1	1995	G7M	C5-C6-N1	3.80	119.69	111.84
37	2	591	A2M	C2-N3-C4	3.80	121.10	111.83
42	1	239	PSU	O2-C2-N1	-3.80	118.88	122.79
29	S1	1192	PSU	C3'-C2'-C1'	3.78	106.15	101.69
29	S1	1246	PSU	O2-C2-N1	-3.77	118.90	122.79
37	2	1264	PSU	O2-C2-N1	-3.77	118.90	122.79
29	S1	33	PSU	O2-C2-N1	-3.76	118.91	122.79
42	1	858	A2M	C1'-N9-C8	3.76	135.44	127.09
38	7	69	PSU	C3'-C2'-C1'	3.75	106.12	101.69
38	7	43	A2M	C1'-N9-C8	3.75	135.41	127.09
29	S1	661	OMU	C5-C4-N3	3.74	120.04	114.80
38	7	162	A2M	N3-C4-N9	3.73	133.52	127.17
37	2	1419	OMU	C5-C4-N3	3.73	120.03	114.80
29	S1	1539	PSU	O2-C2-N1	-3.73	118.94	122.79
29	S1	1979	OMU	C5-C4-N3	3.73	120.02	114.80
42	1	1190	OMG	N9-C8-N7	-3.72	106.49	113.40
37	2	1413	PSU	C6-N1-C2	-3.72	119.23	122.69
29	S1	1879	OMG	N9-C8-N7	-3.72	106.50	113.40
37	2	1060	PSU	O2-C2-N1	-3.72	118.95	122.79
37	2	1152	OMU	C5-C4-N3	3.72	120.01	114.80
42	1	1626	OMG	N9-C8-N7	-3.72	106.51	113.40
29	S1	2151	OMG	N9-C8-N7	-3.70	106.53	113.40
42	1	1664	PSU	O2-C2-N1	-3.70	118.98	122.79
38	7	69	PSU	O2-C2-N1	-3.69	118.98	122.79
37	2	626	PSU	C6-N1-C2	-3.69	119.27	122.69
29	S1	1192	PSU	O2-C2-N1	-3.68	118.99	122.79
37	2	597	PSU	O2-C2-N1	-3.68	118.99	122.79
29	S1	1841	PSU	O2-C2-N1	-3.68	119.00	122.79
42	1	1371	OMU	C1'-N1-C2	3.67	124.19	117.59
29	S1	607	PSU	O2-C2-N1	-3.67	119.00	122.79
42	1	235	A2M	C1'-N9-C8	3.67	135.24	127.09
37	2	382	A2M	N3-C4-N9	3.67	133.41	127.17
42	1	697	A2M	C1'-N9-C8	3.67	135.23	127.09
37	2	560	OMU	C5-C4-N3	3.66	119.92	114.80
37	2	78	PSU	O2-C2-N1	-3.65	119.02	122.79
29	S1	1550	OMG	N9-C8-N7	-3.65	106.63	113.40
37	2	655	OMG	N9-C8-N7	-3.65	106.63	113.40
37	2	527	A2M	C2'-C1'-N9	-3.65	107.75	113.75
29	S1	1533	PSU	O2-C2-N1	-3.64	119.03	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	641	OMG	N9-C8-N7	-3.64	106.66	113.40
37	2	527	A2M	C1'-N9-C8	3.63	135.15	127.09
37	2	1303	PSU	O2-C2-N1	-3.63	119.05	122.79
29	S1	1865	OMG	N9-C8-N7	-3.63	106.67	113.40
37	2	572	A2M	N3-C4-N9	3.63	133.34	127.17
42	1	305	A2M	C1'-N9-C8	3.61	135.11	127.09
29	S1	512	A2M	C2-N3-C4	3.61	120.64	111.83
37	2	1303	PSU	C3'-C2'-C1'	3.61	105.94	101.69
42	1	955	A2M	C2-N3-C4	3.60	120.62	111.83
29	S1	8	OMU	C5-C4-N3	3.60	119.84	114.80
37	2	527	A2M	O4'-C1'-N9	3.60	114.99	108.09
42	1	305	A2M	C3'-C2'-C1'	-3.59	95.92	102.81
29	S1	607	PSU	C3'-C2'-C1'	3.59	105.92	101.69
42	1	959[A]	OMG	N9-C8-N7	-3.58	106.75	113.40
37	2	1078	OMG	N9-C8-N7	-3.58	106.76	113.40
37	2	472	PSU	O2-C2-N1	-3.58	119.10	122.79
37	2	628	A2M	N3-C4-N9	3.57	133.25	127.17
37	2	1194	PSU	C6-N1-C2	-3.57	119.37	122.69
42	1	940	PSU	C6-N1-C2	-3.57	119.38	122.69
37	2	1058	PSU	O2-C2-N1	-3.56	119.12	122.79
37	2	437	PSU	C6-N1-C2	-3.56	119.39	122.69
37	2	570	A2M	C5-N7-C8	3.56	109.04	103.45
42	1	1524	OMG	N9-C8-N7	-3.56	106.80	113.40
42	1	927	A2M	C2-N3-C4	3.55	120.51	111.83
42	1	845	OMU	C5-C4-N3	3.54	119.76	114.80
42	1	856	OMG	C5-C4-N3	-3.54	122.75	128.39
37	2	1046	OMG	N9-C8-N7	-3.54	106.83	113.40
42	1	858	A2M	C2-N3-C4	3.53	120.45	111.83
29	S1	1478	OMG	N9-C8-N7	-3.52	106.87	113.40
29	S1	1647	OMG	N9-C8-N7	-3.52	106.87	113.40
37	2	1372	A2M	N3-C4-N9	3.51	133.14	127.17
37	2	1403	PSU	O2-C2-N1	-3.50	119.18	122.79
29	S1	2021	A2M	C5-N7-C8	3.50	108.94	103.45
37	2	591	A2M	C4-C5-N7	-3.47	106.62	110.58
37	2	527	A2M	C2-N3-C4	3.47	120.30	111.83
37	2	512	PSU	C6-N1-C2	-3.47	119.47	122.69
29	S1	600	OMG	N9-C8-N7	-3.47	106.97	113.40
42	1	305	A2M	C5-C4-N3	-3.46	121.95	126.72
42	1	1540	OMG	C5-C4-N3	-3.46	122.89	128.39
38	7	43	A2M	C2-N3-C4	3.45	120.25	111.83
29	S1	104	PSU	C6-N1-C2	-3.44	119.50	122.69
42	1	927	A2M	C5-N7-C8	3.44	108.86	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	678	A2M	C2-N3-C4	3.44	120.23	111.83
37	2	593	PSU	O2-C2-N1	-3.43	119.25	122.79
42	1	681	A2M	C2-N3-C4	3.43	120.21	111.83
37	2	1372	A2M	C5-N7-C8	3.43	108.83	103.45
29	S1	1623	OMG	C6-C5-N7	3.42	136.52	130.29
38	7	162	A2M	C2-N3-C4	3.42	120.19	111.83
37	2	628	A2M	C2-N3-C4	3.42	120.18	111.83
37	2	1360	OMG	N9-C8-N7	-3.41	107.07	113.40
42	1	681	A2M	C1'-N9-C8	3.41	134.66	127.09
29	S1	512	A2M	N3-C2-N1	-3.40	123.44	128.58
38	7	74	PSU	O2-C2-N1	-3.40	119.29	122.79
37	2	1253	OMG	N9-C8-N7	-3.39	107.11	113.40
29	S1	668	A2M	C5-N7-C8	3.39	108.78	103.45
38	7	162	A2M	C2'-C1'-N9	3.38	119.32	113.75
37	2	572	A2M	C2-N3-C4	3.38	120.09	111.83
37	2	1354	PSU	C6-N1-C2	-3.38	119.56	122.69
42	1	678	A2M	C5-N7-C8	3.37	108.75	103.45
29	S1	455	PSU	C6-N1-C2	-3.37	119.57	122.69
37	2	628	A2M	C5-N7-C8	3.36	108.74	103.45
42	1	856	OMG	C2'-C1'-N9	-3.36	107.86	114.24
37	2	1384	A2M	C2-N3-C4	3.35	120.02	111.83
42	1	955	A2M	C5-N7-C8	3.35	108.71	103.45
37	2	510	PSU	C6-N1-C2	-3.34	119.59	122.69
29	S1	512	A2M	C4-C5-N7	-3.33	106.77	110.58
42	1	697	A2M	C2-N3-C4	3.33	119.97	111.83
42	1	235	A2M	C2-N3-C4	3.33	119.96	111.83
42	1	407	A2M	C1'-N9-C8	3.32	134.47	127.09
42	1	407	A2M	C5-N7-C8	3.32	108.67	103.45
29	S1	2021	A2M	C2-N3-C4	3.32	119.94	111.83
38	7	75	OMG	C6-C5-N7	3.32	136.34	130.29
29	S1	1566	PSU	C6-N1-C2	-3.32	119.61	122.69
37	2	71	OMG	C6-C5-N7	3.31	136.32	130.29
29	S1	609	PSU	O2-C2-N1	-3.31	119.37	122.79
29	S1	2046	PSU	O2-C2-N1	-3.30	119.39	122.79
29	S1	1156	PSU	O2-C2-N1	-3.29	119.39	122.79
42	1	407	A2M	C2-N3-C4	3.29	119.87	111.83
37	2	1185	A2M	C2-N3-C4	3.29	119.87	111.83
29	S1	1995	G7M	O6-C6-C5	-3.29	120.66	128.01
37	2	591	A2M	N3-C2-N1	-3.29	123.61	128.58
29	S1	1829	OMG	N9-C8-N7	-3.29	107.31	113.40
37	2	1372	A2M	C2-N3-C4	3.28	119.85	111.83
37	2	95	A2M	C2-N3-C4	3.28	119.84	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	534	OMG	N9-C8-N7	-3.28	107.32	113.40
42	1	1524	OMG	C2-N1-C6	-3.27	119.17	125.11
38	7	75	OMG	C2'-C1'-N9	-3.27	108.04	114.24
42	1	1664	PSU	C3'-C2'-C1'	3.26	105.54	101.69
37	2	527	A2M	C5-N7-C8	3.26	108.57	103.45
37	2	1403	PSU	C3'-C2'-C1'	3.26	105.53	101.69
37	2	593	PSU	C3'-C2'-C1'	3.25	105.53	101.69
29	S1	668	A2M	C2-N3-C4	3.24	119.74	111.83
37	2	1185	A2M	C5-N7-C8	3.23	108.52	103.45
37	2	604	A2M	C2-N3-C4	3.23	119.71	111.83
42	1	1539	A2M	C2-N3-C4	3.23	119.71	111.83
37	2	1253	OMG	C2-N1-C6	-3.22	119.26	125.11
42	1	870	PSU	C6-N1-C2	-3.22	119.70	122.69
37	2	604	A2M	C5-N7-C8	3.22	108.52	103.45
42	1	1011	PSU	C6-C5-C4	3.22	120.35	118.17
29	S1	609	PSU	C3'-C2'-C1'	3.22	105.48	101.69
37	2	570	A2M	C2-N3-C4	3.21	119.68	111.83
42	1	1539	A2M	C1'-N9-C8	3.21	134.23	127.09
37	2	382	A2M	C2-N3-C4	3.21	119.68	111.83
37	2	1382	PSU	C6-N1-C2	-3.21	119.72	122.69
29	S1	12	PSU	C6-N1-C2	-3.19	119.73	122.69
42	1	858	A2M	C5-N7-C8	3.19	108.46	103.45
38	7	43	A2M	C5-N7-C8	3.18	108.45	103.45
37	2	1185	A2M	C1'-N9-C8	3.18	134.16	127.09
42	1	955	A2M	C1'-N9-C8	3.18	134.15	127.09
42	1	697	A2M	C5-N7-C8	3.16	108.41	103.45
42	1	1533	PSU	C3'-C2'-C1'	3.15	105.41	101.69
42	1	1011	PSU	C6-N1-C2	-3.14	119.77	122.69
29	S1	1979	OMU	O4-C4-C5	-3.14	119.75	125.16
37	2	604	A2M	C1'-N9-C8	3.12	134.01	127.09
37	2	655	OMG	C2-N1-C6	-3.11	119.46	125.11
37	2	95	A2M	C5-N7-C8	3.11	108.34	103.45
42	1	305	A2M	N3-C4-N9	3.11	132.46	127.17
37	2	572	A2M	C5-N7-C8	3.11	108.34	103.45
29	S1	1544	5MC	C5-C6-N1	-3.11	119.94	123.31
42	1	1539	A2M	C5-N7-C8	3.10	108.32	103.45
29	S1	1841	PSU	C3'-C2'-C1'	3.10	105.34	101.69
37	2	1361	PSU	C6-N1-C2	-3.09	119.82	122.69
42	1	235	A2M	C5-N7-C8	3.09	108.30	103.45
42	1	940	PSU	O2-C2-N1	-3.07	119.62	122.79
37	2	641	OMG	C2-N1-C6	-3.07	119.55	125.11
29	S1	1995	G7M	C2-N1-C6	-3.06	119.56	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1478	OMG	C2-N1-C6	-3.04	119.59	125.11
29	S1	2151	OMG	C2-N1-C6	-3.04	119.59	125.11
37	2	1253	OMG	C5-C6-N1	3.04	121.00	113.25
37	2	1384	A2M	C5-N7-C8	3.01	108.19	103.45
29	S1	1879	OMG	C2-N1-C6	-3.01	119.65	125.11
42	1	845	OMU	O2-C2-N3	-3.01	115.94	121.49
29	S1	2061	5MC	C5-C4-N3	-3.00	118.68	121.75
42	1	672	PSU	C3'-C2'-C1'	3.00	105.23	101.69
42	1	1659	OMU	O4-C4-C5	-2.99	120.00	125.16
29	S1	1550	OMG	C2-N1-C6	-2.99	119.69	125.11
37	2	534	OMG	C2-N1-C6	-2.98	119.70	125.11
37	2	1360	OMG	C2-N1-C6	-2.98	119.71	125.11
42	1	1626	OMG	C2-N1-C6	-2.98	119.71	125.11
42	1	1528	PSU	C3'-C2'-C1'	2.98	105.20	101.69
37	2	1078	OMG	C2-N1-C6	-2.97	119.72	125.11
37	2	1229	OMG	C2-N1-C6	-2.97	119.72	125.11
42	1	856	OMG	C5-C6-N1	2.97	120.82	113.25
37	2	95	A2M	C1'-N9-C8	2.96	133.67	127.09
37	2	73	OMU	O4-C4-C5	-2.96	120.06	125.16
42	1	407	A2M	C2'-C1'-N9	-2.95	108.89	113.75
38	7	162	A2M	C5-N7-C8	2.95	108.09	103.45
37	2	1046	OMG	C2-N1-C6	-2.95	119.77	125.11
42	1	847	OMU	O4-C4-C5	-2.94	120.08	125.16
37	2	1419	OMU	O4-C4-C5	-2.94	120.09	125.16
42	1	239	PSU	C3'-C2'-C1'	2.93	105.15	101.69
42	1	1190	OMG	C2-N1-C6	-2.93	119.81	125.11
29	S1	661	OMU	O4-C4-C5	-2.92	120.12	125.16
29	S1	600	OMG	C2-N1-C6	-2.92	119.81	125.11
29	S1	2061	5MC	C5-C6-N1	-2.92	120.15	123.31
42	1	1181	PSU	C3'-C2'-C1'	2.91	105.13	101.69
29	S1	1829	OMG	C2-N1-C6	-2.91	119.83	125.11
29	S1	2046	PSU	C3'-C2'-C1'	2.91	105.12	101.69
38	7	7	OMU	O4-C4-C5	-2.91	120.14	125.16
42	1	959[A]	OMG	N9-C4-N3	2.90	131.76	125.95
29	S1	600	OMG	N9-C4-N3	2.90	131.75	125.95
37	2	655	OMG	C5-C6-N1	2.90	120.62	113.25
29	S1	1647	OMG	C2-N1-C6	-2.89	119.86	125.11
37	2	1359	OMU	O4-C4-C5	-2.89	120.17	125.16
37	2	1229	OMG	C5-C6-N1	2.89	120.61	113.25
37	2	1231	OMG	C2-N1-C6	-2.89	119.87	125.11
40	4	74	OMG	C2-N1-C6	-2.89	119.88	125.11
37	2	667	OMU	O4-C4-C5	-2.88	120.19	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	959[B]	OMG	C2-N1-C6	-2.88	119.89	125.11
42	1	1626	OMG	C5-C6-N1	2.85	120.50	113.25
41	3	13	OMU	O4-C4-C5	-2.85	120.25	125.16
29	S1	1865	OMG	O6-C6-C5	-2.84	119.03	126.53
29	S1	1623	OMG	C2'-C1'-N9	-2.84	108.84	114.24
29	S1	1865	OMG	C2-N1-C6	-2.84	119.96	125.11
29	S1	2151	OMG	N9-C4-N3	2.84	131.62	125.95
38	7	74	PSU	C3'-C2'-C1'	2.83	105.03	101.69
42	1	681	A2M	C5-N7-C8	2.83	107.90	103.45
37	2	1078	OMG	C5-C6-N1	2.82	120.42	113.25
37	2	1360	OMG	C5-C6-N1	2.81	120.40	113.25
37	2	641	OMG	C5-C6-N1	2.81	120.40	113.25
29	S1	1879	OMG	C5-C6-N1	2.80	120.39	113.25
42	1	1524	OMG	C5-C6-N1	2.79	120.36	113.25
29	S1	8	OMU	O4-C4-C5	-2.79	120.34	125.16
42	1	1540	OMG	C5-C6-N1	2.79	120.34	113.25
37	2	560	OMU	O4-C4-C5	-2.78	120.36	125.16
42	1	1107	OMU	O4-C4-C5	-2.78	120.37	125.16
42	1	1190	OMG	C5-C6-N1	2.77	120.29	113.25
37	2	1231	OMG	C5-C6-N1	2.77	120.29	113.25
29	S1	1543	C4J	N3-C2-N1	2.76	120.09	116.72
37	2	570	A2M	O2'-C2'-C1'	2.76	114.23	108.99
42	1	1371	OMU	O4-C4-C5	-2.76	120.41	125.16
37	2	382	A2M	C5-N7-C8	2.76	107.78	103.45
37	2	534	OMG	C5-C6-N1	2.75	120.26	113.25
29	S1	1550	OMG	C5-C6-N1	2.74	120.23	113.25
37	2	641	OMG	N2-C2-N1	2.74	122.54	116.76
29	S1	12	PSU	C6-C5-C4	2.74	120.02	118.17
40	4	74	OMG	C5-C6-N1	2.73	120.21	113.25
37	2	570	A2M	C1'-N9-C8	2.73	133.15	127.09
37	2	597	PSU	C3'-C2'-C1'	2.72	104.90	101.69
29	S1	2048	PSU	C5-C6-N1	-2.72	118.36	122.14
37	2	591	A2M	C4-N9-C8	2.72	108.60	105.74
29	S1	104	PSU	O2-C2-N1	-2.72	119.98	122.79
42	1	1524	OMG	N2-C2-N1	2.71	122.49	116.76
37	2	71	OMG	C4-C5-N7	-2.71	106.37	110.67
29	S1	1647	OMG	C5-C6-N1	2.71	120.15	113.25
37	2	512	PSU	C6-C5-C4	2.71	120.00	118.17
29	S1	2151	OMG	C5-C6-N1	2.70	120.14	113.25
29	S1	1478	OMG	C5-C6-N1	2.70	120.13	113.25
29	S1	512	A2M	C4-N9-C8	2.70	108.57	105.74
29	S1	455	PSU	O2-C2-N1	-2.69	120.01	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	959[A]	OMG	C2-N1-C6	-2.69	120.23	125.11
37	2	1077	OMU	O4-C4-C5	-2.69	120.53	125.16
37	2	1144	PSU	C5-C6-N1	-2.69	118.41	122.14
37	2	626	PSU	O2-C2-N1	-2.68	120.02	122.79
37	2	1078	OMG	N2-C2-N1	2.68	122.42	116.76
29	S1	1647	OMG	N9-C4-N3	2.68	131.31	125.95
42	1	845	OMU	C6-C5-C4	2.68	122.96	119.53
29	S1	1865	OMG	C5-C6-N1	2.68	120.06	113.25
42	1	856	OMG	C6-C5-N7	2.67	135.15	130.29
37	2	1152	OMU	O4-C4-C5	-2.67	120.56	125.16
42	1	927	A2M	C1'-N9-C8	2.67	133.02	127.09
37	2	1060	PSU	C3'-C2'-C1'	2.67	104.83	101.69
29	S1	1829	OMG	N9-C4-N3	2.66	131.28	125.95
37	2	512	PSU	O2-C2-N1	-2.66	120.04	122.79
37	2	1194	PSU	O2-C2-N1	-2.66	120.04	122.79
29	S1	1623	OMG	C4-C5-N7	-2.66	106.46	110.67
42	1	858	A2M	C4'-O4'-C1'	-2.66	103.60	109.47
37	2	1046	OMG	C5-C6-N1	2.66	120.02	113.25
37	2	472	PSU	C5-C6-N1	-2.66	118.45	122.14
37	2	641	OMG	O6-C6-C5	-2.65	119.55	126.53
29	S1	2061	5MC	C2'-C1'-N1	-2.64	105.89	113.25
38	7	75	OMG	C4-C5-N7	-2.64	106.48	110.67
29	S1	1879	OMG	N9-C4-N3	2.64	131.24	125.95
42	1	1540	OMG	C2-N1-C6	-2.64	120.33	125.11
29	S1	600	OMG	C5-C6-N1	2.64	119.97	113.25
37	2	1229	OMG	O6-C6-C5	-2.64	119.57	126.53
29	S1	1192	PSU	C5-C6-N1	-2.63	118.49	122.14
37	2	1354	PSU	O2-C2-N1	-2.60	120.11	122.79
29	S1	1829	OMG	C5-C6-N1	2.60	119.86	113.25
42	1	1539	A2M	C2'-C1'-N9	2.59	118.01	113.75
37	2	437	PSU	C6-C5-C4	2.58	119.92	118.17
42	1	1171	PSU	C5-C4-N3	2.58	122.23	116.55
37	2	591	A2M	C5-N7-C8	2.58	107.51	103.45
41	3	13	OMU	O2-C2-N3	-2.58	116.73	121.49
42	1	678	A2M	C2'-C1'-N9	2.58	117.99	113.75
37	2	472	PSU	C3'-C2'-C1'	2.57	104.72	101.69
29	S1	33	PSU	C3'-C2'-C1'	2.57	104.72	101.69
42	1	959[A]	OMG	C5-C6-N1	2.57	119.78	113.25
29	S1	1865	OMG	N9-C4-N3	2.57	131.08	125.95
37	2	1248	OMC	O2-C2-N3	-2.56	118.29	122.33
42	1	856	OMG	C2-N1-C6	-2.56	120.47	125.11
42	1	1524	OMG	O6-C6-C5	-2.56	119.77	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1360	OMG	O6-C6-C5	-2.55	119.79	126.53
29	S1	1647	OMG	O6-C6-C5	-2.55	119.79	126.53
29	S1	12	PSU	O2-C2-N1	-2.55	120.15	122.79
29	S1	1550	OMG	O6-C6-C5	-2.55	119.79	126.53
29	S1	1539	PSU	C3'-C2'-C1'	2.55	104.70	101.69
37	2	1253	OMG	O6-C6-C5	-2.54	119.81	126.53
37	2	1060	PSU	C5-C6-N1	-2.54	118.61	122.14
42	1	1626	OMG	N2-C2-N1	2.54	122.12	116.76
37	2	534	OMG	N9-C4-N3	2.54	131.03	125.95
29	S1	1478	OMG	O6-C6-C5	-2.53	119.84	126.53
29	S1	104	PSU	C6-C5-C4	2.53	119.88	118.17
37	2	510	PSU	O2-C2-N1	-2.52	120.19	122.79
42	1	959[A]	OMG	O6-C6-C5	-2.52	119.88	126.53
37	2	1403	PSU	C5-C6-N1	-2.51	118.65	122.14
29	S1	609	PSU	C5-C6-N1	-2.51	118.66	122.14
37	2	1231	OMG	O6-C6-C5	-2.51	119.91	126.53
42	1	1540	OMG	O6-C6-C5	-2.50	119.92	126.53
37	2	1354	PSU	C6-C5-C4	2.50	119.86	118.17
37	2	78	PSU	C3'-C2'-C1'	2.50	104.64	101.69
37	2	1152	OMU	O2-C2-N1	-2.50	119.55	122.80
40	4	74	OMG	O6-C6-C5	-2.50	119.94	126.53
42	1	1533	PSU	C5-C6-N1	-2.49	118.68	122.14
29	S1	1550	OMG	N9-C4-N3	2.49	130.94	125.95
37	2	1360	OMG	N9-C4-N3	2.49	130.94	125.95
42	1	1540	OMG	N2-C2-N1	2.49	122.02	116.76
42	1	856	OMG	N1-C2-N3	-2.49	118.77	123.32
42	1	1402	PSU	C6-N1-C2	-2.49	120.39	122.69
42	1	239	PSU	C5-C6-N1	-2.48	118.69	122.14
42	1	955	A2M	C2'-C1'-N9	2.48	117.83	113.75
29	S1	1879	OMG	O6-C6-C5	-2.48	119.99	126.53
40	4	74	OMG	N9-C4-N3	2.48	130.91	125.95
29	S1	2151	OMG	O6-C6-C5	-2.47	120.01	126.53
42	1	1011	PSU	O2-C2-N1	-2.47	120.24	122.79
37	2	1231	OMG	C2'-C1'-N9	-2.47	109.56	114.24
42	1	856	OMG	N2-C2-N1	2.47	121.97	116.76
42	1	1017	PSU	C5-C6-N1	-2.47	118.72	122.14
37	2	593	PSU	C5-C6-N1	-2.46	118.72	122.14
42	1	959[B]	OMG	C5-C6-N1	2.46	119.52	113.25
37	2	1413	PSU	O2-C2-N1	-2.46	120.26	122.79
41	3	13	OMU	C1'-N1-C6	-2.45	115.54	120.78
42	1	678	A2M	C6-C5-C4	2.45	120.52	117.18
37	2	1144	PSU	C3'-C2'-C1'	2.45	104.58	101.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1829	OMG	O6-C6-C5	-2.45	120.06	126.53
37	2	655	OMG	C8-N7-C5	2.44	108.61	104.26
37	2	1046	OMG	N9-C4-N3	2.44	130.84	125.95
37	2	1058	PSU	C3'-C2'-C1'	2.44	104.57	101.69
29	S1	2048	PSU	C3'-C2'-C1'	2.44	104.57	101.69
42	1	1190	OMG	O6-C6-C5	-2.44	120.09	126.53
40	4	74	OMG	N2-C2-N1	2.44	121.90	116.76
29	S1	1539	PSU	C5-C6-N1	-2.43	118.76	122.14
42	1	1171	PSU	C6-N1-C2	-2.43	120.43	122.69
37	2	95	A2M	C2'-C1'-N9	2.42	117.74	113.75
38	7	69	PSU	C5-C6-N1	-2.42	118.78	122.14
42	1	672	PSU	C5-C6-N1	-2.41	118.80	122.14
29	S1	1478	OMG	N9-C4-N3	2.40	130.76	125.95
42	1	1527	OMC	O2-C2-N3	-2.40	118.54	122.33
42	1	959[B]	OMG	O6-C6-C5	-2.40	120.19	126.53
37	2	604	A2M	C6-C5-C4	2.40	120.45	117.18
37	2	437	PSU	O2-C2-N1	-2.40	120.31	122.79
42	1	847	OMU	O2-C2-N1	-2.40	119.67	122.80
37	2	1046	OMG	C8-N7-C5	2.40	108.53	104.26
42	1	305	A2M	C2-N3-C4	2.39	117.68	111.83
37	2	95	A2M	C6-C5-C4	2.39	120.44	117.18
42	1	1190	OMG	N9-C4-N3	2.39	130.74	125.95
29	S1	1533	PSU	C3'-C2'-C1'	2.39	104.51	101.69
37	2	572	A2M	O4'-C1'-C2'	-2.38	102.48	106.59
42	1	1181	PSU	C5-C6-N1	-2.38	118.84	122.14
42	1	305	A2M	C5-N7-C8	2.37	107.17	103.45
37	2	1318	PSU	O2-C2-N1	-2.37	120.34	122.79
42	1	1626	OMG	C6-C5-N7	2.37	134.59	130.29
37	2	1308	5MC	C3'-C2'-C1'	2.37	105.94	101.46
29	S1	1879	OMG	C8-N7-C5	2.36	108.47	104.26
42	1	1190	OMG	C8-N7-C5	2.36	108.47	104.26
29	S1	1246	PSU	C5-C6-N1	-2.36	118.87	122.14
42	1	1371	OMU	O2-C2-N3	-2.36	117.14	121.49
42	1	1171	PSU	O2-C2-N3	-2.35	117.69	121.86
29	S1	512	A2M	C5-N7-C8	2.35	107.14	103.45
29	S1	600	OMG	O6-C6-C5	-2.34	120.35	126.53
37	2	1229	OMG	N2-C2-N1	2.34	121.70	116.76
37	2	1046	OMG	O6-C6-C5	-2.34	120.36	126.53
42	1	422	PSU	C5-C6-N1	-2.33	118.91	122.14
37	2	534	OMG	O6-C6-C5	-2.33	120.38	126.53
42	1	1626	OMG	O6-C6-C5	-2.33	120.38	126.53
29	S1	1657	PSU	C5-C6-N1	-2.33	118.91	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	570	A2M	C6-C5-C4	2.32	120.35	117.18
29	S1	8	OMU	O2-C2-N1	-2.32	119.78	122.80
37	2	1185	A2M	C6-C5-C4	2.32	120.34	117.18
29	S1	2151	OMG	C8-N7-C5	2.32	108.39	104.26
29	S1	600	OMG	C8-N7-C5	2.31	108.38	104.26
37	2	78	PSU	C5-C6-N1	-2.31	118.94	122.14
37	2	1078	OMG	O6-C6-C5	-2.31	120.44	126.53
37	2	655	OMG	C6-C5-N7	2.30	134.48	130.29
37	2	1317	OMC	O2-C2-N3	-2.30	118.70	122.33
37	2	1077	OMU	O2-C2-N1	-2.30	119.81	122.80
42	1	1524	OMG	C8-N7-C5	2.30	108.35	104.26
29	S1	1543	C4J	C5-C4-N3	2.30	120.32	116.15
37	2	1229	OMG	C8-N7-C5	2.29	108.35	104.26
42	1	959[A]	OMG	C8-N7-C5	2.29	108.35	104.26
37	2	1264	PSU	C5-C6-N1	-2.29	118.96	122.14
37	2	1229	OMG	N9-C4-N3	2.29	130.54	125.95
42	1	1659	OMU	C1'-N1-C2	2.29	121.70	117.59
37	2	597	PSU	C5-C6-N1	-2.28	118.97	122.14
29	S1	1841	PSU	C5-C6-N1	-2.28	118.97	122.14
37	2	1231	OMG	N9-C4-N3	2.28	130.51	125.95
37	2	1303	PSU	C5-C6-N1	-2.27	118.99	122.14
42	1	1528	PSU	C5-C6-N1	-2.27	118.99	122.14
37	2	1058	PSU	C5-C6-N1	-2.27	118.99	122.14
42	1	1540	OMG	C6-C5-N7	2.27	134.41	130.29
37	2	1078	OMG	C8-N7-C5	2.27	108.30	104.26
42	1	856	OMG	O6-C6-C5	-2.27	120.55	126.53
37	2	655	OMG	N2-C2-N1	2.26	121.54	116.76
42	1	1107	OMU	O2-C2-N1	-2.26	119.85	122.80
37	2	662	PSU	O2-C2-N1	-2.26	120.46	122.79
37	2	655	OMG	C4-C5-N7	-2.26	107.09	110.67
37	2	1231	OMG	C8-N7-C5	2.26	108.28	104.26
29	S1	1533	PSU	C5-C6-N1	-2.26	119.01	122.14
29	S1	1647	OMG	C8-N7-C5	2.25	108.27	104.26
29	S1	455	PSU	C6-C5-C4	2.25	119.69	118.17
42	1	1402	PSU	C5-C4-N3	2.25	121.50	116.55
29	S1	1550	OMG	C8-N7-C5	2.24	108.26	104.26
37	2	641	OMG	C2'-C1'-N9	-2.24	109.99	114.24
29	S1	1995	G7M	N9-C8-N7	-2.24	107.05	112.48
42	1	422	PSU	O3'-C3'-C2'	2.23	118.96	111.82
42	1	1626	OMG	C8-N7-C5	2.22	108.22	104.26
40	4	74	OMG	C8-N9-C4	2.22	110.19	106.03
42	1	1540	OMG	N1-C2-N3	-2.22	119.26	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1478	OMG	C8-N7-C5	2.22	108.21	104.26
42	1	927	A2M	C6-C5-C4	2.22	120.20	117.18
37	2	1078	OMG	C6-C5-N7	2.21	134.31	130.29
29	S1	1979	OMU	O2-C2-N1	-2.21	119.92	122.80
38	7	74	PSU	C5-C6-N1	-2.20	119.09	122.14
29	S1	1995	G7M	C6-C5-N7	-2.20	129.42	132.17
37	2	655	OMG	O6-C6-C5	-2.19	120.74	126.53
29	S1	512	A2M	C6-C5-N7	2.19	136.32	132.09
37	2	1229	OMG	N1-C2-N3	-2.19	119.32	123.32
37	2	591	A2M	C2'-C1'-N9	-2.18	110.16	113.75
42	1	959[B]	OMG	N2-C2-N1	2.18	121.37	116.76
37	2	641	OMG	C8-N7-C5	2.18	108.14	104.26
42	1	858	A2M	O4'-C1'-N9	2.17	112.26	108.09
37	2	628	A2M	C4-C5-N7	-2.17	108.10	110.58
40	4	74	OMG	C8-N7-C5	2.16	108.11	104.26
42	1	870	PSU	O2-C2-N1	-2.15	120.57	122.79
42	1	1171	PSU	O4-C4-N3	-2.15	116.07	120.11
37	2	1361	PSU	C5-C4-N3	2.15	121.27	116.55
42	1	1539	A2M	O3'-C3'-C2'	-2.14	105.19	111.19
42	1	678	A2M	C1'-N9-C8	2.14	131.84	127.09
37	2	1372	A2M	C4-C5-N7	-2.14	108.14	110.58
42	1	1010	OMC	CM2-O2'-C2'	2.14	119.96	114.47
29	S1	1865	OMG	C8-N7-C5	2.13	108.06	104.26
29	S1	661	OMU	O2-C2-N1	-2.13	120.02	122.80
42	1	955	A2M	C6-C5-C4	2.13	120.09	117.18
42	1	407	A2M	C5'-C4'-C3'	-2.13	107.55	115.21
38	7	75	OMG	O6-C6-C5	-2.12	120.92	126.53
37	2	641	OMG	C6-C5-N7	2.12	134.15	130.29
37	2	1046	OMG	N2-C2-N1	2.12	121.24	116.76
29	S1	1156	PSU	C5-C6-N1	-2.12	119.20	122.14
42	1	695	OMC	O2-C2-N3	-2.12	118.99	122.33
29	S1	512	A2M	C2-N1-C6	2.12	122.21	118.73
42	1	1540	OMG	C8-N9-C4	2.12	109.99	106.03
42	1	959[B]	OMG	C5-C4-N9	2.12	109.44	105.66
42	1	1524	OMG	C4-C5-N7	-2.12	107.31	110.67
42	1	1171	PSU	C5-C6-N1	-2.12	119.20	122.14
42	1	1171	PSU	O4'-C1'-C2'	2.12	108.08	105.15
37	2	1231	OMG	N2-C2-N1	2.11	121.22	116.76
42	1	858	A2M	O4'-C4'-C3'	-2.11	100.96	105.15
42	1	856	OMG	C8-N7-C5	2.10	108.01	104.26
37	2	1185	A2M	C2'-C1'-N9	-2.10	110.29	113.75
37	2	1253	OMG	N9-C4-N3	2.10	130.16	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1382	PSU	O4'-C1'-C2'	2.10	108.05	105.15
37	2	667	OMU	O2-C2-N1	-2.09	120.07	122.80
29	S1	1829	OMG	C8-N7-C5	2.09	107.99	104.26
37	2	570	A2M	C3'-C2'-C1'	2.09	106.81	102.81
29	S1	1865	OMG	N2-C2-N1	2.09	121.17	116.76
29	S1	1623	OMG	O6-C6-C5	-2.08	121.04	126.53
42	1	870	PSU	C6-C5-C4	2.08	119.58	118.17
29	S1	607	PSU	O4'-C1'-C2'	2.08	108.03	105.15
37	2	591	A2M	C6-C5-N7	2.07	136.08	132.09
42	1	1371	OMU	C1'-N1-C6	-2.07	116.35	120.78
37	2	1360	OMG	C8-N7-C5	2.07	107.95	104.26
37	2	1229	OMG	C8-N9-C4	2.07	109.90	106.03
42	1	1626	OMG	C4-C5-N7	-2.07	107.39	110.67
37	2	1382	PSU	O2-C2-N1	-2.07	120.66	122.79
29	S1	1544	5MC	CM5-C5-C6	-2.07	120.06	122.85
29	S1	607	PSU	C5-C6-N1	-2.06	119.28	122.14
29	S1	2046	PSU	C5-C6-N1	-2.06	119.28	122.14
42	1	845	OMU	O4-C4-C5	-2.06	121.61	125.16
42	1	1190	OMG	N2-C2-N1	2.06	121.11	116.76
37	2	73	OMU	C2'-C1'-N1	-2.06	110.34	114.24
37	2	1231	OMG	N1-C2-N3	-2.05	119.56	123.32
37	2	1078	OMG	C4-C5-N7	-2.05	107.42	110.67
37	2	591	A2M	N9-C8-N7	-2.05	111.03	113.94
37	2	593	PSU	O2-C2-N3	-2.05	118.23	121.86
42	1	845	OMU	C5-C6-N1	-2.04	118.52	121.84
42	1	305	A2M	O2'-C2'-C1'	2.04	112.87	108.99
29	S1	2021	A2M	O2'-C2'-C1'	2.04	112.86	108.99
29	S1	2061	5MC	O2-C2-N3	-2.04	119.11	122.33
29	S1	1995	G7M	C5-C4-N9	2.04	110.23	105.88
37	2	71	OMG	O6-C6-C5	-2.04	121.16	126.53
37	2	1419	OMU	C1'-N1-C2	2.03	121.24	117.59
40	4	74	OMG	N1-C2-N3	-2.03	119.60	123.32
42	1	845	OMU	C6-N1-C2	-2.03	118.53	121.00
42	1	1402	PSU	O4-C4-N3	-2.03	116.30	120.11
37	2	71	OMG	C5-C6-N1	2.03	118.41	113.25
38	7	7	OMU	O2-C2-N1	-2.03	120.16	122.80
29	S1	2021	A2M	C4-C5-N7	-2.02	108.27	110.58
37	2	1359	OMU	O2-C2-N1	-2.02	120.17	122.80
42	1	1540	OMG	C8-N7-C5	2.02	107.86	104.26
29	S1	1865	OMG	N1-C2-N3	-2.02	119.63	123.32
37	2	534	OMG	N2-C2-N1	2.02	121.01	116.76
37	2	1360	OMG	N1-C2-N3	-2.01	119.64	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	1011	PSU	O4'-C1'-C2'	2.00	107.92	105.15
42	1	959[A]	OMG	N1-C2-N3	-2.00	119.66	123.32
37	2	641	OMG	C4-C5-N7	-2.00	107.50	110.67

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	2	71	OMG	C1'-C2'-O2'-CM2
37	2	73	OMU	C1'-C2'-O2'-CM2
37	2	78	PSU	O4'-C4'-C5'-O5'
37	2	437	PSU	C3'-C4'-C5'-O5'
37	2	437	PSU	O4'-C4'-C5'-O5'
37	2	443	OMC	C2'-C1'-N1-C2
37	2	443	OMC	C2'-C1'-N1-C6
37	2	510	PSU	O4'-C1'-C5-C4
37	2	510	PSU	O4'-C1'-C5-C6
37	2	510	PSU	O4'-C4'-C5'-O5'
37	2	534	OMG	O4'-C4'-C5'-O5'
37	2	570	A2M	C1'-C2'-O2'-CM'
37	2	591	A2M	C1'-C2'-O2'-CM'
37	2	604	A2M	C1'-C2'-O2'-CM'
37	2	667	OMU	C1'-C2'-O2'-CM2
37	2	1046	OMG	O4'-C4'-C5'-O5'
37	2	1046	OMG	C1'-C2'-O2'-CM2
37	2	1060	PSU	O4'-C4'-C5'-O5'
37	2	1361	PSU	O4'-C1'-C5-C4
37	2	1361	PSU	O4'-C1'-C5-C6
38	7	75	OMG	O4'-C4'-C5'-O5'
38	7	75	OMG	C1'-C2'-O2'-CM2
38	7	162	A2M	C1'-C2'-O2'-CM'
41	3	13	OMU	O4'-C1'-N1-C2
41	3	13	OMU	O4'-C1'-N1-C6
42	1	407	A2M	O4'-C4'-C5'-O5'
42	1	672	PSU	O4'-C4'-C5'-O5'
42	1	681	A2M	O4'-C4'-C5'-O5'
42	1	695	OMC	C3'-C4'-C5'-O5'
42	1	695	OMC	O4'-C4'-C5'-O5'
42	1	845	OMU	O4'-C1'-N1-C2
42	1	845	OMU	O4'-C1'-N1-C6
42	1	959[A]	OMG	O4'-C4'-C5'-O5'
42	1	1010	OMC	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
42	1	1107	OMU	O4'-C4'-C5'-O5'
42	1	1171	PSU	O4'-C1'-C5-C4
42	1	1171	PSU	O4'-C1'-C5-C6
42	1	1181	PSU	C3'-C4'-C5'-O5'
42	1	1371	OMU	O4'-C1'-N1-C2
42	1	1371	OMU	O4'-C1'-N1-C6
42	1	1371	OMU	C3'-C4'-C5'-O5'
42	1	1402	PSU	O4'-C1'-C5-C4
42	1	1402	PSU	O4'-C1'-C5-C6
42	1	1402	PSU	O4'-C4'-C5'-O5'
42	1	1540	OMG	O4'-C4'-C5'-O5'
29	S1	33	PSU	O4'-C1'-C5-C4
29	S1	33	PSU	O4'-C1'-C5-C6
29	S1	104	PSU	C3'-C4'-C5'-O5'
29	S1	104	PSU	O4'-C4'-C5'-O5'
29	S1	455	PSU	C2'-C1'-C5-C4
29	S1	455	PSU	O4'-C1'-C5-C4
29	S1	455	PSU	O4'-C1'-C5-C6
29	S1	512	A2M	O4'-C4'-C5'-O5'
29	S1	512	A2M	C1'-C2'-O2'-CM'
29	S1	600	OMG	O4'-C4'-C5'-O5'
29	S1	607	PSU	O4'-C1'-C5-C6
29	S1	607	PSU	C4'-C5'-O5'-P
29	S1	668	A2M	C1'-C2'-O2'-CM'
29	S1	1543	C4J	N3-C3-C31-C32
29	S1	1543	C4J	C3-C31-C32-N33
29	S1	1543	C4J	N33-C32-C34-O36
29	S1	1544	5MC	O4'-C4'-C5'-O5'
29	S1	1544	5MC	C3'-C4'-C5'-O5'
29	S1	1623	OMG	C1'-C2'-O2'-CM2
29	S1	1657	PSU	O4'-C1'-C5-C6
29	S1	1841	PSU	O4'-C1'-C5-C4
29	S1	1841	PSU	O4'-C1'-C5-C6
29	S1	1979	OMU	C1'-C2'-O2'-CM2
29	S1	2021	A2M	C1'-C2'-O2'-CM'
29	S1	2046	PSU	O4'-C1'-C5-C4
29	S1	2046	PSU	O4'-C1'-C5-C6
29	S1	2151	OMG	O4'-C4'-C5'-O5'
37	2	510	PSU	C3'-C4'-C5'-O5'
37	2	512	PSU	O4'-C4'-C5'-O5'
37	2	534	OMG	C3'-C4'-C5'-O5'
38	7	75	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
42	1	407	A2M	C3'-C4'-C5'-O5'
42	1	959[A]	OMG	C3'-C4'-C5'-O5'
42	1	1107	OMU	C3'-C4'-C5'-O5'
42	1	1402	PSU	C3'-C4'-C5'-O5'
42	1	1528	PSU	O4'-C4'-C5'-O5'
42	1	1540	OMG	C3'-C4'-C5'-O5'
42	1	1664	PSU	C3'-C4'-C5'-O5'
29	S1	668	A2M	C3'-C4'-C5'-O5'
29	S1	1550	OMG	O4'-C4'-C5'-O5'
29	S1	1550	OMG	C3'-C4'-C5'-O5'
29	S1	1566	PSU	C3'-C4'-C5'-O5'
29	S1	1566	PSU	O4'-C4'-C5'-O5'
29	S1	2140	OMC	C3'-C4'-C5'-O5'
29	S1	2140	OMC	O4'-C4'-C5'-O5'
29	S1	2151	OMG	C3'-C4'-C5'-O5'
37	2	570	A2M	O4'-C4'-C5'-O5'
37	2	570	A2M	C3'-C4'-C5'-O5'
37	2	597	PSU	O4'-C4'-C5'-O5'
37	2	1185	A2M	C3'-C4'-C5'-O5'
42	1	1011	PSU	O4'-C4'-C5'-O5'
42	1	1181	PSU	O4'-C4'-C5'-O5'
42	1	1371	OMU	O4'-C4'-C5'-O5'
29	S1	33	PSU	C3'-C4'-C5'-O5'
29	S1	512	A2M	C3'-C4'-C5'-O5'
29	S1	607	PSU	O4'-C4'-C5'-O5'
29	S1	1543	C4J	N33-C32-C34-O35
37	2	78	PSU	C3'-C4'-C5'-O5'
37	2	1046	OMG	C3'-C4'-C5'-O5'
37	2	1060	PSU	C3'-C4'-C5'-O5'
42	1	672	PSU	C3'-C4'-C5'-O5'
37	2	1308	5MC	C2'-C1'-N1-C6
29	S1	8	OMU	C2'-C1'-N1-C6
42	1	681	A2M	C3'-C4'-C5'-O5'
29	S1	600	OMG	C3'-C4'-C5'-O5'
29	S1	607	PSU	C3'-C4'-C5'-O5'
37	2	512	PSU	C3'-C4'-C5'-O5'
37	2	1185	A2M	O4'-C4'-C5'-O5'
42	1	1528	PSU	C3'-C4'-C5'-O5'
42	1	1664	PSU	O4'-C4'-C5'-O5'
37	2	570	A2M	C2'-C1'-N9-C8
38	7	74	PSU	C3'-C4'-C5'-O5'
42	1	422	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
42	1	422	PSU	O4'-C4'-C5'-O5'
42	1	1527	OMC	O4'-C4'-C5'-O5'
29	S1	668	A2M	O4'-C4'-C5'-O5'
29	S1	1995	G7M	O4'-C4'-C5'-O5'
42	1	1527	OMC	C3'-C4'-C5'-O5'
42	1	1626	OMG	O4'-C4'-C5'-O5'
29	S1	1543	C4J	C31-C3-N3-C4
38	7	74	PSU	O4'-C4'-C5'-O5'
42	1	1011	PSU	C3'-C4'-C5'-O5'
29	S1	1995	G7M	C3'-C4'-C5'-O5'
29	S1	1543	C4J	C3-C31-C32-C34
37	2	570	A2M	C2'-C1'-N9-C4
29	S1	33	PSU	O4'-C4'-C5'-O5'
37	2	1361	PSU	C4'-C5'-O5'-P
37	2	1308	5MC	O4'-C1'-N1-C6
29	S1	8	OMU	O4'-C1'-N1-C6
37	2	597	PSU	C3'-C4'-C5'-O5'
37	2	1144	PSU	O4'-C4'-C5'-O5'
37	2	1308	5MC	C2'-C1'-N1-C2
42	1	235	A2M	C3'-C2'-O2'-CM'
37	2	560	OMU	C4'-C5'-O5'-P
29	S1	1543	C4J	C4'-C5'-O5'-P
29	S1	607	PSU	O4'-C1'-C5-C4
29	S1	1657	PSU	O4'-C1'-C5-C4
37	2	443	OMC	C4'-C5'-O5'-P
37	2	443	OMC	O4'-C1'-N1-C6
37	2	583	OMC	O4'-C4'-C5'-O5'
42	1	870	PSU	O4'-C4'-C5'-O5'
37	2	443	OMC	O4'-C1'-N1-C2
29	S1	8	OMU	C2'-C1'-N1-C2
37	2	1077	OMU	C3'-C2'-O2'-CM2
42	1	1524	OMG	C3'-C2'-O2'-CM2
41	3	13	OMU	C4'-C5'-O5'-P
42	1	1539	A2M	O4'-C4'-C5'-O5'
29	S1	2021	A2M	C3'-C4'-C5'-O5'
37	2	1308	5MC	O4'-C1'-N1-C2
42	1	1181	PSU	C4'-C5'-O5'-P
37	2	1058	PSU	O4'-C4'-C5'-O5'
42	1	1533	PSU	O4'-C4'-C5'-O5'
29	S1	8	OMU	O4'-C1'-N1-C2
29	S1	1543	C4J	C31-C3-N3-C2
29	S1	1865	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
42	1	305	A2M	O4'-C1'-N9-C8
42	1	305	A2M	O4'-C1'-N9-C4
29	S1	8	OMU	C3'-C2'-O2'-CM2
29	S1	668	A2M	C2'-C1'-N9-C8
29	S1	18	OMC	O4'-C4'-C5'-O5'
37	2	570	A2M	O4'-C1'-N9-C8
29	S1	1829	OMG	O4'-C4'-C5'-O5'
37	2	1361	PSU	C2'-C1'-C5-C6
42	1	1402	PSU	C2'-C1'-C5-C6
29	S1	8	OMU	O4'-C4'-C5'-O5'
37	2	510	PSU	C4'-C5'-O5'-P
37	2	1248	OMC	C2'-C1'-N1-C2
37	2	71	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

54 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	1	1181	PSU	1	0
37	2	604	A2M	3	0
37	2	472	PSU	1	0
29	S1	1156	PSU	2	0
42	1	695	OMC	1	0
37	2	1372	A2M	1	0
29	S1	2046	PSU	2	0
37	2	1303	PSU	1	0
42	1	845	OMU	2	0
29	S1	600	OMG	1	0
29	S1	1657	PSU	1	0
29	S1	1979	OMU	2	0
29	S1	661	OMU	2	0
42	1	959[A]	OMG	1	0
37	2	667	OMU	1	0
29	S1	1192	PSU	1	0
38	7	69	PSU	1	0
42	1	1659	OMU	1	0
40	4	74	OMG	1	0
42	1	959[B]	OMG	3	0
37	2	71	OMG	1	0
38	7	74	PSU	1	0
29	S1	609	PSU	2	0
42	1	407	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	1	1539	A2M	1	0
37	2	73	OMU	1	0
42	1	422	PSU	1	0
42	1	847	OMU	1	0
41	3	13	OMU	2	0
37	2	1046	OMG	1	0
29	S1	2061	5MC	4	0
42	1	672	PSU	1	0
42	1	1664	PSU	2	0
42	1	239	PSU	1	0
37	2	1058	PSU	1	0
29	S1	1879	OMG	1	0
38	7	7	OMU	1	0
37	2	1264	PSU	2	0
37	2	1308	5MC	1	0
42	1	955	A2M	1	0
37	2	591	A2M	2	0
42	1	1010	OMC	1	0
29	S1	1623	OMG	1	0
42	1	681	A2M	1	0
29	S1	607	PSU	1	0
37	2	560	OMU	1	0
37	2	512	PSU	2	0
29	S1	512	A2M	2	0
29	S1	1246	PSU	1	0
42	1	305	A2M	5	0
37	2	570	A2M	1	0
37	2	655	OMG	1	0
29	S1	1995	G7M	1	0
29	S1	1841	PSU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 188 ligands modelled in this entry, 188 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

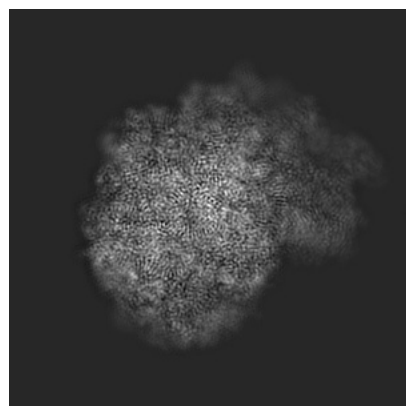
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15124. These allow visual inspection of the internal detail of the map and identification of artifacts.

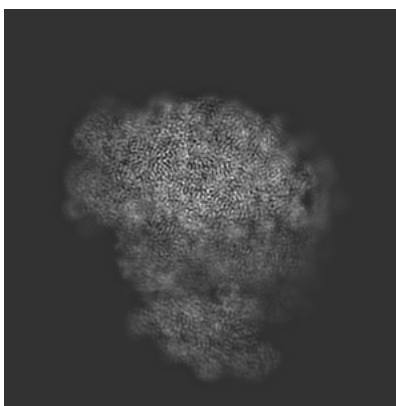
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

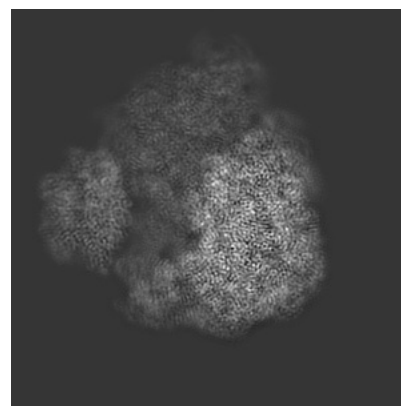
6.1.1 Primary map



X

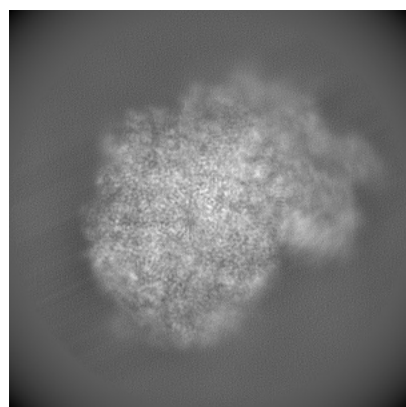


Y

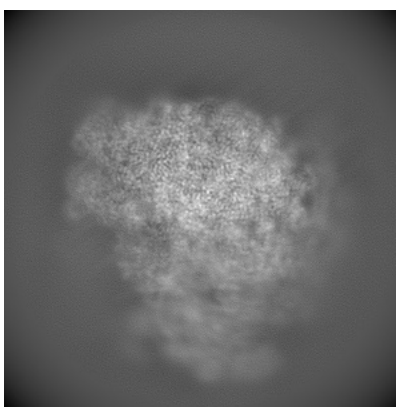


Z

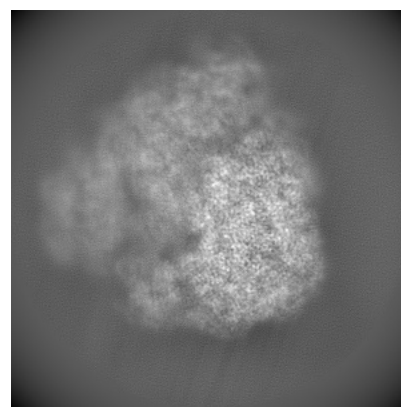
6.1.2 Raw map



X



Y

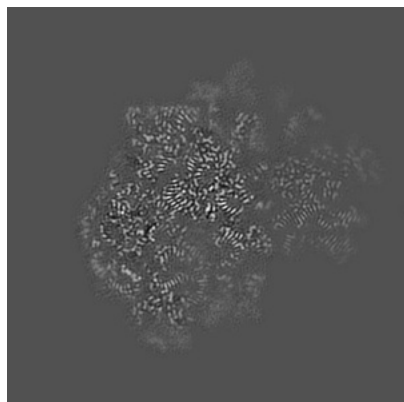


Z

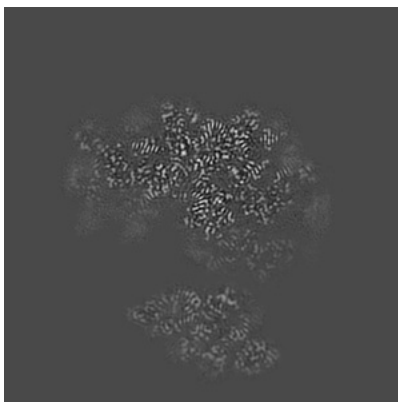
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

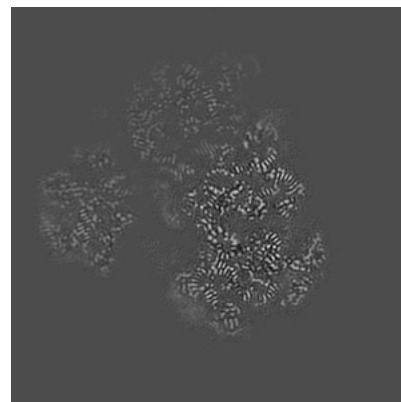
6.2.1 Primary map



X Index: 220

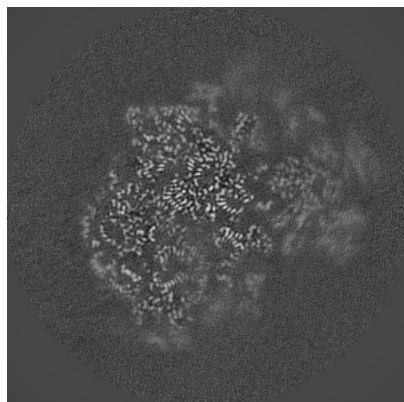


Y Index: 220

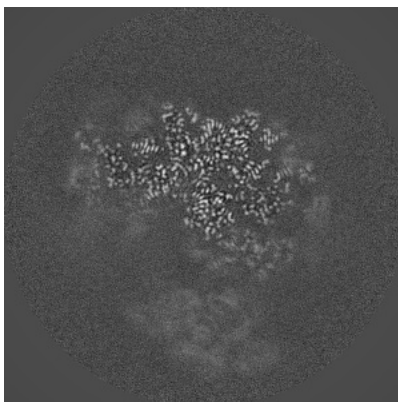


Z Index: 220

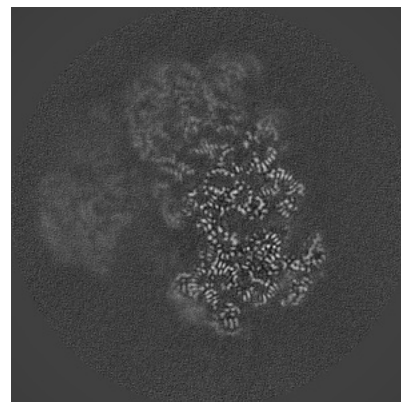
6.2.2 Raw map



X Index: 220



Y Index: 220

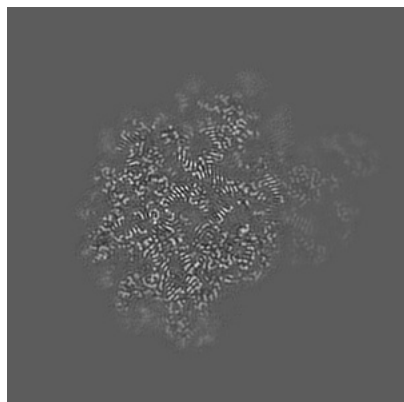


Z Index: 220

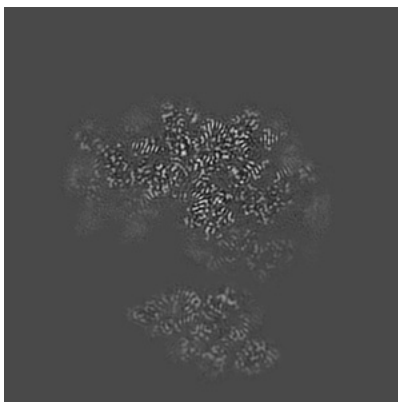
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

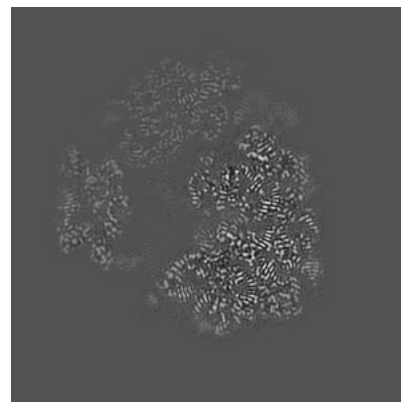
6.3.1 Primary map



X Index: 255

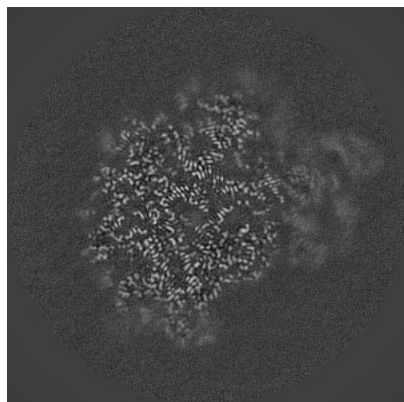


Y Index: 220

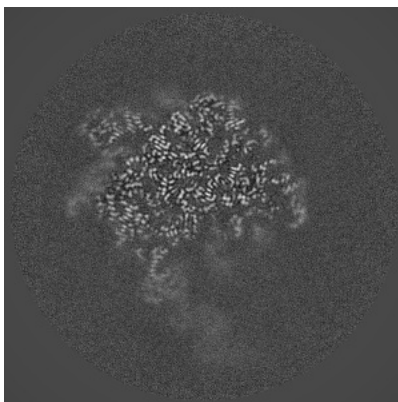


Z Index: 198

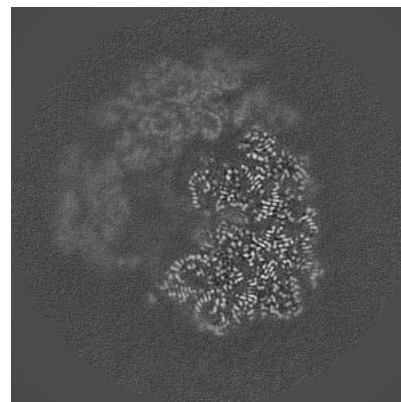
6.3.2 Raw map



X Index: 255



Y Index: 162

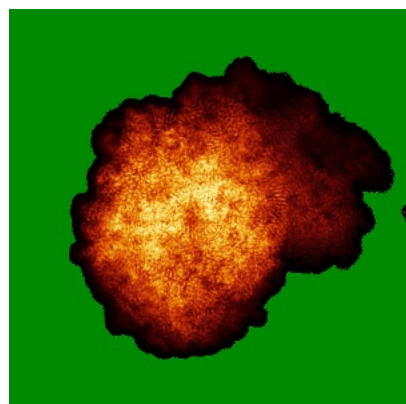


Z Index: 199

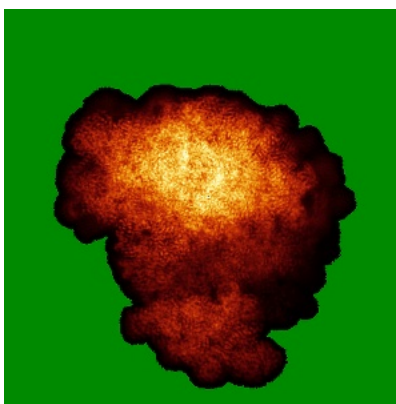
The images above show the largest variance slices of the map in three orthogonal directions.

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

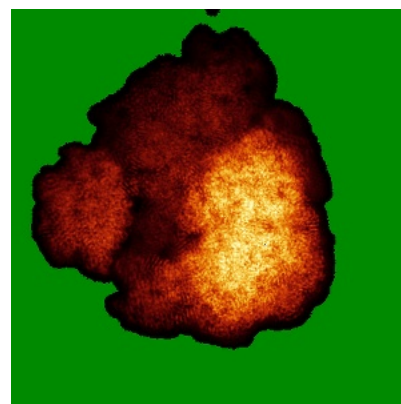
6.4.1 Primary map



X

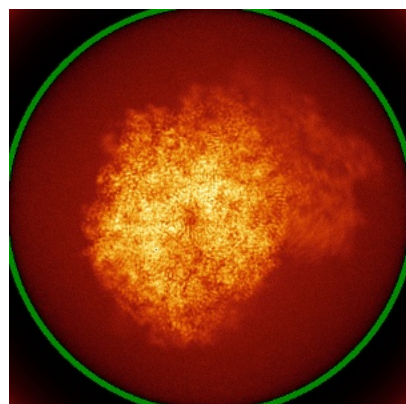


Y

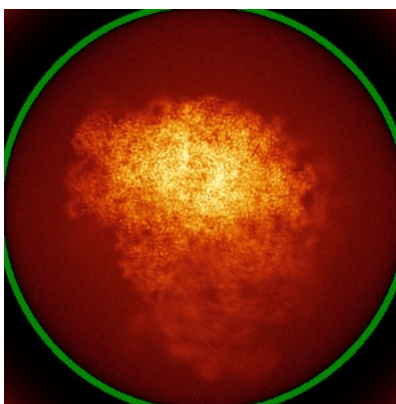


Z

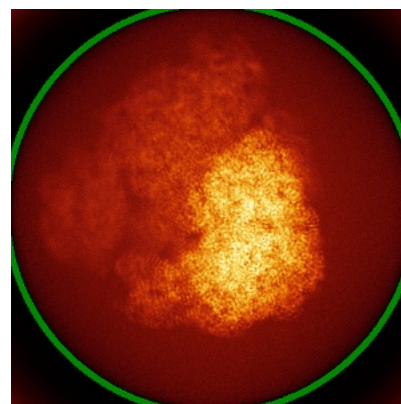
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



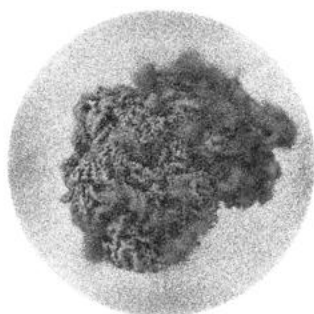
Y



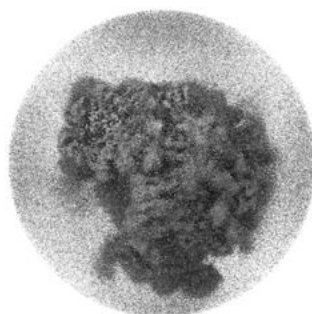
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

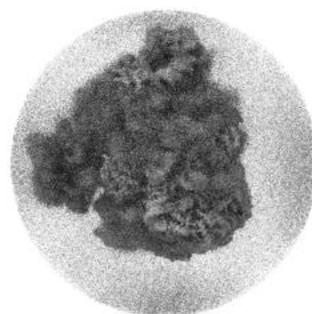
6.5.2 Raw map



X



Y



Z

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

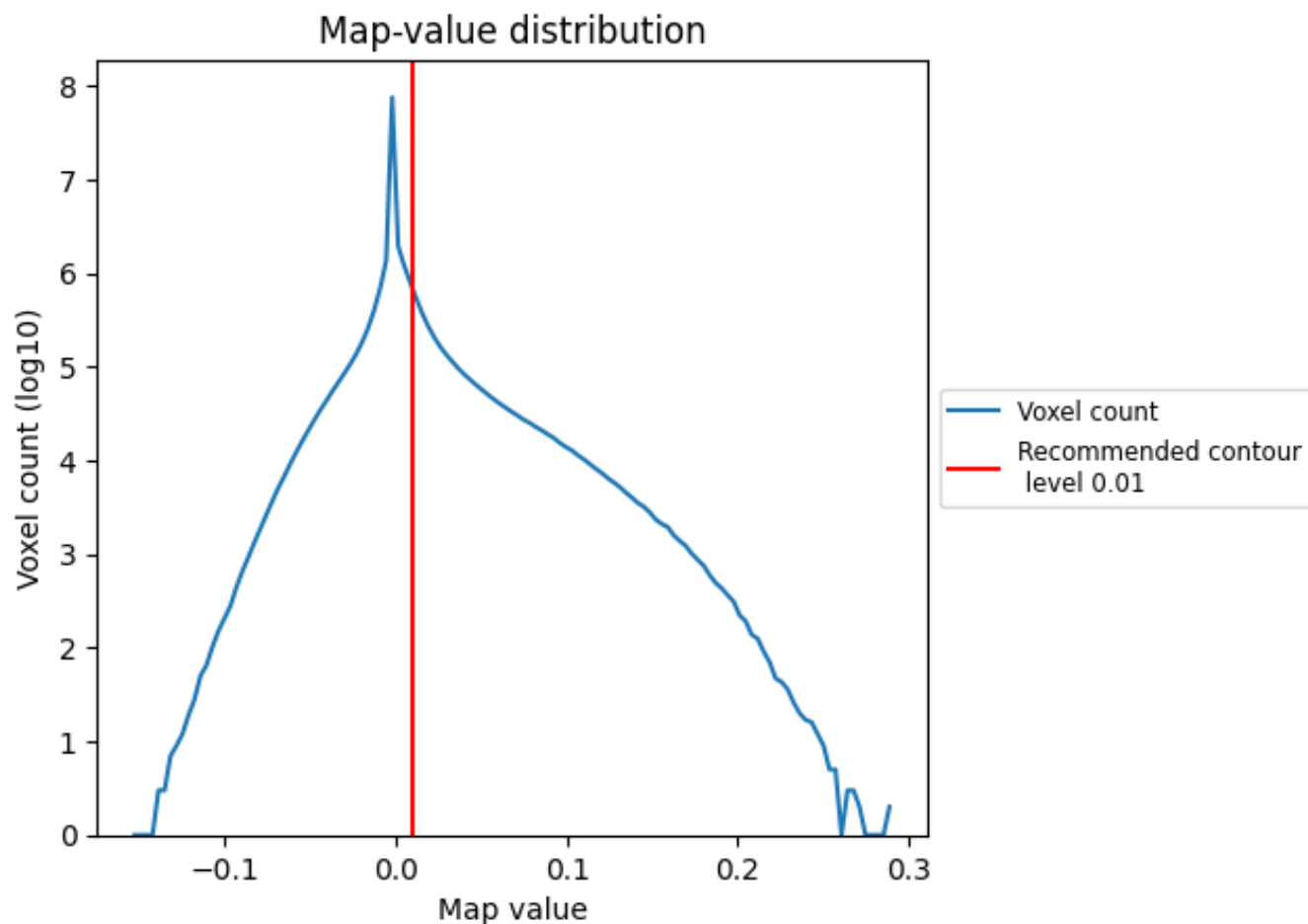
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

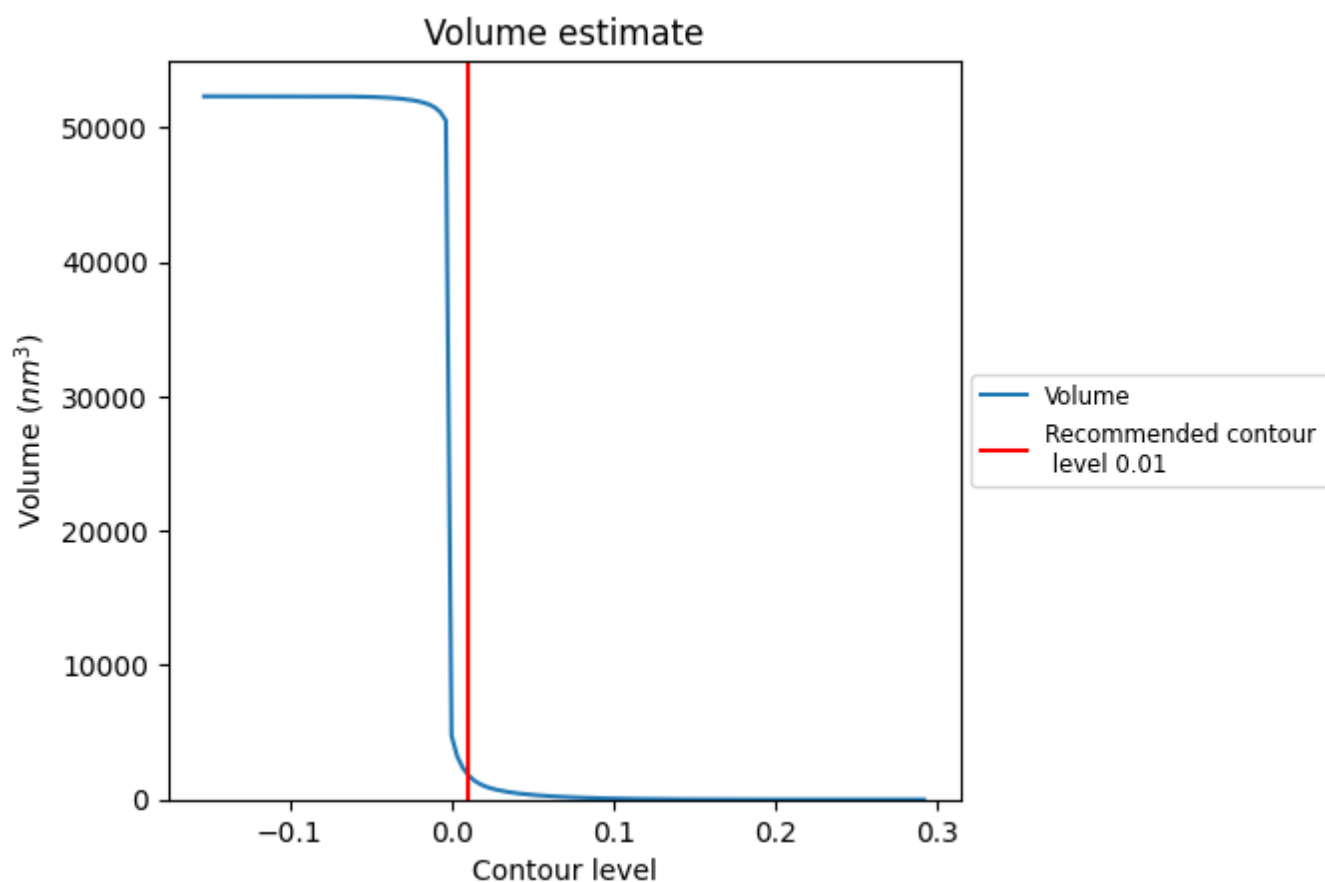
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

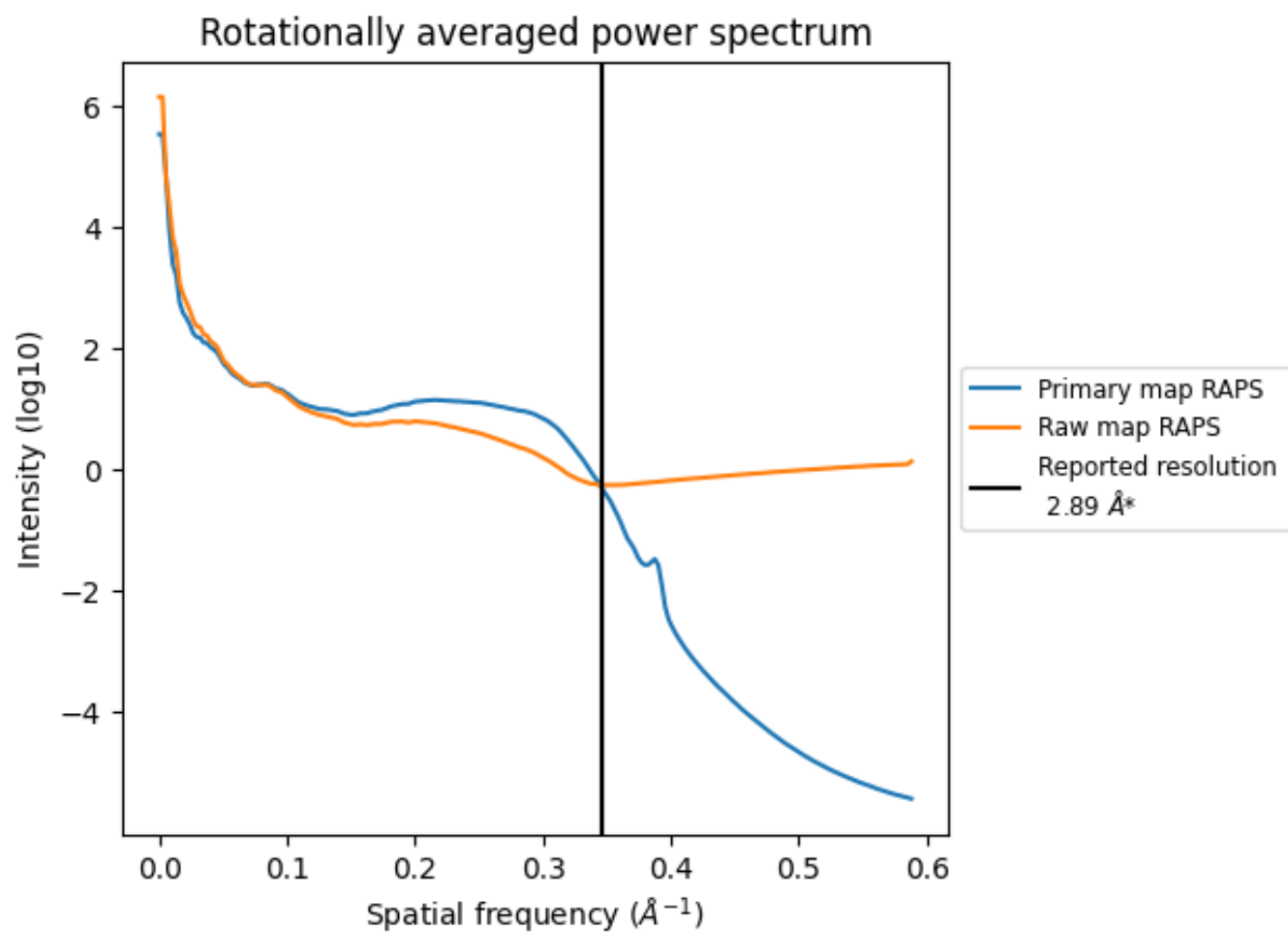
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1903 nm^3 ; this corresponds to an approximate mass of 1719 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 ⓘ

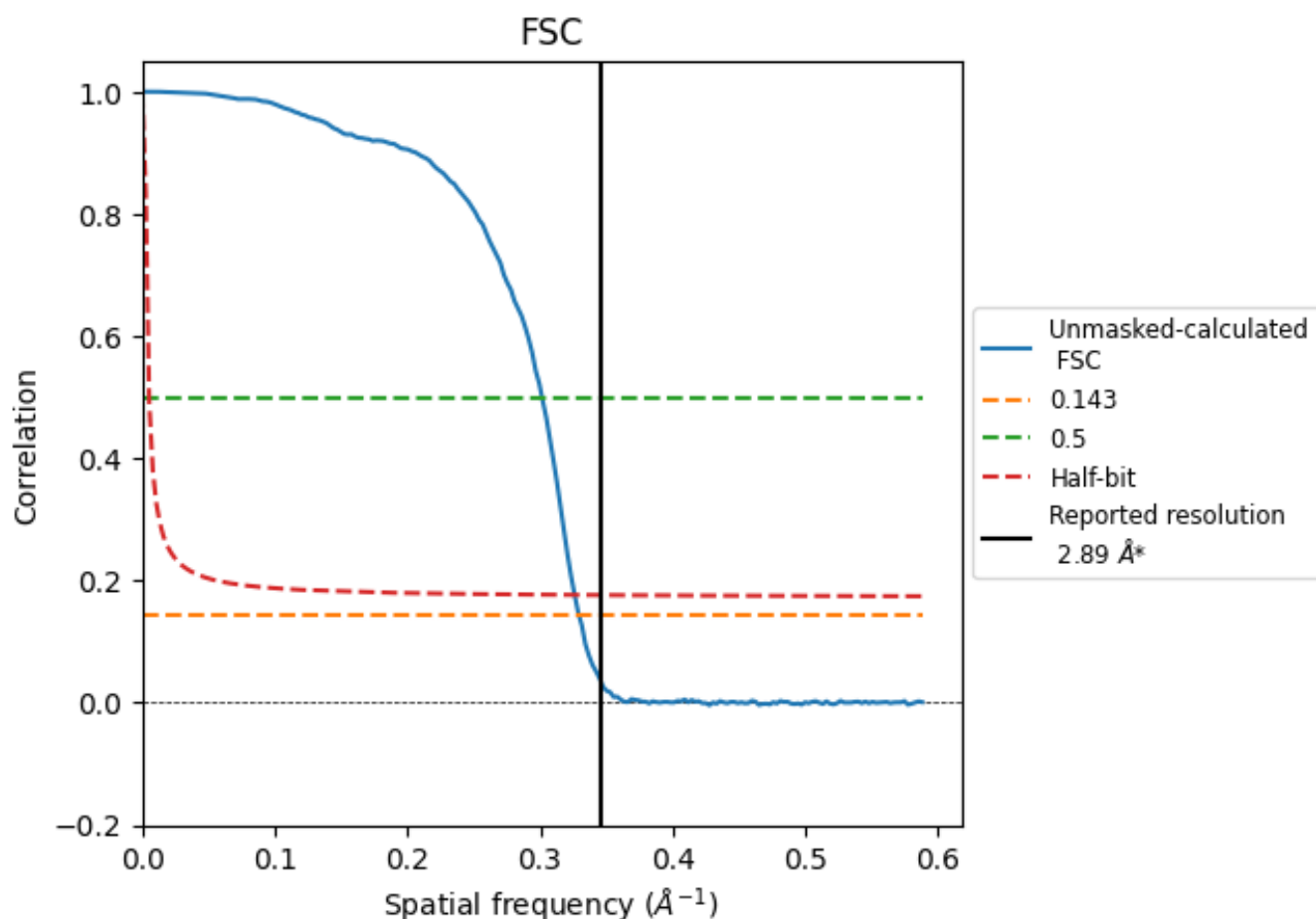


*Reported resolution corresponds to spatial frequency of 0.346 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.346 Å⁻¹

8.2 Resolution estimates [i](#)

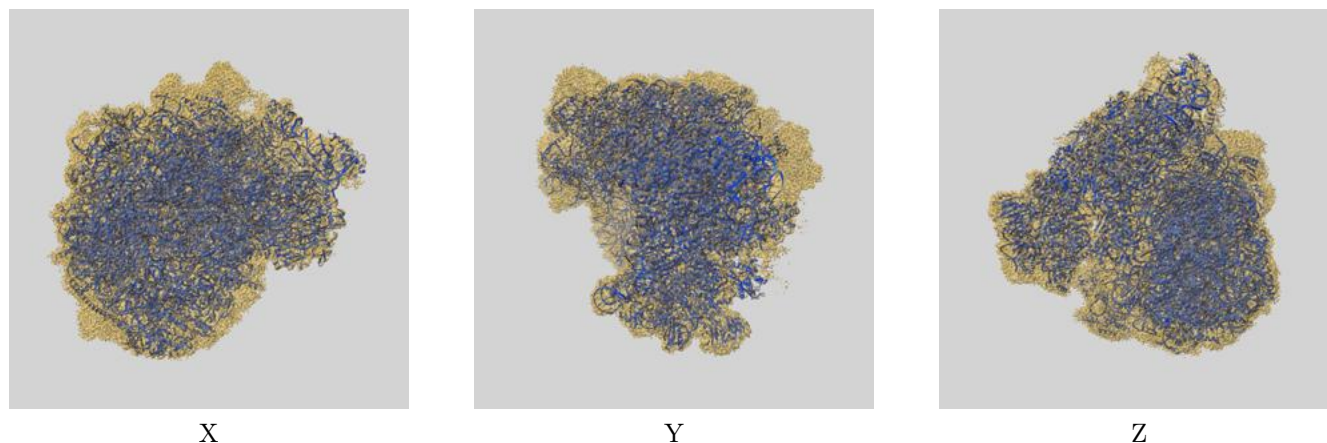
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.04	3.32	3.07

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

9 Map-model fit [i](#)

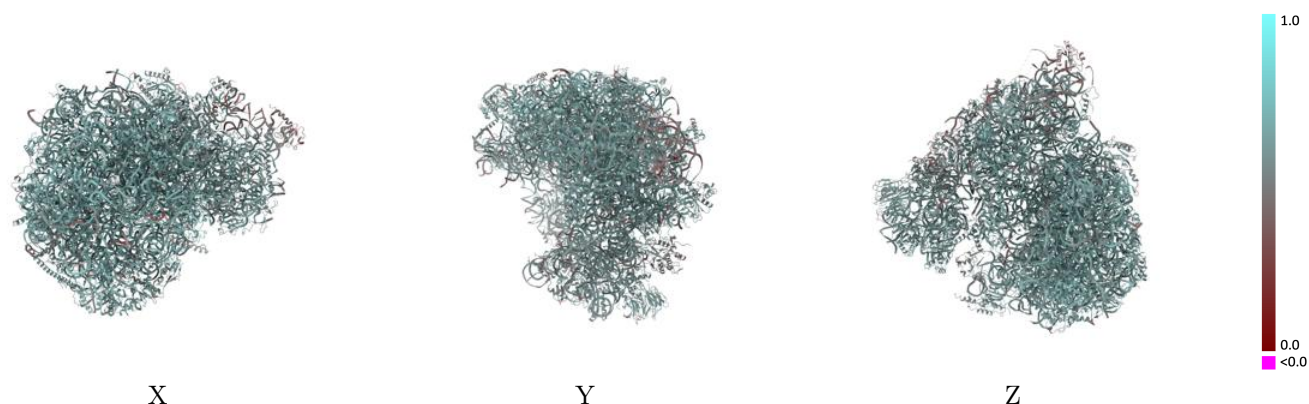
This section contains information regarding the fit between EMDB map EMD-15124 and PDB model 8A3W. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



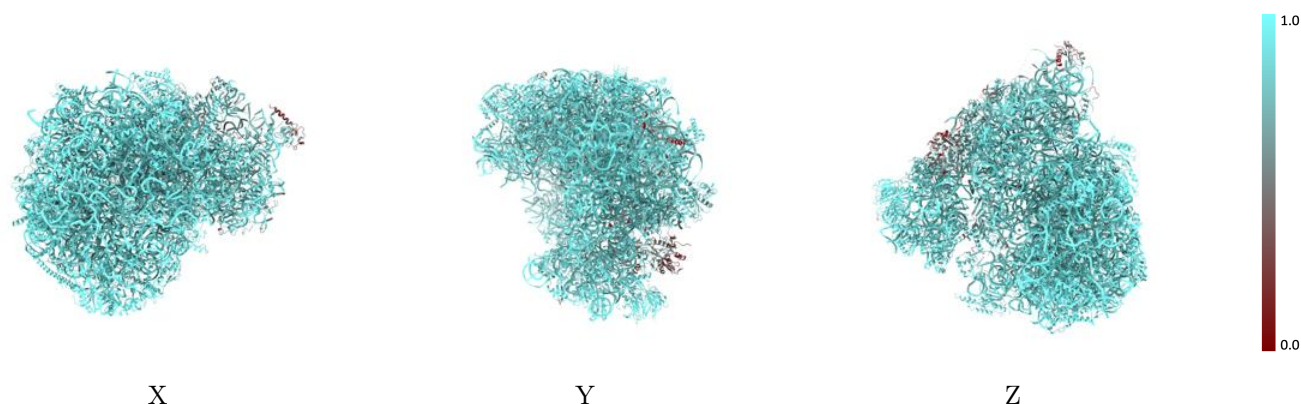
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



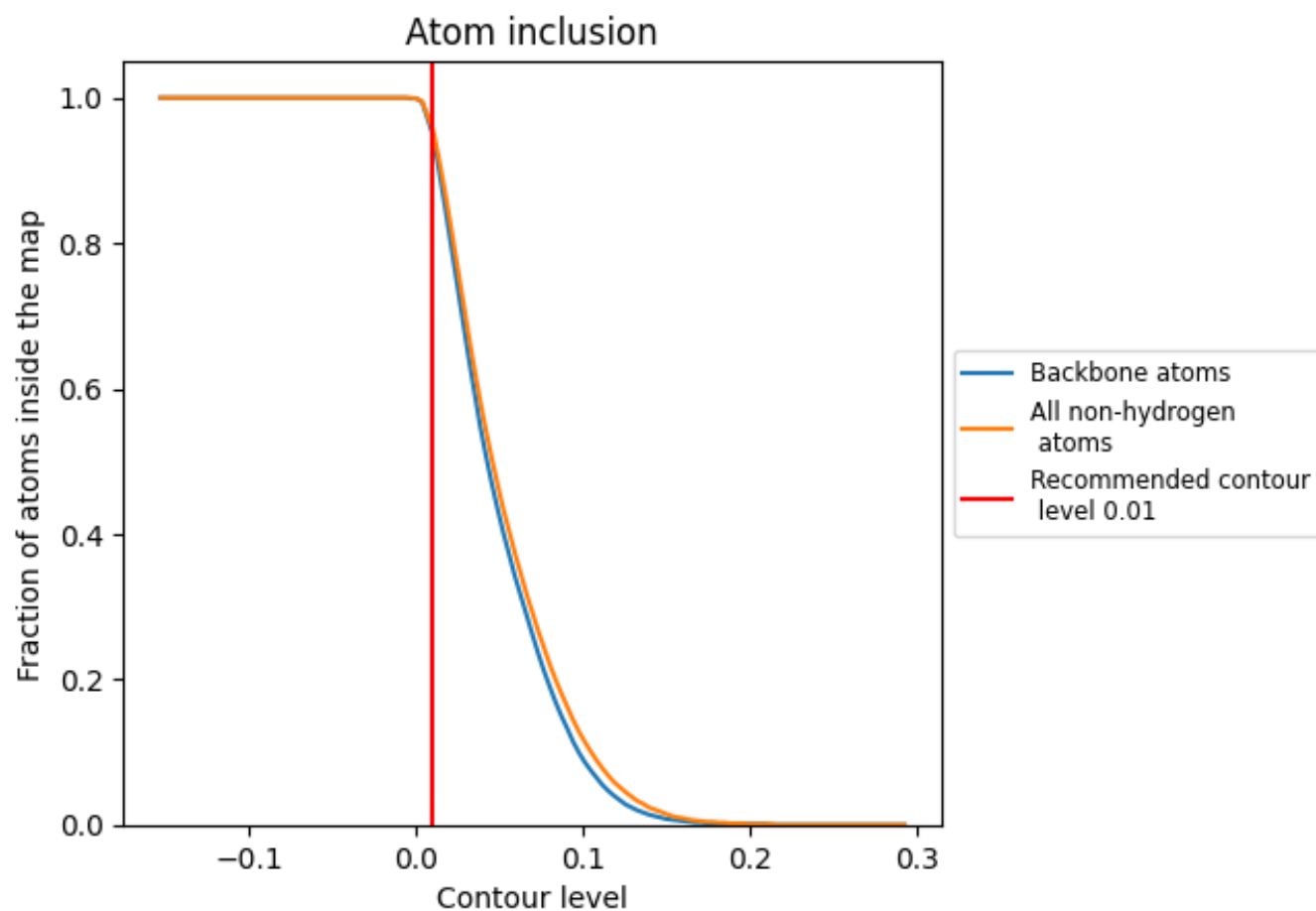
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9570	 0.6070
1	 0.9940	 0.6260
2	 0.9950	 0.6320
3	 0.9930	 0.6170
4	 0.9940	 0.6100
5	 0.9980	 0.6360
6	 0.9860	 0.5860
7	 0.9950	 0.6330
8	 0.9950	 0.5830
A	 0.9960	 0.6570
B	 0.9980	 0.6500
C	 0.9980	 0.6510
D	 0.9890	 0.5400
E	 0.9550	 0.5610
F	 0.9930	 0.6110
G	 0.9940	 0.6280
H	 0.9900	 0.6350
I	 0.9900	 0.6360
J	 0.9980	 0.6450
K	 0.9920	 0.6130
L	 0.9940	 0.6520
M	 0.9970	 0.6620
O	 0.9930	 0.5900
P	 0.9970	 0.6510
Q	 0.9930	 0.6160
R	 0.9890	 0.6310
S	 0.9910	 0.6290
S1	 0.9470	 0.5790
S4	 0.8940	 0.5140
SA	 0.8050	 0.5800
SB	 0.5340	 0.4940
SC	 0.9190	 0.5400
SD	 0.8200	 0.5450
SE	 0.8660	 0.6010
SF	 0.7520	 0.5740



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Chain	Atom inclusion	Q-score
SG	 0.7990	 0.5780
SH	 0.9550	 0.5990
SI	 0.8500	 0.5790
SJ	 0.9300	 0.6260
SK	 0.8990	 0.6070
SL	 0.9820	 0.6110
SM	 0.9530	 0.5660
SN	 0.9320	 0.5410
SO	 0.8740	 0.5890
SP	 0.8650	 0.5990
SR	 0.9680	 0.5970
SS	 0.9630	 0.5810
ST	 0.9320	 0.6130
SU	 0.8760	 0.6190
SV	 0.9610	 0.5870
SW	 0.9510	 0.5870
SX	 0.9930	 0.6120
SY	 0.4200	 0.5030
SZ	 0.8380	 0.5770
Sa	 0.9790	 0.5880
Sb	 0.8120	 0.5750
Sc	 0.8300	 0.5680
Sd	 0.9420	 0.5800
Se	 0.7240	 0.5690
Sg	 0.9640	 0.5670
Sh	 0.4360	 0.4140
T	 0.9940	 0.6550
U	 0.9850	 0.5590
V	 0.9960	 0.6420
W	 0.9920	 0.6350
X	 0.9940	 0.6410
Y	 0.9950	 0.6130
Z	 0.9880	 0.6210
a	 0.9960	 0.6250
b	 0.9920	 0.6350
c	 0.9940	 0.6340
d	 0.9880	 0.5800
e	 0.9350	 0.5920
f	 0.9960	 0.6480
g	 0.9890	 0.6490
h	 0.9880	 0.6330
i	 0.9830	 0.6180

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Chain	Atom inclusion	Q-score
j	 1.0000	 0.6630
k	 0.9900	 0.5940
l	 0.9930	 0.6550
n	 0.3860	 0.4500
o	 0.9910	 0.6240
p	 0.9940	 0.6330