



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:38 AM UTC

PDB ID : 8A98 / pdb_00008a98
EMDB ID : EMD-15272
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :
snoRNA MUTANT
Authors : Rajan, K.S.; Yonath, A.; Bashan, A.
Deposited on : 2022-06-28
Resolution : 2.46 Å (reported)
Based on initial models : 6AZ1, 5T2A, 6AZ3

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:

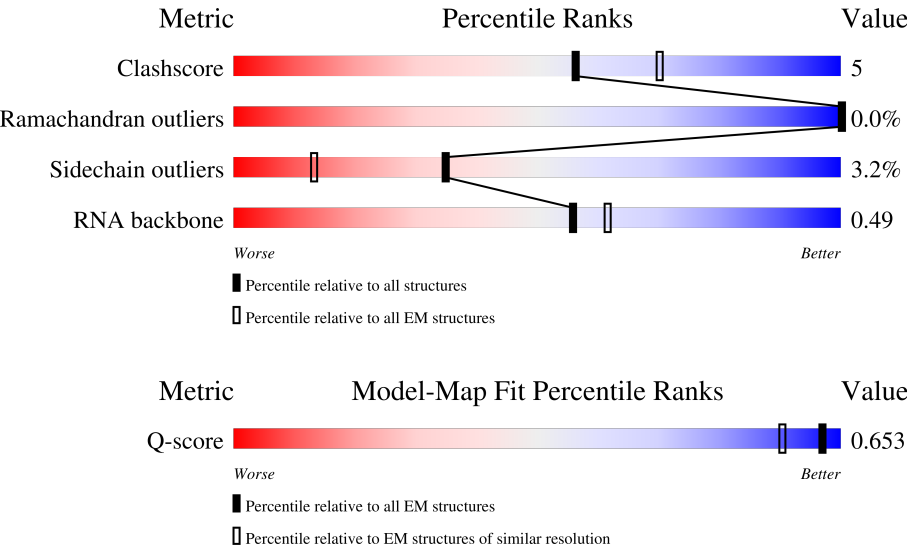
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

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

The reported resolution of this entry is 2.46 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.



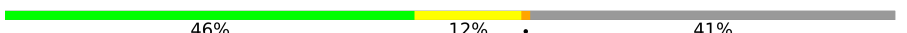
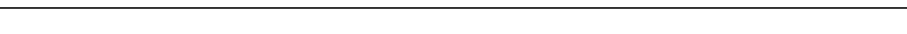
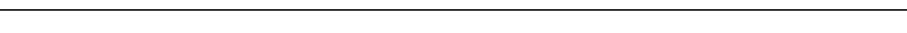
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6014 (1.96 - 2.96)

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	SW	152	
2	SZ	137	
3	SY	164	

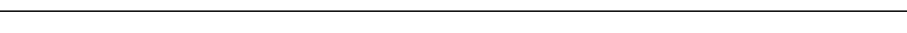
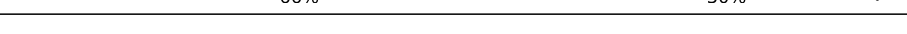
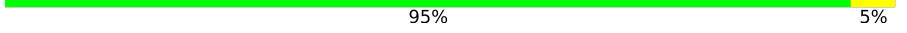
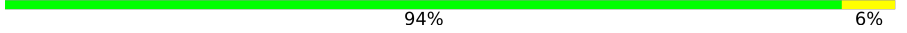
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Mol	Chain	Length	Quality of chain
4	SX	161	
5	SV	143	
6	SU	173	
7	ST	151	
8	SS	57	
9	SR	153	
10	SB	246	
11	SC	219	
12	SD	190	
13	SE	273	
14	SK	220	
15	S4	19	
16	Sg	312	
17	Sa	120	
18	Sc	86	
19	Se	66	
20	S1	2204	
21	SQ	141	
22	SP	143	
23	SO	144	
24	SN	168	
25	Sd	87	
26	SM	116	
27	SL	149	
28	SJ	130	

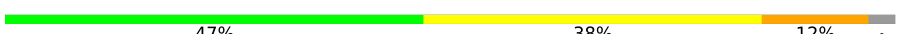
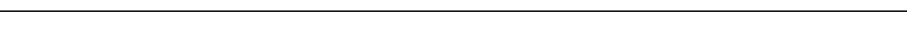
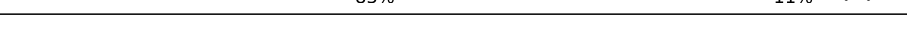
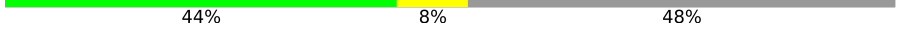
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Mol	Chain	Length	Quality of chain
29	SI	200	
30	SH	190	
31	SG	249	
32	SF	265	
33	SA	264	
34	Sb	112	
35	Sh	235	
36	f	133	
37	d	104	
38	c	252	
39	a	127	
40	b	70	
41	1	1782	
42	2	1526	
43	4	183	
44	7	171	
45	B	419	
46	8	123	
47	5	135	
48	A	260	
49	O	305	
50	G	264	
51	H	222	
52	M	204	
53	I	220	

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Mol	Chain	Length	Quality of chain
54	P	198	
55	Q	254	
56	R	179	
57	E	190	
58	6	73	
59	T	166	
60	S	159	
61	K	175	
62	D	188	
63	L	145	
64	Y	134	
65	Z	147	
66	F	195	
67	h	168	
68	g	144	
69	J	139	
70	V	145	
71	W	143	
72	U	129	
73	i	105	
74	p	106	
75	o	92	
76	X	124	
77	k	83	
78	l	51	

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Mol	Chain	Length	Quality of chain
79	n	34	74%21%
80	C	373	90%8%
81	3	216	41%25%7% 25%
82	e	188	77%14% 8%
83	j	83	87%10%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 197779 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 S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	SW	105	Total	C	N	O	S	0	0
			787	506	152	125	4		

- Molecule 2 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SZ	122	Total	C	N	O	S	1	0
			967	620	184	160	3		

- Molecule 3 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SY	83	Total	C	N	O	S	0	0
			604	371	110	119	4		

- Molecule 4 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SX	139	Total	C	N	O	S	0	0
			1071	682	204	181	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SX	37	SER	THR	conflict	UNP E9AEE8

- Molecule 5 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SV	113	Total	C	N	O	S	0	0
			843	535	159	145	4		

- Molecule 6 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SU	148	Total	C	N	O	S	0	0
			1170	739	235	191	5		

- Molecule 7 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	ST	141	Total	C	N	O	S	0	0
			1145	723	228	186	8		

- Molecule 8 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SS	55	Total	C	N	O	S	0	0
			428	265	87	72	4		

- Molecule 9 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SR	119	Total	C	N	O	S	0	0
			892	567	167	154	4		

- Molecule 10 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SB	209	Total	C	N	O	S	2	0
			1643	1046	297	288	12		

- Molecule 11 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SC	212	Total	C	N	O	S	2	0
			1619	1028	296	282	13		

- Molecule 12 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SD	182	Total	C	N	O	S	1	0
			1513	951	308	246	8		

- Molecule 13 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SE	260	Total	C	N	O	S	2	0
			2056	1304	396	347	9		

- Molecule 14 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SK	180	Total	C	N	O	S	0	0
			1424	895	300	227	2		

- Molecule 15 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S4	19	Total	C	N	O	P	0	0
			404	181	76	129	18		

- Molecule 16 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Sg	300	Total	C	N	O	S	0	0
			2251	1415	399	424	13		

- Molecule 17 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Sa	71	Total	C	N	O	S	0	0
			541	345	93	100	3		

- Molecule 18 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Sc	84	Total	C	N	O	S	0	0
			638	396	123	111	8		

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Se	52	Total	C	N	O	S	0	0
			404	253	87	63	1		

- Molecule 20 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S1	1727	Total	C	N	O	P	0	0
			36928	16523	6655	12024	1726		

- Molecule 21 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SQ	28	Total	C	N	O	S	0	0
			179	111	33	33	2		

- Molecule 22 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SP	142	Total	C	N	O	S	3	0
			1115	704	222	186	3		

- Molecule 23 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SO	136	Total	C	N	O	S	1	0
			1012	625	197	182	8		

- Molecule 24 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SN	101	Total	C	N	O	S	0	0
			813	521	143	142	7		

- Molecule 25 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Sd	65	Total	C	N	O	S	0	0
			466	286	94	82	4		

- Molecule 26 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SM	102	Total	C	N	O	S	1	0
			811	506	149	154	2		

- Molecule 27 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SL	143	Total	C	N	O	S	0	0
			1130	727	209	191	3		

- Molecule 28 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SJ	129	Total	C	N	O	S	0	0
			1014	643	188	175	8		

- Molecule 29 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SI	200	Total	C	N	O	S	0	0
			1613	1026	307	272	8		

- Molecule 30 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SH	184	Total	C	N	O	S	0	0
			1437	894	277	259	7		

- Molecule 31 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SG	233	Total	C	N	O	S	1	0
			1809	1131	370	305	3		

- Molecule 32 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SF	220	Total	C	N	O	S	0	0
			1656	1063	299	284	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SA	225	Total	C	N	O	S	2	0
			1834	1148	353	322	11		

- Molecule 34 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sb	100	Total	C	N	O	S	0	0
			779	484	162	126	7		

- Molecule 35 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sh	94	Total	C	N	O	S	0	0
			657	406	125	124	2		

- Molecule 36 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	122	Total	C	N	O	S	0	0
			988	621	196	167	4		

- Molecule 37 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	90	Total	C	N	O	S	0	0
			625	388	114	118	5		

- Molecule 38 is a protein called Putative 60S ribosomal protein L7.

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

- Molecule 39 is a protein called Putative 60S ribosomal protein L35.

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

- Molecule 40 is a protein called 60S ribosomal protein L29.

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

- Molecule 41 is a RNA chain called LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1	1579	Total	C	N	O	P	0	0
			33802	15099	6193	10932	1578		

- Molecule 42 is a RNA chain called LSub_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	2	1047	Total	C	N	O	P	0	0
			22358	10009	4022	7280	1047		

- Molecule 43 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	4	183	Total	C	N	O	P	0	0
			3906	1742	706	1275	183		

- Molecule 44 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	7	160	Total	C	N	O	P	0	0
			3399	1520	599	1121	159		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	87	U	A	conflict	GB 1207899567

- Molecule 45 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	B	402	Total	C	N	O	S	7	0
			3200	2019	636	532	13		

- Molecule 46 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	8	118	Total	C	N	O	P	0	0
			2511	1123	448	822	118		

- Molecule 47 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5	111	Total	C	N	O	P	0	0
			2373	1058	431	773	111		

- Molecule 48 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A	255	Total	C	N	O	S	5	0
			1973	1229	407	326	11		

- Molecule 49 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	O	252	Total	C	N	O	S	3	0
			1970	1259	373	333	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	G	233	Total	C	N	O	S	2	0
			1850	1160	370	313	7		

- Molecule 51 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	H	221	Total	C	N	O	S	1	0
			1771	1121	352	291	7		

- Molecule 52 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	M	203	Total	C	N	O	S	0	0
			1714	1080	362	264	8		

- Molecule 53 is a protein called eL13_chain_I.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	I	205	Total	C	N	O	S	0	0
			1593	993	318	274	8		

- Molecule 54 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	P	197	Total	C	N	O	S	0	0
			1539	968	307	258	6		

- Molecule 55 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Q	189	Total	C	N	O	S	0	0
			1482	916	319	241	6		

- Molecule 56 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	R	178	Total	C	N	O	S	0	0
			1447	921	277	244	5		

- Molecule 57 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	E	186	Total	C	N	O	S	0	0
			1439	911	267	255	6		

- Molecule 58 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	6	71	Total	C	N	O	P	0	0
			1484	663	267	483	71		

- Molecule 59 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	T	153	Total	C	N	O	S	0	0
			1233	770	244	208	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	S	152	Total	C	N	O	S	0	0
			1203	764	236	200	3		

- Molecule 61 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	K	153	Total	C	N	O	S	0	0
			1193	746	234	206	7		

- Molecule 62 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	D	159	Total	C	N	O	S	0	0
			1140	723	212	197	8		

- Molecule 63 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	L	144	Total	C	N	O	S	0	0
			1124	707	226	185	6		

- Molecule 64 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Y	132	Total	C	N	O	S	1	0
			1046	667	211	165	3		

- Molecule 65 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Z	139	Total	C	N	O	S	0	0
			1052	642	221	184	5		

- Molecule 66 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	F	142	Total	C	N	O	S	0	0
			1045	665	194	184	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
67	h	126	Total	C	N	O	S	1	0
			1016	626	222	162	6		

- Molecule 68 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	g	138	Total	C	N	O	S	0	0
			1101	684	233	179	5		

- Molecule 69 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	J	129	Total	C	N	O	S	0	0
			968	614	183	165	6		

- Molecule 70 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	V	118	Total	C	N	O	S	0	0
			939	595	176	165	3		

- Molecule 71 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	W	118	Total	C	N	O	S	0	0
			948	591	197	156	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
72	U	112	Total	C	N	O	S	0	0
			879	572	154	151	2		

- Molecule 73 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	i	95	Total	C	N	O	S	0	0
			738	467	148	121	2		

- Molecule 74 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	p	96	Total	C	N	O	S	0	0
			722	460	144	116	2		

- Molecule 75 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o	90	Total	C	N	O	S	0	0
			696	432	144	114	6		

- Molecule 76 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	X	65	Total	C	N	O	S	0	0
			553	362	106	81	4		

- Molecule 77 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	k	73	Total	C	N	O	S	0	0
			546	342	104	97	3		

- Molecule 78 is a protein called Putative 60S ribosomal protein L39.

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

- Molecule 79 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	n	33	Total	C	N	O	S	0	0
			259	161	60	37	1		

- Molecule 80 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	C	366	Total	C	N	O	S	0	0
			2797	1745	554	483	15		

- Molecule 81 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	3	161	Total	C	N	O	P	0	0
			3419	1529	596	1133	161		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
82	e	173	Total	C	N	O	S	0	0
			1298	821	254	220	3		

- Molecule 83 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	j	80	Total	C	N	O	S	0	0
			662	403	151	102	6		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	SS	1	Total	Mg	0
			1	1	
84	S1	23	Total	Mg	0
			23	23	
84	SL	1	Total	Mg	0
			1	1	
84	1	61	Total	Mg	0
			61	61	
84	2	31	Total	Mg	0
			31	31	
84	4	3	Total	Mg	0
			3	3	
84	7	4	Total	Mg	0
			4	4	
84	8	1	Total	Mg	0
			1	1	
84	5	1	Total	Mg	0
			1	1	
84	6	1	Total	Mg	0
			1	1	
84	T	1	Total	Mg	0
			1	1	
84	J	1	Total	Mg	0
			1	1	
84	3	1	Total	Mg	0
			1	1	

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

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

- Molecule 86 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
86	1	5	Total 5	Na 5	0
86	2	3	Total 3	Na 3	0

- Molecule 87 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
87	1	2	Total 2	K 2	0

- Molecule 88 is water.

Mol	Chain	Residues	Atoms		AltConf
88	SZ	1	Total 1	O 1	0
88	SY	1	Total 1	O 1	0
88	SX	7	Total 7	O 7	0
88	ST	5	Total 5	O 5	0
88	SS	1	Total 1	O 1	0
88	SR	2	Total 2	O 2	0
88	SB	3	Total 3	O 3	0
88	SC	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
88	SD	1	Total 1	O 1	0
88	SE	1	Total 1	O 1	0
88	SK	1	Total 1	O 1	0
88	S4	1	Total 1	O 1	0
88	Sg	3	Total 3	O 3	0
88	Sa	1	Total 1	O 1	0
88	Sc	2	Total 2	O 2	0
88	S1	237	Total 237	O 237	0
88	SP	3	Total 3	O 3	0
88	SO	2	Total 2	O 2	0
88	SN	3	Total 3	O 3	0
88	Sd	1	Total 1	O 1	0
88	SH	4	Total 4	O 4	0
88	SF	2	Total 2	O 2	0
88	Sb	2	Total 2	O 2	0
88	f	16	Total 16	O 16	0
88	d	3	Total 3	O 3	0
88	c	4	Total 4	O 4	0
88	a	3	Total 3	O 3	0
88	1	918	Total 918	O 918	0
88	2	536	Total 536	O 536	0

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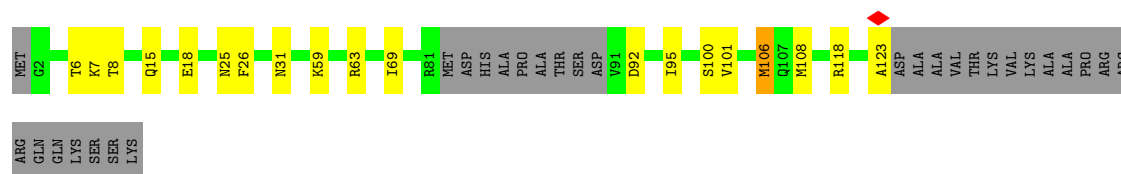
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Mol	Chain	Residues	Atoms		AltConf
88	4	73	Total 73	O 73	0
88	7	85	Total 85	O 85	0
88	B	29	Total 29	O 29	0
88	8	17	Total 17	O 17	0
88	5	37	Total 37	O 37	0
88	A	30	Total 30	O 30	0
88	G	4	Total 4	O 4	0
88	H	9	Total 9	O 9	0
88	M	28	Total 28	O 28	0
88	I	21	Total 21	O 21	0
88	P	12	Total 12	O 12	0
88	Q	6	Total 6	O 6	0
88	R	1	Total 1	O 1	0
88	E	1	Total 1	O 1	0
88	6	3	Total 3	O 3	0
88	T	14	Total 14	O 14	0
88	S	4	Total 4	O 4	0
88	K	1	Total 1	O 1	0
88	L	17	Total 17	O 17	0
88	h	12	Total 12	O 12	0
88	g	9	Total 9	O 9	0

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Mol	Chain	Residues	Atoms		AltConf
88	J	1	Total 1	O 1	0
88	V	6	Total 6	O 6	0
88	W	2	Total 2	O 2	0
88	i	1	Total 1	O 1	0
88	p	13	Total 13	O 13	0
88	o	2	Total 2	O 2	0
88	X	2	Total 2	O 2	0
88	k	2	Total 2	O 2	0
88	l	6	Total 6	O 6	0
88	C	21	Total 21	O 21	0
88	3	31	Total 31	O 31	0
88	e	9	Total 9	O 9	0
88	j	13	Total 13	O 13	0



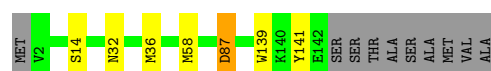
- Molecule 6: Putative 40S ribosomal protein S11

Chain SU: 77% 9% 14%



- Molecule 7: Putative 40S ribosomal protein S13

Chain ST: 89% 7%



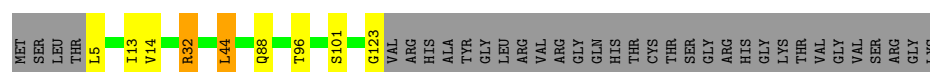
- Molecule 8: Putative ribosomal protein S29

Chain SS: 81% 14%



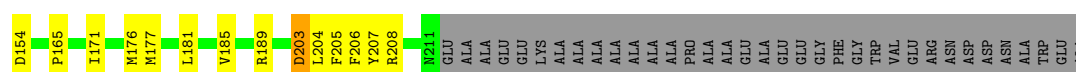
- Molecule 9: Putative 40S ribosomal protein S18

Chain SR: 72% 5% 22%



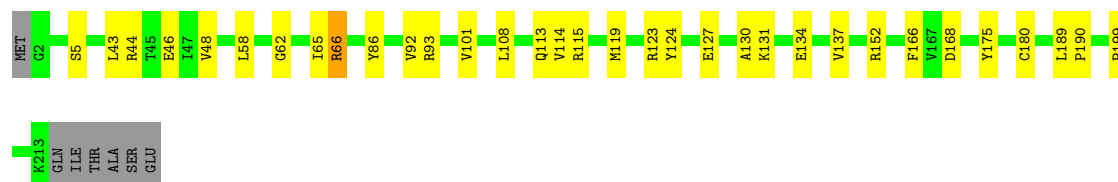
- Molecule 10: 40S ribosomal protein SA

Chain SB: 66% 18% 15%



- Molecule 11: Putative 40S ribosomal protein S3

Chain SC: 82% 15%



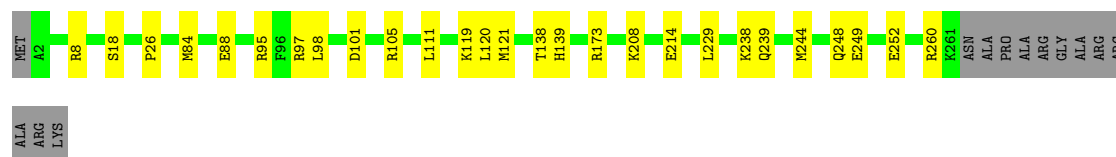
- Molecule 12: Putative 40S ribosomal protein S9

Chain SD: 84% 12% .



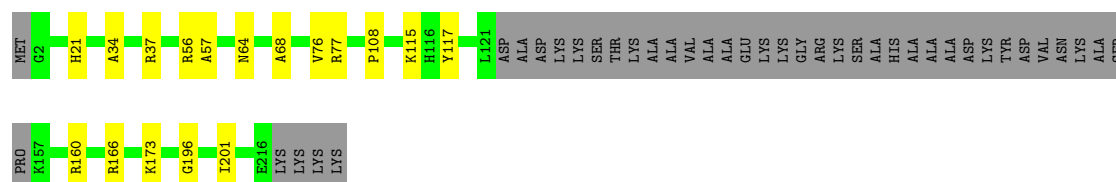
- Molecule 13: 40S ribosomal protein S4

Chain SE: 85% 10% 5%



- Molecule 14: 40S ribosomal protein S8

Chain SK: 74% 8% 18%



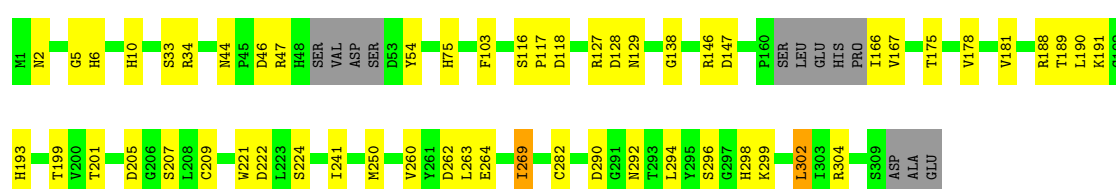
- Molecule 15: E-site_tRNA_chain_S4

Chain S4: 58% 32% 11%

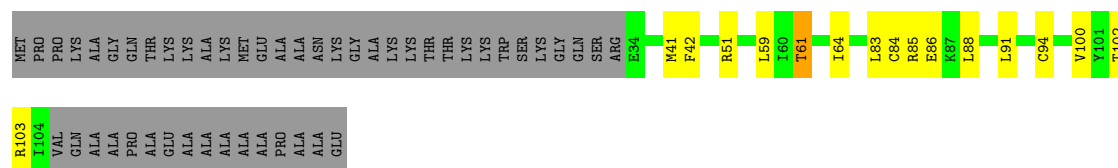


- Molecule 16: Small ribosomal subunit protein RACK1

Chain Sg: 79% 17% . .



Chain Sa: 46% 12% . 41%



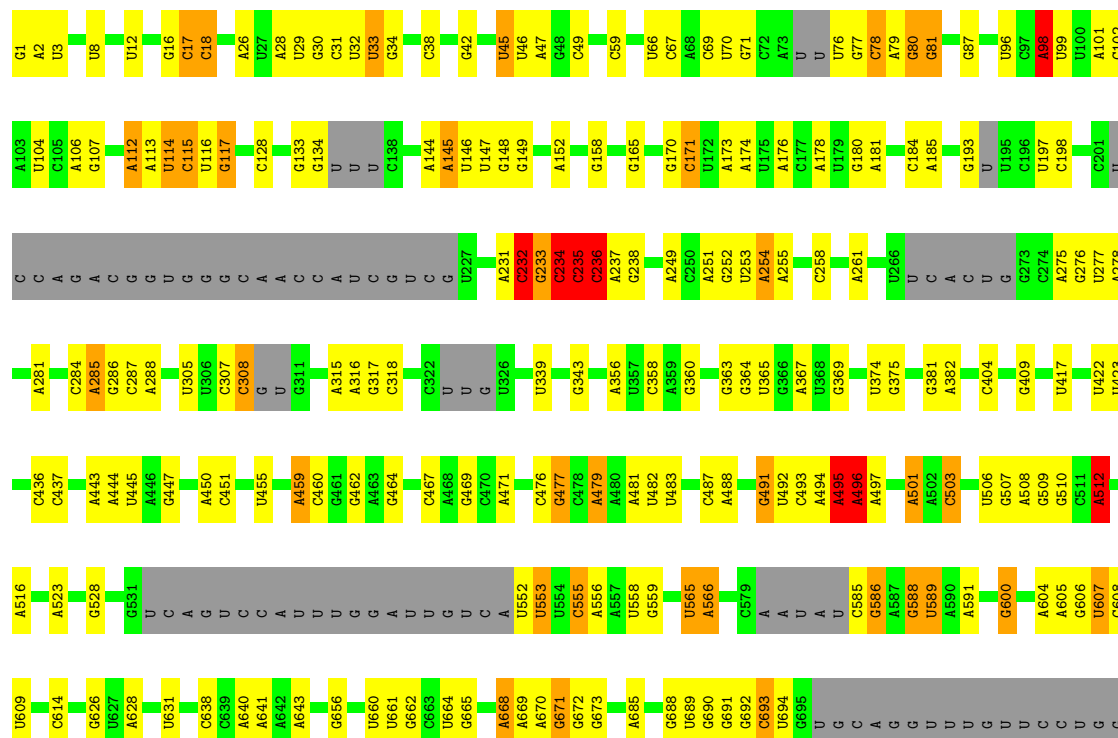
Chain Sc: 80% 17%



Chain Se:

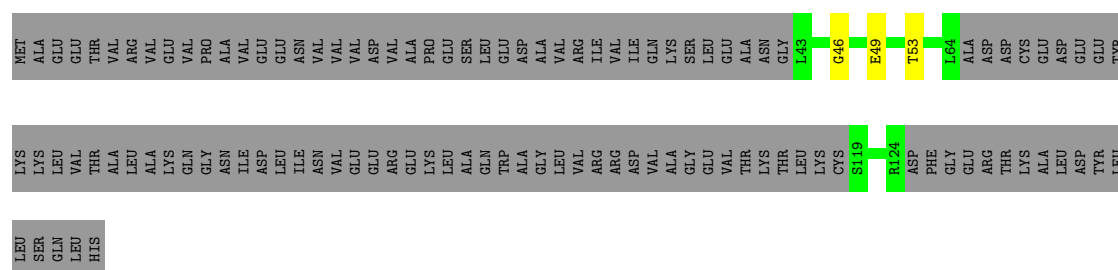


Chain S1:

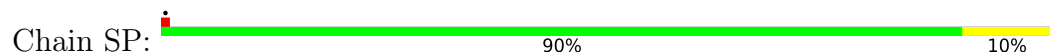


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A1882	U1774	C	A	G	A1503	A	G	G1276	G1139	U	A	U	G	A761
G1883	U1775	C	U	C	A1504	U	C	A1277	G1139	C	C	U	C	C762
G1889	U1776	A	C	C	C1510	C	C	U1278	G1142	G	U	G	U	A763
A1890	U1777	U	U	C	C1511	U	C	G1279	G1143	C	U	C	C	C764
A1891	G1782	C	U	C	A1512	C	C	C1281	G1144	U	U	C	C	C765
A	U1789	A	A	U	A1515	A	U	U1287	A1145	G	G	U	G	C766
A	U1795	A	U	U	G1519	U	U	U1288	A1146	U	U	U	U	C767
C	G1796	C	G	U	G1523	U	U	A1289	G1147	U	U	U	U	C768
G	A1797	C	C	U	G1524	U	A	G1295	G1148	U	U	U	U	C769
A	U1800	A	A	C	U1533	U	C	G1296	G1149	U	U	U	U	C770
U	U1807	C	U	U	U1537	U	C	A1297	U1155	G	U	U	U	C771
U	G1801	C	U	U	U1538	U	C	U1298	U1156	U	U	U	U	C772
U	G1807	C	U	U	U1539	U	C	C	C1168	U	U	U	U	C773
U	U1816	C	U	U	C4J1543	U	C	U	C1169	U	U	U	U	C774
G	G1820	C	G	U	A1545	U	C	U	A1170	U	U	U	U	C775
G	G1821	C	G	U	A1546	U	C	U	A1171	U	U	U	U	C776
C	A1822	C	G	U	C1547	U	C	U	G1172	U	U	U	U	C777
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U	U1836	C	G	U	U1566	U	C	U	A1199	U	U	U	U	C787
U	U1837	C	G	U	U1567	U	C	U	G1206	U	U	U	U	C788
U	U1838	C	G	U	C1568	U	C	U	U1207	U	U	U	U	C789
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U	U1841	C	G	U	C1572	U	C	U	G1219	U	U	U	U	C792
U	A1847	C	G	U	G1574	U	C	U	A1224	U	U	U	U	C793
U	U1848	C	G	U	G1575	U	C	U	A1235	U	U	U	U	C794
U	U1849	C	G	U	A1576	U	C	U	G1114	U	U	U	U	C795
U	U1850	C	G	U	U1577	U	C	U	G1115	U	U	U	U	C796
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U	G1858	C	G	U	A1579	U	C	U	A1117	U	U	U	U	C798
U	G1859	C	G	U	G1580	U	C	U	G1118	U	U	U	U	C799
U	G1865	C	G	U	G1581	U	C	U	U1119	U	U	U	U	C800
U	G1866	C	G	U	A1586	U	C	U	U1120	U	U	U	U	C801
U	A1870	C	G	U	G1589	U	C	U	G1121	U	U	U	U	C802
U	C1871	C	G	U	G1595	U	C	U	A1252	U	U	U	U	C803
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U	G1875	C	G	U	U1597	U	C	U	C1271	U	U	U	U	C805
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U	G1877	C	G	U	U1599	U	C	U	A1273	U	U	U	U	C807
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U	G1879	C	G	U	G1700	U	C	U	G1123	U	U	U	U	C809
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U	G1884	C	G	U	A1709	U	C	U	U1498	U	U	U	U	C814
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U	G1886	C	G	U	U1711	U	C	U	A	U	U	U	U	C816
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U	G1889	C	G	U	U1764	U	C	U	C1765	U	U	U	U	C819
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U	G1891	C	G	U	G1767	U	C	U	G1767	U	U	U	U	C821
U	G1892	C	G	U	U	U	C	U	U	U	U	U	U	C822
U	G1893	C	G	U	C	U	C	U	A	U	U	U	U	C823
U	G1894	C	G	U	U1770	U	C	U	A	U	U	U	U	C824
U	G1895	C	G	U	A1771	U	C	U	A	U	U	U	U	C825
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U	G1898	C	G	U	U	U	C	U	A	U	U	U	U	C828
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U	G1914	C	G	U	U	U	C	U	A	U	U	U	U	C844
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U	G1916	C	G	U	U	U	C	U	A	U	U	U	U	C846
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U	G1918	C	G	U	U	U	C	U	A	U	U	U	U	C848
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U	G1928	C	G	U	U	U	C	U	A	U	U	U	U	C858
U	G1929	C	G	U	U	U	C	U	A	U	U	U	U	C859
U	G1930	C	G	U	U	U	C	U	A	U	U	U	U	C860
U	G1931	C	G	U	U	U	C	U	A	U	U	U	U	C861
U	G1932	C	G	U	U	U	C	U	A	U	U	U	U	C862
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U	G1934	C	G	U	U	U	C	U	A	U	U	U	U	C864
U	G1935	C	G	U	U	U	C	U	A	U	U	U	U	C865
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U	G1937	C	G	U	U	U	C	U	A	U	U	U	U	C867
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U	G1949	C	G	U	U	U	C	U	A	U	U	U	U	C879
U	G1950	C	G	U	U	U	C	U	A	U	U	U	U	C880
U	G1951	C	G	U	U	U	C	U	A	U	U	U	U	C881
U	G1952	C	G	U	U	U	C	U	A	U	U	U	U	C882
U	G1953	C	G	U	U									

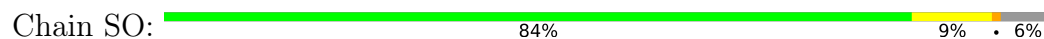
- Molecule 21: 40S ribosomal protein S12



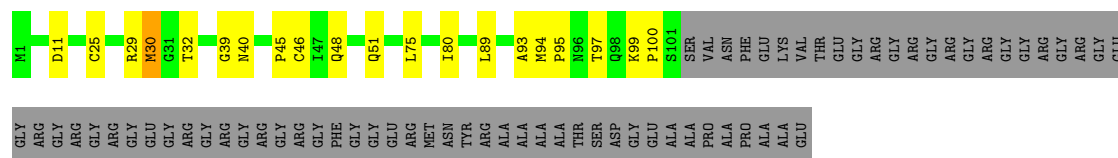
- Molecule 22: Putative 40S ribosomal protein S23



- Molecule 23: 40S ribosomal protein S14



- Molecule 24: Putative 40S ribosomal protein S10



- Molecule 25: Putative 40S ribosomal protein S33





- Molecule 26: Putative ribosomal protein S20

Chain SM: 78% 9% 12%



- Molecule 27: Putative 40S ribosomal protein S16

Chain SL: 91% 5% . .



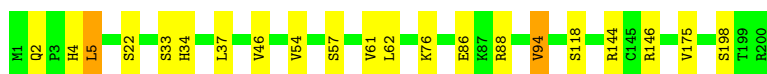
- Molecule 28: Putative 40S ribosomal protein S15A

Chain SJ: 94% 5% .



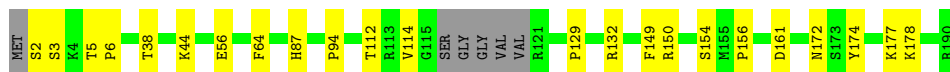
- Molecule 29: 40S ribosomal protein S7

Chain SI: 90% 10% .



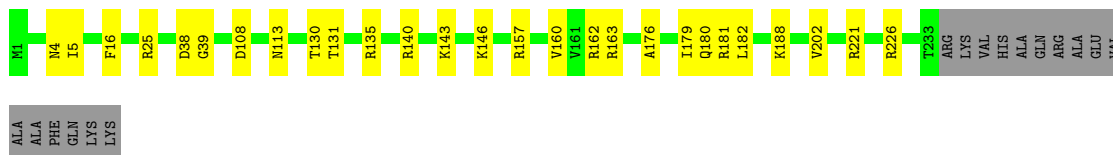
- Molecule 30: 40S ribosomal protein S5

Chain SH: 85% 12% .

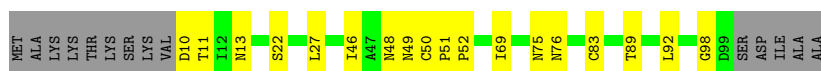


- Molecule 31: 40S ribosomal protein S6

Chain SG: 83% 11% 6%

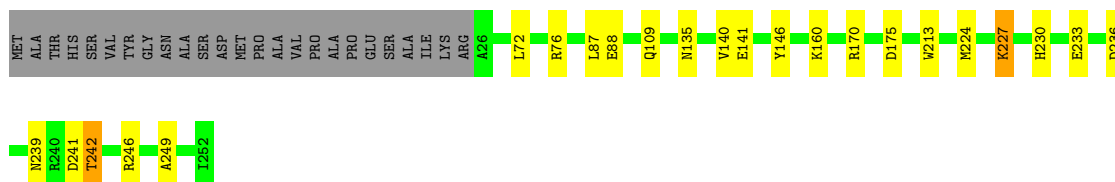


- Molecule 32: 40S ribosomal protein S2



• Molecule 38: Putative 60S ribosomal protein L7

Chain c: 81% 8% 10%



• Molecule 39: Putative 60S ribosomal protein L35

Chain a: 86% 9% 5%



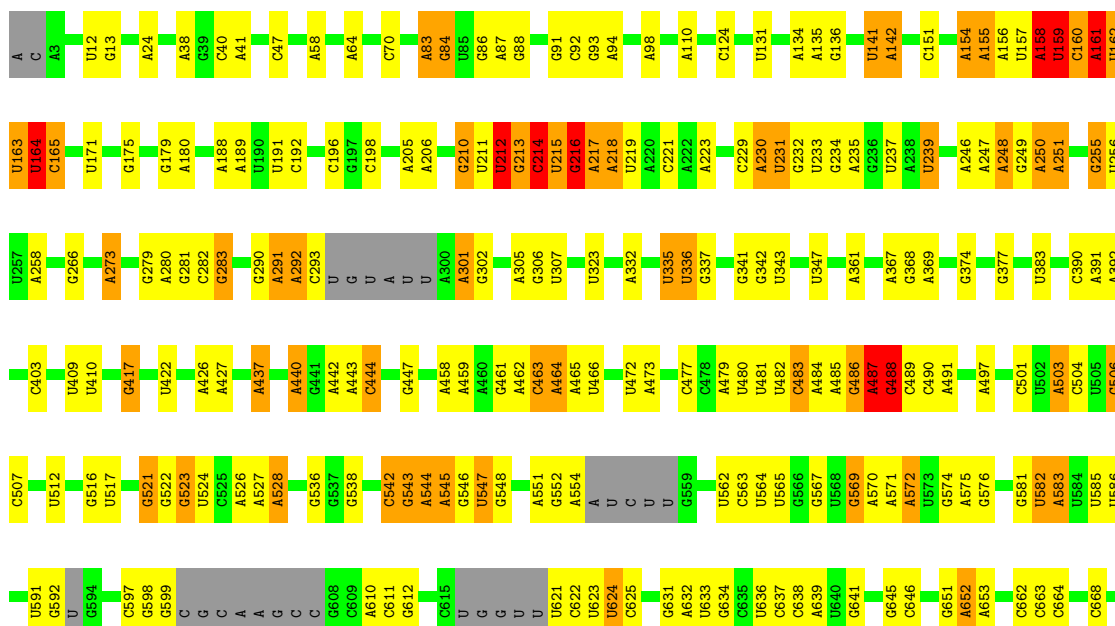
• Molecule 40: 60S ribosomal protein L29

Chain b: 90% 6% 4%



• Molecule 41: LSUa_rRNA_chain_1

Chain 1: 58% 23% 7% 11%

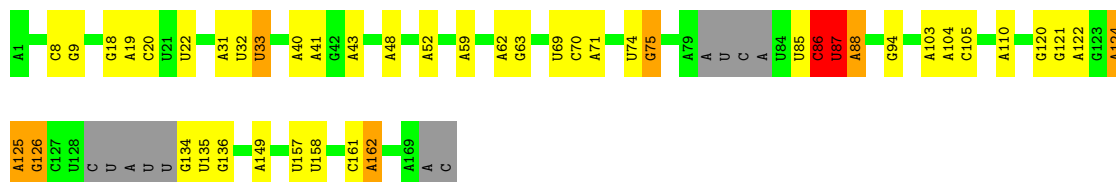






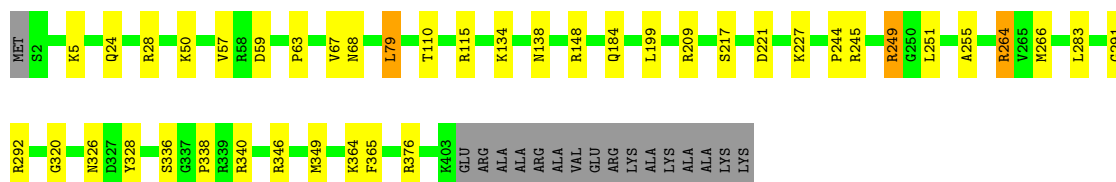
• Molecule 44: 5.8S_rRNA_chain_7

Chain 7: 67% 21% 6%



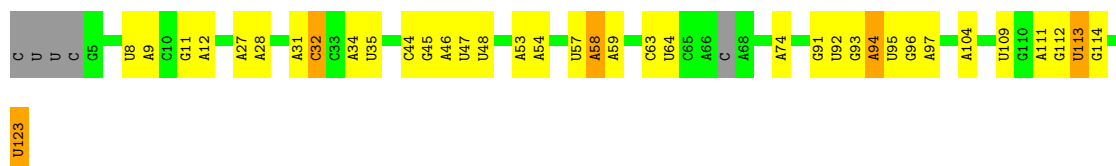
• Molecule 45: Putative ribosomal protein L3

Chain B: 86% 9%



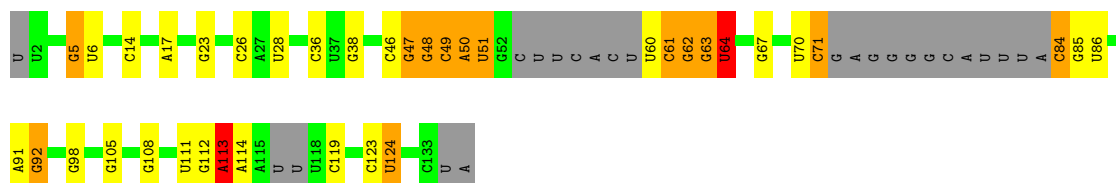
• Molecule 46: 5S_rRNA_chain_8

Chain 8: 66% 26%



• Molecule 47: SR4_chain_5

Chain 5: 54% 17% 10% 18%

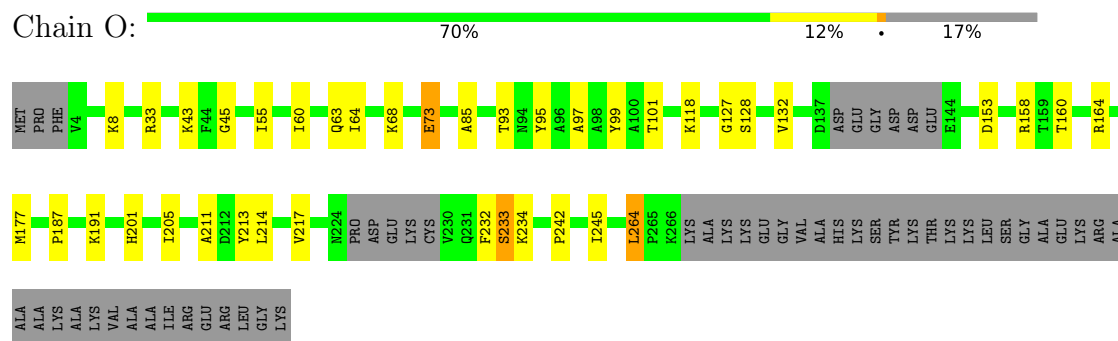


• Molecule 48: Putative 60S ribosomal protein L2

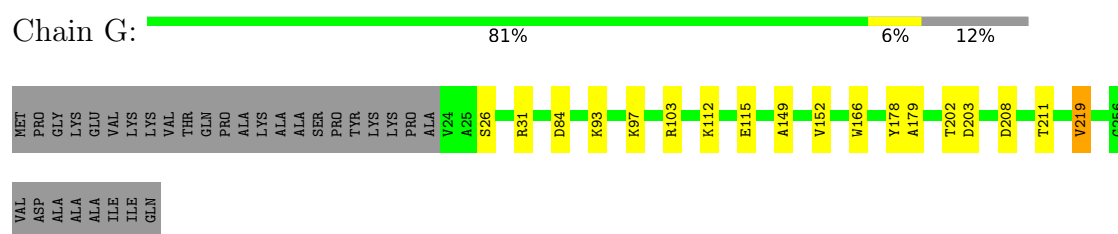
Chain A: 89% 8%



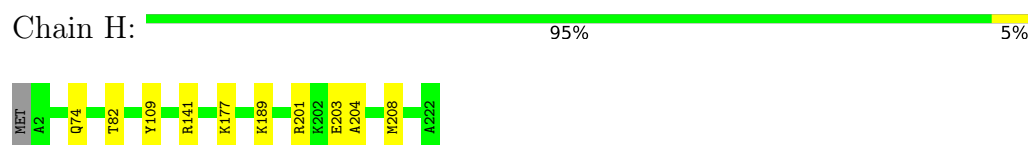
• Molecule 49: Putative 60S ribosomal protein L5



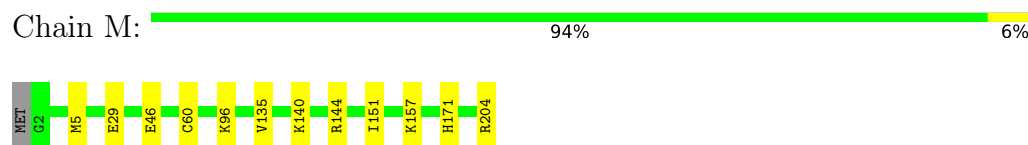
• Molecule 50: 60S ribosomal protein L7a



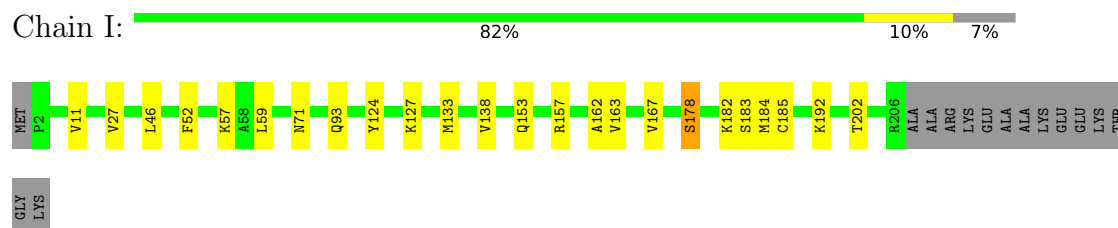
• Molecule 51: Putative 60S ribosomal protein L13a



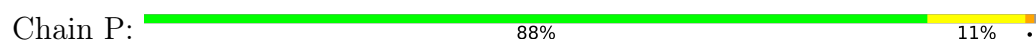
• Molecule 52: Ribosomal protein L15



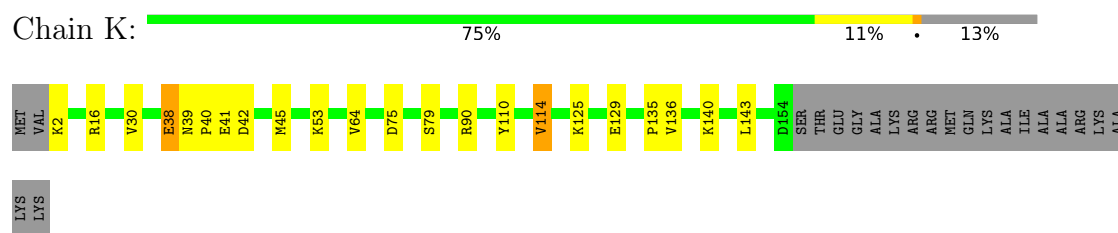
• Molecule 53: eL13_chain_I



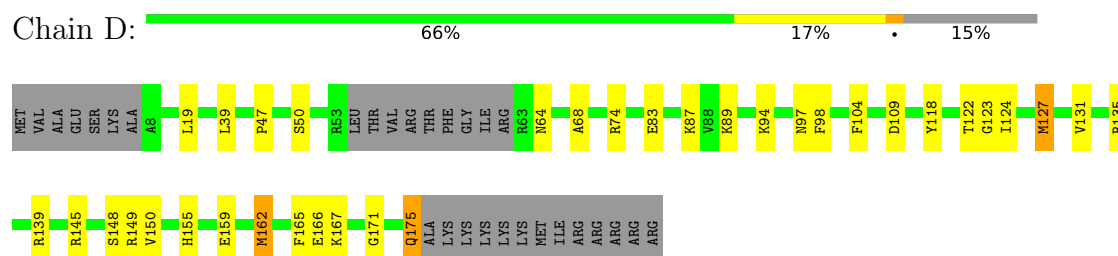
• Molecule 54: 60S ribosomal protein L18



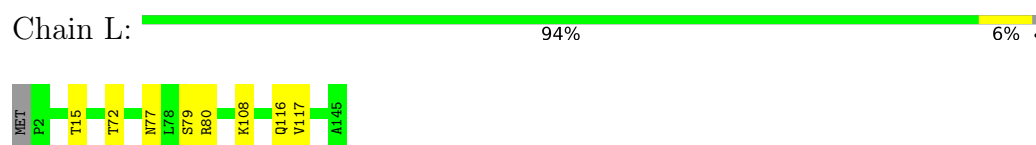
- Molecule 61: Putative 40S ribosomal protein L14



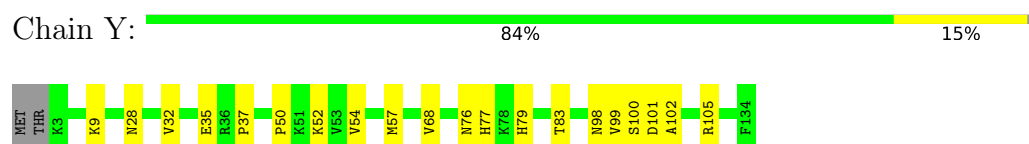
- Molecule 62: 60S ribosomal protein L11



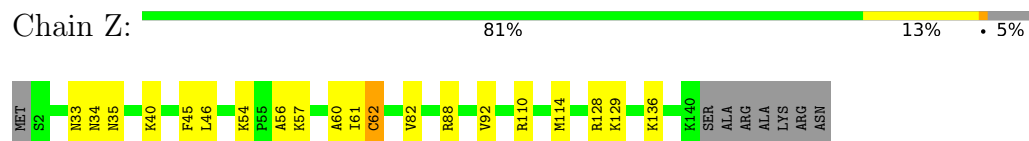
- Molecule 63: Putative 60S ribosomal protein L27A/L29



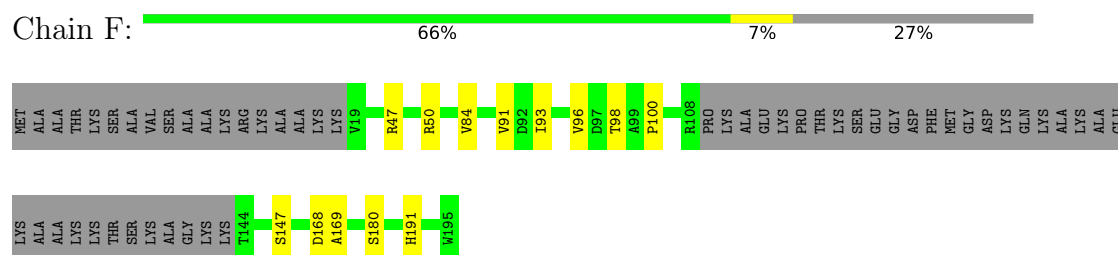
- Molecule 64: 60S ribosomal protein L27



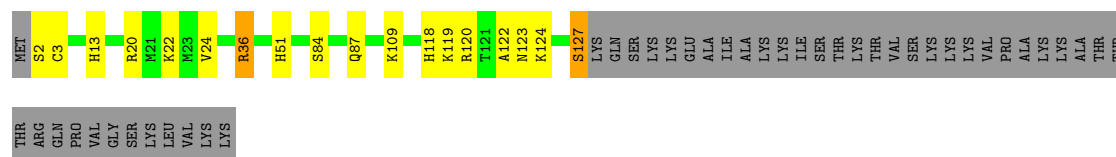
- Molecule 65: Putative 60S ribosomal protein L28



- Molecule 66: Putative 60S ribosomal protein L6



• Molecule 67: Putative 60S ribosomal protein L34

Chain h:  64% 10% 25%

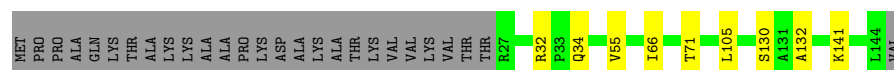
• Molecule 68: Putative ribosomal protein l35a

Chain g:  83% 11% 6%

• Molecule 69: Putative 60S ribosomal protein L23

Chain J:  88% 5% 7%

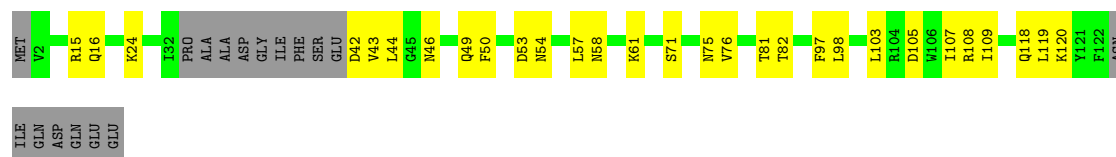
• Molecule 70: Putative 60S ribosomal protein L23a

Chain V:  75% 6% 19%

• Molecule 71: Putative 60S ribosomal protein L26

Chain W:  69% 13% 17%

• Molecule 72: Putative 60S ribosomal protein L22

Chain U:  64% 22% 13%

• Molecule 73: Putative 60S Ribosomal protein L36

Chain i:  76% 14% 10%



- Molecule 74: Putative 60S ribosomal protein L44

Chain p: 82% 8% 9%



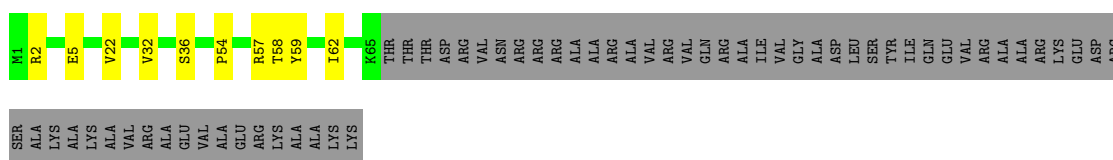
- Molecule 75: 60S ribosomal protein L37a

Chain o: 80% 15%



- Molecule 76: Putative ribosomal protein L24

Chain X: 44% 8% 48%



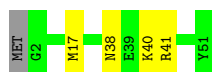
- Molecule 77: Putative ribosomal protein L38

Chain k: 75% 11% 12%



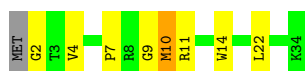
- Molecule 78: Putative 60S ribosomal protein L39

Chain l: 90% 8%



- Molecule 79: 60S ribosomal protein L41

Chain n: 74% 21%



- Molecule 80: Putative ribosomal protein L1a

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	345376	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	0.367	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.004	Depositor
Map size ($\text{\AA}$)	374.0, 374.0, 374.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: 1MA, ZN, PSU, NA, MA6, OMU, K, G7M, OMG, OMC, 5MC, A2M, C4J, MG

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	SW	0.25	0/804	0.29	0/1090
2	SZ	0.15	0/988	0.29	0/1322
3	SY	0.12	0/610	0.35	0/829
4	SX	0.28	0/1100	0.38	0/1485
5	SV	0.20	0/850	0.31	0/1141
6	SU	0.18	0/1196	0.30	0/1613
7	ST	0.18	0/1168	0.35	0/1567
8	SS	0.28	0/433	0.40	0/578
9	SR	0.28	0/908	0.34	0/1232
10	SB	0.16	0/1679	0.30	0/2273
11	SC	0.21	0/1647	0.34	0/2208
12	SD	0.15	0/1541	0.32	0/2066
13	SE	0.16	0/2100	0.32	0/2830
14	SK	0.20	0/1445	0.33	0/1937
15	S4	0.28	0/450	0.41	0/698
16	Sg	0.29	0/2306	0.46	1/3144 (0.0%)
17	Sa	0.27	0/546	0.45	0/738
18	Sc	0.16	0/651	0.33	0/877
19	Se	0.15	0/410	0.35	0/544
20	S1	0.32	2/40111 (0.0%)	0.43	43/62469 (0.1%)
21	SQ	0.15	0/178	0.28	0/242
22	SP	0.25	0/1144	0.41	0/1533
23	SO	0.38	0/1027	0.55	0/1382
24	SN	0.24	0/836	0.39	0/1134
25	Sd	0.24	0/468	0.38	0/630
26	SM	0.22	0/821	0.32	0/1112
27	SL	0.27	0/1151	0.34	0/1547
28	SJ	0.17	0/1031	0.30	0/1382
29	SI	0.15	0/1643	0.29	0/2215
30	SH	0.27	0/1459	0.34	0/1958
31	SG	0.14	0/1833	0.26	0/2458
32	SF	0.18	0/1692	0.32	0/2294

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SA	0.16	0/1862	0.30	0/2505
34	Sb	0.18	0/796	0.33	0/1070
35	Sh	0.14	0/664	0.38	0/904
36	f	0.35	0/1008	0.42	0/1351
37	d	0.29	0/635	0.36	0/871
38	c	0.31	0/1812	0.40	0/2440
39	a	0.28	0/965	0.34	0/1295
40	b	0.31	0/531	0.40	0/712
41	1	0.45	1/37000 (0.0%)	0.50	42/57678 (0.1%)
42	2	0.45	2/23546 (0.0%)	0.52	33/36681 (0.1%)
43	4	0.39	0/4341	0.42	0/6767
44	7	0.46	0/3669	0.48	5/5710 (0.1%)
45	B	0.34	0/3283	0.47	0/4421
46	8	0.28	0/2806	0.32	0/4367
47	5	0.47	0/2650	0.59	5/4123 (0.1%)
48	A	0.34	0/2029	0.47	0/2722
49	O	0.24	0/2007	0.37	0/2696
50	G	0.31	0/1883	0.44	0/2535
51	H	0.35	0/1810	0.48	1/2435 (0.0%)
52	M	0.36	0/1754	0.47	0/2342
53	I	0.30	0/1626	0.42	1/2186 (0.0%)
54	P	0.31	0/1564	0.40	0/2092
55	Q	0.32	0/1500	0.43	0/2000
56	R	0.35	0/1481	0.49	0/1997
57	E	0.27	0/1458	0.44	0/1971
58	6	0.33	0/1658	0.52	0/2580
59	T	0.34	0/1257	0.46	0/1683
60	S	0.29	0/1230	0.40	0/1658
61	K	0.24	0/1212	0.34	0/1634
62	D	0.26	0/1159	0.48	0/1565
63	L	0.33	0/1151	0.44	0/1538
64	Y	0.26	0/1070	0.39	0/1437
65	Z	0.26	0/1066	0.36	0/1431
66	F	0.27	0/1065	0.40	1/1451 (0.1%)
67	h	0.47	2/1035 (0.2%)	0.54	4/1378 (0.3%)
68	g	0.38	0/1124	0.48	0/1511
69	J	0.39	0/985	0.54	0/1329
70	V	0.30	0/954	0.41	0/1284
71	W	0.30	0/962	0.43	0/1284
72	U	0.24	0/892	0.37	0/1192
73	i	0.25	0/750	0.38	0/1003
74	p	0.31	0/733	0.44	0/977
75	o	0.37	0/708	0.54	0/944

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	X	0.29	0/574	0.42	0/774
77	k	0.26	0/554	0.41	0/751
78	l	0.35	0/453	0.42	0/606
79	n	0.60	0/263	0.87	1/348 (0.3%)
80	C	0.42	0/2847	0.61	1/3836 (0.0%)
81	3	0.47	0/3792	0.67	19/5895 (0.3%)
82	e	0.45	0/1314	0.70	0/1761
83	j	0.39	0/676	0.53	0/902
All	All	0.36	7/206390 (0.0%)	0.46	157/303151 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	36[A]	ARG	C-O	7.47	1.33	1.24
67	h	36[B]	ARG	C-O	7.47	1.33	1.24
20	S1	512	A2M	O3'-P	5.25	1.61	1.56
42	2	527	A2M	O3'-P	5.16	1.61	1.56
42	2	572	A2M	O3'-P	5.14	1.61	1.56
20	S1	479	A2M	O3'-P	5.08	1.61	1.56
41	1	858	A2M	O3'-P	5.02	1.61	1.56

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	214	C	P-O3'-C3'	-10.62	104.27	120.20
42	2	508	A	P-O3'-C3'	-10.09	105.07	120.20
41	1	487	A	P-O3'-C3'	-9.04	106.65	120.20
20	S1	232	C	P-O3'-C3'	-9.03	106.66	120.20
42	2	497	G	P-O3'-C3'	-8.80	107.00	120.20
42	2	507	G	P-O3'-C3'	-8.74	107.10	120.20
41	1	164	U	P-O3'-C3'	-8.52	107.43	120.20
42	2	510	PSU	P-O3'-C3'	-8.34	107.69	120.20
20	S1	780	A	P-O3'-C3'	-8.31	107.73	120.20
41	1	1393	A	P-O3'-C3'	-8.29	107.77	120.20
20	S1	783	A	P-O3'-C3'	-8.16	107.96	120.20
20	S1	234	C	P-O3'-C3'	-8.13	108.00	120.20
41	1	212	U	P-O3'-C3'	-8.11	108.04	120.20
41	1	1392	G	P-O3'-C3'	-8.01	108.19	120.20
20	S1	2061	5MC	P-O3'-C3'	-7.99	108.22	120.20
81	3	183	G	P-O3'-C3'	-7.95	108.28	120.20
41	1	1382	G	P-O3'-C3'	-7.88	108.37	120.20
20	S1	784	C	P-O3'-C3'	-7.75	108.58	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	159	U	P-O3'-C3'	-7.74	108.59	120.20
41	1	646	C	P-O3'-C3'	-7.72	108.63	120.20
42	2	504	PSU	P-O3'-C3'	-7.67	108.69	120.20
42	2	512	U	P-O3'-C3'	-7.63	108.75	120.20
41	1	1761	A	P-O3'-C3'	-7.61	108.78	120.20
81	3	58	U	P-O3'-C3'	-7.56	108.86	120.20
81	3	40	A	P-O3'-C3'	-7.55	108.88	120.20
44	7	88	A	P-O3'-C3'	-7.49	108.96	120.20
41	1	160	C	P-O3'-C3'	-7.49	108.97	120.20
41	1	1245	G	P-O3'-C3'	-7.43	109.05	120.20
41	1	216	G	P-O3'-C3'	-7.42	109.07	120.20
41	1	211	U	P-O3'-C3'	-7.34	109.19	120.20
20	S1	2065	G	P-O3'-C3'	-7.33	109.20	120.20
44	7	86	C	P-O3'-C3'	-7.32	109.23	120.20
42	2	783	A	P-O3'-C3'	-7.26	109.31	120.20
20	S1	782	C	P-O3'-C3'	-7.22	109.36	120.20
20	S1	1577	U	P-O3'-C3'	-7.22	109.37	120.20
41	1	490	C	P-O3'-C3'	-7.18	109.43	120.20
20	S1	231	A	P-O3'-C3'	-7.16	109.47	120.20
42	2	500	PSU	P-O3'-C3'	-7.14	109.49	120.20
44	7	87	U	P-O3'-C3'	-7.14	109.49	120.20
41	1	251	A	P-O3'-C3'	-7.12	109.52	120.20
66	F	100	PRO	CA-N-CD	-7.12	102.03	112.00
20	S1	235	C	P-O3'-C3'	-7.11	109.53	120.20
20	S1	1462	G	P-O3'-C3'	-7.11	109.53	120.20
42	2	518	G	P-O3'-C3'	-7.11	109.53	120.20
41	1	1395	U	P-O3'-C3'	-7.10	109.54	120.20
47	5	64	U	P-O3'-C3'	-7.09	109.56	120.20
20	S1	233	G	P-O3'-C3'	-7.03	109.66	120.20
42	2	62	A	P-O3'-C3'	-7.02	109.67	120.20
20	S1	509	G	P-O3'-C3'	-7.00	109.70	120.20
41	1	1762	A	P-O3'-C3'	-7.00	109.71	120.20
20	S1	508	A	P-O3'-C3'	-6.95	109.77	120.20
81	3	146	G	P-O3'-C3'	-6.90	109.85	120.20
20	S1	492	U	P-O3'-C3'	-6.89	109.86	120.20
81	3	59	U	P-O3'-C3'	-6.87	109.90	120.20
20	S1	2059	C	P-O3'-C3'	-6.83	109.96	120.20
20	S1	236	C	P-O3'-C3'	-6.82	109.97	120.20
42	2	501	A	P-O3'-C3'	-6.82	109.97	120.20
42	2	444	A	P-O3'-C3'	-6.80	110.00	120.20
42	2	786	A	P-O3'-C3'	-6.79	110.01	120.20
42	2	74	A	P-O3'-C3'	-6.72	110.12	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	516	A	P-O3'-C3'	-6.69	110.17	120.20
20	S1	510	G	P-O3'-C3'	-6.69	110.17	120.20
81	3	45	U	P-O3'-C3'	-6.69	110.17	120.20
41	1	1244	G	P-O3'-C3'	-6.68	110.18	120.20
41	1	213	G	P-O3'-C3'	-6.64	110.24	120.20
42	2	517	A	P-O3'-C3'	-6.62	110.27	120.20
20	S1	117	G	P-O3'-C3'	-6.62	110.27	120.20
20	S1	779	A	P-O3'-C3'	-6.61	110.28	120.20
20	S1	506	U	P-O3'-C3'	-6.61	110.29	120.20
44	7	70	C	P-O3'-C3'	-6.60	110.29	120.20
47	5	92	G	P-O3'-C3'	-6.58	110.32	120.20
81	3	144	U	P-O3'-C3'	-6.58	110.32	120.20
42	2	63	U	P-O3'-C3'	-6.58	110.33	120.20
41	1	161	A	P-O3'-C3'	-6.54	110.39	120.20
20	S1	1576	A	P-O3'-C3'	-6.53	110.41	120.20
41	1	1255	G	P-O3'-C3'	-6.52	110.42	120.20
42	2	441	C	P-O3'-C3'	-6.46	110.51	120.20
42	2	61	C	P-O3'-C3'	-6.45	110.52	120.20
67	h	36[A]	ARG	CA-C-O	6.40	127.78	120.54
67	h	36[B]	ARG	CA-C-O	6.40	127.78	120.54
20	S1	493	C	P-O3'-C3'	-6.40	110.60	120.20
51	H	109	TYR	CB-CA-C	6.40	121.41	110.79
20	S1	2058	G	P-O3'-C3'	-6.37	110.64	120.20
42	2	496	G	P-O3'-C3'	-6.37	110.65	120.20
20	S1	113	A	P-O3'-C3'	-6.36	110.66	120.20
47	5	113	A	P-O3'-C3'	-6.35	110.68	120.20
42	2	58	G	P-O3'-C3'	-6.35	110.68	120.20
20	S1	116	U	P-O3'-C3'	-6.33	110.71	120.20
20	S1	496	A	P-O3'-C3'	-6.33	110.71	120.20
16	Sg	299	LYS	N-CA-C	-6.30	104.41	111.28
41	1	484	A	P-O3'-C3'	-6.28	110.78	120.20
81	3	142	G	P-O3'-C3'	-6.22	110.87	120.20
81	3	145	U	P-O3'-C3'	-6.22	110.87	120.20
42	2	514	U	P-O3'-C3'	-6.20	110.90	120.20
81	3	143	A	P-O3'-C3'	-6.20	110.90	120.20
20	S1	1463	G	P-O3'-C3'	-6.18	110.93	120.20
20	S1	495	A	P-O3'-C3'	-6.14	111.00	120.20
41	1	1396	G	P-O3'-C3'	-6.14	111.00	120.20
20	S1	114	U	P-O3'-C3'	-6.10	111.05	120.20
81	3	46	C	P-O3'-C3'	-6.07	111.09	120.20
42	2	495	G	P-O3'-C3'	-6.06	111.10	120.20
41	1	1381	G	P-O3'-C3'	-6.04	111.14	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1461	G	P-O3'-C3'	-6.02	111.16	120.20
20	S1	115	C	P-O3'-C3'	-5.96	111.26	120.20
41	1	215	U	P-O3'-C3'	-5.90	111.35	120.20
41	1	1760	C	P-O3'-C3'	-5.87	111.40	120.20
20	S1	781	A	P-O3'-C3'	-5.84	111.44	120.20
41	1	247	A	P-O3'-C3'	-5.83	111.45	120.20
20	S1	112	A	P-O3'-C3'	-5.80	111.49	120.20
41	1	1763	A	P-O3'-C3'	-5.80	111.50	120.20
41	1	938	G	P-O3'-C3'	-5.73	111.60	120.20
41	1	250	A	P-O3'-C3'	-5.72	111.61	120.20
81	3	141	A	P-O3'-C3'	-5.72	111.62	120.20
81	3	188	C	P-O3'-C3'	-5.71	111.63	120.20
42	2	59	U	P-O3'-C3'	-5.71	111.63	120.20
42	2	1512	G	P-O3'-C3'	-5.70	111.66	120.20
41	1	488	G	P-O3'-C3'	-5.69	111.66	120.20
41	1	481	U	P-O3'-C3'	-5.67	111.69	120.20
20	S1	2056	C	P-O3'-C3'	-5.67	111.70	120.20
81	3	43	C	P-O3'-C3'	-5.63	111.75	120.20
42	2	800	G	P-O3'-C3'	-5.63	111.76	120.20
41	1	645	G	P-O3'-C3'	-5.61	111.79	120.20
47	5	84	C	P-O3'-C3'	-5.54	111.90	120.20
81	3	41	A	P-O3'-C3'	-5.53	111.90	120.20
81	3	196	U	P-O3'-C3'	-5.52	111.92	120.20
20	S1	1578	G	P-O3'-C3'	-5.51	111.93	120.20
41	1	1602	C	P-O3'-C3'	-5.49	111.96	120.20
41	1	158	A	P-O3'-C3'	-5.46	112.00	120.20
41	1	983	U	C2'-C3'-O3'	5.45	117.67	109.50
81	3	38	U	P-O3'-C3'	-5.45	112.03	120.20
20	S1	1464	G	P-O3'-C3'	-5.44	112.04	120.20
41	1	246	A	P-O3'-C3'	-5.43	112.06	120.20
41	1	248	A	P-O3'-C3'	-5.42	112.07	120.20
47	5	63	G	P-O3'-C3'	-5.42	112.07	120.20
41	1	1601	U	P-O3'-C3'	-5.40	112.10	120.20
42	2	506	PSU	P-O3'-C3'	-5.40	112.10	120.20
42	2	493	G	P-O3'-C3'	-5.40	112.11	120.20
20	S1	491	G	P-O3'-C3'	-5.38	112.13	120.20
81	3	186	U	P-O3'-C3'	-5.38	112.13	120.20
20	S1	1580	G	P-O3'-C3'	-5.37	112.14	120.20
42	2	515	U	P-O3'-C3'	-5.35	112.18	120.20
81	3	187	U	C2'-C3'-O3'	5.30	117.45	109.50
42	2	782	G	P-O3'-C3'	-5.29	112.27	120.20
42	2	347	A	P-O3'-C3'	-5.28	112.28	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	n	7	PRO	CB-CA-C	-5.24	103.98	112.62
44	7	71	A	P-O3'-C3'	-5.23	112.36	120.20
53	I	163	VAL	N-CA-C	-5.21	108.76	113.71
41	1	1391	U	P-O3'-C3'	-5.20	112.40	120.20
20	S1	1581	G	P-O3'-C3'	-5.20	112.40	120.20
42	2	491	C	P-O3'-C3'	-5.19	112.42	120.20
41	1	447	G	O4'-C1'-N9	5.17	115.95	108.20
67	h	36[A]	ARG	O-C-N	-5.15	117.35	123.22
67	h	36[B]	ARG	O-C-N	-5.15	117.35	123.22
80	C	107	PHE	CA-CB-CG	5.12	118.92	113.80
20	S1	778	G	P-O3'-C3'	-5.08	112.58	120.20
20	S1	1923	A	O4'-C1'-N9	5.05	115.78	108.20
42	2	60	A	P-O3'-C3'	-5.01	112.68	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	SW	787	0	772	5	0
2	SZ	967	0	1013	5	0
3	SY	604	0	589	11	0
4	SX	1071	0	1068	9	0
5	SV	843	0	861	10	0
6	SU	1170	0	1180	9	0
7	ST	1145	0	1211	6	0
8	SS	428	0	418	7	0
9	SR	892	0	871	8	0
10	SB	1643	0	1658	32	0
11	SC	1619	0	1671	18	0
12	SD	1513	0	1588	15	0
13	SE	2056	0	2155	17	0
14	SK	1424	0	1501	10	0
15	S4	404	0	211	4	0
16	Sg	2251	0	2116	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Sa	541	0	561	8	0
18	Sc	638	0	624	7	0
19	Se	404	0	434	4	0
20	S1	36928	0	18662	318	0
21	SQ	179	0	160	2	0
22	SP	1115	0	1162	9	0
23	SO	1012	0	1023	11	0
24	SN	813	0	787	17	0
25	Sd	466	0	476	5	0
26	SM	811	0	854	5	0
27	SL	1130	0	1190	5	0
28	SJ	1014	0	1044	6	0
29	SI	1613	0	1669	11	0
30	SH	1437	0	1464	11	0
31	SG	1809	0	1889	18	0
32	SF	1656	0	1706	14	0
33	SA	1834	0	1920	20	0
34	Sb	779	0	793	7	0
35	Sh	657	0	615	14	0
36	f	988	0	1023	0	0
37	d	625	0	567	10	0
38	c	1779	0	1822	16	0
39	a	955	0	983	11	0
40	b	520	0	531	2	0
41	1	33802	0	17053	269	0
42	2	22358	0	11347	234	0
43	4	3906	0	1975	27	0
44	7	3399	0	1721	16	0
45	B	3200	0	3297	28	0
46	8	2511	0	1272	24	0
47	5	2373	0	1205	25	0
48	A	1973	0	2040	20	0
49	O	1970	0	2011	24	0
50	G	1850	0	1956	10	0
51	H	1771	0	1854	7	0
52	M	1714	0	1793	7	0
53	I	1593	0	1614	12	0
54	P	1539	0	1648	20	0
55	Q	1482	0	1500	15	0
56	R	1447	0	1481	17	0
57	E	1439	0	1489	29	0
58	6	1484	0	758	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	T	1233	0	1278	8	0
60	S	1203	0	1240	9	0
61	K	1193	0	1219	13	0
62	D	1140	0	1071	22	0
63	L	1124	0	1151	5	0
64	Y	1046	0	1084	15	0
65	Z	1052	0	1072	16	0
66	F	1045	0	1052	6	0
67	h	1016	0	1070	15	0
68	g	1101	0	1138	12	0
69	J	968	0	1023	2	0
70	V	939	0	992	8	0
71	W	948	0	1019	12	0
72	U	879	0	896	17	0
73	i	738	0	785	12	0
74	p	722	0	732	5	0
75	o	696	0	716	10	0
76	X	553	0	555	4	0
77	k	546	0	537	5	0
78	l	440	0	461	4	0
79	n	259	0	269	7	0
80	C	2797	0	2875	20	0
81	3	3419	0	1733	41	0
82	e	1298	0	1360	24	0
83	j	662	0	669	6	0
84	1	61	0	0	0	0
84	2	31	0	0	0	0
84	3	1	0	0	0	0
84	4	3	0	0	0	0
84	5	1	0	0	0	0
84	6	1	0	0	0	0
84	7	4	0	0	0	0
84	8	1	0	0	0	0
84	J	1	0	0	0	0
84	S1	23	0	0	0	0
84	SL	1	0	0	0	0
84	SS	1	0	0	0	0
84	T	1	0	0	0	0
85	Sb	1	0	0	0	0
85	Sc	1	0	0	0	0
85	j	1	0	0	0	0
85	o	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	1	5	0	0	0	0
86	2	3	0	0	0	0
87	1	2	0	0	0	0
88	1	918	0	0	27	0
88	2	536	0	0	34	0
88	3	31	0	0	0	0
88	4	73	0	0	5	0
88	5	37	0	0	0	0
88	6	3	0	0	0	0
88	7	85	0	0	3	0
88	8	17	0	0	4	0
88	A	30	0	0	4	0
88	B	29	0	0	4	0
88	C	21	0	0	0	0
88	E	1	0	0	0	0
88	G	4	0	0	0	0
88	H	9	0	0	0	0
88	I	21	0	0	1	0
88	J	1	0	0	0	0
88	K	1	0	0	0	0
88	L	17	0	0	0	0
88	M	28	0	0	1	0
88	P	12	0	0	0	0
88	Q	6	0	0	0	0
88	R	1	0	0	0	0
88	S	4	0	0	0	0
88	S1	237	0	0	34	0
88	S4	1	0	0	0	0
88	SB	3	0	0	1	0
88	SC	1	0	0	0	0
88	SD	1	0	0	0	0
88	SE	1	0	0	0	0
88	SF	2	0	0	0	0
88	SH	4	0	0	0	0
88	SK	1	0	0	0	0
88	SN	3	0	0	2	0
88	SO	2	0	0	1	0
88	SP	3	0	0	0	0
88	SR	2	0	0	1	0
88	SS	1	0	0	0	0
88	ST	5	0	0	0	0
88	SX	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	SY	1	0	0	0	0
88	SZ	1	0	0	0	0
88	Sa	1	0	0	1	0
88	Sb	2	0	0	0	0
88	Sc	2	0	0	0	0
88	Sd	1	0	0	0	0
88	Sg	3	0	0	1	0
88	T	14	0	0	0	0
88	V	6	0	0	0	0
88	W	2	0	0	1	0
88	X	2	0	0	0	0
88	a	3	0	0	1	0
88	c	4	0	0	0	0
88	d	3	0	0	0	0
88	e	9	0	0	1	0
88	f	16	0	0	0	0
88	g	9	0	0	1	0
88	h	12	0	0	0	0
88	i	1	0	0	0	0
88	j	13	0	0	0	0
88	k	2	0	0	0	0
88	l	6	0	0	1	0
88	o	2	0	0	0	0
88	p	13	0	0	0	0
All	All	197779	0	142853	1623	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 5.

All (1623) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S1:955:A:N6	20:S1:980:G:H1	1.46	1.13
41:1:1776:G:H1	42:2:6:A:N6	1.49	1.09
20:S1:1574:G:H1	20:S1:1613:C:H5	1.10	0.97
81:3:156:G:H1	81:3:175:A:H2	1.12	0.95
47:5:64:U:H5	47:5:92:G:H1	1.06	0.95
42:2:818:U:H3	42:2:958:A:H61	1.15	0.92
41:1:959:OMG:H5'	41:1:959:OMG:H8	1.34	0.91
42:2:501:A:H62	42:2:507:G:H2'	1.37	0.90
41:1:124:C:H42	41:1:142:A:H61	1.21	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:3:156:G:N1	81:3:175:A:C2	2.39	0.89
42:2:1457:C:H41	42:2:1465:G:H1	1.15	0.89
20:S1:2059:C:H5	20:S1:2166:A:H61	1.20	0.84
41:1:1776:G:N2	42:2:6:A:N1	2.25	0.84
10:SB:203:ASP:O	10:SB:208[A]:ARG:NH2	2.11	0.83
10:SB:24:MET:HG3	10:SB:176:MET:HG2	1.60	0.82
42:2:1455:U:H3	42:2:1467:G:H1	1.26	0.82
20:S1:1612:C:O2'	20:S1:1613:C:O2	1.96	0.82
20:S1:776:A:H2'	20:S1:779:A:H4'	1.61	0.81
47:5:48:G:H4'	47:5:49:C:H4'	1.63	0.81
39:a:94:ARG:NH1	88:a:201:HOH:O	2.13	0.81
16:Sg:6:HIS:HB2	16:Sg:302:LEU:HD13	1.63	0.80
20:S1:528:G:H1	20:S1:553:U:H5	1.29	0.80
42:2:768:G:H21	70:V:34:GLN:HE22	1.32	0.77
20:S1:780:A:H61	20:S1:840:A:H62	1.31	0.77
41:1:638:C:H5	41:1:1433:G:H1	1.31	0.76
20:S1:1577:U:H3'	20:S1:1578:G:H21	1.50	0.76
44:7:124:A:N7	44:7:124:A:N6	2.33	0.76
20:S1:1922:A:H1'	20:S1:1923:A:H5'	1.69	0.75
81:3:156:G:N1	81:3:175:A:H2	1.80	0.75
41:1:216:G:H5''	65:Z:128:ARG:HD2	1.68	0.75
41:1:1148:A:H61	60:S:111:GLN:HE21	1.35	0.74
46:8:44:C:O2	62:D:74:ARG:NH1	2.19	0.74
37:d:27:LEU:HD22	37:d:89:THR:HG21	1.69	0.74
41:1:1676:G:H1	41:1:1723:A:H61	1.32	0.74
20:S1:955:A:N1	20:S1:980:G:N2	2.30	0.74
42:2:452:G:N3	88:2:1722:HOH:O	2.21	0.74
42:2:569:G:O2'	42:2:571:G:OP2	2.05	0.74
20:S1:1909:C:H5	20:S1:1930:G:H1	1.36	0.74
20:S1:2078:A:OP2	88:S1:2401:HOH:O	2.06	0.74
42:2:499:G:H1	42:2:510:PSU:HN3	1.36	0.74
48:A:39:GLY:HA2	48:A:93:LYS:HE2	1.70	0.74
20:S1:974:G:H3'	20:S1:975:G:H21	1.51	0.73
41:1:336:U:OP2	73:i:35:VAL:N	2.21	0.73
41:1:504:C:H3'	41:1:552:G:H21	1.52	0.73
13:SE:84:MET:HE2	13:SE:120:LEU:HB2	1.70	0.73
20:S1:2160:G:H21	42:2:502:A:H1'	1.54	0.73
71:W:71:TYR:O	88:W:201:HOH:O	2.06	0.73
57:E:45:LEU:HD23	57:E:56:VAL:HG12	1.71	0.72
71:W:35:GLU:OE2	71:W:35:GLU:N	2.17	0.72
41:1:682:C:OP1	88:1:1901:HOH:O	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S1:1504:A:O2'	34:Sb:89:ARG:NH2	2.22	0.72
20:S1:2060:C:H2'	20:S1:2061:5MC:HM53	1.71	0.72
20:S1:552:U:O2'	20:S1:553:U:O2	2.06	0.72
20:S1:1101:A:N1	88:S1:2429:HOH:O	2.23	0.72
41:1:1245:G:C2	41:1:1382:G:N2	2.57	0.72
40:b:6:ASN:ND2	41:1:1005:U:OP2	2.22	0.72
42:2:792:G:H1	42:2:801:C:H5	1.37	0.71
10:SB:88:ARG:HD3	10:SB:207:TYR:HA	1.70	0.71
45:B:245[B]:ARG:NH1	88:B:502:HOH:O	2.21	0.71
20:S1:2050:U:OP1	88:S1:2402:HOH:O	2.08	0.71
20:S1:1931:G:H4'	20:S1:1932:A:H5'	1.71	0.71
43:4:9:G:OP2	44:7:9:G:O2'	2.08	0.71
41:1:1152:A:OP2	88:1:1902:HOH:O	2.09	0.71
42:2:459:A:H2'	42:2:460:A:C8	2.26	0.71
20:S1:69:C:H42	20:S1:79:A:H61	1.39	0.70
41:1:1273:U:H2'	41:1:1274:G:H5''	1.71	0.70
41:1:160:C:H3'	41:1:161:A:H8	1.55	0.70
20:S1:1287:U:H2'	20:S1:1288:G:C8	2.26	0.70
41:1:1246:C:C2	41:1:1382:G:N2	2.59	0.70
16:Sg:146:ARG:NH1	16:Sg:147:ASP:OD2	2.24	0.70
41:1:1271:G:N7	88:1:1924:HOH:O	2.25	0.70
47:5:50:A:H61	47:5:62:G:H1	1.39	0.70
73:i:32:ARG:HA	73:i:35:VAL:HG21	1.74	0.70
88:1:2764:HOH:O	78:l:17:MET:SD	2.50	0.70
41:1:377:G:N7	88:1:1925:HOH:O	2.25	0.69
10:SB:206:PHE:O	10:SB:208[A]:ARG:NH2	2.25	0.69
13:SE:260:ARG:NH2	20:S1:877:U:O2	2.24	0.69
41:1:188:A:OP1	71:W:121:ARG:NH1	2.24	0.69
41:1:463:C:H5'	41:1:464:A:H5''	1.74	0.69
20:S1:605:A:OP2	88:S1:2403:HOH:O	2.10	0.69
41:1:417:G:O2'	41:1:442:A:N6	2.25	0.69
47:5:26:C:N3	47:5:124:U:O2'	2.22	0.69
20:S1:2061:5MC:H4'	79:n:9:GLY:O	1.92	0.69
39:a:113:ARG:NH2	41:1:151:C:OP1	2.25	0.69
56:R:23:GLU:N	56:R:23:GLU:OE2	2.26	0.69
64:Y:54:VAL:H	64:Y:57:MET:HE3	1.57	0.69
35:Sh:151:ALA:HA	35:Sh:154:MET:HE1	1.75	0.69
42:2:494:C:H4'	42:2:518:G:H21	1.56	0.69
63:L:72:THR:HG22	63:L:108:LYS:HB3	1.75	0.69
24:SN:25:CYS:SG	88:SN:203:HOH:O	2.50	0.69
43:4:94:G:N7	88:4:302:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:g:63:THR:HG22	68:g:66:ASP:H	1.56	0.69
82:e:46:LYS:C	82:e:48:PHE:H	2.00	0.69
24:SN:46:CYS:SG	88:SN:203:HOH:O	2.49	0.68
42:2:1055:A:N3	88:2:1726:HOH:O	2.25	0.68
75:o:5:THR:HG21	75:o:9:GLY:H	1.58	0.68
46:8:53:A:H3'	49:O:234:LYS:HE2	1.75	0.68
42:2:1439:U:OP2	88:2:1702:HOH:O	2.10	0.68
62:D:166:GLU:O	62:D:167:LYS:HG2	1.93	0.68
57:E:125:VAL:HG21	57:E:131:VAL:HG21	1.75	0.68
42:2:1381:G:OP1	88:2:1701:HOH:O	2.10	0.68
60:S:50:GLU:OE2	60:S:50:GLU:N	2.27	0.68
73:i:62:GLU:OE2	73:i:65:ARG:NH1	2.27	0.68
20:S1:1369:U:H3	20:S1:1412:G:H1	1.40	0.67
41:1:1352:C:H2'	41:1:1353:A:C8	2.29	0.67
42:2:510:PSU:H2'	42:2:511:C:C6	2.28	0.67
42:2:1309:G:OP2	88:2:1703:HOH:O	2.10	0.67
42:2:337:A:N1	55:Q:153:ARG:NH2	2.43	0.67
52:M:5:MET:HE1	73:i:39:HIS:CD2	2.30	0.67
41:1:1029:G:N2	41:1:1030:U:O4	2.26	0.67
14:SK:34:ALA:HB2	14:SK:56:ARG:HD2	1.76	0.67
46:8:27:A:O2'	46:8:123:U:OP1	2.11	0.67
67:h:118:HIS:HA	67:h:122:ALA:HB3	1.75	0.67
20:S1:1960:G:OP2	88:S1:2404:HOH:O	2.12	0.67
8:SS:53:PHE:HB3	26:SM:77:PHE:HB3	1.77	0.67
57:E:28:THR:HG23	57:E:33:THR:HG22	1.77	0.67
60:S:128:LEU:HD23	60:S:128:LEU:H	1.58	0.67
13:SE:101:ASP:HB2	13:SE:239:GLN:HE22	1.59	0.67
20:S1:1770:G:OP2	20:S1:1770:G:N2	2.28	0.67
62:D:135:ARG:NH1	62:D:155:HIS:O	2.27	0.67
46:8:47:U:OP2	88:8:301:HOH:O	2.12	0.67
4:SX:68:ILE:HD12	9:SR:44:LEU:HD11	1.77	0.66
17:Sa:84:CYS:SG	88:Sa:201:HOH:O	2.53	0.66
43:4:136:G:N7	88:4:303:HOH:O	2.27	0.66
5:SV:118:ARG:O	10:SB:19:GLN:NE2	2.24	0.66
20:S1:1288:G:H1	20:S1:1426:U:H5	1.42	0.66
42:2:1350:G:OP1	88:2:1705:HOH:O	2.12	0.66
42:2:1275:A:H2	42:2:1291:G:H1	1.43	0.66
41:1:347:U:OP1	73:i:87:LYS:NZ	2.29	0.66
41:1:1600:U:H5	42:2:18:A:N1	1.93	0.66
10:SB:106:PHE:N	88:SB:301:HOH:O	2.28	0.66
42:2:558:A:OP1	42:2:560:OMU:H5	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:1:1901:HOH:O	42:2:1311:U:OP2	2.13	0.66
24:SN:95:PRO:HB2	24:SN:100:PRO:HD3	1.77	0.66
42:2:1382:PSU:OP2	88:2:1701:HOH:O	2.14	0.66
8:SS:7:TRP:O	20:S1:1851:U:O2'	2.09	0.66
47:5:50:A:N1	47:5:62:G:N2	2.44	0.66
41:1:569:G:OP2	88:1:1905:HOH:O	2.13	0.66
42:2:55:C:N3	67:h:2:SER:OG	2.26	0.66
42:2:617:G:N7	88:2:1732:HOH:O	2.28	0.66
20:S1:1796:U:H2'	20:S1:1797:A:C8	2.31	0.65
41:1:886:G:H2'	41:1:908:G:H22	1.60	0.65
47:5:47:G:H2'	47:5:48:G:N3	2.12	0.65
49:O:217:VAL:HG21	49:O:232:PHE:HD2	1.61	0.65
11:SC:180:CYS:SG	88:S1:2616:HOH:O	2.54	0.65
20:S1:861:A:OP2	88:S1:2405:HOH:O	2.13	0.65
20:S1:951:U:H3	20:S1:984:G:H1	1.44	0.65
48:A:174:ARG:O	88:A:301:HOH:O	2.14	0.65
82:e:35:ARG:O	82:e:39:ASN:ND2	2.30	0.65
16:Sg:44:ASN:HB2	16:Sg:47:ARG:HG3	1.77	0.65
41:1:1748:G:OP2	88:1:1904:HOH:O	2.13	0.65
41:1:954:U:OP1	88:1:1906:HOH:O	2.13	0.65
42:2:516:A:H2'	42:2:517:A:C8	2.31	0.65
41:1:1553:G:N7	88:1:1931:HOH:O	2.28	0.65
42:2:1184:C:OP1	88:2:1706:HOH:O	2.14	0.65
20:S1:70:U:H3	20:S1:78:C:H41	1.44	0.65
2:SZ:106:ALA:O	20:S1:503:C:N4	2.28	0.65
17:Sa:61:THR:HB	17:Sa:64:ILE:HD12	1.77	0.65
18:Sc:38:CYS:O	18:Sc:42:ARG:NH1	2.30	0.65
20:S1:1635:U:OP1	88:S1:2406:HOH:O	2.13	0.65
31:SG:160:VAL:HG21	31:SG:179:ILE:HD11	1.77	0.65
13:SE:173:ARG:NH1	20:S1:789:G:OP1	2.30	0.64
20:S1:585:C:HO2'	20:S1:586:G:H8	1.46	0.64
57:E:10:LEU:HD23	57:E:73:LYS:HG3	1.79	0.64
72:U:107:ILE:HD11	72:U:119:LEU:HB3	1.77	0.64
20:S1:780:A:N6	20:S1:840:A:H62	1.95	0.64
20:S1:916:G:H1	55:Q:164:LEU:HD21	1.61	0.64
41:1:1659:OMU:OP1	88:1:1907:HOH:O	2.14	0.64
56:R:132:PRO:HG2	56:R:135:GLU:HG3	1.78	0.64
57:E:90:LYS:HG2	57:E:144:VAL:HG22	1.80	0.64
20:S1:1289:A:H62	20:S1:1425:U:H3	1.46	0.64
41:1:291:A:H2'	41:1:292:A:C8	2.32	0.64
35:Sh:136:SER:HA	35:Sh:180:PRO:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2:1342:G:H2'	42:2:1343:A:C8	2.32	0.64
14:SK:64:ASN:OD1	20:S1:305:U:O2'	2.15	0.64
26:SM:48:HIS:HB2	26:SM:87:ASP:HB2	1.80	0.64
41:1:210:G:O6	65:Z:57:LYS:NZ	2.31	0.64
41:1:527:A:O2'	41:1:528:A:O5'	2.15	0.64
41:1:1245:G:N2	41:1:1382:G:N2	2.46	0.64
42:2:1271:G:H1	42:2:1294:G:H22	1.46	0.64
20:S1:875:A:H62	20:S1:887:U:H5	1.46	0.64
41:1:483:C:H4'	41:1:486:G:H21	1.63	0.63
11:SC:46:GLU:HG3	11:SC:86:TYR:HE2	1.63	0.63
16:Sg:5:GLY:HA3	16:Sg:54:TYR:HB2	1.80	0.63
43:4:54:G:N2	43:4:57:A:OP2	2.28	0.63
17:Sa:51:ARG:NH2	17:Sa:86:GLU:OE1	2.31	0.63
25:Sd:33:THR:HG21	25:Sd:41:GLN:HG3	1.80	0.63
33:SA:37:ASN:HD21	33:SA:184:LYS:HG2	1.64	0.63
20:S1:1553:G:OP1	88:S1:2407:HOH:O	2.16	0.63
41:1:521:G:H2'	41:1:522:G:C8	2.34	0.63
42:2:1271:G:H1	42:2:1294:G:H1	1.45	0.63
78:l:41:ARG:NH2	88:l:101:HOH:O	2.30	0.63
38:c:76:ARG:NH2	38:c:88:GLU:OE2	2.32	0.63
42:2:1066:G:OP2	88:2:1709:HOH:O	2.15	0.63
56:R:175:ARG:NH2	58:6:45:G:N7	2.47	0.63
20:S1:694:U:H3	20:S1:751:G:H1	1.46	0.63
10:SB:92:LYS:HE2	10:SB:204:LEU:HB3	1.80	0.62
80:C:295:GLU:OE2	80:C:295:GLU:N	2.20	0.62
41:1:487:A:H4'	41:1:488:G:H8	1.64	0.62
43:4:16:G:H2'	43:4:17:A:C8	2.34	0.62
41:1:487:A:H4'	41:1:488:G:C8	2.34	0.62
20:S1:1224:A:H62	20:S1:1271:C:H5	1.47	0.62
47:5:47:G:O2'	47:5:50:A:OP1	2.13	0.62
41:1:1037:A:N1	88:1:1936:HOH:O	2.31	0.62
42:2:613:A:OP2	88:2:1711:HOH:O	2.16	0.62
41:1:569:G:N2	88:1:1905:HOH:O	2.33	0.62
42:2:557:G:OP1	88:2:1710:HOH:O	2.16	0.62
7:ST:14:SER:HB2	20:S1:1206:C:H5''	1.81	0.62
73:i:90:ARG:O	73:i:94:GLU:HG3	2.00	0.62
20:S1:1132:G:H2'	20:S1:1133:U:C6	2.35	0.61
41:1:846:G:H2'	41:1:847:OMU:H6	1.83	0.61
41:1:886:G:H1'	41:1:909:A:N6	2.15	0.61
44:7:31:A:O2'	44:7:33:U:OP2	2.12	0.61
41:1:1730:A:OP2	70:V:32:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2:453:A:N6	42:2:456:G:O6	2.31	0.61
41:1:162:U:H4'	41:1:163:U:OP1	2.00	0.61
41:1:836:G:OP1	54:P:149:ARG:NH1	2.33	0.61
56:R:75:ASN:HD21	56:R:145:HIS:HE1	1.47	0.61
39:a:102:ASN:HD21	39:a:106:ARG:HH21	1.47	0.61
44:7:124:A:N6	44:7:125:A:N7	2.49	0.61
18:Sc:57:CYS:H	18:Sc:62:LYS:HA	1.65	0.61
20:S1:2166:A:OP2	88:S1:2410:HOH:O	2.16	0.61
41:1:1425:C:O3'	65:Z:88:ARG:NH2	2.29	0.61
42:2:451:U:O2'	88:2:1704:HOH:O	2.11	0.61
20:S1:2153:A:H4'	79:n:22:LEU:HD21	1.82	0.61
20:S1:2168:A:OP1	79:n:2:GLY:HA2	2.00	0.61
42:2:809:C:H2'	42:2:810:G:N2	2.16	0.61
20:S1:148:G:H2'	20:S1:149:G:C8	2.36	0.61
20:S1:1829:OMG:OP1	88:S1:2409:HOH:O	2.16	0.61
38:c:241:ASP:OD1	38:c:242:THR:N	2.32	0.61
41:1:212:U:H2'	41:1:213:G:C8	2.35	0.61
41:1:1245:G:H8	41:1:1245:G:H5''	1.66	0.61
42:2:959:A:H2'	42:2:960:C:C6	2.36	0.61
32:SF:50:LYS:HG2	32:SF:259:LEU:HD13	1.83	0.61
42:2:818:U:H3	42:2:958:A:N6	1.94	0.61
20:S1:1186:A:H2'	20:S1:1187:A:C8	2.36	0.60
41:1:791:C:OP2	41:1:792:G:N1	2.34	0.60
80:C:304:LYS:HD2	80:C:305:LEU:H	1.66	0.60
10:SB:88:ARG:NH2	10:SB:204:LEU:O	2.30	0.60
42:2:587:A:N7	88:2:1735:HOH:O	2.31	0.60
42:2:1089:A:OP1	88:2:1713:HOH:O	2.16	0.60
66:F:50:ARG:NH1	66:F:180:SER:OG	2.34	0.60
11:SC:66[B]:ARG:NH1	24:SN:100:PRO:O	2.34	0.60
20:S1:955:A:H61	20:S1:980:G:H1	0.70	0.60
41:1:1541:C:OP1	88:1:1909:HOH:O	2.16	0.60
41:1:1619:U:OP1	88:1:1908:HOH:O	2.16	0.60
41:1:572:A:O4'	80:C:313:PHE:HE2	1.83	0.60
57:E:184:THR:OG1	57:E:185:ASN:N	2.34	0.60
2:SZ:15:SER:HA	20:S1:879:A:H61	1.66	0.60
20:S1:1281:C:HO2'	28:SJ:2:THR:N	1.99	0.60
64:Y:76:ASN:HD22	64:Y:77:HIS:N	1.98	0.60
9:SR:88:GLN:HA	9:SR:96:THR:HG23	1.84	0.60
10:SB:83:ARG:NH2	10:SB:132:THR:OG1	2.35	0.60
41:1:483:C:H5''	41:1:483:C:H6	1.65	0.60
41:1:1238:C:H5'	41:1:1239:U:H5'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2:1399:G:OP1	88:2:1710:HOH:O	2.16	0.60
12:SD:65:HIS:HD2	12:SD:67:ARG:H	1.49	0.60
20:S1:836:C:H3'	20:S1:837:G:H21	1.67	0.60
20:S1:1833:OMU:OP2	88:S1:2408:HOH:O	2.16	0.60
9:SR:123:GLY:O	88:SR:201:HOH:O	2.16	0.60
37:d:22:SER:OG	37:d:98:GLY:O	2.16	0.60
42:2:1239:A:OP1	88:2:1708:HOH:O	2.15	0.60
68:g:122:ASN:ND2	88:g:201:HOH:O	2.35	0.60
20:S1:670:A:OP2	88:S1:2411:HOH:O	2.16	0.59
41:1:792:G:O2'	41:1:793:U:OP2	2.19	0.59
42:2:540:C:OP2	69:J:73:LYS:NZ	2.33	0.59
10:SB:34:SER:HB2	10:SB:154:ASP:HA	1.84	0.59
20:S1:1117:A:H2'	20:S1:1118:G:C8	2.37	0.59
41:1:522:G:H2'	41:1:523:G:C8	2.37	0.59
16:Sg:116:SER:OG	16:Sg:118:ASP:OD1	2.18	0.59
20:S1:1920:A:O2'	20:S1:1921:A:OP2	2.14	0.59
41:1:1725:U:O2'	41:1:1726:G:O4'	2.20	0.59
20:S1:1603:U:H2'	20:S1:1604:C:C6	2.38	0.59
41:1:512:U:N3	56:R:30:GLU:OE2	2.21	0.59
41:1:585:U:H5	41:1:624:U:H3	1.50	0.59
15:S4:2:C:H2'	15:S4:3:G:H8	1.66	0.59
38:c:246:ARG:HG2	41:1:1394:A:C5	2.37	0.59
39:a:5:MET:HE2	39:a:5:MET:HA	1.83	0.59
42:2:434:A:OP1	88:2:1714:HOH:O	2.17	0.59
20:S1:1829:OMG:OP2	88:S1:2412:HOH:O	2.17	0.59
39:a:114:GLN:HE21	53:I:93:GLN:HE22	1.50	0.59
42:2:958:A:H2'	42:2:959:A:C8	2.38	0.59
14:SK:57:ALA:HB2	14:SK:196:GLY:HA2	1.84	0.59
20:S1:363:G:H4'	20:S1:367:A:C8	2.38	0.59
41:1:576:G:O6	80:C:324:ARG:HG3	2.03	0.59
41:1:1722:U:H2'	41:1:1723:A:C4	2.37	0.59
42:2:512:U:H2'	42:2:513:C:C6	2.38	0.59
75:o:58:ASP:OD2	81:3:194:A:N6	2.36	0.59
20:S1:1114:G:H1	20:S1:1207:U:H3	1.48	0.59
42:2:511:C:H2'	42:2:512:U:C6	2.38	0.59
43:4:98:A:H2'	43:4:99:A:C8	2.37	0.59
12:SD:87:GLU:OE2	12:SD:87:GLU:N	2.27	0.59
20:S1:916:G:H4'	20:S1:917:C:H5'	1.85	0.59
28:SJ:18:GLU:HG2	28:SJ:69:LEU:HB3	1.85	0.59
42:2:434:A:OP2	88:2:1707:HOH:O	2.15	0.59
47:5:50:A:N6	47:5:62:G:H1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1:212:U:H2'	41:1:213:G:H8	1.68	0.58
41:1:709:A:OP1	54:P:115:SER:OG	2.21	0.58
42:2:1183:C:OP1	88:2:1715:HOH:O	2.17	0.58
20:S1:951:U:O2	20:S1:984:G:N2	2.30	0.58
20:S1:957:G:H1	20:S1:978:C:H42	1.51	0.58
20:S1:1430:C:N4	20:S1:1439:G:N7	2.46	0.58
41:1:488:G:H2'	41:1:489:C:C6	2.39	0.58
20:S1:1138:G:H2'	20:S1:1139:G:C8	2.38	0.58
30:SH:112:THR:HG23	30:SH:114:VAL:HG12	1.84	0.58
41:1:1274:G:O2'	41:1:1275:G:H8	1.86	0.58
42:2:590:U:H2'	42:2:591:A2M:H8	1.85	0.58
82:e:22:ALA:H	82:e:25:ARG:HG2	1.67	0.58
15:S4:2:C:H2'	15:S4:3:G:C8	2.39	0.58
68:g:111:HIS:HD2	68:g:118:ARG:HE	1.52	0.58
20:S1:76:U:H1'	20:S1:77:G:C8	2.38	0.58
49:O:55:ILE:HG12	49:O:60:ILE:HG23	1.85	0.58
38:c:224:MET:HB3	38:c:236:ASP:OD2	2.03	0.58
20:S1:757:C:H4'	20:S1:758:G:O5'	2.03	0.58
42:2:351:C:H5'	55:Q:89:MET:HE2	1.85	0.58
42:2:809:C:H3'	42:2:810:G:H5''	1.86	0.58
20:S1:1289:A:N6	20:S1:1425:U:H3	2.01	0.58
41:1:791:C:H4'	41:1:792:G:C5	2.38	0.58
47:5:71:C:H5	47:5:85:G:H1	1.51	0.58
5:SV:25:ASN:H	5:SV:31:ASN:HD21	1.52	0.58
20:S1:96:U:OP1	88:S1:2413:HOH:O	2.17	0.58
41:1:179:G:H2'	41:1:180:A:C8	2.39	0.58
49:O:68:LYS:NZ	49:O:73:GLU:OE2	2.34	0.58
41:1:1777:U:H3	42:2:5:A:H61	1.52	0.57
42:2:780:G:H2'	42:2:781:G:H8	1.67	0.57
56:R:77:LEU:HD11	56:R:93:VAL:HG12	1.85	0.57
67:h:119:LYS:HD3	67:h:120:ARG:H	1.69	0.57
41:1:472:U:H2'	41:1:473:A:C8	2.40	0.57
16:Sg:260:VAL:HG23	16:Sg:269:ILE:HG13	1.85	0.57
20:S1:71:G:H1	20:S1:77:G:H22	1.50	0.57
35:Sh:177:LEU:HD12	35:Sh:180:PRO:HB3	1.87	0.57
41:1:1242:U:OP1	61:K:16:ARG:NH2	2.38	0.57
42:2:956:C:H41	67:h:127:SER:HA	1.69	0.57
20:S1:640:A:H2'	20:S1:641:A:C8	2.39	0.57
42:2:586:G:N7	88:2:1738:HOH:O	2.32	0.57
11:SC:48:VAL:HG12	11:SC:86:TYR:HB2	1.87	0.57
20:S1:2103:G:O2'	20:S1:2104:G:N2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1:885:U:H2'	41:1:886:G:O4'	2.05	0.57
2:SZ:17:PHE:HZ	2:SZ:26:LYS:HD3	1.70	0.57
3:SY:74:ASN:OD1	10:SB:60:LYS:NZ	2.37	0.57
20:S1:318:C:OP1	88:S1:2414:HOH:O	2.18	0.57
42:2:494:C:H4'	42:2:518:G:N2	2.19	0.57
45:B:320:GLY:O	45:B:340:ARG:NH1	2.36	0.57
52:M:157:LYS:O	88:M:301:HOH:O	2.17	0.57
61:K:135:PRO:HB3	61:K:140:LYS:HB3	1.86	0.57
16:Sg:190:LEU:HD21	16:Sg:221:TRP:CE2	2.39	0.57
41:1:403:C:OP2	83:j:56:ARG:NH2	2.29	0.57
41:1:506:G:H5''	80:C:349:ARG:HD3	1.86	0.57
42:2:1404:G:H5''	48:A:220:GLY:HA3	1.85	0.57
20:S1:16:G:H2'	20:S1:17:C:C6	2.40	0.57
20:S1:45:U:O2'	20:S1:46:U:H2'	2.04	0.57
42:2:969:A:H5'	42:2:970:A:OP1	2.05	0.57
49:O:55:ILE:HG21	49:O:164:ARG:HH21	1.70	0.57
74:p:13:GLY:HA2	74:p:18:ASN:HA	1.86	0.57
1:SW:89:ASP:OD1	1:SW:89:ASP:N	2.36	0.57
82:e:160:HIS:N	88:e:201:HOH:O	2.37	0.57
12:SD:77:ARG:O	12:SD:81:GLU:HG2	2.05	0.57
16:Sg:221:TRP:NE1	88:Sg:401:HOH:O	2.35	0.57
61:K:75:ASP:N	61:K:75:ASP:OD1	2.33	0.57
81:3:43:C:O5'	81:3:43:C:H6	1.88	0.57
24:SN:95:PRO:HG2	24:SN:100:PRO:HG3	1.87	0.56
41:1:503:A:N6	41:1:554:A:OP1	2.37	0.56
2:SZ:44:GLN:OE1	2:SZ:47:ARG:NH2	2.34	0.56
20:S1:1574:G:N1	20:S1:1613:C:H5	1.92	0.56
37:d:10:ASP:HA	37:d:13:ASN:HD22	1.69	0.56
41:1:141:U:H1'	41:1:142:A:H5''	1.87	0.56
56:R:70:LYS:O	56:R:74:ARG:NH2	2.38	0.56
72:U:49:GLN:OE1	72:U:49:GLN:N	2.25	0.56
41:1:1255:G:H2'	41:1:1256:A:C8	2.41	0.56
42:2:1024:U:H2'	42:2:1025:G:C8	2.41	0.56
42:2:1500:U:OP1	45:B:134:LYS:NZ	2.34	0.56
57:E:16:VAL:O	57:E:52:ARG:NH2	2.38	0.56
59:T:41:LEU:HD13	59:T:150:MET:HE1	1.87	0.56
41:1:1011:PSU:O2'	41:1:1012:C:OP2	2.22	0.56
75:o:84:ARG:HG2	75:o:84:ARG:HH11	1.70	0.56
16:Sg:103:PHE:HE2	16:Sg:138:GLY:HA2	1.69	0.56
20:S1:1278:U:H5	20:S1:1445:A:N7	2.02	0.56
41:1:458:A:H2'	41:1:459:A:O4'	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2:68:A:O2'	42:2:69:A:O5'	2.21	0.56
46:8:32:C:OP1	62:D:139:ARG:NH1	2.38	0.56
48:A:36:GLU:HG3	48:A:91:GLY:HA2	1.88	0.56
32:SF:125:ILE:HD12	32:SF:227:PHE:HB2	1.87	0.56
41:1:1561:A:H2'	41:1:1562:C:H6	1.70	0.56
42:2:1065:C:OP1	88:2:1716:HOH:O	2.18	0.56
16:Sg:175:THR:HG22	16:Sg:191:LYS:HB3	1.85	0.56
20:S1:285:A:H62	20:S1:816:C:H2'	1.70	0.56
41:1:507:C:OP2	80:C:353:ARG:NH1	2.39	0.56
42:2:1263:C:H42	42:2:1302:A:H61	1.54	0.56
42:2:1386:C:OP1	45:B:249[A]:ARG:NH2	2.39	0.56
41:1:886:G:H1'	41:1:909:A:H61	1.69	0.56
42:2:1499:G:H1	42:2:1522:U:H5	1.53	0.56
20:S1:1460:G:H1	22:SP:20:ASN:HD22	1.54	0.56
20:S1:1554:A:OP1	88:S1:2415:HOH:O	2.18	0.56
20:S1:1914:U:O2'	20:S1:1915:U:H6	1.89	0.56
38:c:227:LYS:NZ	41:1:1215:C:OP1	2.38	0.56
47:5:49:C:H5''	47:5:63:G:N2	2.20	0.56
20:S1:1881:G:H2'	20:S1:1882:A:C8	2.41	0.55
8:SS:22:CYS:SG	8:SS:25:CYS:N	2.78	0.55
33:SA:112:MET:HA	33:SA:112:MET:HE2	1.87	0.55
48:A:80:GLU:HG3	75:o:66:GLY:HA3	1.88	0.55
66:F:96:VAL:HG13	66:F:98:THR:HG23	1.88	0.55
41:1:1238:C:H42	56:R:179:ALA:HB1	1.70	0.55
82:e:77:ASP:HB3	82:e:161:PHE:HE1	1.70	0.55
6:SU:112:TYR:O	6:SU:114:ARG:N	2.40	0.55
31:SG:162:ARG:HD3	31:SG:176:ALA:HB2	1.88	0.55
42:2:478:A:H2'	42:2:479:C:O2	2.06	0.55
42:2:1291:G:H2'	42:2:1292:U:O4'	2.07	0.55
72:U:49:GLN:H	72:U:49:GLN:CD	2.14	0.55
79:n:10:MET:O	79:n:11:ARG:C	2.49	0.55
3:SY:82:ILE:O	10:SB:1:MET:N	2.37	0.55
20:S1:1271:C:N3	88:S1:2454:HOH:O	2.32	0.55
42:2:347:A:H2'	42:2:348:A:C8	2.41	0.55
42:2:553:G:O2'	42:2:556:U:OP2	2.22	0.55
42:2:1270:C:OP2	42:2:1270:C:H3'	2.06	0.55
11:SC:114:VAL:HG11	11:SC:137:VAL:HG11	1.89	0.55
42:2:1436:A:O2'	42:2:1438:U:OP1	2.18	0.55
48:A:140:ASN:ND2	48:A:143:THR:HG23	2.21	0.55
54:P:100:ALA:H	63:L:116:GLN:NE2	2.04	0.55
4:SX:169:GLN:OE1	4:SX:169:GLN:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S1:558:U:H2'	20:S1:559:G:C8	2.42	0.55
41:1:959:OMG:H5'	41:1:959:OMG:C8	2.30	0.55
42:2:1271:G:H22	42:2:1294:G:H22	1.53	0.55
58:6:40:C:H3'	61:K:90:ARG:HG3	1.88	0.55
59:T:5:SER:H	59:T:147:GLN:HE22	1.53	0.55
61:K:41:GLU:N	61:K:41:GLU:OE2	2.39	0.55
20:S1:71:G:H1	20:S1:77:G:H1	1.53	0.55
33:SA:139:LEU:HD13	33:SA:217:VAL:HB	1.89	0.55
52:M:204:ARG:NH2	80:C:109:ARG:HG2	2.22	0.55
5:SV:26:PHE:HD2	5:SV:59:LYS:HG2	1.71	0.55
20:S1:1595:G:H2'	20:S1:1595:G:N3	2.22	0.55
41:1:40:C:OP1	88:1:1910:HOH:O	2.18	0.55
41:1:179:G:H2'	41:1:180:A:H8	1.71	0.55
83:j:28:HIS:CD2	83:j:31:TRP:H	2.24	0.55
41:1:1381:G:H2'	41:1:1382:G:C8	2.42	0.55
14:SK:76:VAL:HG12	14:SK:108:PRO:HG2	1.89	0.54
16:Sg:262:ASP:HB3	16:Sg:264:GLU:OE2	2.06	0.54
28:SJ:68:ARG:HG2	32:SF:242:TRP:CE2	2.43	0.54
41:1:1251:U:H1'	51:H:74:GLN:NE2	2.22	0.54
41:1:1676:G:H1	41:1:1723:A:N6	2.04	0.54
57:E:125:VAL:HG12	57:E:126:PRO:HD2	1.89	0.54
65:Z:56:ALA:HB3	65:Z:60:ALA:HB3	1.89	0.54
24:SN:45:PRO:HB2	24:SN:48:GLN:HG3	1.89	0.54
41:1:790:C:H4'	41:1:791:C:OP1	2.05	0.54
43:4:11:G:N7	88:4:307:HOH:O	2.34	0.54
9:SR:13:ILE:HD12	62:D:118:TYR:CE2	2.41	0.54
43:4:15:G:O2'	43:4:16:G:O5'	2.18	0.54
44:7:75:OMG:N2	88:7:306:HOH:O	2.40	0.54
41:1:1274:G:O2'	41:1:1275:G:O5'	2.25	0.54
44:7:161:C:H2'	44:7:162:A2M:H8	1.89	0.54
62:D:122:THR:OG1	62:D:123:GLY:N	2.40	0.54
42:2:613:A:OP1	45:B:264[B]:ARG:NH2	2.41	0.54
76:X:5:GLU:OE2	76:X:57:ARG:NH2	2.41	0.54
42:2:1505:A:HO2'	42:2:1506:G:H8	1.55	0.54
81:3:191:C:H5'	81:3:192:G:H4'	1.88	0.54
41:1:823:G:N2	88:1:1933:HOH:O	2.30	0.54
42:2:78:PSU:H6	42:2:78:PSU:H5'	1.73	0.54
46:8:27:A:OP2	88:8:303:HOH:O	2.18	0.54
52:M:5:MET:HE1	73:i:39:HIS:HD2	1.72	0.54
62:D:94:LYS:O	62:D:97:ASN:HB2	2.07	0.54
77:k:52:LYS:O	77:k:56:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S1:1577:U:H3'	20:S1:1578:G:N2	2.22	0.54
42:2:453:A:H2'	42:2:454:A:H4'	1.88	0.54
42:2:780:G:H2'	42:2:781:G:C8	2.43	0.54
41:1:696:A:H2'	41:1:697:A2M:C8	2.38	0.54
41:1:889:G:HO2'	81:3:124:U:HO2'	1.51	0.54
54:P:100:ALA:H	63:L:116:GLN:HE21	1.56	0.54
20:S1:87:G:N2	20:S1:495:A:OP1	2.41	0.53
20:S1:604:A:OP2	88:S1:2403:HOH:O	2.18	0.53
42:2:1272:G:O2'	42:2:1273:C:H5'	2.08	0.53
49:O:85:ALA:HB2	49:O:264:LEU:HD23	1.90	0.53
20:S1:1914:U:O2'	20:S1:1915:U:O5'	2.23	0.53
23:SO:86:LEU:HD12	23:SO:117:MET:HE2	1.89	0.53
33:SA:175:LYS:O	33:SA:179:SER:OG	2.20	0.53
41:1:1489:U:H2'	41:1:1490:G:C8	2.43	0.53
42:2:1027:C:OP2	88:2:1717:HOH:O	2.19	0.53
42:2:1457:C:H3'	42:2:1458:G:H5''	1.89	0.53
52:M:140:LYS:HD2	52:M:144:ARG:NH2	2.23	0.53
9:SR:101:SER:O	9:SR:101:SER:OG	2.26	0.53
35:Sh:153:VAL:HG23	35:Sh:154:MET:SD	2.48	0.53
44:7:32:U:H5''	44:7:33:U:OP2	2.09	0.53
50:G:179:ALA:HB2	50:G:219:VAL:HG22	1.89	0.53
20:S1:71:G:H22	20:S1:77:G:H22	1.55	0.53
20:S1:106:A:H2'	20:S1:107:G:C8	2.43	0.53
23:SO:21:TYR:HA	23:SO:85:ALA:O	2.08	0.53
42:2:498:A:H61	42:2:511:C:H42	1.55	0.53
44:7:19:A:OP1	88:7:301:HOH:O	2.19	0.53
41:1:886:G:H2'	41:1:908:G:N2	2.24	0.53
41:1:1019:G:H2'	41:1:1020:C:C6	2.44	0.53
42:2:1042:G:H2'	42:2:1043:C:H6	1.73	0.53
42:2:1403:PSU:H5'	42:2:1403:PSU:C6	2.43	0.53
72:U:15:ARG:HA	72:U:58:ASN:HD22	1.73	0.53
6:SU:30:ASN:ND2	6:SU:32:ASN:H	2.06	0.53
6:SU:30:ASN:HD22	6:SU:32:ASN:H	1.57	0.53
20:S1:785:G:O4'	20:S1:787:G:N2	2.41	0.53
20:S1:1171:A:H2'	20:S1:1172:G:C8	2.44	0.53
57:E:149:ASP:HB3	57:E:152:GLN:HB2	1.90	0.53
1:SW:60:PRO:O	20:S1:1595:G:N2	2.24	0.53
11:SC:134:GLU:HG2	11:SC:152:ARG:HB3	1.91	0.53
20:S1:1420:U:H2'	20:S1:1421:C:C6	2.44	0.53
20:S1:2039:C:H2'	20:S1:2040:C:O2	2.09	0.53
41:1:544:A:OP2	41:1:1392:G:H8	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2:1457:C:H5	42:2:1465:G:H22	1.57	0.53
20:S1:71:G:H22	20:S1:77:G:N2	2.07	0.53
42:2:1184:C:OP2	88:2:1715:HOH:O	2.19	0.53
20:S1:784:C:H2'	20:S1:787:G:N2	2.23	0.53
20:S1:1850:U:OP2	88:S1:2417:HOH:O	2.19	0.53
27:SL:60:VAL:O	30:SH:3:SER:OG	2.26	0.53
42:2:382:A2M:O5'	42:2:382:A2M:H8	2.09	0.53
42:2:985:A:H1'	42:2:986:U:H2'	1.90	0.53
43:4:10:U:H2'	43:4:10:U:O2	2.09	0.53
4:SX:60:ILE:HG21	4:SX:86:TYR:HE1	1.74	0.53
41:1:1776:G:H1	42:2:6:A:H61	0.69	0.53
41:1:1776:G:H2'	41:1:1777:U:C6	2.44	0.53
20:S1:2010:G:H1	20:S1:2026:U:H3	1.57	0.52
20:S1:2085:A:HO2'	20:S1:2086:A:H8	1.54	0.52
24:SN:75:LEU:HD13	24:SN:80:ILE:HG13	1.91	0.52
42:2:500:PSU:H2'	42:2:501:A:N3	2.24	0.52
8:SS:10:ARG:HH12	20:S1:1973:C:H5	1.57	0.52
16:Sg:222:ASP:OD2	16:Sg:224:SER:OG	2.26	0.52
25:Sd:44:VAL:HG22	25:Sd:59:ILE:HG22	1.90	0.52
47:5:85:G:O5'	47:5:85:G:H8	1.91	0.52
6:SU:30:ASN:HD22	6:SU:30:ASN:C	2.17	0.52
10:SB:31:ARG:CZ	10:SB:32:ASN:HB3	2.39	0.52
20:S1:285:A:H2'	20:S1:817:A:H2	1.74	0.52
20:S1:671:G:O2'	20:S1:1279:G:H5'	2.10	0.52
20:S1:685:A:OP2	88:S1:2416:HOH:O	2.18	0.52
20:S1:1920:A:O2'	20:S1:1921:A:H8	1.92	0.52
41:1:1597:G:OP2	88:1:1911:HOH:O	2.19	0.52
42:2:1467:G:H2'	42:2:1468:G:C8	2.45	0.52
72:U:46:ASN:H	72:U:49:GLN:NE2	2.08	0.52
20:S1:1512:A:O2'	20:S1:2040:C:H5	1.91	0.52
20:S1:1219:G:N7	88:S1:2455:HOH:O	2.33	0.52
41:1:83:A:H4'	41:1:84:G:OP1	2.09	0.52
41:1:597:C:H2'	41:1:598:G:H8	1.73	0.52
53:I:133:MET:O	88:I:301:HOH:O	2.19	0.52
20:S1:78:C:H6	20:S1:501:A:H61	1.58	0.52
30:SH:129:PRO:HA	30:SH:132:ARG:HG3	1.91	0.52
58:6:37:C:N4	58:6:38:C:H41	2.07	0.52
20:S1:1523:A:H2'	20:S1:1524:G:C8	2.44	0.52
35:Sh:148:THR:HG22	35:Sh:196:ARG:HH21	1.74	0.52
35:Sh:210:GLU:CD	35:Sh:210:GLU:H	2.18	0.52
41:1:636:U:H2'	41:1:637:C:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:h:119:LYS:O	67:h:122:ALA:N	2.42	0.52
20:S1:236:C:H2'	20:S1:237:A:C8	2.45	0.52
26:SM:35:GLN:O	26:SM:39:ARG:HG3	2.10	0.52
38:c:246:ARG:HG2	41:1:1394:A:C4	2.44	0.52
41:1:497:A:OP1	41:1:576:G:N2	2.43	0.52
5:SV:63:ARG:NH2	20:S1:1801:G:OP1	2.43	0.52
6:SU:116:GLN:HE21	6:SU:118:ARG:HE	1.58	0.52
20:S1:479:A2M:O5'	20:S1:479:A2M:H8	2.10	0.52
20:S1:1621:OMU:OP2	88:S1:2418:HOH:O	2.19	0.52
20:S1:2064:C:H2'	20:S1:2065:G:H5''	1.92	0.52
20:S1:2122:G:H2'	20:S1:2123:A:O4'	2.10	0.52
35:Sh:177:LEU:HB2	35:Sh:180:PRO:HG3	1.91	0.52
42:2:495:G:O2'	42:2:496:G:H5'	2.10	0.52
44:7:20:C:OP1	80:C:194:LYS:HE2	2.10	0.52
46:8:74:A:H61	46:8:109:U:H5	1.57	0.52
54:P:5:LEU:HD22	54:P:8:ILE:HD12	1.90	0.52
64:Y:28:ASN:HD21	64:Y:77:HIS:CE1	2.27	0.52
81:3:174:C:H1'	81:3:175:A:C8	2.45	0.52
20:S1:251:A:O2'	20:S1:783:A:H2'	2.09	0.52
42:2:1457:C:N4	42:2:1465:G:H1	1.95	0.52
11:SC:131:LYS:HD3	11:SC:190:PRO:HA	1.90	0.51
20:S1:2085:A:O2'	20:S1:2086:A:H8	1.93	0.51
31:SG:157:ARG:HH11	31:SG:182:LEU:HD21	1.75	0.51
41:1:837:A:H4'	41:1:838:G:O5'	2.08	0.51
42:2:1510:U:H5	45:B:326:ASN:HD22	1.57	0.51
72:U:107:ILE:HD12	72:U:108:ARG:H	1.74	0.51
5:SV:6:THR:HG22	5:SV:8:THR:H	1.76	0.51
35:Sh:189:GLU:HA	35:Sh:193:THR:HG23	1.93	0.51
41:1:213:G:H2'	41:1:214:C:O4'	2.10	0.51
42:2:1268:G:H2'	42:2:1269:G:O4'	2.11	0.51
71:W:36:LEU:HD22	71:W:40:TYR:HE2	1.75	0.51
13:SE:208:LYS:HG3	13:SE:214:GLU:OE1	2.10	0.51
41:1:696:A:H2'	41:1:697:A2M:H8	1.93	0.51
42:2:653:C:H2'	42:2:654:U:H6	1.75	0.51
54:P:29:LEU:HG	80:C:282:LEU:HD11	1.93	0.51
57:E:141:ASP:OD1	57:E:141:ASP:N	2.41	0.51
5:SV:101:VAL:HG23	5:SV:106:MET:HG2	1.92	0.51
12:SD:65:HIS:CD2	12:SD:67:ARG:H	2.28	0.51
20:S1:1673:A:H4'	20:S1:1674:A:O5'	2.10	0.51
31:SG:25:ARG:HG3	31:SG:25:ARG:HH11	1.76	0.51
41:1:88:G:OP2	88:1:1913:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2:134:C:H5	42:2:344:G:H1	1.58	0.51
42:2:452:G:O2'	42:2:453:A:H3'	2.10	0.51
42:2:1271:G:H22	42:2:1294:G:N2	2.09	0.51
42:2:1498:G:H4'	45:B:138:ASN:HB3	1.92	0.51
64:Y:50:PRO:HD3	64:Y:68:VAL:HG12	1.93	0.51
20:S1:2158:A:H2'	20:S1:2159:A:O4'	2.10	0.51
41:1:1245:G:N1	41:1:1382:G:N1	2.59	0.51
32:SF:67:PHE:HZ	32:SF:148:ILE:HG22	1.76	0.51
45:B:227:LYS:HD2	45:B:338:PRO:HB3	1.93	0.51
49:O:187:PRO:HD2	49:O:201:HIS:CE1	2.46	0.51
77:k:37:ARG:O	77:k:37:ARG:NE	2.43	0.51
10:SB:74:PRO:HG3	10:SB:189:ARG:HH22	1.75	0.51
20:S1:964:U:H5'	20:S1:965:G:H5'	1.92	0.51
23:SO:81:CYS:SG	33:SA:24:MET:HE3	2.50	0.51
33:SA:185:GLU:N	33:SA:185:GLU:OE1	2.44	0.51
7:ST:36:MET:CE	7:ST:58:MET:HE2	2.41	0.51
20:S1:1287:U:H2'	20:S1:1288:G:H8	1.75	0.51
42:2:768:G:H21	70:V:34:GLN:NE2	2.02	0.51
16:Sg:103:PHE:CE2	16:Sg:138:GLY:HA2	2.46	0.51
20:S1:692:G:H22	20:S1:753:A:H2	1.58	0.51
20:S1:1572:C:H2'	20:S1:1573:A:H8	1.76	0.51
20:S1:2055:A:OP1	88:S1:2419:HOH:O	2.19	0.51
24:SN:95:PRO:O	24:SN:99:LYS:HB2	2.11	0.51
37:d:75:ASN:HD22	37:d:76:ASN:H	1.59	0.51
41:1:967:G:H5'	41:1:968:A:OP1	2.11	0.51
43:4:48:U:H4'	57:E:118:LYS:HE2	1.93	0.51
67:h:84:SER:H	67:h:87:GLN:NE2	2.09	0.51
81:3:153:G:H1	81:3:178:G:N2	2.08	0.51
81:3:156:G:C2	81:3:175:A:H2	2.28	0.51
41:1:789:U:O2'	41:1:792:G:O6	2.29	0.51
82:e:74:ARG:NH1	82:e:74:ARG:HB3	2.26	0.51
16:Sg:298:HIS:CE1	16:Sg:304:ARG:HD2	2.47	0.50
20:S1:80:G:O5'	20:S1:81:G:H5''	2.11	0.50
41:1:542:C:O2'	41:1:543:G:H5''	2.10	0.50
42:2:1189:A:H2'	42:2:1190:U:O2	2.11	0.50
54:P:182:ARG:HA	54:P:188:ARG:HB3	1.93	0.50
80:C:154:GLU:OE1	80:C:156:SER:OG	2.28	0.50
20:S1:1966:A:N1	20:S1:1983:U:H5	2.09	0.50
22:SP:52:LEU:HB2	22:SP:71[A]:ARG:HG3	1.92	0.50
41:1:735:U:O2'	41:1:736:C:O4'	2.29	0.50
42:2:615:G:H2'	42:2:616:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:U:103:LEU:O	72:U:107:ILE:HG22	2.11	0.50
16:Sg:264:GLU:CD	16:Sg:264:GLU:H	2.19	0.50
41:1:638:C:H5	41:1:1433:G:N1	2.05	0.50
42:2:501:A:H8	42:2:508:A:H62	1.58	0.50
57:E:111:VAL:HB	57:E:121:ARG:HB2	1.92	0.50
67:h:22:LYS:HB3	67:h:36[B]:ARG:HD3	1.93	0.50
72:U:107:ILE:HD12	72:U:120:LYS:O	2.12	0.50
20:S1:691:G:H22	20:S1:754:G:N2	2.09	0.50
20:S1:975:G:H2'	20:S1:976:A:O4'	2.10	0.50
47:5:70:U:H2'	47:5:71:C:C2	2.47	0.50
82:e:31:LYS:HD2	82:e:31:LYS:C	2.36	0.50
20:S1:1708:A:N1	20:S1:1764:U:H5	2.09	0.50
20:S1:2092:G:H2'	20:S1:2093:U:C6	2.47	0.50
24:SN:94:MET:SD	24:SN:94:MET:N	2.84	0.50
41:1:503:A:H61	41:1:554:A:P	2.34	0.50
45:B:221:ASP:OD2	45:B:346:ARG:NH1	2.45	0.50
50:G:31:ARG:NH2	64:Y:52:LYS:HE3	2.26	0.50
81:3:156:G:C6	81:3:175:A:N1	2.80	0.50
20:S1:1295:G:H1	20:S1:1419:U:H3	1.60	0.50
38:c:160:LYS:HE2	80:C:318:ASN:ND2	2.27	0.50
42:2:1457:C:OP1	45:B:148:ARG:NH2	2.45	0.50
60:S:148:ARG:HD2	60:S:153:TYR:CZ	2.46	0.50
64:Y:101:ASP:OD1	64:Y:102:ALA:N	2.42	0.50
20:S1:1835:U:OP2	88:S1:2408:HOH:O	2.19	0.50
41:1:216:G:C6	65:Z:136:LYS:HG3	2.47	0.50
42:2:1114:G:OP1	49:O:8:LYS:HE2	2.12	0.50
46:8:12:A:OP1	49:O:33:ARG:NH1	2.45	0.50
48:A:20:GLY:HA2	48:A:23[A]:ARG:HD3	1.94	0.50
73:i:61:GLN:HG2	73:i:97:LEU:HD13	1.92	0.50
13:SE:244:MET:HG2	13:SE:249:GLU:HB2	1.94	0.50
20:S1:782:C:H3'	20:S1:783:A:H8	1.76	0.50
22:SP:101:LEU:HB3	22:SP:124:LYS:HB2	1.94	0.50
41:1:1010:C:OP1	88:2:1708:HOH:O	2.20	0.50
42:2:497:G:H2'	42:2:498:A:O4'	2.12	0.50
42:2:958:A:H2'	42:2:959:A:H8	1.75	0.50
42:2:1131:A:OP2	88:2:1718:HOH:O	2.19	0.50
48:A:176:GLU:HG3	75:o:29:LEU:HD21	1.93	0.50
64:Y:9:LYS:NZ	64:Y:83:THR:O	2.32	0.50
20:S1:992:C:N3	88:S1:2458:HOH:O	2.35	0.50
20:S1:1569:G:H5'	24:SN:51:GLN:HE22	1.75	0.50
56:R:46:MET:HB3	60:S:146:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:E:20:VAL:HG12	57:E:25:VAL:HG12	1.93	0.50
20:S1:1914:U:HO2'	20:S1:1915:U:P	2.35	0.49
41:1:929:G:OP2	88:1:1912:HOH:O	2.19	0.49
43:4:92:U:H2'	43:4:93:U:C6	2.47	0.49
58:6:7:A:H1'	68:g:99:THR:OG1	2.12	0.49
82:e:17:ALA:O	82:e:21:ALA:HB3	2.12	0.49
14:SK:117:TYR:O	14:SK:166:ARG:NH1	2.46	0.49
20:S1:784:C:H2'	20:S1:787:G:C2	2.47	0.49
30:SH:174:TYR:O	30:SH:178:LYS:HG2	2.12	0.49
42:2:590:U:H2'	42:2:591:A2M:C8	2.42	0.49
42:2:1271:G:O2'	42:2:1272:G:H8	1.94	0.49
42:2:1275:A:H2'	42:2:1276:A:O4'	2.11	0.49
75:o:67:GLY:HA3	75:o:70:THR:O	2.12	0.49
3:SY:8:ASN:C	3:SY:8:ASN:HD22	2.12	0.49
13:SE:97:ARG:HB2	13:SE:111:LEU:HD11	1.94	0.49
20:S1:819:G:P	31:SG:221:ARG:HH22	2.34	0.49
20:S1:1121:C:H2'	20:S1:1122:G:C8	2.47	0.49
29:SI:88:ARG:HG3	29:SI:88:ARG:HH11	1.76	0.49
32:SF:91:GLU:OE1	32:SF:198:LYS:HD3	2.13	0.49
41:1:1239:U:OP1	51:H:141:ARG:NH1	2.46	0.49
42:2:1370:U:OP2	88:2:1720:HOH:O	2.20	0.49
45:B:244:PRO:O	45:B:251:LEU:HD22	2.12	0.49
54:P:135:MET:HE2	54:P:135:MET:HA	1.94	0.49
81:3:40:A:C2	81:3:41:A:H1'	2.47	0.49
20:S1:2200:A:N6	34:Sb:88:VAL:HG13	2.27	0.49
24:SN:39:GLY:C	24:SN:40:ASN:HD22	2.20	0.49
42:2:804:U:O4	88:2:1719:HOH:O	2.19	0.49
42:2:1452:U:H4'	42:2:1453:U:H5'	1.95	0.49
46:8:59:A:OP2	88:8:302:HOH:O	2.19	0.49
81:3:156:G:O6	81:3:175:A:N1	2.45	0.49
20:S1:2057:C:H3'	20:S1:2058:G:H5'	1.93	0.49
32:SF:63:LEU:HD12	32:SF:66:ILE:HD12	1.93	0.49
41:1:159:U:H2'	41:1:160:C:C6	2.48	0.49
41:1:734:U:H2'	41:1:735:U:C6	2.48	0.49
41:1:1638:C:H2'	41:1:1639:U:C6	2.47	0.49
43:4:50:G:O2'	43:4:59:G:O6	2.29	0.49
20:S1:902:G:O2'	20:S1:903:G:H8	1.94	0.49
88:S1:2414:HOH:O	31:SG:180:GLN:NE2	2.31	0.49
31:SG:146:LYS:HD3	31:SG:146:LYS:C	2.38	0.49
37:d:48:ASN:OD1	37:d:49:ASN:N	2.46	0.49
41:1:652:A:H2'	41:1:653:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1:1672:U:O4	88:1:1914:HOH:O	2.20	0.49
75:o:52:VAL:HB	81:3:198:A:H5'	1.93	0.49
4:SX:38:LEU:HD21	4:SX:94:ARG:HG3	1.95	0.49
34:Sb:86:ARG:HG3	34:Sb:89:ARG:NH1	2.28	0.49
37:d:75:ASN:ND2	37:d:76:ASN:H	2.11	0.49
58:6:68:A:H5''	66:F:47:ARG:CZ	2.43	0.49
5:SV:100:SER:HB2	5:SV:123:ALA:HB2	1.94	0.49
20:S1:1510:C:H2'	20:S1:1510:C:O2	2.12	0.49
20:S1:2159:A:O2'	20:S1:2160:G:H8	1.96	0.49
33:SA:128:GLU:OE1	33:SA:138:ARG:NH1	2.46	0.49
41:1:898:A:H2'	41:1:899:A:C8	2.47	0.49
41:1:1265:A:H2'	41:1:1266:A:H8	1.78	0.49
41:1:1363:A:H4'	41:1:1364:A:H5''	1.95	0.49
42:2:1042:G:H2'	42:2:1043:C:C6	2.47	0.49
42:2:1389:G:OP2	88:2:1721:HOH:O	2.20	0.49
43:4:21:C:HO2'	43:4:22:G:H8	1.61	0.49
46:8:58:A:OP2	88:8:302:HOH:O	2.18	0.49
66:F:168:ASP:OD1	66:F:169:ALA:N	2.45	0.49
72:U:50:PHE:CE2	72:U:97:PHE:HB2	2.47	0.49
4:SX:68:ILE:HD11	9:SR:44:LEU:HD21	1.93	0.49
16:Sg:290:ASP:OD2	16:Sg:292:ASN:ND2	2.46	0.49
20:S1:833:G:H2'	20:S1:834:U:O4'	2.12	0.49
20:S1:1615:G:H2'	20:S1:1616:A:O4'	2.13	0.49
20:S1:2159:A:O2'	20:S1:2160:G:O5'	2.29	0.49
22:SP:39:ASN:HD22	22:SP:40:PRO:HD2	1.78	0.49
22:SP:135:ARG:HE	22:SP:135:ARG:HA	1.77	0.49
41:1:229:C:H2'	41:1:230:A:O4'	2.13	0.49
64:Y:28:ASN:HD21	64:Y:77:HIS:HE1	1.61	0.49
20:S1:1765:C:O2'	20:S1:1766:G:H5'	2.13	0.49
41:1:483:C:H5''	41:1:483:C:C6	2.47	0.49
41:1:781:A:OP1	54:P:141:LYS:HG3	2.13	0.49
75:o:6:VAL:O	75:o:7:LYS:HG2	2.13	0.49
20:S1:255:A:N7	20:S1:962:A:H2	2.11	0.48
28:SJ:18:GLU:OE2	28:SJ:18:GLU:HA	2.12	0.48
41:1:1382:G:O5'	41:1:1382:G:H8	1.96	0.48
42:2:1520:C:O2'	42:2:1521:A:O5'	2.31	0.48
43:4:140:G:N7	88:4:308:HOH:O	2.35	0.48
58:6:47:G:H4'	68:g:26:ARG:HA	1.94	0.48
20:S1:78:C:H6	20:S1:501:A:N6	2.09	0.48
25:Sd:28:LYS:HB3	25:Sd:43:ARG:HG2	1.95	0.48
41:1:235:A:N3	41:1:255:G:O2'	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1:491:A:O2'	58:6:65:C:H5	1.95	0.48
41:1:1238:C:N4	56:R:179:ALA:HB1	2.28	0.48
41:1:1761:A:O3'	41:1:1762:A:H8	1.97	0.48
56:R:75:ASN:HD21	56:R:145:HIS:CE1	2.31	0.48
20:S1:1170:A:H2'	20:S1:1171:A:C8	2.48	0.48
41:1:215:U:P	65:Z:129:LYS:HZ3	2.36	0.48
20:S1:1774:U:O2'	20:S1:1775:C:H6	1.96	0.48
32:SF:64:GLU:N	32:SF:64:GLU:OE1	2.46	0.48
33:SA:200:VAL:HG22	33:SA:212:LEU:HB3	1.96	0.48
46:8:93:G:H2'	46:8:94:A:C8	2.48	0.48
46:8:112:G:O2'	46:8:113:U:O5'	2.31	0.48
61:K:125:LYS:O	61:K:129:GLU:HG3	2.13	0.48
81:3:105:C:H2'	81:3:106:U:C6	2.48	0.48
82:e:46:LYS:O	82:e:48:PHE:N	2.45	0.48
13:SE:248:GLN:O	13:SE:252:GLU:HG3	2.14	0.48
29:SI:2:GLN:HB3	29:SI:4:HIS:CE1	2.49	0.48
41:1:217:A:C4'	41:1:218:A:H5'	2.43	0.48
41:1:1588:G:O2'	41:1:1590:G:OP2	2.28	0.48
42:2:809:C:H3'	42:2:810:G:C5'	2.44	0.48
42:2:1403:PSU:H5'	42:2:1403:PSU:H6	1.77	0.48
42:2:1506:G:N7	82:e:35:ARG:NH1	2.61	0.48
3:SY:8:ASN:O	3:SY:8:ASN:ND2	2.31	0.48
10:SB:76:ASP:HB3	10:SB:123:ARG:HB2	1.96	0.48
18:Sc:39:PRO:HD3	18:Sc:78:CYS:SG	2.54	0.48
20:S1:450:A:H2'	20:S1:451:C:C6	2.48	0.48
40:b:49:LYS:NZ	41:1:812:A:OP1	2.42	0.48
41:1:292:A:H2'	41:1:293:C:O4'	2.14	0.48
41:1:636:U:H2'	41:1:637:C:H6	1.78	0.48
41:1:1245:G:N1	41:1:1382:G:C2	2.81	0.48
41:1:1600:U:C5	42:2:18:A:N1	2.79	0.48
42:2:652:C:H2'	42:2:653:C:C6	2.48	0.48
48:A:104:LEU:HD12	48:A:162:SER:HB2	1.95	0.48
55:Q:160:ALA:O	55:Q:164:LEU:HB2	2.14	0.48
58:6:36:C:H2'	58:6:37:C:C6	2.48	0.48
61:K:143:LEU:HD13	68:g:17:LEU:HB2	1.94	0.48
11:SC:5:SER:HA	20:S1:1931:G:O2'	2.14	0.48
16:Sg:128:ASP:OD1	16:Sg:128:ASP:N	2.40	0.48
20:S1:2184:MA6:H8	20:S1:2184:MA6:O5'	2.14	0.48
29:SI:86:GLU:HG3	29:SI:94:VAL:HG13	1.94	0.48
31:SG:140:ARG:HB3	31:SG:143:LYS:HG3	1.95	0.48
39:a:38:THR:HG22	70:V:71:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:U:50:PHE:O	72:U:54:ASN:HB2	2.14	0.48
4:SX:110:ARG:NH1	20:S1:1940:G:N2	2.61	0.48
11:SC:93:ARG:NH2	11:SC:124:TYR:OH	2.47	0.48
20:S1:133:G:H2'	20:S1:134:G:C8	2.49	0.48
41:1:159:U:H2'	41:1:160:C:O4'	2.14	0.48
41:1:562:U:H2'	41:1:565:U:H5	1.79	0.48
48:A:37:ARG:O	48:A:92:GLN:HG3	2.14	0.48
49:O:211:ALA:HB2	49:O:245:ILE:HD12	1.96	0.48
12:SD:177:LYS:O	12:SD:181:ARG:HD3	2.14	0.48
49:O:64:ILE:HD11	49:O:177:MET:HE1	1.96	0.48
57:E:100:ILE:HD11	57:E:114:PHE:HD1	1.79	0.48
10:SB:80:CYS:HA	10:SB:102:HIS:O	2.14	0.48
20:S1:67:C:H5	20:S1:81:G:H21	1.62	0.48
20:S1:588:G:H4'	20:S1:589:U:H5'	1.96	0.48
41:1:938:G:H2'	41:1:939:C:C6	2.49	0.48
41:1:1443:U:O2'	41:1:1444:A:H3'	2.13	0.48
41:1:1730:A:H8	88:2:2184:HOH:O	1.97	0.48
42:2:653:C:H2'	42:2:654:U:C6	2.49	0.48
42:2:1108:U:H2'	42:2:1109:C:H6	1.79	0.48
42:2:1512:G:OP1	42:2:1512:G:H2'	2.14	0.48
47:5:60:U:O2'	47:5:61:C:O5'	2.29	0.48
57:E:91:VAL:HG23	57:E:143:ILE:HB	1.94	0.48
82:e:46:LYS:C	82:e:48:PHE:N	2.66	0.48
7:ST:36:MET:HE3	7:ST:58:MET:HE2	1.95	0.47
10:SB:92:LYS:O	10:SB:96:HIS:ND1	2.47	0.47
13:SE:26:PRO:HD3	20:S1:491:G:OP1	2.14	0.47
20:S1:859:G:OP2	88:S1:2420:HOH:O	2.20	0.47
20:S1:2048:OMU:OP1	34:Sb:93:VAL:HG23	2.14	0.47
31:SG:38:ASP:OD1	31:SG:39:GLY:N	2.47	0.47
33:SA:146:LYS:HB3	33:SA:210:ARG:HB2	1.97	0.47
41:1:694:U:H2'	41:1:695:OMC:C6	2.49	0.47
42:2:496:G:H2'	42:2:497:G:O4'	2.14	0.47
44:7:8:C:OP1	88:7:302:HOH:O	2.20	0.47
20:S1:374:U:H2'	20:S1:375:G:C8	2.48	0.47
20:S1:994:U:H2'	20:S1:995:U:C6	2.49	0.47
41:1:237:U:OP1	71:W:57:ARG:NH1	2.40	0.47
41:1:472:U:H2'	41:1:473:A:H8	1.77	0.47
42:2:1267:U:H2'	42:2:1268:G:C8	2.49	0.47
45:B:209:ARG:HH12	45:B:292:ARG:NH2	2.12	0.47
71:W:39:LYS:HD3	71:W:40:TYR:CE2	2.49	0.47
20:S1:49:C:OP2	88:S1:2422:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2:337:A:O2'	42:2:338:C:O5'	2.22	0.47
81:3:156:G:H22	81:3:175:A:H2	1.61	0.47
12:SD:70:LEU:HD12	12:SD:71:GLU:H	1.80	0.47
20:S1:232:C:H2'	20:S1:233:G:C8	2.49	0.47
42:2:383:U:H5	42:2:388:A:N7	2.12	0.47
42:2:969:A:C2	48:A:95:PRO:HD3	2.49	0.47
42:2:1343:A:H2'	42:2:1344:C:C6	2.50	0.47
48:A:176:GLU:N	88:A:301:HOH:O	2.47	0.47
57:E:95:TYR:HD1	57:E:96:ALA:N	2.13	0.47
60:S:39:TYR:CZ	60:S:63:ILE:HD11	2.49	0.47
64:Y:54:VAL:HG22	64:Y:57:MET:HE2	1.96	0.47
83:j:31:TRP:O	83:j:33:ARG:N	2.47	0.47
1:SW:63:LEU:HD13	1:SW:85:THR:HB	1.97	0.47
7:ST:87:ASP:OD1	7:ST:87:ASP:N	2.35	0.47
16:Sg:282:CYS:SG	16:Sg:296:SER:HB2	2.54	0.47
20:S1:1618:U:H2'	20:S1:1619:G:C8	2.50	0.47
24:SN:45:PRO:HG2	24:SN:48:GLN:HE21	1.79	0.47
25:Sd:38:ASN:OD1	25:Sd:38:ASN:N	2.41	0.47
30:SH:154:SER:HB3	30:SH:156:PRO:HD2	1.97	0.47
41:1:70:C:O2'	53:I:71:ASN:OD1	2.31	0.47
23:SO:22:GLY:C	23:SO:86:LEU:HD23	2.40	0.47
29:SI:76:LYS:HB2	29:SI:76:LYS:HE3	1.71	0.47
35:Sh:191:ASN:OD1	35:Sh:191:ASN:N	2.47	0.47
39:a:107:LYS:HB2	39:a:107:LYS:HE2	1.73	0.47
41:1:215:U:P	65:Z:129:LYS:NZ	2.87	0.47
42:2:1452:U:H3'	42:2:1454:A:N6	2.30	0.47
48:A:177:LYS:N	88:A:301:HOH:O	2.21	0.47
71:W:6:CYS:C	71:W:8:SER:H	2.23	0.47
72:U:16:GLN:NE2	72:U:58:ASN:H	2.13	0.47
10:SB:181:LEU:O	10:SB:185:VAL:HG23	2.15	0.47
11:SC:123:ARG:O	11:SC:127:GLU:HG2	2.15	0.47
13:SE:88:GLU:HG2	13:SE:95:ARG:HG2	1.95	0.47
20:S1:1579:A:H1'	20:S1:1581:G:C8	2.49	0.47
20:S1:1612:C:O2'	20:S1:1613:C:O5'	2.33	0.47
31:SG:140:ARG:HG3	31:SG:181:ARG:HD3	1.97	0.47
32:SF:92:MET:HE1	32:SF:112:ALA:HB1	1.97	0.47
32:SF:249:ARG:HH12	32:SF:254:GLU:HA	1.80	0.47
38:c:249:ALA:HB3	41:1:1394:A:C2	2.50	0.47
41:1:569:G:O2'	41:1:572:A:N7	2.45	0.47
41:1:700:A:H2'	41:1:701:G:C8	2.48	0.47
41:1:770:G:C2	54:P:99:MET:HE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2:1271:G:O2'	42:2:1272:G:O5'	2.32	0.47
50:G:112:LYS:HA	50:G:115:GLU:HG3	1.97	0.47
52:M:96:LYS:HG2	52:M:171:HIS:CE1	2.50	0.47
61:K:38:GLU:HG3	61:K:39:ASN:N	2.29	0.47
62:D:94:LYS:NZ	62:D:175:GLN:O	2.47	0.47
76:X:2:ARG:HG2	76:X:2:ARG:HH11	1.80	0.47
81:3:145:U:H5''	81:3:145:U:H6	1.80	0.47
82:e:43:GLU:O	82:e:44:LYS:C	2.57	0.47
6:SU:54:GLY:O	6:SU:56:GLY:N	2.45	0.47
20:S1:665:G:O6	22:SP:2:THR:HG22	2.15	0.47
21:SQ:49:GLU:O	21:SQ:53:THR:HG23	2.14	0.47
57:E:110:GLU:OE1	57:E:122:ARG:HG3	2.13	0.47
61:K:110:TYR:O	61:K:114:VAL:HG13	2.15	0.47
20:S1:777:A:C6	20:S1:842:U:H3'	2.49	0.47
20:S1:1781:U:O2'	20:S1:1782:G:N7	2.36	0.47
27:SL:55:MET:HB3	27:SL:55:MET:HE3	1.83	0.47
37:d:46:ILE:HD11	37:d:69:ILE:HD11	1.95	0.47
42:2:1272:G:C2	42:2:1273:C:C5	3.03	0.47
49:O:191:LYS:HB3	49:O:191:LYS:HE3	1.77	0.47
54:P:40:THR:HG22	54:P:42:SER:H	1.80	0.47
58:6:67:C:OP1	68:g:96:ARG:NH2	2.46	0.47
20:S1:1870:A:H2'	20:S1:1871:C:C6	2.50	0.47
41:1:663:C:H2'	41:1:664:C:C6	2.50	0.47
42:2:501:A:H3'	42:2:507:G:H1	1.80	0.47
42:2:1006:G:H2'	42:2:1007:U:C6	2.50	0.47
42:2:1447:A:O2'	42:2:1448:A:H8	1.96	0.47
47:5:84:C:H3'	47:5:85:G:C8	2.50	0.47
54:P:26:ILE:HG12	80:C:281:MET:HE1	1.96	0.47
79:n:11:ARG:HB3	79:n:14:TRP:CD1	2.50	0.47
7:ST:139:TRP:CZ3	7:ST:141:TYR:HB2	2.50	0.46
10:SB:31:ARG:C	10:SB:31:ARG:HD2	2.40	0.46
20:S1:1581:G:H8	20:S1:1608:A:H62	1.61	0.46
20:S1:2202:PSU:H2'	33:SA:118:LYS:HB2	1.97	0.46
33:SA:128:GLU:HG2	33:SA:138:ARG:HG3	1.96	0.46
43:4:17:A:H2'	43:4:18:U:C6	2.50	0.46
50:G:97:LYS:HE3	50:G:97:LYS:HB2	1.74	0.46
55:Q:136:ARG:HE	55:Q:136:ARG:HB3	1.57	0.46
57:E:119:ARG:HH21	57:E:121:ARG:HG2	1.79	0.46
62:D:83:GLU:O	62:D:87:LYS:HG2	2.14	0.46
14:SK:21:HIS:HB2	20:S1:99:U:O2	2.15	0.46
20:S1:145:A:H61	20:S1:180:G:H21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S1:147:U:H5	20:S1:178:A:N1	2.12	0.46
24:SN:11:ASP:N	24:SN:11:ASP:OD1	2.47	0.46
37:d:83:CYS:SG	37:d:92:LEU:HD12	2.55	0.46
41:1:1272:U:H2'	41:1:1273:U:C6	2.49	0.46
43:4:19:C:H2'	43:4:20:U:C6	2.50	0.46
54:P:129:THR:H	54:P:132:GLN:HE21	1.61	0.46
82:e:28:ARG:O	82:e:31:LYS:HB3	2.16	0.46
5:SV:92:ASP:HA	5:SV:95:ILE:HD12	1.97	0.46
20:S1:285:A:H3'	20:S1:285:A:N3	2.30	0.46
20:S1:1586:A:H62	20:S1:1603:U:H3	1.62	0.46
20:S1:1680:G:OP2	88:S1:2421:HOH:O	2.20	0.46
38:c:146:TYR:CZ	38:c:239:ASN:HB2	2.51	0.46
41:1:93:G:H2'	41:1:94:A:C8	2.50	0.46
41:1:487:A:N3	41:1:487:A:H3'	2.30	0.46
41:1:1144:G:OP1	88:1:1917:HOH:O	2.20	0.46
42:2:505:A:H3'	42:2:506:PSU:H6	1.80	0.46
46:8:31:A:H2'	46:8:32:C:C6	2.50	0.46
54:P:82:LYS:HB3	54:P:82:LYS:HE3	1.66	0.46
55:Q:190:ARG:HE	55:Q:190:ARG:HA	1.79	0.46
62:D:39:LEU:HB3	62:D:47:PRO:HG3	1.98	0.46
3:SY:44:VAL:HG13	10:SB:4:VAL:HG13	1.96	0.46
16:Sg:75:HIS:CE1	16:Sg:117:PRO:HA	2.50	0.46
17:Sa:85:ARG:HA	17:Sa:85:ARG:HD3	1.71	0.46
20:S1:1920:A:O2'	20:S1:1921:A:C8	2.69	0.46
38:c:175:ASP:OD1	38:c:175:ASP:N	2.47	0.46
41:1:1366:A:H5'	88:1:1979:HOH:O	2.16	0.46
42:2:1520:C:O2'	42:2:1521:A:N3	2.44	0.46
57:E:62:SER:O	57:E:64:ILE:N	2.47	0.46
8:SS:26:SER:O	8:SS:26:SER:OG	2.33	0.46
18:Sc:64:LEU:HD12	18:Sc:65:CYS:HB2	1.98	0.46
20:S1:1567:C:HO2'	20:S1:1568:C:H6	1.60	0.46
20:S1:1580:G:OP2	21:SQ:46:GLY:HA2	2.15	0.46
31:SG:108:ASP:OD2	31:SG:108:ASP:N	2.37	0.46
33:SA:88:PHE:HB3	33:SA:100:THR:HB	1.97	0.46
41:1:759:A:O2'	41:1:761:A:N1	2.48	0.46
42:2:1390:G:OP2	88:2:1721:HOH:O	2.21	0.46
6:SU:98:THR:HG21	20:S1:369:G:H4'	1.97	0.46
20:S1:2059:C:H5	20:S1:2166:A:N6	2.00	0.46
41:1:154:A:H4'	41:1:155:A:O5'	2.13	0.46
41:1:845:OMU:O5'	41:1:845:OMU:H6	2.15	0.46
42:2:1069:A:H2'	42:2:1070:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2:1398:C:H2'	42:2:1399:G:C8	2.51	0.46
42:2:1419:OMU:H1'	42:2:1419:OMU:HM23	1.66	0.46
68:g:13:LYS:HD2	68:g:16:GLN:HE22	1.80	0.46
3:SY:82:ILE:HG22	10:SB:1:MET:N	2.31	0.46
11:SC:62:GLY:O	11:SC:65:ILE:HG22	2.15	0.46
16:Sg:146:ARG:O	16:Sg:146:ARG:HG2	2.15	0.46
19:Se:58:ASN:HB3	20:S1:638:C:H4'	1.97	0.46
20:S1:261:A:H2	20:S1:966:G:H22	1.61	0.46
20:S1:1566:PSU:O2'	20:S1:1567:C:H5'	2.16	0.46
41:1:597:C:H2'	41:1:598:G:C8	2.51	0.46
41:1:1240:U:H2'	41:1:1241:A:C8	2.51	0.46
42:2:381:U:H2'	42:2:382:A2M:C8	2.46	0.46
42:2:406:G:H2'	42:2:407:C:C6	2.51	0.46
42:2:756:C:H2'	42:2:757:A:C8	2.50	0.46
42:2:1334:C:O3'	88:2:1712:HOH:O	2.16	0.46
42:2:1519:U:H2'	42:2:1520:C:C6	2.51	0.46
47:5:91:A:H2'	47:5:92:G:O4'	2.15	0.46
51:H:204:ALA:O	51:H:208:MET:HG2	2.16	0.46
6:SU:30:ASN:HD22	6:SU:31:GLU:N	2.13	0.46
11:SC:113:GLN:OE1	11:SC:114:VAL:N	2.49	0.46
11:SC:175:TYR:OH	20:S1:1839:G:OP1	2.29	0.46
19:Se:38:LEU:HD11	19:Se:42:ARG:NH2	2.31	0.46
20:S1:17:C:H2'	20:S1:18:OMC:C6	2.51	0.46
20:S1:819:G:H5'	20:S1:820:C:H2'	1.98	0.46
20:S1:1956:C:O2	20:S1:1956:C:H2'	2.16	0.46
24:SN:97:THR:O	24:SN:97:THR:HG22	2.16	0.46
41:1:159:U:H2'	41:1:160:C:H6	1.81	0.46
41:1:1574:C:H2'	41:1:1575:G:C8	2.51	0.46
44:7:86:C:H3'	44:7:87:U:C5'	2.46	0.46
62:D:148:SER:OG	62:D:149:ARG:N	2.49	0.46
82:e:45:ARG:HA	82:e:47:LYS:HD3	1.98	0.46
3:SY:8:ASN:O	3:SY:9:GLU:HG2	2.15	0.46
3:SY:17:TYR:O	3:SY:17:TYR:CG	2.69	0.46
29:SI:34:HIS:CG	29:SI:37:LEU:HD12	2.51	0.46
41:1:440:A:OP2	88:1:1916:HOH:O	2.20	0.46
41:1:739:U:H2'	41:1:740:C:C6	2.51	0.46
45:B:59:ASP:OD1	45:B:364:LYS:HD2	2.16	0.46
45:B:291:GLY:HA3	45:B:328:TYR:CZ	2.51	0.46
47:5:123:C:H2'	47:5:124:U:H5''	1.97	0.46
62:D:39:LEU:HD12	62:D:39:LEU:HA	1.84	0.46
64:Y:35:GLU:CD	64:Y:35:GLU:N	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:Z:110:ARG:O	65:Z:114:MET:HG2	2.16	0.46
72:U:98:LEU:HD22	72:U:107:ILE:HG21	1.97	0.46
9:SR:88:GLN:O	9:SR:96:THR:OG1	2.27	0.46
29:SI:61:VAL:HG11	29:SI:175:VAL:HG21	1.98	0.46
73:i:79:ARG:HD2	73:i:79:ARG:HA	1.61	0.46
83:j:28:HIS:HD2	83:j:31:TRP:H	1.63	0.46
4:SX:99:ARG:HD3	20:S1:1938:C:C4	2.50	0.45
23:SO:124:ASP:O	33:SA:109:THR:HG21	2.16	0.45
47:5:48:G:H4'	47:5:49:C:O5'	2.15	0.45
55:Q:190:ARG:HE	55:Q:190:ARG:CA	2.29	0.45
82:e:43:GLU:H	82:e:46:LYS:HG2	1.81	0.45
17:Sa:102:THR:OG1	17:Sa:103:ARG:N	2.49	0.45
20:S1:1256:U:OP2	23:SO:136:LYS:NZ	2.48	0.45
26:SM:39:ARG:NH1	26:SM:101:PHE:HB3	2.31	0.45
32:SF:182:VAL:HB	32:SF:209:TYR:HB2	1.97	0.45
41:1:231:U:H2'	41:1:232:G:C8	2.52	0.45
41:1:1265:A:H2'	41:1:1266:A:C8	2.50	0.45
45:B:184:GLN:OE1	88:B:501:HOH:O	2.20	0.45
51:H:201:ARG:NH2	58:6:15:C:O2	2.49	0.45
55:Q:85:ARG:HH11	55:Q:85:ARG:HG3	1.81	0.45
57:E:84:THR:HG22	57:E:85:LYS:HG2	1.98	0.45
65:Z:61:ILE:HG21	65:Z:92:VAL:HG21	1.98	0.45
74:p:24:LYS:HG3	74:p:73:GLN:O	2.16	0.45
79:n:11:ARG:HD3	79:n:14:TRP:NE1	2.31	0.45
13:SE:8:ARG:HD3	13:SE:18:SER:O	2.17	0.45
20:S1:417:U:O4	88:S1:2424:HOH:O	2.21	0.45
20:S1:902:G:O2'	20:S1:903:G:O5'	2.33	0.45
27:SL:104:ASN:OD1	27:SL:107:GLU:HG3	2.17	0.45
28:SJ:68:ARG:HG2	32:SF:242:TRP:NE1	2.31	0.45
38:c:109:GLN:HG3	38:c:140:VAL:HG12	1.99	0.45
41:1:719:U:O2'	41:1:720:A:H5''	2.17	0.45
42:2:509:C:O5'	42:2:509:C:H6	1.98	0.45
46:8:34:A:H2'	46:8:35:U:O4'	2.15	0.45
82:e:21:ALA:O	82:e:22:ALA:HB3	2.17	0.45
20:S1:71:G:N2	20:S1:77:G:H22	2.14	0.45
42:2:349:C:H2'	42:2:350:U:C6	2.51	0.45
42:2:1412:U:H2'	42:2:1413:PSU:C6	2.52	0.45
46:8:9:A:O2'	49:O:63:GLN:NE2	2.49	0.45
57:E:47:VAL:HG12	57:E:54:PHE:HD1	1.81	0.45
65:Z:33:ASN:HD22	65:Z:34:ASN:N	2.14	0.45
81:3:42:U:H2'	81:3:43:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SC:166:PHE:CD2	11:SC:199:PRO:HG2	2.51	0.45
12:SD:122:HIS:HD2	19:Se:33:ARG:HH11	1.63	0.45
20:S1:752:C:O2	88:S1:2425:HOH:O	2.21	0.45
41:1:163:U:H2'	41:1:163:U:O2	2.17	0.45
41:1:1558:U:OP2	88:1:1915:HOH:O	2.20	0.45
42:2:497:G:C2	42:2:513:C:C2	3.04	0.45
48:A:140:ASN:HD21	48:A:143:THR:HG23	1.80	0.45
81:3:64:U:H2'	81:3:65:U:C6	2.51	0.45
14:SK:68:ALA:HB2	14:SK:201:ILE:HD11	1.97	0.45
20:S1:114:U:H2'	20:S1:115:C:C6	2.52	0.45
20:S1:958:G:N2	20:S1:977:G:H1	2.14	0.45
20:S1:1496:U:H2'	20:S1:1497:U:C6	2.51	0.45
20:S1:1657:PSU:H6	20:S1:1657:PSU:OP1	1.99	0.45
20:S1:1795:G:C2	20:S1:1796:U:H1'	2.52	0.45
42:2:507:G:O2'	42:2:508:A:N7	2.50	0.45
42:2:528:U:OP1	42:2:1411:G:O2'	2.31	0.45
42:2:665:A2M:H2'	42:2:666:C:C6	2.51	0.45
42:2:1520:C:O2'	42:2:1521:A:H2'	2.16	0.45
44:7:40:A:H2'	44:7:41:A:C8	2.52	0.45
59:T:137:THR:HG23	59:T:138:PRO:HD2	1.98	0.45
72:U:61:LYS:HE3	72:U:61:LYS:HB2	1.84	0.45
81:3:156:G:N2	81:3:175:A:H2	2.14	0.45
15:S4:4:C:H3'	15:S4:5:G:H8	1.82	0.45
20:S1:98:A2M:O5'	20:S1:98:A2M:H8	2.16	0.45
39:a:120:LYS:HD2	39:a:120:LYS:HA	1.71	0.45
41:1:342:G:N3	41:1:342:G:H5'	2.31	0.45
43:4:1:G:C4	58:6:3:A:H1'	2.52	0.45
46:8:96:G:H2'	46:8:97:A:C8	2.51	0.45
56:R:97:ARG:HG2	61:K:30:VAL:O	2.16	0.45
60:S:18:LYS:HD2	60:S:18:LYS:HA	1.75	0.45
61:K:40:PRO:HB2	61:K:41:GLU:OE2	2.16	0.45
20:S1:66:U:H6	31:SG:163:ARG:HH11	1.63	0.45
20:S1:691:G:H1	20:S1:754:G:H22	1.65	0.45
20:S1:957:G:H2'	20:S1:958:G:C8	2.52	0.45
34:Sb:91:ARG:HH12	34:Sb:98:ILE:HB	1.81	0.45
35:Sh:171:ASN:OD1	35:Sh:171:ASN:N	2.45	0.45
42:2:782:G:O2'	42:2:786:A:H5'	2.16	0.45
47:5:84:C:H2'	47:5:85:G:C1'	2.47	0.45
49:O:99:TYR:CD2	49:O:205:ILE:HD12	2.52	0.45
49:O:201:HIS:O	49:O:205:ILE:HG12	2.17	0.45
78:l:38:ASN:HB3	78:l:41:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S1:1459:G:O2'	20:S1:1460:G:H5'	2.16	0.45
20:S1:2103:G:O2'	20:S1:2104:G:H5'	2.17	0.45
20:S1:2185:MA6:H8	20:S1:2185:MA6:H5''	1.99	0.45
41:1:479:A:H2'	41:1:480:U:C6	2.51	0.45
41:1:1011:PSU:HO2'	41:1:1012:C:P	2.40	0.45
41:1:1169:A:H2'	41:1:1170:G:C8	2.51	0.45
41:1:1177:U:H2'	41:1:1178:U:H6	1.81	0.45
42:2:504:PSU:H2'	42:2:505:A:N3	2.32	0.45
42:2:511:C:H2'	42:2:512:U:H6	1.80	0.45
46:8:8:U:H2'	46:8:9:A:C8	2.51	0.45
48:A:140:ASN:HD22	48:A:143:THR:H	1.64	0.45
57:E:41:LEU:HD23	57:E:41:LEU:HA	1.77	0.45
67:h:119:LYS:O	67:h:123:ASN:N	2.49	0.45
1:SW:54:ARG:NH1	20:S1:1974:A:OP2	2.50	0.45
20:S1:792:G:H8	20:S1:833:G:H22	1.64	0.45
20:S1:1504:A:O3'	34:Sb:89:ARG:NH2	2.50	0.45
20:S1:1581:G:C8	20:S1:1607:G:C2	3.04	0.45
41:1:442:A:H1'	41:1:444:C:C4	2.51	0.45
41:1:543:G:H3'	41:1:1392:G:C8	2.52	0.45
41:1:662:C:H2'	41:1:663:C:C6	2.51	0.45
42:2:1510:U:H5	45:B:326:ASN:ND2	2.14	0.45
46:8:8:U:H2'	46:8:9:A:H8	1.82	0.45
46:8:111:A:O2'	46:8:112:G:H5'	2.17	0.45
11:SC:115:ARG:O	11:SC:119:MET:HG2	2.16	0.44
20:S1:459:A:H5''	20:S1:460:C:H5	1.81	0.44
20:S1:1246:PSU:H5'	20:S1:1246:PSU:H6	1.82	0.44
20:S1:1914:U:O2'	20:S1:1915:U:C6	2.69	0.44
42:2:604:A2M:H2'	42:2:605:C:O4'	2.17	0.44
42:2:1117:G:H5'	88:2:2137:HOH:O	2.17	0.44
54:P:100:ALA:N	63:L:116:GLN:HE21	2.15	0.44
54:P:188:ARG:HD2	54:P:188:ARG:N	2.32	0.44
62:D:165:PHE:HE1	62:D:171:GLY:HA3	1.82	0.44
13:SE:138:THR:HG22	13:SE:139:HIS:N	2.32	0.44
14:SK:115:LYS:HD3	14:SK:115:LYS:HA	1.70	0.44
20:S1:133:G:H2'	20:S1:134:G:H8	1.81	0.44
20:S1:656:G:H5'	20:S1:662:G:N2	2.33	0.44
20:S1:790:U:O2	31:SG:226:ARG:NH2	2.41	0.44
20:S1:1148:G:H2'	20:S1:1149:G:C8	2.53	0.44
41:1:335:U:H3'	73:i:35:VAL:HG23	2.00	0.44
42:2:454:A:N3	42:2:454:A:H2'	2.33	0.44
44:7:134:G:H2'	44:7:135:U:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:8:48:U:OP2	62:D:139:ARG:NH2	2.41	0.44
53:I:192:LYS:HB3	53:I:192:LYS:HE3	1.77	0.44
81:3:188:C:H3'	81:3:189:U:H6	1.82	0.44
11:SC:130:ALA:HA	11:SC:190:PRO:HD3	1.99	0.44
41:1:516:G:H2'	41:1:517:U:H6	1.83	0.44
41:1:1276:U:H2'	41:1:1277:G:C8	2.52	0.44
49:O:95:TYR:HE1	49:O:205:ILE:HD13	1.82	0.44
53:I:52:PHE:CD1	53:I:153:GLN:HB2	2.52	0.44
62:D:104:PHE:CZ	62:D:131:VAL:HG11	2.52	0.44
67:h:51:HIS:HE1	81:3:31:U:OP1	2.01	0.44
71:W:108:LEU:HD12	71:W:113:LYS:HG2	1.98	0.44
10:SB:95:GLN:HE21	10:SB:96:HIS:CE1	2.36	0.44
20:S1:555:C:H2'	20:S1:556:A:C8	2.53	0.44
20:S1:790:U:O2	20:S1:790:U:N3	2.50	0.44
24:SN:93:ALA:O	24:SN:95:PRO:HD3	2.16	0.44
41:1:141:U:C1'	41:1:142:A:H5''	2.48	0.44
41:1:157:U:H4'	41:1:158:A:O4'	2.18	0.44
41:1:720:A:C8	41:1:721:U:H2'	2.52	0.44
42:2:506:PSU:H3'	42:2:507:G:C8	2.52	0.44
42:2:1436:A:OP1	88:2:1702:HOH:O	2.21	0.44
57:E:102:VAL:HA	57:E:110:GLU:O	2.18	0.44
71:W:80:ASP:OD2	71:W:81:LYS:HG2	2.18	0.44
77:k:23:VAL:HG11	77:k:60:ILE:HD11	1.99	0.44
10:SB:124:VAL:HG22	10:SB:146:PRO:HG2	1.98	0.44
11:SC:168:ASP:HB2	11:SC:189:LEU:HD21	1.99	0.44
17:Sa:41:MET:HE3	17:Sa:41:MET:HB3	1.87	0.44
20:S1:255:A:H61	20:S1:972:A:N6	2.16	0.44
20:S1:1427:U:H5	88:S1:2622:HOH:O	2.01	0.44
20:S1:1830:G:H2'	20:S1:1831:U:C6	2.52	0.44
67:h:51:HIS:HD2	81:3:193:C:H5	1.64	0.44
81:3:59:U:H2'	81:3:60:U:O4'	2.17	0.44
1:SW:108:GLN:HE21	1:SW:108:GLN:HB3	1.59	0.44
12:SD:27:MET:HE3	12:SD:27:MET:HA	1.99	0.44
20:S1:236:C:H2'	20:S1:237:A:H8	1.81	0.44
20:S1:1635:U:OP2	20:S1:1636:U:O2'	2.29	0.44
41:1:1563:U:H2'	41:1:1564:C:O4'	2.18	0.44
41:1:1565:A:C6	82:e:74:ARG:HD3	2.53	0.44
41:1:1749:G:H2'	41:1:1751:A:N7	2.33	0.44
45:B:24:GLN:NE2	45:B:28:ARG:HE	2.16	0.44
48:A:93:LYS:H	48:A:93:LYS:HG2	1.56	0.44
71:W:80:ASP:OD2	71:W:81:LYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4: SX:38: LEU:O	4: SX:39: LYS:HB2	2.18	0.44
7: ST:32: ASN:O	7: ST:36: MET:HB2	2.18	0.44
41:1:160: C:H3'	41:1:161: A:C8	2.43	0.44
41:1:163: U:H5	41:1:292: A:H61	1.61	0.44
41:1:1186: A:H2'	41:1:1187: A:C8	2.52	0.44
42:2:504: PSU:H2'	42:2:505: A:O4'	2.18	0.44
61: K:42: ASP:OD2	61: K:45: MET:HG2	2.18	0.44
64: Y:32: VAL:HB	64: Y:37: PRO:HA	2.00	0.44
65: Z:45: PHE:CZ	65: Z:46: LEU:HD23	2.52	0.44
81:3:49: A:N1	81:3:180: U:H5	2.15	0.44
81:3:111: A:C2	81:3:116: U:N3	2.80	0.44
82: e:25: ARG:O	82: e:26: LYS:C	2.60	0.44
3: SY:9: GLU:HG2	32: SF:159: LYS:O	2.17	0.44
12: SD:48: LEU:HD21	12: SD:98: LEU:HB3	2.00	0.44
18: Sc:60: CYS:SG	18: Sc:61: SER:N	2.89	0.44
20: S1:777: A:H61	20: S1:841: U:H2'	1.82	0.44
39: a:104: LYS:O	39: a:105: ASN:HB2	2.18	0.44
41:1:996: A:H2'	41:1:997: C:C6	2.52	0.44
41:1:1365: A:O2'	41:1:1366: A:O4'	2.13	0.44
62: D:127: MET:HE2	62: D:127: MET:HB2	1.77	0.44
20: S1:1709: A:H2'	20: S1:1710: U:C6	2.53	0.44
26: SM:75: ASP:OD2	26: SM:75: ASP:N	2.51	0.44
35: Sh:210: GLU:CD	35: Sh:210: GLU:N	2.76	0.44
41:1:1574: C:H2'	41:1:1575: G:H8	1.83	0.44
42:2:501: A:H3'	42:2:507: G:N1	2.32	0.44
42:2:811: U:H5	42:2:1007: U:O2	1.99	0.44
42:2:1141: G:H4'	42:2:1142: A:H5''	1.99	0.44
42:2:1501: G:H5'	82: e:25: ARG:CZ	2.48	0.44
47:5:51: U:H3	47:5:61: C:H42	1.66	0.44
50: G:103[A]: ARG:HH11	50: G:103[A]: ARG:HG2	1.83	0.44
53: I:127: LYS:HD2	53: I:162: ALA:HB1	1.99	0.44
2: SZ:93: GLU:OE2	2: SZ:94: PRO:HD2	2.18	0.43
20: S1:80: G:H3'	20: S1:81: G:C5'	2.48	0.43
20: S1:585: C:O2'	20: S1:586: G:H8	2.00	0.43
20: S1:760: G:H3'	20: S1:761: A:H8	1.83	0.43
20: S1:1569: G:H1'	24: SN:29: ARG:HH22	1.83	0.43
23: SO:89: LYS:HA	23: SO:89: LYS:HD3	1.72	0.43
41:1:497: A:P	41:1:576: G:H21	2.41	0.43
41:1:736: C:O2'	41:1:737: U:H6	2.01	0.43
41:1:1245: G:N1	41:1:1382: G:N2	2.65	0.43
41:1:1451: C:H2'	41:1:1452: C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SS:4:LEU:HG	20:S1:1596:U:O2'	2.18	0.43
12:SD:152:GLU:HA	12:SD:155:ILE:HD12	2.00	0.43
20:S1:779:A:O2'	20:S1:780:A:H8	2.02	0.43
20:S1:956:A:H61	20:S1:979:U:H5	1.65	0.43
20:S1:1466:G:N2	20:S1:1482:G:H2'	2.33	0.43
54:P:129:THR:H	54:P:132:GLN:NE2	2.16	0.43
57:E:85:LYS:HE3	57:E:185:ASN:ND2	2.33	0.43
81:3:190:G:H2'	81:3:191:C:O4'	2.18	0.43
16:Sg:129:ASN:N	16:Sg:129:ASN:HD22	2.16	0.43
16:Sg:241:ILE:HG23	16:Sg:250:MET:HG3	2.00	0.43
20:S1:1578:G:H8	20:S1:1608:A:H2	1.67	0.43
20:S1:1889:G:H5''	20:S1:1890:A:OP1	2.18	0.43
29:SI:4:HIS:CD2	29:SI:5:LEU:HD23	2.53	0.43
41:1:736:C:O2'	41:1:737:U:P	2.76	0.43
41:1:1264:A:H4'	41:1:1265:A:OP1	2.18	0.43
49:O:97:ALA:O	49:O:101:THR:OG1	2.33	0.43
68:g:111:HIS:CD2	68:g:118:ARG:HE	2.34	0.43
20:S1:285:A:N6	20:S1:816:C:H2'	2.32	0.43
43:4:19:C:H2'	43:4:20:U:H6	1.83	0.43
46:8:27:A:H2'	46:8:28:A:C8	2.53	0.43
56:R:92:MET:HE2	56:R:112:LEU:HD21	1.99	0.43
67:h:120:ARG:HA	67:h:124:LYS:H	1.84	0.43
82:e:6:LEU:HD12	82:e:6:LEU:H	1.83	0.43
10:SB:74:PRO:O	10:SB:99:THR:HA	2.18	0.43
11:SC:44:ARG:NH1	11:SC:46:GLU:OE2	2.52	0.43
30:SH:87:HIS:HB2	30:SH:94:PRO:HG3	1.99	0.43
41:1:1565:A:N6	82:e:74:ARG:HH11	2.17	0.43
42:2:957:C:H2'	42:2:958:A:O4'	2.18	0.43
42:2:1089:A:H2'	42:2:1090:G:C8	2.54	0.43
42:2:1275:A:H8	42:2:1275:A:OP2	2.01	0.43
42:2:1383:G:O2'	42:2:1386:C:OP2	2.27	0.43
73:i:38:LYS:HB2	73:i:38:LYS:HE2	1.86	0.43
76:X:54:PRO:HA	76:X:59:TYR:CG	2.54	0.43
81:3:155:A:H2'	81:3:156:G:C8	2.54	0.43
4:SX:122:GLU:OE2	4:SX:122:GLU:N	2.49	0.43
12:SD:90:ASP:OD1	12:SD:90:ASP:N	2.50	0.43
13:SE:105:ARG:NH2	20:S1:889:A:OP2	2.36	0.43
13:SE:119:LYS:HD3	13:SE:121:MET:HE3	2.01	0.43
20:S1:30:G:H2'	20:S1:31:C:C6	2.53	0.43
20:S1:1858:G:N1	20:S1:1978:A:H1'	2.33	0.43
31:SG:179:ILE:HG22	31:SG:182:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1:994:U:H5	41:1:1521:G:OP1	2.02	0.43
41:1:1414:A:OP1	54:P:17:HIS:HE1	2.02	0.43
42:2:1300:U:H2'	42:2:1301:G:O4'	2.18	0.43
43:4:62:C:H42	57:E:118:LYS:HG2	1.84	0.43
43:4:88:G:OP2	88:4:301:HOH:O	2.21	0.43
59:T:7:LYS:HB3	59:T:7:LYS:HE2	1.66	0.43
74:p:6:LYS:HE2	74:p:95:ASP:N	2.34	0.43
81:3:38:U:H3	81:3:191:C:H5	1.66	0.43
20:S1:978:C:H2'	20:S1:979:U:O4'	2.18	0.43
20:S1:1460:G:H1	22:SP:20:ASN:ND2	2.15	0.43
20:S1:1770:G:H21	20:S1:1770:G:P	2.41	0.43
41:1:442:A:H1'	41:1:444:C:N3	2.33	0.43
42:2:619:A:N3	42:2:1262:G:O2'	2.37	0.43
42:2:756:C:H2'	42:2:757:A:H8	1.84	0.43
45:B:110:THR:OG1	45:B:115[B]:ARG:NH1	2.52	0.43
48:A:109:GLU:HG2	48:A:138:SER:HA	2.01	0.43
53:I:184:MET:HG3	53:I:185:CYS:N	2.34	0.43
64:Y:99:VAL:HG23	64:Y:105:ARG:HG3	2.01	0.43
71:W:52:GLU:HG3	71:W:105:LYS:HB3	2.01	0.43
8:SS:11:GLN:HB3	24:SN:30:MET:HE1	2.00	0.43
12:SD:91:LYS:HD2	12:SD:91:LYS:HA	1.85	0.43
20:S1:1579:A:H4'	20:S1:1580:G:O5'	2.19	0.43
20:S1:1605:U:O2'	20:S1:1606:C:H5'	2.19	0.43
25:Sd:69:GLU:CD	25:Sd:69:GLU:H	2.26	0.43
35:Sh:143:ILE:C	35:Sh:143:ILE:HD12	2.44	0.43
42:2:464:G:H2'	42:2:465:A:H8	1.83	0.43
42:2:502:A:C5'	42:2:507:G:H22	2.31	0.43
42:2:982:G:H3'	42:2:983:G:H5''	2.01	0.43
57:E:31:ARG:HE	57:E:31:ARG:HB3	1.72	0.43
69:J:19:LEU:HB2	69:J:54:ALA:HB3	2.01	0.43
10:SB:83:ARG:HG3	10:SB:85:TYR:H	1.83	0.43
14:SK:173:LYS:HA	14:SK:173:LYS:HD3	1.89	0.43
20:S1:307:C:H2'	20:S1:308:C:C4	2.54	0.43
20:S1:496:A:H2'	20:S1:496:A:N3	2.34	0.43
20:S1:781:A:H5''	20:S1:781:A:N3	2.33	0.43
20:S1:1656:G:H3'	20:S1:1657:PSU:H5'	2.01	0.43
41:1:544:A:H2'	41:1:545:A:C8	2.53	0.43
41:1:621:U:H2'	41:1:622:C:C6	2.54	0.43
42:2:502:A:H5'	42:2:507:G:H22	1.84	0.43
42:2:1521:A:N3	42:2:1521:A:H2'	2.34	0.43
44:7:18:G:H2'	44:7:19:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:49:C:C4	47:5:50:A:N6	2.87	0.43
48:A:194:ASN:ND2	88:A:303:HOH:O	2.46	0.43
10:SB:94:SER:OG	10:SB:99:THR:O	2.23	0.43
16:Sg:75:HIS:ND1	16:Sg:117:PRO:HA	2.34	0.43
16:Sg:190:LEU:HD11	16:Sg:221:TRP:CD2	2.53	0.43
20:S1:307:C:H2'	20:S1:308:C:C5	2.54	0.43
20:S1:1288:G:H22	20:S1:1426:U:H5	1.67	0.43
20:S1:2006:A:OP1	27:SL:139:SER:OG	2.35	0.43
33:SA:37:ASN:OD1	33:SA:37:ASN:N	2.52	0.43
42:2:95:A2M:HM'3	42:2:95:A2M:H1'	1.74	0.43
42:2:513:C:H2'	42:2:514:U:C6	2.54	0.43
42:2:603:A:H5'	59:T:137:THR:CG2	2.48	0.43
42:2:752:G:H2'	42:2:753:C:C6	2.54	0.43
45:B:266:MET:HG2	51:H:82:THR:HG22	2.01	0.43
81:3:204:A:H2'	81:3:205:A:C8	2.54	0.43
12:SD:63:GLU:OE2	12:SD:63:GLU:HA	2.19	0.42
20:S1:144:A:C8	31:SG:188:LYS:HD3	2.54	0.42
38:c:72:LEU:HD23	38:c:72:LEU:HA	1.81	0.42
41:1:547:U:OP1	56:R:7:ARG:NE	2.52	0.42
41:1:623:U:N3	41:1:624:U:O4	2.52	0.42
43:4:149:U:H4'	43:4:150:A:OP1	2.18	0.42
56:R:42:ARG:HA	56:R:42:ARG:HD2	1.85	0.42
63:L:77:ASN:HD22	63:L:80:ARG:HE	1.65	0.42
65:Z:61:ILE:HD13	65:Z:61:ILE:HA	1.85	0.42
20:S1:691:G:H2'	20:S1:692:G:H8	1.83	0.42
20:S1:1471:U:H2'	20:S1:1472:U:C6	2.54	0.42
20:S1:1572:C:H2'	20:S1:1573:A:C8	2.53	0.42
29:SI:144:ARG:HH21	29:SI:146:ARG:NE	2.17	0.42
37:d:51:PRO:HA	37:d:52:PRO:HD3	1.96	0.42
41:1:943:U:H2'	41:1:944:A:O4'	2.19	0.42
41:1:1750:G:C6	77:k:74:HIS:CE1	3.06	0.42
42:2:515:U:C2	42:2:518:G:N7	2.88	0.42
42:2:622:G:H2'	42:2:623:A:C8	2.54	0.42
42:2:966:U:O2'	42:2:967:G:H5'	2.19	0.42
42:2:1505:A:C6	42:2:1517:G:C6	3.07	0.42
43:4:47:G:O2'	43:4:48:U:O5'	2.37	0.42
70:V:141:LYS:HE3	70:V:141:LYS:HB3	1.67	0.42
3:SY:44:VAL:HA	3:SY:50:ILE:HA	2.01	0.42
10:SB:52:ILE:HG21	10:SB:165:PRO:HB2	2.01	0.42
17:Sa:91:LEU:HD21	17:Sa:94:CYS:HB3	2.01	0.42
20:S1:1123:G:H1'	20:S1:1191:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1:12:U:H2'	41:1:13:G:H8	1.84	0.42
45:B:346:ARG:NH1	45:B:349:MET:HG3	2.34	0.42
48:A:206:PRO:HG3	48:A:213:GLY:HA3	2.00	0.42
49:O:213:TYR:O	49:O:217:VAL:HG22	2.19	0.42
67:h:109:LYS:NZ	67:h:109:LYS:HB2	2.33	0.42
82:e:46:LYS:HA	82:e:46:LYS:HD2	1.58	0.42
82:e:81:MET:HE3	82:e:81:MET:HB3	1.83	0.42
19:Se:30:PRO:O	19:Se:35:LEU:HB2	2.19	0.42
20:S1:1882:A:H2'	20:S1:1883:G:O4'	2.19	0.42
38:c:135:ASN:ND2	41:1:1038:U:OP1	2.53	0.42
41:1:1779:G:H5''	88:1:2767:HOH:O	2.19	0.42
42:2:515:U:H2'	42:2:517:A:OP2	2.20	0.42
42:2:979:A:O2'	42:2:980:A:H8	2.02	0.42
42:2:1522:U:H2'	42:2:1523:C:C6	2.54	0.42
55:Q:90:PRO:HB2	55:Q:93:GLU:HG2	2.01	0.42
81:3:43:C:H2'	81:3:44:C:O4'	2.20	0.42
20:S1:1705:C:H42	20:S1:1770:G:H1	1.67	0.42
41:1:486:G:O5'	41:1:486:G:H8	2.01	0.42
42:2:628:A2M:HM'3	42:2:628:A2M:H8	2.02	0.42
42:2:959:A:O2'	42:2:960:C:OP1	2.31	0.42
49:O:127:GLY:HA3	49:O:201:HIS:HB3	2.01	0.42
3:SY:41:ILE:HG12	10:SB:67:VAL:HG22	2.02	0.42
10:SB:13:MET:HB2	10:SB:58:TRP:CD1	2.54	0.42
20:S1:1498:G:H2'	20:S1:1499:A:C8	2.54	0.42
20:S1:1635:U:H5''	20:S1:1636:U:H3'	2.02	0.42
20:S1:1914:U:O2'	20:S1:1915:U:P	2.77	0.42
28:SJ:3:MET:HE3	28:SJ:3:MET:HB2	1.80	0.42
30:SH:149:PHE:CD2	30:SH:150:ARG:HG3	2.55	0.42
30:SH:172:ASN:HD22	30:SH:172:ASN:HA	1.70	0.42
41:1:1670:A:H61	70:V:32:ARG:NH2	2.17	0.42
42:2:124:G:OP1	55:Q:75:HIS:HD2	2.03	0.42
57:E:49:LYS:HB2	57:E:49:LYS:HE2	1.84	0.42
77:k:48:ASN:OD1	77:k:48:ASN:N	2.53	0.42
14:SK:160:ARG:HA	14:SK:160:ARG:HD2	1.82	0.42
17:Sa:83:LEU:HD22	17:Sa:88:LEU:HD12	2.01	0.42
20:S1:170:G:H2'	20:S1:171:C:H5''	2.02	0.42
20:S1:1994:G:H5''	20:S1:1995:G7M:OP1	2.20	0.42
41:1:637:C:H2'	41:1:638:C:O2	2.19	0.42
41:1:938:G:H4'	42:2:75:A:C5	2.54	0.42
41:1:1245:G:N2	41:1:1383:C:C2	2.88	0.42
41:1:1425:C:C3'	65:Z:88:ARG:HH22	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2:1462:A:H4'	51:H:189:LYS:NZ	2.35	0.42
54:P:23:ASN:HB3	54:P:26:ILE:HB	2.00	0.42
58:6:73:A:C2	68:g:27:ASN:HB2	2.54	0.42
61:K:53:LYS:HE2	61:K:53:LYS:HB2	1.85	0.42
72:U:118:GLN:HE21	72:U:120:LYS:HD2	1.84	0.42
73:i:74:LYS:HE3	73:i:74:LYS:HB3	1.94	0.42
81:3:13:OMU:HM23	81:3:13:OMU:H1'	1.82	0.42
81:3:141:A:H2'	81:3:142:G:O4'	2.20	0.42
12:SD:91:LYS:HB3	12:SD:93:ASP:OD1	2.19	0.42
20:S1:254:A:HO2'	20:S1:255:A:H8	1.64	0.42
20:S1:976:A:H2'	20:S1:977:G:C8	2.55	0.42
20:S1:1684:U:H3	20:S1:1820:G:H22	1.66	0.42
20:S1:1836:G:H5''	20:S1:1837:A:H5'	2.02	0.42
22:SP:73:GLN:HG3	22:SP:80:LYS:HG2	2.02	0.42
41:1:738:C:H2'	41:1:739:U:C6	2.55	0.42
41:1:789:U:O2'	41:1:791:C:OP1	2.23	0.42
41:1:1153:A:H2'	41:1:1155:A:H62	1.85	0.42
42:2:1318:PSU:H1'	45:B:255:ALA:HB3	2.02	0.42
49:O:43:LYS:O	49:O:45:GLY:N	2.52	0.42
49:O:214:LEU:HD22	49:O:242:PRO:HG3	2.01	0.42
53:I:178:SER:O	53:I:182:LYS:HG3	2.19	0.42
53:I:184:MET:HE2	53:I:185:CYS:SG	2.60	0.42
60:S:80:VAL:HG21	60:S:85:LEU:HD22	2.01	0.42
62:D:109:ASP:OD1	62:D:109:ASP:N	2.53	0.42
64:Y:79:HIS:ND1	81:3:10:U:O2'	2.49	0.42
64:Y:98:ASN:OD1	64:Y:98:ASN:C	2.62	0.42
68:g:120:LYS:HE2	68:g:120:LYS:HB2	1.96	0.42
81:3:41:A:O2'	81:3:188:C:N4	2.53	0.42
20:S1:1920:A:HO2'	20:S1:1921:A:P	2.37	0.42
23:SO:91:ARG:HB3	23:SO:125:VAL:HG23	2.00	0.42
35:Sh:194:GLU:HB2	35:Sh:199:THR:HA	2.01	0.42
41:1:164:U:H2'	41:1:165:C:C6	2.54	0.42
41:1:523:G:H2'	41:1:524:U:C6	2.54	0.42
41:1:1245:G:H5''	41:1:1245:G:C8	2.49	0.42
42:2:134:C:O2'	42:2:135:A:H8	2.02	0.42
42:2:382:A2M:HM'3	42:2:382:A2M:H1'	1.80	0.42
42:2:665:A2M:HM'3	42:2:665:A2M:H1'	1.69	0.42
42:2:1343:A:H2'	42:2:1344:C:H6	1.85	0.42
43:4:16:G:H2'	43:4:17:A:H8	1.81	0.42
65:Z:33:ASN:ND2	65:Z:35:ASN:H	2.17	0.42
81:3:201:C:H6	81:3:201:C:H2'	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S1:409:G:OP1	20:S1:859:G:O2'	2.36	0.42
20:S1:1143:U:OP1	33:SA:26:ARG:NH2	2.52	0.42
20:S1:1193:U:H2'	20:S1:1194:C:C6	2.54	0.42
27:SL:11:GLN:HG3	27:SL:28:THR:HB	2.02	0.42
42:2:454:A:O2'	42:2:455:U:OP2	2.38	0.42
44:7:125:A:H3'	44:7:126:G:H8	1.85	0.42
46:8:53:A:H5''	49:O:233:SER:HB3	2.01	0.42
55:Q:66:MET:HE2	55:Q:66:MET:HB2	1.85	0.42
72:U:53:ASP:O	72:U:54:ASN:ND2	2.53	0.42
9:SR:32:ARG:HE	9:SR:32:ARG:HB2	1.71	0.41
20:S1:693:C:H42	20:S1:752:C:N4	2.18	0.41
20:S1:1772:A:H2'	20:S1:1773:U:H6	1.85	0.41
41:1:426:A:H2'	41:1:427:A:C8	2.55	0.41
41:1:1561:A:C4	41:1:1562:C:H5	2.38	0.41
41:1:1592:G:H21	67:h:13:HIS:HD2	1.68	0.41
42:2:625:U:H2'	42:2:626:PSU:C6	2.55	0.41
42:2:1459:U:H1'	42:2:1463:A:N6	2.35	0.41
45:B:110:THR:OG1	45:B:115[A]:ARG:NH1	2.53	0.41
47:5:50:A:C2	47:5:62:G:N2	2.88	0.41
48:A:140:ASN:ND2	48:A:143:THR:H	2.18	0.41
62:D:50:SER:HB3	62:D:68:ALA:HB3	2.02	0.41
20:S1:71:G:H1	20:S1:77:G:N2	2.15	0.41
20:S1:1906:G:H2'	20:S1:1907:A:C8	2.54	0.41
42:2:603:A:H5'	59:T:137:THR:HG23	2.02	0.41
45:B:57:VAL:HB	45:B:365:PHE:HB3	2.03	0.41
47:5:113:A:H2'	47:5:114:A:O4'	2.20	0.41
53:I:57:LYS:NZ	53:I:157:ARG:O	2.38	0.41
72:U:42:ASP:OD1	72:U:43:VAL:HG22	2.20	0.41
74:p:23:PHE:HD2	74:p:72:LEU:HB3	1.85	0.41
80:C:75:ILE:HG13	80:C:76:PRO:HD2	2.02	0.41
6:SU:95:MET:HE3	6:SU:98:THR:HG23	2.01	0.41
16:Sg:33:SER:OG	16:Sg:34:ARG:N	2.52	0.41
20:S1:476:C:H2'	20:S1:477:G:O4'	2.21	0.41
41:1:217:A:C3'	41:1:218:A:H5'	2.51	0.41
42:2:689:A:O2'	42:2:690:C:H6	2.03	0.41
42:2:1113:C:H2'	42:2:1114:G:O4'	2.20	0.41
42:2:1254:G:C8	42:2:1308:5MC:H5''	2.55	0.41
55:Q:85:ARG:HG3	55:Q:85:ARG:NH1	2.33	0.41
66:F:93:ILE:O	66:F:93:ILE:HG13	2.20	0.41
20:S1:436:C:H2'	20:S1:437:C:C6	2.55	0.41
20:S1:977:G:N3	20:S1:977:G:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S1:1923:A:O2'	20:S1:1924:G:N2	2.47	0.41
30:SH:38:THR:HG22	30:SH:56:GLU:OE2	2.20	0.41
41:1:574:G:O2'	41:1:576:G:H2'	2.20	0.41
42:2:495:G:C8	42:2:518:G:C4	3.08	0.41
42:2:781:G:H3'	42:2:782:G:N2	2.36	0.41
43:4:75:C:H5'	45:B:336:SER:HA	2.03	0.41
52:M:135:VAL:HG21	52:M:151:ILE:HG21	2.02	0.41
58:6:38:C:O2'	58:6:40:C:H5	2.02	0.41
74:p:23:PHE:CD2	74:p:72:LEU:HB3	2.55	0.41
81:3:179:U:OP2	81:3:179:U:H3'	2.20	0.41
20:S1:2198:U:H3'	34:Sb:5:ARG:HH21	1.85	0.41
33:SA:178:LEU:HD23	33:SA:178:LEU:HA	1.88	0.41
38:c:249:ALA:HB3	41:1:1394:A:H2	1.85	0.41
41:1:582:U:H4'	41:1:583:A:O4'	2.21	0.41
42:2:790:U:H2'	42:2:791:A:C8	2.55	0.41
42:2:1452:U:H4'	42:2:1453:U:OP2	2.20	0.41
45:B:376[B]:ARG:HG2	88:B:515:HOH:O	2.19	0.41
46:8:92:U:H2'	46:8:93:G:O4'	2.21	0.41
47:5:5:G:H2'	47:5:6:U:C6	2.55	0.41
62:D:87:LYS:NZ	62:D:87:LYS:HB3	2.35	0.41
62:D:98:PHE:CD2	62:D:162:MET:HG3	2.56	0.41
81:3:153:G:N1	81:3:178:G:N2	2.68	0.41
83:j:64:CYS:O	83:j:68:LYS:HG3	2.21	0.41
10:SB:60:LYS:HD2	10:SB:60:LYS:HA	1.61	0.41
20:S1:422:U:OP2	88:S1:2427:HOH:O	2.22	0.41
20:S1:1276:G:O2'	20:S1:1278:U:O2	2.36	0.41
20:S1:1980:U:H4'	20:S1:2019:C:H4'	2.03	0.41
29:SI:62:LEU:HD23	29:SI:62:LEU:HA	1.89	0.41
35:Sh:143:ILE:HD12	35:Sh:143:ILE:O	2.21	0.41
38:c:170:ARG:HD2	38:c:213:TRP:CD1	2.56	0.41
41:1:248:A:OP2	80:C:221:ASN:HB2	2.21	0.41
41:1:527:A:O2'	41:1:528:A:H8	2.03	0.41
41:1:1374:C:H2'	41:1:1375:G:O4'	2.20	0.41
41:1:1746:C:H2'	41:1:1747:U:C6	2.56	0.41
42:2:1270:C:H1'	42:2:1271:G:C8	2.55	0.41
45:B:63:PRO:HA	45:B:68:ASN:ND2	2.35	0.41
50:G:149:ALA:HA	50:G:202:THR:HG22	2.02	0.41
62:D:159:GLU:HA	62:D:162:MET:HE2	2.03	0.41
78:l:38:ASN:C	78:l:40:LYS:H	2.28	0.41
18:Sc:34:MET:HE2	18:Sc:49:SER:HA	2.03	0.41
20:S1:565:U:C4	20:S1:566:A:H1'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S1:1578:G:H8	20:S1:1608:A:C2	2.39	0.41
23:SO:44:GLU:OE1	88:SO:201:HOH:O	2.22	0.41
23:SO:90:MET:HB3	23:SO:90:MET:HE2	1.67	0.41
29:SI:54:VAL:HB	29:SI:57:SER:HB3	2.03	0.41
41:1:273:A:C6	83:j:79:LYS:HA	2.55	0.41
41:1:1576:U:H2'	41:1:1577:U:C6	2.56	0.41
42:2:1457:C:H5''	42:2:1458:G:H21	1.86	0.41
42:2:1463:A:H2'	42:2:1464:A:O4'	2.21	0.41
45:B:50:LYS:HA	45:B:79:LEU:HD23	2.02	0.41
55:Q:154:GLN:CD	55:Q:154:GLN:C	2.88	0.41
56:R:75:ASN:ND2	56:R:145:HIS:HE1	2.16	0.41
80:C:304:LYS:HD2	80:C:305:LEU:N	2.35	0.41
13:SE:229:LEU:HD23	13:SE:229:LEU:HA	1.92	0.41
20:S1:1288:G:N1	20:S1:1426:U:H5	2.15	0.41
41:1:1012:C:P	41:1:1012:C:O4'	2.79	0.41
41:1:1275:G:H4'	56:R:92:MET:SD	2.60	0.41
41:1:1392:G:H3'	41:1:1392:G:N3	2.36	0.41
88:1:2581:HOH:O	53:I:11:VAL:HG22	2.20	0.41
42:2:443:OMC:H6	42:2:443:OMC:H2'	1.71	0.41
42:2:496:G:H2'	42:2:497:G:C4'	2.51	0.41
42:2:1271:G:H1	42:2:1294:G:N2	2.14	0.41
43:4:51:U:H2'	43:4:52:A:H8	1.86	0.41
55:Q:190:ARG:HE	55:Q:190:ARG:C	2.28	0.41
80:C:295:GLU:H	80:C:295:GLU:CD	2.19	0.41
81:3:181:G:H8	81:3:181:G:H5''	1.85	0.41
10:SB:92:LYS:HB2	10:SB:205:PHE:CE1	2.56	0.41
15:S4:5:G:H2'	15:S4:5:G:N3	2.36	0.41
16:Sg:46:ASP:C	16:Sg:46:ASP:OD2	2.64	0.41
20:S1:184:C:H5''	20:S1:185:A:H2'	2.03	0.41
20:S1:512:A2M:HM'3	20:S1:512:A2M:H1'	1.72	0.41
20:S1:777:A:N1	20:S1:842:U:H3'	2.35	0.41
20:S1:1484:A:OP1	22:SP:28:LYS:NZ	2.40	0.41
32:SF:83:ILE:HG21	32:SF:88:LEU:HD13	2.02	0.41
32:SF:168:MET:HE3	32:SF:168:MET:HB3	1.97	0.41
41:1:196:C:O2'	41:1:198:C:OP2	2.39	0.41
41:1:507:C:H5''	80:C:352:ARG:NH2	2.36	0.41
41:1:835:G:N3	41:1:835:G:H2'	2.36	0.41
42:2:653:C:H4'	42:2:1046:OMG:HM22	2.02	0.41
42:2:959:A:H2'	42:2:960:C:H6	1.85	0.41
42:2:1271:G:C2	42:2:1272:G:C8	3.09	0.41
42:2:1309:G:H5'	42:2:1310:A:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:7:121:G:H2'	44:7:122:A:C8	2.56	0.41
50:G:93:LYS:HE3	50:G:93:LYS:HB2	1.75	0.41
50:G:152:VAL:O	50:G:178:TYR:HA	2.21	0.41
50:G:166:TRP:CD1	50:G:166:TRP:H	2.39	0.41
58:6:52:G:H21	58:6:54:A:H62	1.69	0.41
67:h:22:LYS:HB2	67:h:22:LYS:HE2	1.92	0.41
71:W:86:LYS:HB3	71:W:86:LYS:HE3	1.83	0.41
75:o:50:LYS:O	81:3:200:G:N1	2.54	0.41
80:C:59:MET:HE3	80:C:59:MET:HB3	1.97	0.41
81:3:191:C:H5'	81:3:192:G:O5'	2.21	0.41
5:SV:108:MET:HE3	10:SB:54:VAL:HG22	2.03	0.41
12:SD:87:GLU:H	12:SD:87:GLU:CD	2.23	0.41
20:S1:232:C:H2'	20:S1:233:G:H8	1.86	0.41
20:S1:234:C:H2'	20:S1:235:C:C6	2.56	0.41
20:S1:2186:C:OP2	79:n:10:MET:HB2	2.21	0.41
23:SO:54:LYS:HB3	23:SO:54:LYS:HE3	1.77	0.41
31:SG:4:ASN:HB2	31:SG:113:ASN:HD22	1.86	0.41
31:SG:135:ARG:HD3	31:SG:135:ARG:HA	1.92	0.41
33:SA:183:ILE:HD12	33:SA:183:ILE:HA	1.82	0.41
41:1:688:A:H2'	41:1:689:A:C8	2.56	0.41
43:4:47:G:HO2'	43:4:48:U:H6	1.67	0.41
51:H:203:GLU:O	51:H:203:GLU:HG2	2.21	0.41
53:I:59:LEU:HD22	53:I:124:TYR:CG	2.56	0.41
57:E:185:ASN:N	57:E:185:ASN:OD1	2.53	0.41
59:T:43:LYS:HE2	59:T:43:LYS:HB3	1.56	0.41
66:F:191:HIS:CD2	66:F:191:HIS:H	2.39	0.41
75:o:62:LYS:HE2	75:o:62:LYS:HB2	1.79	0.41
5:SV:18:GLU:OE1	5:SV:69:ILE:HG23	2.21	0.40
16:Sg:205:ASP:OD2	16:Sg:207:SER:HB3	2.21	0.40
20:S1:258:C:H42	20:S1:969:A:H61	1.69	0.40
20:S1:760:G:H3'	20:S1:761:A:C8	2.56	0.40
20:S1:1115:G:H2'	20:S1:1116:U:C6	2.56	0.40
20:S1:1296:G:H1	20:S1:1418:U:H3	1.69	0.40
20:S1:1983:U:H2'	20:S1:1984:C:C6	2.56	0.40
33:SA:176:ARG:HE	33:SA:176:ARG:HB3	1.65	0.40
42:2:1467:G:HO2'	42:2:1468:G:P	2.44	0.40
43:4:48:U:H2'	43:4:49:A:C8	2.56	0.40
47:5:48:G:N3	47:5:48:G:H5''	2.35	0.40
54:P:16:ARG:HH12	54:P:55:SER:HB3	1.87	0.40
58:6:37:C:N4	58:6:38:C:N4	2.68	0.40
64:Y:28:ASN:ND2	64:Y:77:HIS:HE1	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:Z:62:CYS:SG	65:Z:82:VAL:HG22	2.60	0.40
70:V:130:SER:C	70:V:132:ALA:H	2.29	0.40
80:C:320:MET:HE3	80:C:320:MET:HB3	1.85	0.40
20:S1:916:G:H22	55:Q:164:LEU:HD22	1.86	0.40
20:S1:1586:A:N6	20:S1:1603:U:H3	2.19	0.40
30:SH:177:LYS:HE2	30:SH:177:LYS:HB2	1.86	0.40
41:1:638:C:H2'	41:1:639:A:C8	2.57	0.40
41:1:848:U:H2'	41:1:849:U:C6	2.56	0.40
42:2:42:A:H4'	67:h:3:CYS:SG	2.61	0.40
42:2:91:C:H5	88:B:502:HOH:O	2.04	0.40
42:2:1254:G:O4'	42:2:1308:5MC:HM52	2.21	0.40
46:8:63:C:H2'	46:8:64:U:C6	2.56	0.40
49:O:153:ASP:OD1	49:O:153:ASP:C	2.64	0.40
50:G:208:ASP:OD1	50:G:208:ASP:N	2.54	0.40
60:S:17:LYS:HD3	60:S:22:HIS:HA	2.03	0.40
16:Sg:302:LEU:HD21	16:Sg:304:ARG:NH2	2.36	0.40
18:Sc:18:MET:HE2	18:Sc:18:MET:HB2	1.86	0.40
20:S1:1510:C:H5	20:S1:1515:A:H61	1.69	0.40
38:c:230:HIS:HB3	38:c:233:GLU:HG3	2.04	0.40
41:1:886:G:O2'	41:1:909:A:N6	2.55	0.40
41:1:1006:U:H2'	41:1:1007:U:C6	2.57	0.40
41:1:1368:G:O2'	41:1:1369:G:H5''	2.21	0.40
41:1:1764:A:H4'	41:1:1765:A:OP2	2.21	0.40
42:2:498:A:H61	42:2:511:C:N4	2.18	0.40
42:2:803:A:H2'	42:2:804:U:C6	2.56	0.40
45:B:283:LEU:HA	45:B:283:LEU:HD12	1.78	0.40
49:O:158:ARG:HG2	49:O:160:THR:HG23	2.03	0.40
57:E:170:ASP:HB3	57:E:173:LYS:HB2	2.02	0.40
62:D:64:ASN:N	62:D:64:ASN:HD22	2.17	0.40
72:U:16:GLN:HE22	72:U:57:LEU:HD12	1.86	0.40
13:SE:238:LYS:H	13:SE:238:LYS:HG2	1.60	0.40
16:Sg:201:THR:HG21	16:Sg:241:ILE:O	2.21	0.40
16:Sg:263:LEU:HD23	16:Sg:263:LEU:HA	1.85	0.40
20:S1:991:G:O6	29:SI:76:LYS:NZ	2.43	0.40
20:S1:2132:C:H2'	20:S1:2133:G:O4'	2.21	0.40
30:SH:5:THR:HA	30:SH:6:PRO:HD3	1.97	0.40
33:SA:32:VAL:HG22	33:SA:98:LEU:HD12	2.03	0.40
37:d:10:ASP:HA	37:d:13:ASN:ND2	2.34	0.40
39:a:53:LYS:HD3	39:a:53:LYS:HA	1.65	0.40
39:a:62:LEU:HD22	70:V:55:VAL:HG11	2.02	0.40
41:1:221:C:H42	41:1:232:G:H1	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1:301:A:H2'	41:1:302:G:O4'	2.22	0.40
41:1:736:C:O2'	41:1:737:U:OP2	2.30	0.40
47:5:85:G:H2'	47:5:86:U:C6	2.55	0.40
59:T:109:PRO:HA	59:T:112:MET:HG2	2.03	0.40
68:g:14:LEU:HD23	68:g:14:LEU:HA	1.74	0.40
76:X:58:THR:O	76:X:62:ILE:HG23	2.22	0.40
80:C:181:ARG:NH2	80:C:204:ARG:O	2.54	0.40
13:SE:84:MET:HE3	13:SE:84:MET:HB3	1.89	0.40
20:S1:2203:U:H5	33:SA:154:ARG:O	2.04	0.40
31:SG:5:ILE:HD12	31:SG:16:PHE:CD1	2.57	0.40
41:1:282:C:H2'	41:1:283:G:H5''	2.02	0.40
41:1:437:A2M:H8	41:1:437:A2M:O5'	2.20	0.40
41:1:465:A:H2'	41:1:466:U:O4'	2.22	0.40
65:Z:33:ASN:HD22	65:Z:35:ASN:H	1.68	0.40
82:e:25:ARG:O	82:e:28:ARG:N	2.55	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	SW	101/152 (66%)	97 (96%)	4 (4%)	0	100	100
2	SZ	121/137 (88%)	116 (96%)	5 (4%)	0	100	100
3	SY	81/164 (49%)	79 (98%)	2 (2%)	0	100	100
4	SX	137/161 (85%)	129 (94%)	8 (6%)	0	100	100
5	SV	109/143 (76%)	105 (96%)	4 (4%)	0	100	100
6	SU	146/173 (84%)	139 (95%)	7 (5%)	0	100	100
7	ST	139/151 (92%)	131 (94%)	8 (6%)	0	100	100
8	SS	53/57 (93%)	49 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	SR	117/153 (76%)	115 (98%)	2 (2%)	0	100	100
10	SB	207/246 (84%)	199 (96%)	8 (4%)	0	100	100
11	SC	212/219 (97%)	206 (97%)	6 (3%)	0	100	100
12	SD	181/190 (95%)	174 (96%)	7 (4%)	0	100	100
13	SE	260/273 (95%)	256 (98%)	4 (2%)	0	100	100
14	SK	176/220 (80%)	173 (98%)	3 (2%)	0	100	100
16	Sg	294/312 (94%)	269 (92%)	25 (8%)	0	100	100
17	Sa	69/120 (58%)	65 (94%)	4 (6%)	0	100	100
18	Sc	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
19	Se	48/66 (73%)	43 (90%)	5 (10%)	0	100	100
21	SQ	24/141 (17%)	24 (100%)	0	0	100	100
22	SP	143/143 (100%)	141 (99%)	2 (1%)	0	100	100
23	SO	135/144 (94%)	130 (96%)	5 (4%)	0	100	100
24	SN	99/168 (59%)	94 (95%)	5 (5%)	0	100	100
25	Sd	63/87 (72%)	57 (90%)	6 (10%)	0	100	100
26	SM	101/116 (87%)	99 (98%)	2 (2%)	0	100	100
27	SL	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
28	SJ	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
29	SI	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
30	SH	180/190 (95%)	175 (97%)	5 (3%)	0	100	100
31	SG	232/249 (93%)	229 (99%)	3 (1%)	0	100	100
32	SF	218/265 (82%)	214 (98%)	4 (2%)	0	100	100
33	SA	225/264 (85%)	224 (100%)	1 (0%)	0	100	100
34	Sb	98/112 (88%)	94 (96%)	4 (4%)	0	100	100
35	Sh	92/235 (39%)	85 (92%)	7 (8%)	0	100	100
36	f	120/133 (90%)	116 (97%)	4 (3%)	0	100	100
37	d	88/104 (85%)	85 (97%)	3 (3%)	0	100	100
38	c	225/252 (89%)	218 (97%)	7 (3%)	0	100	100
39	a	121/127 (95%)	115 (95%)	6 (5%)	0	100	100
40	b	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
45	B	407/419 (97%)	397 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	A	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
49	O	249/305 (82%)	235 (94%)	14 (6%)	0	100	100
50	G	233/264 (88%)	225 (97%)	8 (3%)	0	100	100
51	H	220/222 (99%)	219 (100%)	1 (0%)	0	100	100
52	M	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
53	I	203/220 (92%)	192 (95%)	11 (5%)	0	100	100
54	P	195/198 (98%)	188 (96%)	7 (4%)	0	100	100
55	Q	187/254 (74%)	184 (98%)	3 (2%)	0	100	100
56	R	176/179 (98%)	174 (99%)	2 (1%)	0	100	100
57	E	184/190 (97%)	174 (95%)	10 (5%)	0	100	100
59	T	151/166 (91%)	148 (98%)	3 (2%)	0	100	100
60	S	150/159 (94%)	143 (95%)	7 (5%)	0	100	100
61	K	151/175 (86%)	145 (96%)	6 (4%)	0	100	100
62	D	155/188 (82%)	146 (94%)	9 (6%)	0	100	100
63	L	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
64	Y	131/134 (98%)	128 (98%)	3 (2%)	0	100	100
65	Z	137/147 (93%)	134 (98%)	3 (2%)	0	100	100
66	F	138/195 (71%)	135 (98%)	3 (2%)	0	100	100
67	h	125/168 (74%)	119 (95%)	6 (5%)	0	100	100
68	g	136/144 (94%)	131 (96%)	4 (3%)	1 (1%)	18	24
69	J	127/139 (91%)	125 (98%)	2 (2%)	0	100	100
70	V	116/145 (80%)	114 (98%)	2 (2%)	0	100	100
71	W	116/143 (81%)	113 (97%)	3 (3%)	0	100	100
72	U	108/129 (84%)	105 (97%)	3 (3%)	0	100	100
73	i	91/105 (87%)	88 (97%)	3 (3%)	0	100	100
74	p	94/106 (89%)	81 (86%)	13 (14%)	0	100	100
75	o	88/92 (96%)	78 (89%)	10 (11%)	0	100	100
76	X	63/124 (51%)	61 (97%)	2 (3%)	0	100	100
77	k	71/83 (86%)	69 (97%)	2 (3%)	0	100	100
78	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
79	n	31/34 (91%)	28 (90%)	3 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	C	364/373 (98%)	354 (97%)	10 (3%)	0	100	100
82	e	169/188 (90%)	159 (94%)	9 (5%)	1 (1%)	21	27
83	j	78/83 (94%)	76 (97%)	2 (3%)	0	100	100
All	All	10720/12433 (86%)	10343 (96%)	375 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
82	e	47	LYS
68	g	20	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SW	74/130 (57%)	74 (100%)	0	100	100
2	SZ	100/118 (85%)	97 (97%)	3 (3%)	36	51
3	SY	63/116 (54%)	62 (98%)	1 (2%)	55	69
4	SX	107/131 (82%)	106 (99%)	1 (1%)	70	81
5	SV	83/126 (66%)	80 (96%)	3 (4%)	31	45
6	SU	121/152 (80%)	117 (97%)	4 (3%)	33	48
7	ST	122/132 (92%)	121 (99%)	1 (1%)	73	83
8	SS	42/49 (86%)	40 (95%)	2 (5%)	23	34
9	SR	86/130 (66%)	82 (95%)	4 (5%)	23	35
10	SB	175/202 (87%)	169 (97%)	6 (3%)	32	47
11	SC	168/184 (91%)	161 (96%)	7 (4%)	26	39
12	SD	160/164 (98%)	156 (98%)	4 (2%)	42	56
13	SE	215/225 (96%)	214 (100%)	1 (0%)	81	87
14	SK	138/176 (78%)	136 (99%)	2 (1%)	59	72
16	Sg	235/265 (89%)	220 (94%)	15 (6%)	16	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Sa	58/95 (61%)	54 (93%)	4 (7%)	14	19
18	Sc	68/76 (90%)	66 (97%)	2 (3%)	37	52
19	Se	40/54 (74%)	39 (98%)	1 (2%)	42	56
21	SQ	15/120 (12%)	15 (100%)	0	100	100
22	SP	114/117 (97%)	112 (98%)	2 (2%)	51	65
23	SO	101/113 (89%)	98 (97%)	3 (3%)	36	51
24	SN	85/128 (66%)	82 (96%)	3 (4%)	32	46
25	Sd	46/75 (61%)	43 (94%)	3 (6%)	15	21
26	SM	94/104 (90%)	90 (96%)	4 (4%)	26	38
27	SL	114/120 (95%)	112 (98%)	2 (2%)	51	65
28	SJ	108/111 (97%)	106 (98%)	2 (2%)	50	64
29	SI	174/186 (94%)	167 (96%)	7 (4%)	28	41
30	SH	150/159 (94%)	146 (97%)	4 (3%)	39	54
31	SG	180/208 (86%)	177 (98%)	3 (2%)	53	67
32	SF	170/208 (82%)	165 (97%)	5 (3%)	37	52
33	SA	198/222 (89%)	192 (97%)	6 (3%)	36	51
34	Sb	80/93 (86%)	80 (100%)	0	100	100
35	Sh	59/177 (33%)	54 (92%)	5 (8%)	10	11
36	f	104/115 (90%)	102 (98%)	2 (2%)	50	64
37	d	60/89 (67%)	58 (97%)	2 (3%)	33	48
38	c	174/209 (83%)	170 (98%)	4 (2%)	44	59
39	a	93/118 (79%)	90 (97%)	3 (3%)	34	49
40	b	52/58 (90%)	51 (98%)	1 (2%)	50	64
45	B	331/351 (94%)	322 (97%)	9 (3%)	39	54
48	A	202/204 (99%)	198 (98%)	4 (2%)	48	63
49	O	191/242 (79%)	184 (96%)	7 (4%)	30	44
50	G	192/221 (87%)	187 (97%)	5 (3%)	40	55
51	H	183/188 (97%)	182 (100%)	1 (0%)	81	87
52	M	179/180 (99%)	176 (98%)	3 (2%)	53	67
53	I	165/183 (90%)	158 (96%)	7 (4%)	26	39
54	P	163/164 (99%)	161 (99%)	2 (1%)	63	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	Q	138/198 (70%)	136 (99%)	2 (1%)	59	72
56	R	155/159 (98%)	147 (95%)	8 (5%)	21	30
57	E	157/172 (91%)	144 (92%)	13 (8%)	10	12
59	T	131/143 (92%)	129 (98%)	2 (2%)	57	70
60	S	125/134 (93%)	123 (98%)	2 (2%)	55	69
61	K	121/145 (83%)	115 (95%)	6 (5%)	22	32
62	D	104/162 (64%)	96 (92%)	8 (8%)	12	15
63	L	113/114 (99%)	110 (97%)	3 (3%)	39	54
64	Y	106/116 (91%)	105 (99%)	1 (1%)	70	81
65	Z	106/118 (90%)	103 (97%)	3 (3%)	38	54
66	F	103/153 (67%)	100 (97%)	3 (3%)	37	52
67	h	105/146 (72%)	102 (97%)	3 (3%)	37	52
68	g	112/121 (93%)	107 (96%)	5 (4%)	24	37
69	J	102/111 (92%)	98 (96%)	4 (4%)	28	42
70	V	100/124 (81%)	98 (98%)	2 (2%)	48	63
71	W	102/122 (84%)	99 (97%)	3 (3%)	37	52
72	U	88/114 (77%)	79 (90%)	9 (10%)	7	6
73	i	75/88 (85%)	73 (97%)	2 (3%)	39	54
74	p	66/92 (72%)	64 (97%)	2 (3%)	36	51
75	o	70/74 (95%)	65 (93%)	5 (7%)	13	18
76	X	58/104 (56%)	55 (95%)	3 (5%)	21	30
77	k	56/74 (76%)	50 (89%)	6 (11%)	6	6
78	l	44/47 (94%)	44 (100%)	0	100	100
79	n	24/32 (75%)	22 (92%)	2 (8%)	10	12
80	C	287/301 (95%)	278 (97%)	9 (3%)	35	50
82	e	128/158 (81%)	118 (92%)	10 (8%)	11	14
83	j	67/70 (96%)	66 (98%)	1 (2%)	57	70
All	All	8675/10380 (84%)	8398 (97%)	277 (3%)	35	49

All (277) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SZ	22	LEU

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Mol	Chain	Res	Type
2	SZ	56	VAL
2	SZ	123	LYS
3	SY	40	SER
4	SX	98	LEU
5	SV	7	LYS
5	SV	15	GLN
5	SV	106	MET
6	SU	41	VAL
6	SU	101	ILE
6	SU	121	SER
6	SU	127	SER
7	ST	87	ASP
8	SS	26	SER
8	SS	37	LEU
9	SR	5	LEU
9	SR	14	VAL
9	SR	32	ARG
9	SR	44	LEU
10	SB	10	VAL
10	SB	84	LEU
10	SB	132	THR
10	SB	171	ILE
10	SB	177	MET
10	SB	203	ASP
11	SC	43	LEU
11	SC	58	LEU
11	SC	66[A]	ARG
11	SC	66[B]	ARG
11	SC	92	VAL
11	SC	101	VAL
11	SC	108	LEU
12	SD	73	SER
12	SD	117	LEU
12	SD	151	SER
12	SD	168	THR
13	SE	98	LEU
14	SK	37	ARG
14	SK	77	ARG
16	Sg	2	ASN
16	Sg	10	HIS
16	Sg	127	ARG
16	Sg	166	ILE

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Mol	Chain	Res	Type
16	Sg	167	VAL
16	Sg	178	VAL
16	Sg	181	VAL
16	Sg	188	ARG
16	Sg	189	THR
16	Sg	193	HIS
16	Sg	199	THR
16	Sg	209	CYS
16	Sg	269	ILE
16	Sg	294	LEU
16	Sg	302	LEU
17	Sa	42	PHE
17	Sa	59	LEU
17	Sa	61	THR
17	Sa	100	VAL
18	Sc	13	VAL
18	Sc	75	VAL
19	Se	8	LEU
22	SP	105	PHE
22	SP	138	LYS
23	SO	84	ASN
23	SO	89	LYS
23	SO	90	MET
24	SN	30	MET
24	SN	32	THR
24	SN	89	LEU
25	Sd	30	LEU
25	Sd	41	GLN
25	Sd	44	VAL
26	SM	29	VAL
26	SM	45	VAL
26	SM	76	THR
26	SM	105	SER
27	SL	28	THR
27	SL	75	VAL
28	SJ	30	SER
28	SJ	118	SER
29	SI	5	LEU
29	SI	22	SER
29	SI	33	SER
29	SI	46	VAL
29	SI	94	VAL

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Mol	Chain	Res	Type
29	SI	118	SER
29	SI	198	SER
30	SH	2	SER
30	SH	44	LYS
30	SH	64	PHE
30	SH	161	ASP
31	SG	130	THR
31	SG	131	THR
31	SG	202	VAL
32	SF	61	THR
32	SF	79	VAL
32	SF	158	ASN
32	SF	245	THR
32	SF	262	MET
33	SA	51	THR
33	SA	81	GLU
33	SA	109	THR
33	SA	153	SER
33	SA	188	SER
33	SA	217	VAL
35	Sh	134	ASN
35	Sh	138	VAL
35	Sh	149	THR
35	Sh	191	ASN
35	Sh	196	ARG
36	f	5	THR
36	f	56	LYS
37	d	11	THR
37	d	50	CYS
38	c	87	LEU
38	c	141	GLU
38	c	227	LYS
38	c	242	THR
39	a	4	HIS
39	a	5	MET
39	a	104	LYS
40	b	21	ILE
45	B	5	LYS
45	B	67	VAL
45	B	79	LEU
45	B	199	LEU
45	B	217	SER

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Mol	Chain	Res	Type
45	B	249[A]	ARG
45	B	249[B]	ARG
45	B	264[A]	ARG
45	B	264[B]	ARG
48	A	23[A]	ARG
48	A	23[B]	ARG
48	A	28	LYS
48	A	93	LYS
49	O	73	GLU
49	O	93	THR
49	O	118	LYS
49	O	128	SER
49	O	132	VAL
49	O	233	SER
49	O	264	LEU
50	G	26	SER
50	G	84	ASP
50	G	203	ASP
50	G	211	THR
50	G	219	VAL
51	H	177	LYS
52	M	29	GLU
52	M	46	GLU
52	M	60	CYS
53	I	27	VAL
53	I	46	LEU
53	I	138	VAL
53	I	167	VAL
53	I	178	SER
53	I	183	SER
53	I	202	THR
54	P	42	SER
54	P	89	VAL
55	Q	150	LYS
55	Q	179	LYS
56	R	65	VAL
56	R	66	VAL
56	R	87	CYS
56	R	93	VAL
56	R	98	ASP
56	R	128	VAL
56	R	158	THR

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Mol	Chain	Res	Type
56	R	173	THR
57	E	6	SER
57	E	9	THR
57	E	17	THR
57	E	20	VAL
57	E	39	THR
57	E	93	CYS
57	E	95	TYR
57	E	125	VAL
57	E	128	THR
57	E	131	VAL
57	E	166	VAL
57	E	180	VAL
57	E	184	THR
59	T	11	SER
59	T	93	SER
60	S	46	SER
60	S	145	VAL
61	K	2	LYS
61	K	38	GLU
61	K	64	VAL
61	K	79	SER
61	K	114	VAL
61	K	136	VAL
62	D	19	LEU
62	D	89	LYS
62	D	124	ILE
62	D	127	MET
62	D	145	ARG
62	D	150	VAL
62	D	162	MET
62	D	175	GLN
63	L	15	THR
63	L	79	SER
63	L	117	VAL
64	Y	100	SER
65	Z	40	LYS
65	Z	54	LYS
65	Z	62	CYS
66	F	84	VAL
66	F	91	VAL
66	F	147	SER

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Mol	Chain	Res	Type
67	h	20	ARG
67	h	24	VAL
67	h	127	SER
68	g	14	LEU
68	g	18	SER
68	g	63	THR
68	g	75	VAL
68	g	116	MET
69	J	111	MET
69	J	120	VAL
69	J	132	SER
69	J	133	THR
70	V	66	ILE
70	V	105	LEU
71	W	5	LYS
71	W	74	LYS
71	W	91	THR
72	U	24	LYS
72	U	44	LEU
72	U	71	SER
72	U	75	ASN
72	U	76	VAL
72	U	81	THR
72	U	82	THR
72	U	105	ASP
72	U	109	ILE
73	i	31	ASP
73	i	51	VAL
74	p	24	LYS
74	p	77	CYS
75	o	5	THR
75	o	10	VAL
75	o	21	ASN
75	o	29	LEU
75	o	61	SER
76	X	22	VAL
76	X	32	VAL
76	X	36	SER
77	k	12	LEU
77	k	15	CYS
77	k	23	VAL
77	k	47	VAL

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Mol	Chain	Res	Type
77	k	73	SER
77	k	74	HIS
79	n	4	VAL
79	n	10	MET
80	C	68	THR
80	C	107	PHE
80	C	134	SER
80	C	142	GLN
80	C	156	SER
80	C	176	ILE
80	C	321	LYS
80	C	337	THR
80	C	346	VAL
82	e	14	ILE
82	e	23	GLU
82	e	32	ARG
82	e	46	LYS
82	e	47	LYS
82	e	51	VAL
82	e	54	THR
82	e	88	SER
82	e	114	LEU
82	e	172	SER
83	j	80	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (227) such sidechains are listed below:

Mol	Chain	Res	Type
1	SW	45	HIS
1	SW	108	GLN
1	SW	110	ASN
1	SW	121	HIS
2	SZ	34	HIS
2	SZ	95	ASN
2	SZ	119	ASN
3	SY	34	HIS
4	SX	80	GLN
4	SX	116	ASN
4	SX	153	GLN
5	SV	31	ASN
6	SU	11	HIS
6	SU	24	GLN

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Mol	Chain	Res	Type
6	SU	26	GLN
6	SU	30	ASN
6	SU	91	HIS
6	SU	104	ASN
6	SU	107	HIS
6	SU	116	GLN
6	SU	134	GLN
6	SU	142	GLN
7	ST	49	GLN
7	ST	65	ASN
7	ST	134	GLN
9	SR	98	HIS
10	SB	33	GLN
10	SB	95	GLN
10	SB	102	HIS
11	SC	144	GLN
12	SD	65	HIS
12	SD	122	HIS
12	SD	138	GLN
13	SE	64	GLN
13	SE	71	ASN
13	SE	72	HIS
13	SE	185	ASN
13	SE	203	ASN
13	SE	231	ASN
13	SE	239	GLN
13	SE	240	GLN
14	SK	52	ASN
14	SK	169	HIS
14	SK	178	GLN
16	Sg	10	HIS
16	Sg	44	ASN
16	Sg	58	ASN
16	Sg	64	HIS
16	Sg	106	HIS
16	Sg	129	ASN
16	Sg	182	ASN
17	Sa	82	GLN
19	Se	17	GLN
19	Se	60	GLN
22	SP	20	ASN
22	SP	39	ASN

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Mol	Chain	Res	Type
22	SP	97	ASN
22	SP	127	ASN
23	SO	36	HIS
24	SN	12	ASN
24	SN	40	ASN
24	SN	48	GLN
24	SN	51	GLN
24	SN	70	HIS
24	SN	96	ASN
27	SL	32	GLN
27	SL	43	GLN
27	SL	76	HIS
27	SL	89	GLN
28	SJ	42	GLN
28	SJ	70	ASN
28	SJ	98	GLN
28	SJ	120	ASN
29	SI	99	GLN
29	SI	101	GLN
30	SH	134	ASN
30	SH	172	ASN
30	SH	189	ASN
31	SG	15	GLN
31	SG	27	GLN
31	SG	35	ASN
31	SG	86	ASN
31	SG	113	ASN
32	SF	76	HIS
32	SF	122	HIS
32	SF	158	ASN
32	SF	255	HIS
33	SA	97	ASN
33	SA	228	GLN
33	SA	245	GLN
34	Sb	27	ASN
35	Sh	220	ASN
36	f	21	HIS
37	d	13	ASN
37	d	38	GLN
37	d	75	ASN
37	d	96	ASN
38	c	176	ASN

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Mol	Chain	Res	Type
38	c	177	GLN
38	c	184	ASN
39	a	69	ASN
39	a	93	HIS
39	a	102	ASN
39	a	105	ASN
40	b	28	HIS
40	b	31	ASN
45	B	94	GLN
45	B	135	GLN
45	B	151	ASN
45	B	167	GLN
45	B	174	HIS
45	B	289	GLN
45	B	326	ASN
48	A	17	GLN
48	A	139	HIS
48	A	140	ASN
48	A	194	ASN
48	A	205	ASN
48	A	216	HIS
48	A	218	HIS
49	O	63	GLN
49	O	184	ASN
50	G	39	GLN
50	G	169	ASN
50	G	174	ASN
50	G	205	ASN
50	G	238	GLN
51	H	44	GLN
51	H	68	ASN
51	H	74	GLN
51	H	90	HIS
51	H	118	ASN
51	H	159	ASN
51	H	212	ASN
52	M	8	ASN
52	M	99	GLN
52	M	112	ASN
52	M	171	HIS
53	I	36	GLN
53	I	93	GLN

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Mol	Chain	Res	Type
53	I	153	GLN
54	P	17	HIS
54	P	18	HIS
54	P	132	GLN
55	Q	27	ASN
55	Q	33	GLN
55	Q	75	HIS
55	Q	137	ASN
55	Q	143	HIS
56	R	85	GLN
56	R	116	HIS
56	R	121	HIS
56	R	143	GLN
56	R	145	HIS
56	R	148	ASN
57	E	42	GLN
57	E	133	GLN
57	E	152	GLN
59	T	110	ASN
59	T	147	GLN
60	S	33	ASN
60	S	110	HIS
60	S	111	GLN
61	K	51	ASN
62	D	45	GLN
62	D	64	ASN
62	D	97	ASN
62	D	142	HIS
63	L	11	GLN
63	L	25	HIS
63	L	62	HIS
63	L	77	ASN
63	L	102	GLN
63	L	116	GLN
64	Y	21	HIS
64	Y	28	ASN
64	Y	76	ASN
64	Y	77	HIS
65	Z	33	ASN
65	Z	71	ASN
65	Z	76	GLN
66	F	154	GLN

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Mol	Chain	Res	Type
66	F	191	HIS
67	h	7	GLN
67	h	13	HIS
67	h	19	ASN
67	h	51	HIS
67	h	87	GLN
67	h	101	GLN
67	h	111	HIS
68	g	16	GLN
68	g	25	ASN
68	g	111	HIS
68	g	122	ASN
68	g	143	GLN
70	V	34	GLN
70	V	39	HIS
70	V	51	ASN
70	V	133	HIS
70	V	140	ASN
72	U	16	GLN
72	U	54	ASN
72	U	58	ASN
72	U	118	GLN
73	i	15	ASN
73	i	18	HIS
73	i	39	HIS
73	i	61	GLN
74	p	3	ASN
75	o	21	ASN
75	o	33	GLN
75	o	34	HIS
75	o	75	ASN
76	X	63	HIS
78	l	18	ASN
78	l	19	GLN
78	l	33	ASN
78	l	43	HIS
80	C	142	GLN
80	C	183	ASN
80	C	292	GLN
82	e	39	ASN
82	e	127	ASN
82	e	147	GLN

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Mol	Chain	Res	Type
83	j	28	HIS
83	j	30	GLN
83	j	76	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	S4	17/19 (89%)	6 (35%)	0
20	S1	1702/2204 (77%)	357 (20%)	15 (0%)
41	1	1564/1782 (87%)	318 (20%)	24 (1%)
42	2	1036/1526 (67%)	217 (20%)	17 (1%)
43	4	182/183 (99%)	35 (19%)	2 (1%)
44	7	157/171 (91%)	24 (15%)	0
46	8	116/123 (94%)	13 (11%)	1 (0%)
47	5	107/135 (79%)	26 (24%)	3 (2%)
58	6	70/73 (95%)	29 (41%)	5 (7%)
81	3	156/216 (72%)	33 (21%)	3 (1%)
All	All	5107/6432 (79%)	1058 (20%)	70 (1%)

All (1058) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	S4	2	C
15	S4	5	G
15	S4	7	A
15	S4	69	G
15	S4	70	C
15	S4	76	A
20	S1	2	A
20	S1	3	U
20	S1	17	C
20	S1	26	A
20	S1	32	U
20	S1	33	PSU
20	S1	34	G
20	S1	42	G
20	S1	45	U
20	S1	47	A
20	S1	59	C
20	S1	78	C
20	S1	80	G

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Mol	Chain	Res	Type
20	S1	81	G
20	S1	98	A2M
20	S1	101	A
20	S1	102	C
20	S1	112	A
20	S1	117	G
20	S1	128	C
20	S1	145	A
20	S1	146	U
20	S1	152	A
20	S1	158	G
20	S1	165	G
20	S1	171	C
20	S1	173	A
20	S1	174	A
20	S1	176	A
20	S1	181	A
20	S1	193	G
20	S1	197	U
20	S1	198	C
20	S1	232	C
20	S1	234	C
20	S1	235	C
20	S1	236	C
20	S1	238	G
20	S1	249	A
20	S1	252	G
20	S1	253	U
20	S1	254	A
20	S1	275	A
20	S1	276	G
20	S1	278	A
20	S1	281	A
20	S1	284	C
20	S1	285	A
20	S1	286	G
20	S1	287	C
20	S1	288	A
20	S1	308	C
20	S1	315	A
20	S1	316	A
20	S1	317	G

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Mol	Chain	Res	Type
20	S1	339	U
20	S1	343	G
20	S1	356	A
20	S1	358	C
20	S1	360	G
20	S1	364	G
20	S1	365	U
20	S1	381	G
20	S1	382	A
20	S1	404	C
20	S1	423	U
20	S1	443	A
20	S1	444	A
20	S1	445	U
20	S1	447	G
20	S1	459	A
20	S1	462	G
20	S1	464	G
20	S1	467	C
20	S1	469	G
20	S1	471	A
20	S1	477	G
20	S1	481	A
20	S1	482	U
20	S1	483	U
20	S1	487	C
20	S1	488	A
20	S1	495	A
20	S1	496	A
20	S1	497	A
20	S1	501	A
20	S1	503	C
20	S1	507	G
20	S1	512	A2M
20	S1	516	A
20	S1	523	A
20	S1	553	U
20	S1	555	C
20	S1	565	U
20	S1	566	A
20	S1	586	G
20	S1	588	G

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Mol	Chain	Res	Type
20	S1	589	U
20	S1	591	A
20	S1	600	OMG
20	S1	606	G
20	S1	607	PSU
20	S1	608	C
20	S1	614	C
20	S1	626	G
20	S1	628	A
20	S1	631	U
20	S1	643	A
20	S1	660	U
20	S1	664	U
20	S1	668	A2M
20	S1	669	A
20	S1	671	G
20	S1	672	G
20	S1	673	G
20	S1	688	G
20	S1	689	U
20	S1	690	G
20	S1	693	C
20	S1	746	C
20	S1	750	U
20	S1	752	C
20	S1	753	A
20	S1	757	C
20	S1	758	G
20	S1	778	G
20	S1	779	A
20	S1	782	C
20	S1	783	A
20	S1	785	G
20	S1	787	G
20	S1	788	A
20	S1	789	G
20	S1	790	U
20	S1	791	G
20	S1	792	G
20	S1	811	C
20	S1	815	U
20	S1	816	C

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Mol	Chain	Res	Type
20	S1	819	G
20	S1	820	C
20	S1	821	A
20	S1	834	U
20	S1	839	G
20	S1	842	U
20	S1	843	U
20	S1	856	A
20	S1	863	C
20	S1	866	G
20	S1	867	A
20	S1	875	A
20	S1	876	G
20	S1	883	G
20	S1	884	A
20	S1	886	U
20	S1	887	U
20	S1	894	G
20	S1	895	A
20	S1	897	A2M
20	S1	903	G
20	S1	905	A
20	S1	914	G
20	S1	916	G
20	S1	917	C
20	S1	955	A
20	S1	957	G
20	S1	965	G
20	S1	970	U
20	S1	972	A
20	S1	973	U
20	S1	974	G
20	S1	977	G
20	S1	978	C
20	S1	990	U
20	S1	991	G
20	S1	992	C
20	S1	993	U
20	S1	994	U
20	S1	1101	A
20	S1	1102	G
20	S1	1105	A

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Mol	Chain	Res	Type
20	S1	1109	A
20	S1	1119	U
20	S1	1123	G
20	S1	1129	A
20	S1	1133	U
20	S1	1139	G
20	S1	1142	G
20	S1	1146	G
20	S1	1155	U
20	S1	1168	C
20	S1	1180	A
20	S1	1189	G
20	S1	1191	A
20	S1	1192	PSU
20	S1	1199	A
20	S1	1207	U
20	S1	1213	A
20	S1	1235	A
20	S1	1239	A
20	S1	1245	A
20	S1	1246	PSU
20	S1	1252	A
20	S1	1273	A
20	S1	1275	C
20	S1	1279	G
20	S1	1287	U
20	S1	1289	A
20	S1	1427	U
20	S1	1431	A
20	S1	1432	C
20	S1	1442	U
20	S1	1443	U
20	S1	1444	G
20	S1	1449	U
20	S1	1452	A
20	S1	1466	G
20	S1	1490	A
20	S1	1498	G
20	S1	1502	G
20	S1	1503	A
20	S1	1510	C
20	S1	1511	C

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Mol	Chain	Res	Type
20	S1	1519	G
20	S1	1537	U
20	S1	1543	C4J
20	S1	1544	5MC
20	S1	1546	A
20	S1	1548	A
20	S1	1551	G
20	S1	1552	G
20	S1	1554	A
20	S1	1565	A
20	S1	1567	C
20	S1	1568	C
20	S1	1569	G
20	S1	1570	G
20	S1	1573	A
20	S1	1574	G
20	S1	1578	G
20	S1	1579	A
20	S1	1580	G
20	S1	1589	G
20	S1	1595	G
20	S1	1597	G
20	S1	1598	U
20	S1	1606	C
20	S1	1607	G
20	S1	1608	A
20	S1	1611	C
20	S1	1612	C
20	S1	1613	C
20	S1	1616	A
20	S1	1622	G
20	S1	1636	U
20	S1	1637	U
20	S1	1643	G
20	S1	1653	U
20	S1	1657	PSU
20	S1	1658	U
20	S1	1666	U
20	S1	1667	U
20	S1	1670	G
20	S1	1673	A
20	S1	1677	G

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Mol	Chain	Res	Type
20	S1	1700	G
20	S1	1705	C
20	S1	1706	A
20	S1	1767	G
20	S1	1771	A
20	S1	1775	C
20	S1	1782	G
20	S1	1789	U
20	S1	1795	G
20	S1	1796	U
20	S1	1797	A
20	S1	1801	G
20	S1	1807	G
20	S1	1816	U
20	S1	1822	A
20	S1	1825	A
20	S1	1828	A
20	S1	1829	OMG
20	S1	1833	OMU
20	S1	1834	G
20	S1	1836	G
20	S1	1837	A
20	S1	1847	A
20	S1	1848	U
20	S1	1872	A
20	S1	1875	G
20	S1	1890	A
20	S1	1891	A
20	S1	1907	A
20	S1	1909	C
20	S1	1915	U
20	S1	1919	C
20	S1	1920	A
20	S1	1921	A
20	S1	1922	A
20	S1	1923	A
20	S1	1924	G
20	S1	1928	G
20	S1	1931	G
20	S1	1932	A
20	S1	1933	A
20	S1	1938	C

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Mol	Chain	Res	Type
20	S1	1944	C
20	S1	1948	U
20	S1	1950	G
20	S1	1955	A
20	S1	1956	C
20	S1	1976	U
20	S1	1977	U
20	S1	1978	A
20	S1	1979	OMU
20	S1	1984	C
20	S1	1988	C
20	S1	1995	G7M
20	S1	2004	G
20	S1	2010	G
20	S1	2012	A
20	S1	2021	A2M
20	S1	2027	G
20	S1	2053	A
20	S1	2054	C
20	S1	2055	A
20	S1	2057	C
20	S1	2058	G
20	S1	2065	G
20	S1	2066	U
20	S1	2069	U
20	S1	2086	A
20	S1	2097	C
20	S1	2099	G
20	S1	2100	A
20	S1	2102	A
20	S1	2104	G
20	S1	2105	C
20	S1	2157	A
20	S1	2160	G
20	S1	2163	G
20	S1	2165	A
20	S1	2169	A
20	S1	2170	G
20	S1	2172	U
20	S1	2173	A
20	S1	2183	G
20	S1	2185	MA6

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Mol	Chain	Res	Type
20	S1	2186	C
20	S1	2195	G
20	S1	2196	G
20	S1	2197	A
20	S1	2198	U
20	S1	2199	C
20	S1	2202	PSU
20	S1	2203	U
41	1	24	A
41	1	38	A
41	1	41	A
41	1	47	C
41	1	58	A
41	1	64	A
41	1	84	G
41	1	86	G
41	1	87	A
41	1	91	G
41	1	92	C
41	1	98	A
41	1	110	A
41	1	131	U
41	1	134	A
41	1	135	A
41	1	136	G
41	1	141	U
41	1	142	A
41	1	154	A
41	1	155	A
41	1	156	A
41	1	158	A
41	1	159	U
41	1	161	A
41	1	162	U
41	1	163	U
41	1	164	U
41	1	165	C
41	1	171	U
41	1	175	G
41	1	189	A
41	1	191	U
41	1	192	C

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Mol	Chain	Res	Type
41	1	205	A
41	1	206	A
41	1	210	G
41	1	212	U
41	1	214	C
41	1	216	G
41	1	217	A
41	1	218	A
41	1	219	U
41	1	223	A
41	1	230	A
41	1	231	U
41	1	233	U
41	1	234	G
41	1	239	PSU
41	1	249	G
41	1	250	A
41	1	251	A
41	1	255	G
41	1	256	U
41	1	258	A
41	1	266	G
41	1	273	A
41	1	279	G
41	1	280	A
41	1	281	G
41	1	283	G
41	1	290	G
41	1	291	A
41	1	292	A
41	1	301	A
41	1	305	A
41	1	306	G
41	1	307	U
41	1	323	U
41	1	332	A
41	1	335	U
41	1	336	U
41	1	337	G
41	1	341	G
41	1	343	U
41	1	361	A

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Mol	Chain	Res	Type
41	1	367	A
41	1	368	G
41	1	369	A
41	1	374	G
41	1	383	U
41	1	390	C
41	1	391	A
41	1	392	A
41	1	409	U
41	1	410	U
41	1	417	G
41	1	440	A
41	1	443	A
41	1	444	C
41	1	461	G
41	1	462	A
41	1	463	C
41	1	464	A
41	1	477	C
41	1	482	U
41	1	483	C
41	1	485	A
41	1	486	G
41	1	487	A
41	1	488	G
41	1	501	C
41	1	503	A
41	1	506	G
41	1	521	G
41	1	523	G
41	1	526	A
41	1	528	A
41	1	536	G
41	1	538	G
41	1	542	C
41	1	543	G
41	1	544	A
41	1	545	A
41	1	546	G
41	1	547	U
41	1	548	G
41	1	551	A

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Mol	Chain	Res	Type
41	1	563	C
41	1	564	U
41	1	567	G
41	1	569	G
41	1	570	A
41	1	571	A
41	1	572	A
41	1	575	A
41	1	582	U
41	1	583	A
41	1	586	U
41	1	591	U
41	1	592	G
41	1	599	G
41	1	610	A
41	1	611	C
41	1	612	G
41	1	624	U
41	1	625	C
41	1	631	G
41	1	632	A
41	1	633	U
41	1	634	G
41	1	641	G
41	1	651	G
41	1	652	A
41	1	668	C
41	1	681	A2M
41	1	692	A
41	1	709	A
41	1	713	A
41	1	728	C
41	1	729	A
41	1	735	U
41	1	736	C
41	1	737	U
41	1	750	G
41	1	753	A
41	1	754	G
41	1	761	A
41	1	763	U
41	1	767	U

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Mol	Chain	Res	Type
41	1	769	U
41	1	771	U
41	1	788	A
41	1	789	U
41	1	790	C
41	1	791	C
41	1	792	G
41	1	793	U
41	1	803	C
41	1	818	C
41	1	821	C
41	1	822	C
41	1	823	G
41	1	824	U
41	1	832	G
41	1	836	G
41	1	838	G
41	1	850	G
41	1	868	A
41	1	880	C
41	1	886	G
41	1	912	C
41	1	925	U
41	1	930	U
41	1	959	OMG
41	1	960	A
41	1	965	A
41	1	967	G
41	1	968	A
41	1	972	A
41	1	975	G
41	1	976	A
41	1	983	U
41	1	984	A
41	1	988	G
41	1	995	C
41	1	1010	C
41	1	1011	PSU
41	1	1012	C
41	1	1029	G
41	1	1031	A
41	1	1045	G

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Mol	Chain	Res	Type
41	1	1102	U
41	1	1105	A
41	1	1108	G
41	1	1114	A
41	1	1116	A
41	1	1118	A
41	1	1128	A
41	1	1134	C
41	1	1135	U
41	1	1148	A
41	1	1150	A
41	1	1156	A
41	1	1159	A
41	1	1165	A
41	1	1174	G
41	1	1181	PSU
41	1	1188	G
41	1	1210	A
41	1	1216	U
41	1	1235	A
41	1	1239	U
41	1	1242	U
41	1	1243	G
41	1	1249	A
41	1	1250	U
41	1	1251	U
41	1	1252	C
41	1	1253	U
41	1	1254	C
41	1	1257	U
41	1	1261	U
41	1	1265	A
41	1	1269	G
41	1	1270	U
41	1	1271	G
41	1	1275	G
41	1	1278	G
41	1	1352	C
41	1	1353	A
41	1	1354	C
41	1	1364	A
41	1	1369	G

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Mol	Chain	Res	Type
41	1	1370	A
41	1	1371	OMU
41	1	1375	G
41	1	1378	U
41	1	1379	A
41	1	1380	A
41	1	1389	A
41	1	1390	G
41	1	1392	G
41	1	1393	A
41	1	1394	A
41	1	1395	U
41	1	1401	U
41	1	1412	G
41	1	1413	U
41	1	1414	A
41	1	1420	G
41	1	1421	G
41	1	1422	A
41	1	1435	A
41	1	1438	A
41	1	1445	G
41	1	1453	G
41	1	1464	G
41	1	1490	G
41	1	1504	A
41	1	1509	C
41	1	1524	OMG
41	1	1527	OMC
41	1	1536	C
41	1	1540	OMG
41	1	1543	A
41	1	1545	G
41	1	1557	A
41	1	1559	A
41	1	1560	U
41	1	1561	A
41	1	1564	C
41	1	1586	G
41	1	1590	G
41	1	1605	G
41	1	1613	C

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Mol	Chain	Res	Type
41	1	1625	A
41	1	1654	A
41	1	1655	U
41	1	1661	U
41	1	1662	G
41	1	1663	U
41	1	1666	G
41	1	1667	G
41	1	1669	A
41	1	1671	G
41	1	1672	U
41	1	1673	G
41	1	1675	A
41	1	1723	A
41	1	1726	G
41	1	1727	A
41	1	1728	A
41	1	1730	A
41	1	1738	C
41	1	1739	A
41	1	1744	A
41	1	1747	U
41	1	1753	U
41	1	1761	A
41	1	1762	A
41	1	1763	A
41	1	1764	A
41	1	1766	G
41	1	1774	A
41	1	1775	U
41	1	1779	G
41	1	1780	G
42	2	7	C
42	2	22	A
42	2	25	A
42	2	33	A
42	2	61	C
42	2	63	U
42	2	68	A
42	2	69	A
42	2	75	A
42	2	78	PSU

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Mol	Chain	Res	Type
42	2	90	G
42	2	91	C
42	2	118	G
42	2	135	A
42	2	136	A
42	2	338	C
42	2	339	A
42	2	340	A
42	2	342	U
42	2	343	U
42	2	349	C
42	2	368	G
42	2	377	A
42	2	380	G
42	2	386	U
42	2	388	A
42	2	390	A
42	2	404	A
42	2	443	OMC
42	2	444	A
42	2	453	A
42	2	454	A
42	2	455	U
42	2	456	G
42	2	485	G
42	2	490	A
42	2	492	G
42	2	495	G
42	2	496	G
42	2	497	G
42	2	498	A
42	2	499	G
42	2	500	PSU
42	2	501	A
42	2	502	A
42	2	505	A
42	2	506	PSU
42	2	507	G
42	2	508	A
42	2	509	C
42	2	513	C
42	2	518	G

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Mol	Chain	Res	Type
42	2	519	G
42	2	520	U
42	2	526	A
42	2	527	A2M
42	2	529	G
42	2	530	C
42	2	534	OMG
42	2	544	U
42	2	552	C
42	2	553	G
42	2	554	C
42	2	556	U
42	2	559	A
42	2	561	G
42	2	571	G
42	2	580	U
42	2	582	U
42	2	602	A
42	2	618	A
42	2	620	C
42	2	621	G
42	2	639	G
42	2	643	A
42	2	647	A
42	2	648	A
42	2	649	G
42	2	650	A
42	2	657	U
42	2	658	G
42	2	665	A2M
42	2	685	G
42	2	688	G
42	2	690	C
42	2	750	U
42	2	760	U
42	2	761	A
42	2	769	A
42	2	774	A
42	2	777	A
42	2	780	G
42	2	781	G
42	2	784	U

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Mol	Chain	Res	Type
42	2	785	U
42	2	786	A
42	2	797	C
42	2	798	G
42	2	810	G
42	2	811	U
42	2	814	A
42	2	960	C
42	2	964	G
42	2	968	U
42	2	969	A
42	2	970	A
42	2	972	C
42	2	979	A
42	2	982	G
42	2	983	G
42	2	985	A
42	2	986	U
42	2	1011	G
42	2	1012	U
42	2	1019	A
42	2	1022	U
42	2	1030	A
42	2	1033	G
42	2	1034	G
42	2	1041	G
42	2	1046	OMG
42	2	1055	A
42	2	1064	A
42	2	1075	G
42	2	1079	U
42	2	1083	A
42	2	1101	A
42	2	1116	A
42	2	1118	A
42	2	1121	A
42	2	1123	A
42	2	1126	C
42	2	1131	A
42	2	1132	A
42	2	1146	A
42	2	1147	C

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Mol	Chain	Res	Type
42	2	1156	G
42	2	1157	U
42	2	1165	G
42	2	1180	A
42	2	1181	G
42	2	1189	A
42	2	1215	A
42	2	1234	G
42	2	1237	A
42	2	1238	G
42	2	1239	A
42	2	1241	U
42	2	1248	OMC
42	2	1252	G
42	2	1255	A
42	2	1265	PSU
42	2	1267	U
42	2	1270	C
42	2	1271	G
42	2	1272	G
42	2	1273	C
42	2	1274	C
42	2	1275	A
42	2	1301	G
42	2	1303	PSU
42	2	1305	C
42	2	1308	5MC
42	2	1309	G
42	2	1314	C
42	2	1325	A
42	2	1327	C
42	2	1332	C
42	2	1373	C
42	2	1374	A
42	2	1380	C
42	2	1385	G
42	2	1389	G
42	2	1403	PSU
42	2	1409	A
42	2	1416	U
42	2	1421	C
42	2	1428	U

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Mol	Chain	Res	Type
42	2	1433	G
42	2	1436	A
42	2	1438	U
42	2	1441	C
42	2	1443	A
42	2	1444	G
42	2	1445	A
42	2	1447	A
42	2	1448	A
42	2	1450	G
42	2	1451	A
42	2	1452	U
42	2	1453	U
42	2	1454	A
42	2	1455	U
42	2	1458	G
42	2	1461	C
42	2	1462	A
42	2	1464	A
42	2	1465	G
42	2	1466	C
42	2	1468	G
42	2	1496	G
42	2	1497	C
42	2	1498	G
42	2	1501	G
42	2	1502	G
42	2	1503	G
42	2	1510	U
42	2	1511	U
42	2	1512	G
42	2	1513	G
42	2	1514	U
42	2	1517	G
42	2	1520	C
42	2	1521	A
42	2	1522	U
42	2	1524	A
42	2	1525	C
43	4	8	U
43	4	9	G
43	4	14	G

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Mol	Chain	Res	Type
43	4	16	G
43	4	22	G
43	4	24	A
43	4	25	G
43	4	40	G
43	4	48	U
43	4	50	G
43	4	55	A
43	4	58	G
43	4	85	C
43	4	86	U
43	4	87	G
43	4	102	G
43	4	107	U
43	4	114	A
43	4	120	U
43	4	121	C
43	4	127	G
43	4	128	U
43	4	129	G
43	4	131	U
43	4	139	U
43	4	142	A
43	4	145	C
43	4	150	A
43	4	151	A
43	4	155	A
43	4	157	A
43	4	159	G
43	4	168	A
43	4	173	C
43	4	174	A
44	7	22	U
44	7	33	U
44	7	48	A
44	7	52	A
44	7	59	A
44	7	62	A
44	7	63	G
44	7	85	U
44	7	86	C
44	7	87	U

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Mol	Chain	Res	Type
44	7	88	A
44	7	94	G
44	7	103	A
44	7	104	A
44	7	105	C
44	7	110	A
44	7	120	G
44	7	124	A
44	7	125	A
44	7	126	G
44	7	136	G
44	7	149	A
44	7	157	U
44	7	158	U
46	8	11	G
46	8	32	C
46	8	46	A
46	8	54	A
46	8	57	U
46	8	58	A
46	8	91	G
46	8	94	A
46	8	95	U
46	8	104	A
46	8	113	U
46	8	114	G
46	8	123	U
47	5	5	G
47	5	14	C
47	5	17	A
47	5	23	G
47	5	28	U
47	5	36	C
47	5	38	G
47	5	46	C
47	5	47	G
47	5	48	G
47	5	49	C
47	5	50	A
47	5	51	U
47	5	61	C
47	5	62	G

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Mol	Chain	Res	Type
47	5	64	U
47	5	67	G
47	5	71	C
47	5	98	G
47	5	105	G
47	5	108	G
47	5	111	U
47	5	112	G
47	5	113	A
47	5	119	C
47	5	124	U
58	6	7	A
58	6	11	G
58	6	12	C
58	6	14	A
58	6	15	C
58	6	24	C
58	6	25	U
58	6	26	G
58	6	29	G
58	6	31	U
58	6	32	U
58	6	37	C
58	6	38	C
58	6	39	U
58	6	40	C
58	6	41	G
58	6	42	A
58	6	43	A
58	6	52	G
58	6	53	U
58	6	55	U
58	6	56	A
58	6	58	U
58	6	59	C
58	6	64	U
58	6	67	C
58	6	68	A
58	6	72	C
58	6	73	A
81	3	16	G
81	3	34	C

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Mol	Chain	Res	Type
81	3	41	A
81	3	42	U
81	3	59	U
81	3	63	U
81	3	72	A
81	3	107	U
81	3	109	U
81	3	110	U
81	3	118	G
81	3	119	C
81	3	124	U
81	3	125	U
81	3	126	C
81	3	138	U
81	3	145	U
81	3	146	G
81	3	149	A
81	3	150	A
81	3	151	A
81	3	179	U
81	3	181	G
81	3	183	G
81	3	184	A
81	3	188	C
81	3	191	C
81	3	192	G
81	3	194	A
81	3	202	A
81	3	210	G
81	3	213	G
81	3	214	U

All (70) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	S1	1	G
20	S1	277	U
20	S1	494	A
20	S1	607	PSU
20	S1	757	C
20	S1	916	G
20	S1	1108	A

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Mol	Chain	Res	Type
20	S1	1145	A
20	S1	1579	A
20	S1	1612	C
20	S1	1636	U
20	S1	1931	G
20	S1	1983	U
20	S1	2065	G
20	S1	2159	A
41	1	83	A
41	1	141	U
41	1	154	A
41	1	162	U
41	1	163	U
41	1	191	U
41	1	249	G
41	1	443	A
41	1	485	A
41	1	581	G
41	1	728	C
41	1	790	C
41	1	837	A
41	1	947	A
41	1	959	OMG
41	1	967	G
41	1	983	U
41	1	1011	PSU
41	1	1264	A
41	1	1269	G
41	1	1352	C
41	1	1394	A
41	1	1443	U
41	1	1524	OMG
42	2	25	A
42	2	68	A
42	2	134	C
42	2	337	A
42	2	443	OMC
42	2	452	G
42	2	500	PSU
42	2	504	PSU
42	2	646	G
42	2	648	A

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Mol	Chain	Res	Type
42	2	959	A
42	2	985	A
42	2	1156	G
42	2	1403	PSU
42	2	1452	U
42	2	1467	G
42	2	1497	C
43	4	15	G
43	4	149	U
46	8	45	G
47	5	48	G
47	5	105	G
47	5	111	U
58	6	10	C
58	6	38	C
58	6	40	C
58	6	51	A
58	6	72	C
81	3	41	A
81	3	183	G
81	3	187	U

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

152 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	$\# Z > 2$
20	OMU	S1	2048	20	19,22,23	2.95	7 (36%)	25,31,34	1.90	5 (20%)
44	PSU	7	74	44	18,21,22	4.47	8 (44%)	21,30,33	2.00	5 (23%)
20	G7M	S1	1995	20	23,26,27	3.75	11 (47%)	34,39,42	1.73	7 (20%)
42	OMC	2	1159	42	19,22,23	2.81	7 (36%)	25,31,34	0.81	0
41	PSU	1	239	41	18,21,22	4.50	7 (38%)	21,30,33	1.86	5 (23%)
41	OMU	1	1371	41	19,22,23	2.97	8 (42%)	25,31,34	2.21	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	PSU	2	1403	42	18,21,22	4.38	9 (50%)	21,30,33	1.84	4 (19%)
42	OMG	2	1078	42	23,26,27	2.30	8 (34%)	32,38,41	2.46	13 (40%)
20	OMG	S1	1647	20	23,26,27	2.36	9 (39%)	32,38,41	2.46	13 (40%)
41	A2M	1	437	41	22,25,26	3.27	10 (45%)	30,36,39	3.11	11 (36%)
20	OMU	S1	8	20	19,22,23	3.01	8 (42%)	25,31,34	1.86	5 (20%)
20	A2M	S1	2021	20	22,25,26	3.26	9 (40%)	30,36,39	3.05	12 (40%)
42	A2M	2	95	42	22,25,26	3.30	10 (45%)	30,36,39	2.94	12 (40%)
42	PSU	2	1265	42	18,21,22	4.62	7 (38%)	21,30,33	1.85	5 (23%)
20	PSU	S1	1156	20	18,21,22	4.65	7 (38%)	21,30,33	1.90	5 (23%)
20	PSU	S1	33	20	18,21,22	4.65	7 (38%)	21,30,33	1.95	5 (23%)
20	OMU	S1	661	20	19,22,23	2.99	8 (42%)	25,31,34	1.82	4 (16%)
20	OMU	S1	1621	20	19,22,23	2.99	8 (42%)	25,31,34	1.87	5 (20%)
41	PSU	1	1533	42,41	18,21,22	4.31	8 (44%)	21,30,33	2.23	6 (28%)
42	A2M	2	1384	42	22,25,26	3.25	10 (45%)	30,36,39	3.01	13 (43%)
20	OMC	S1	1866	20	19,22,23	2.81	8 (42%)	25,31,34	0.71	0
42	PSU	2	506	42	18,21,22	1.41	3 (16%)	21,30,33	2.27	5 (23%)
42	OMC	2	1397	42	19,22,23	2.73	8 (42%)	25,31,34	0.83	0
41	A2M	1	955	41	22,25,26	3.26	10 (45%)	30,36,39	2.97	12 (40%)
41	PSU	1	870	41,84	18,21,22	4.40	8 (44%)	21,30,33	1.98	5 (23%)
42	OMG	2	1046	42	23,26,27	2.39	9 (39%)	32,38,41	2.48	13 (40%)
20	PSU	S1	607	20	18,21,22	4.69	7 (38%)	21,30,33	1.90	5 (23%)
42	OMG	2	1231	42	23,26,27	2.32	8 (34%)	32,38,41	2.41	13 (40%)
20	5MC	S1	2061	20	19,22,23	1.65	3 (15%)	26,32,35	1.21	2 (7%)
20	OMG	S1	1550	20	23,26,27	2.41	9 (39%)	32,38,41	2.52	12 (37%)
42	PSU	2	662	42,84	18,21,22	4.37	8 (44%)	21,30,33	1.95	5 (23%)
20	PSU	S1	1539	20	18,21,22	4.45	7 (38%)	21,30,33	1.89	4 (19%)
20	C4J	S1	1543	20	25,29,30	2.89	9 (36%)	28,42,45	1.58	5 (17%)
42	PSU	2	1058	42	18,21,22	4.48	8 (44%)	21,30,33	1.90	4 (19%)
20	5MC	S1	1544	20	19,22,23	3.64	8 (42%)	26,32,35	1.06	1 (3%)
41	OMC	1	695	41	19,22,23	2.73	8 (42%)	25,31,34	0.73	0
44	A2M	7	43	44	22,25,26	3.29	10 (45%)	30,36,39	3.07	11 (36%)
41	A2M	1	678	42,41	22,25,26	3.28	9 (40%)	30,36,39	3.04	13 (43%)
42	A2M	2	570	42,41	22,25,26	3.28	10 (45%)	30,36,39	3.17	14 (46%)
42	OMG	2	71	42	23,26,27	2.33	8 (34%)	32,38,41	2.30	14 (43%)
41	PSU	1	672	41,84	18,21,22	4.37	8 (44%)	21,30,33	2.07	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A2M	1	1539	42,41,87,84	22,25,26	3.24	10 (45%)	30,36,39	3.08	14 (46%)
42	5MC	2	524	42,84	19,22,23	3.46	8 (42%)	26,32,35	1.08	2 (7%)
20	OMC	S1	38	20	19,22,23	2.93	8 (42%)	25,31,34	0.76	0
20	A2M	S1	28	20	22,25,26	3.20	9 (40%)	30,36,39	3.06	11 (36%)
20	OMG	S1	1623	20	23,26,27	2.36	8 (34%)	32,38,41	2.58	10 (31%)
42	OMU	2	1419	42	19,22,23	2.92	8 (42%)	25,31,34	1.80	4 (16%)
20	PSU	S1	1657	20	18,21,22	4.44	7 (38%)	21,30,33	1.77	4 (19%)
42	OMG	2	1229	42	23,26,27	2.33	9 (39%)	32,38,41	2.44	13 (40%)
42	A2M	2	527	42	22,25,26	3.32	10 (45%)	30,36,39	3.39	14 (46%)
42	OMC	2	359	42	19,22,23	2.88	8 (42%)	25,31,34	0.66	0
20	OMG	S1	600	20	23,26,27	2.41	9 (39%)	32,38,41	2.55	10 (31%)
41	PSU	1	1171	41	18,21,22	4.29	9 (50%)	21,30,33	1.91	5 (23%)
20	PSU	S1	104	20	18,21,22	4.58	7 (38%)	21,30,33	1.92	5 (23%)
42	A2M	2	665	42	22,25,26	3.28	10 (45%)	30,36,39	2.96	12 (40%)
20	OMG	S1	2151	20	23,26,27	2.42	9 (39%)	32,38,41	2.63	11 (34%)
41	PSU	1	1664	41	18,21,22	4.35	8 (44%)	21,30,33	1.84	4 (19%)
42	A2M	2	628	42	22,25,26	3.31	11 (50%)	30,36,39	2.96	13 (43%)
41	OMG	1	1626	41	23,26,27	2.31	8 (34%)	32,38,41	2.38	14 (43%)
42	PSU	2	1354	42	18,21,22	4.44	7 (38%)	21,30,33	2.05	5 (23%)
42	PSU	2	510	42	18,21,22	1.42	3 (16%)	21,30,33	2.09	5 (23%)
20	A2M	S1	479	20	22,25,26	3.23	10 (45%)	30,36,39	3.07	12 (40%)
20	OMG	S1	1478	20	23,26,27	2.38	8 (34%)	32,38,41	2.51	14 (43%)
42	A2M	2	1372	42	22,25,26	3.31	10 (45%)	30,36,39	3.09	11 (36%)
42	PSU	2	626	42	18,21,22	4.34	8 (44%)	21,30,33	1.89	4 (19%)
42	PSU	2	437	42	18,21,22	4.31	8 (44%)	21,30,33	2.03	5 (23%)
41	PSU	1	940	41	18,21,22	4.40	8 (44%)	21,30,33	1.95	5 (23%)
42	OMU	2	667	42	19,22,23	2.90	8 (42%)	25,31,34	1.91	5 (20%)
42	OMU	2	1077	42	19,22,23	2.94	8 (42%)	25,31,34	1.89	4 (16%)
20	MA6	S1	2185	20	23,26,27	1.53	5 (21%)	33,38,41	2.95	13 (39%)
42	OMC	2	1248	42	19,22,23	2.81	8 (42%)	25,31,34	0.93	1 (4%)
42	OMC	2	443	42	19,22,23	0.85	0	25,31,34	1.06	0
41	A2M	1	681	41	22,25,26	3.26	10 (45%)	30,36,39	3.06	12 (40%)
20	A2M	S1	668	20	22,25,26	3.22	9 (40%)	30,36,39	3.09	12 (40%)
42	OMC	2	1317	42	19,22,23	2.76	8 (42%)	25,31,34	0.89	1 (4%)
42	OMG	2	534	42	23,26,27	2.32	8 (34%)	32,38,41	2.46	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	MA6	S1	2184	20	23,26,27	1.55	6 (26%)	33,38,41	2.93	12 (36%)
42	PSU	2	1318	42	18,21,22	4.38	8 (44%)	21,30,33	1.86	4 (19%)
42	OMU	2	560	42	19,22,23	2.93	7 (36%)	25,31,34	1.84	4 (16%)
44	A2M	7	162	44,41	22,25,26	3.26	10 (45%)	30,36,39	3.16	11 (36%)
42	PSU	2	1382	42	18,21,22	4.38	9 (50%)	21,30,33	1.93	6 (28%)
41	A2M	1	697	41	22,25,26	3.28	10 (45%)	30,36,39	3.08	11 (36%)
42	OMU	2	73	42	19,22,23	2.86	7 (36%)	25,31,34	1.80	5 (20%)
42	OMG	2	641	42	23,26,27	2.33	9 (39%)	32,38,41	2.38	15 (46%)
42	A2M	2	1185	42	22,25,26	3.23	9 (40%)	30,36,39	3.11	13 (43%)
20	PSU	S1	2202	20	18,21,22	4.59	7 (38%)	21,30,33	1.89	5 (23%)
41	OMU	1	847	41	19,22,23	2.82	7 (36%)	25,31,34	2.00	5 (20%)
42	A2M	2	572	42	22,25,26	3.29	10 (45%)	30,36,39	3.12	12 (40%)
81	OMU	3	13	81	19,22,23	2.92	7 (36%)	25,31,34	1.94	5 (20%)
42	PSU	2	472	42	18,21,22	4.49	7 (38%)	21,30,33	1.93	5 (23%)
42	PSU	2	500	42	18,21,22	1.42	3 (16%)	21,30,33	2.23	4 (19%)
20	A2M	S1	512	20	22,25,26	1.48	4 (18%)	30,36,39	2.25	11 (36%)
44	PSU	7	69	44	18,21,22	4.44	8 (44%)	21,30,33	1.92	4 (19%)
41	OMG	1	1190	41	23,26,27	2.36	9 (39%)	32,38,41	2.49	13 (40%)
42	PSU	2	1144	42	18,21,22	4.44	8 (44%)	21,30,33	2.09	4 (19%)
41	PSU	1	422	41	18,21,22	4.47	8 (44%)	21,30,33	2.05	5 (23%)
20	PSU	S1	1533	20	18,21,22	4.45	7 (38%)	21,30,33	1.99	5 (23%)
41	PSU	1	1017	41	18,21,22	4.29	8 (44%)	21,30,33	1.88	5 (23%)
20	PSU	S1	2046	20	18,21,22	4.51	7 (38%)	21,30,33	2.08	5 (23%)
42	OMU	2	1359	42	19,22,23	2.93	8 (42%)	25,31,34	1.91	5 (20%)
41	PSU	1	1402	41	18,21,22	4.29	9 (50%)	21,30,33	2.02	4 (19%)
42	PSU	2	1060	42	18,21,22	4.47	8 (44%)	21,30,33	1.93	4 (19%)
41	OMG	1	856	41	23,26,27	2.31	9 (39%)	32,38,41	2.43	14 (43%)
42	OMG	2	655	42	23,26,27	2.31	8 (34%)	32,38,41	2.40	11 (34%)
41	1MA	1	677	41,84	21,25,26	0.65	0	30,37,40	0.74	1 (3%)
42	5MC	2	1308	42	19,22,23	3.71	8 (42%)	26,32,35	1.28	3 (11%)
20	A2M	S1	98	20	22,25,26	3.21	9 (40%)	30,36,39	3.01	13 (43%)
42	A2M	2	591	42	22,25,26	3.28	10 (45%)	30,36,39	3.00	12 (40%)
20	PSU	S1	12	20	18,21,22	4.49	7 (38%)	21,30,33	2.14	6 (28%)
42	PSU	2	1264	42	18,21,22	4.63	7 (38%)	21,30,33	1.99	5 (23%)
41	PSU	1	1528	41	18,21,22	4.41	8 (44%)	21,30,33	1.89	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	OMG	2	1253	42	23,26,27	2.33	8 (34%)	32,38,41	2.37	12 (37%)
20	OMU	S1	1833	20	19,22,23	3.07	8 (42%)	25,31,34	1.86	5 (20%)
43	OMG	4	74	43	23,26,27	2.27	8 (34%)	32,38,41	2.36	14 (43%)
20	A2M	S1	897	20	22,25,26	3.27	9 (40%)	30,36,39	3.03	13 (43%)
41	PSU	1	1181	41	18,21,22	4.44	7 (38%)	21,30,33	1.92	5 (23%)
41	A2M	1	858	41	22,25,26	3.19	9 (40%)	30,36,39	3.07	12 (40%)
20	OMU	S1	1979	20	19,22,23	2.91	8 (42%)	25,31,34	1.89	5 (20%)
42	A2M	2	604	42,41	22,25,26	3.23	10 (45%)	30,36,39	3.07	11 (36%)
20	PSU	S1	1566	20	18,21,22	1.39	3 (16%)	21,30,33	2.15	5 (23%)
42	A2M	2	382	42	22,25,26	3.27	10 (45%)	30,36,39	2.97	12 (40%)
20	OMU	S1	29	20	19,22,23	3.05	8 (42%)	25,31,34	1.85	5 (20%)
20	PSU	S1	609	20	18,21,22	4.60	7 (38%)	21,30,33	1.97	5 (23%)
20	OMC	S1	18	20	19,22,23	2.90	8 (42%)	25,31,34	0.73	0
20	OMG	S1	1829	20	23,26,27	2.34	9 (39%)	32,38,41	2.48	11 (34%)
41	OMC	1	1527	41	19,22,23	2.70	7 (36%)	25,31,34	0.73	0
41	OMG	1	1540	42,41	23,26,27	2.31	9 (39%)	32,38,41	2.40	13 (40%)
20	PSU	S1	1841	20	18,21,22	4.53	7 (38%)	21,30,33	2.00	5 (23%)
41	OMG	1	1524	41	23,26,27	2.35	8 (34%)	32,38,41	2.57	12 (37%)
41	OMU	1	1659	41	19,22,23	2.84	7 (36%)	25,31,34	1.94	5 (20%)
20	OMU	S1	1777	20	19,22,23	3.00	8 (42%)	25,31,34	1.85	5 (20%)
41	OMG	1	959	41	23,26,27	2.38	9 (39%)	32,38,41	2.67	9 (28%)
20	OMG	S1	1865	20	23,26,27	2.35	9 (39%)	32,38,41	2.51	12 (37%)
42	PSU	2	504	42	18,21,22	1.36	2 (11%)	21,30,33	2.29	5 (23%)
20	PSU	S1	1246	20	18,21,22	4.59	8 (44%)	21,30,33	1.84	4 (19%)
42	PSU	2	597	42	18,21,22	4.31	8 (44%)	21,30,33	2.07	4 (19%)
20	PSU	S1	455	20	18,21,22	4.63	7 (38%)	21,30,33	2.05	5 (23%)
42	PSU	2	1303	42	18,21,22	4.63	8 (44%)	21,30,33	2.07	6 (28%)
42	OMC	2	583	42	19,22,23	2.71	7 (36%)	25,31,34	0.79	1 (4%)
42	PSU	2	593	42	18,21,22	4.33	9 (50%)	21,30,33	2.13	5 (23%)
41	OMU	1	1107	41	19,22,23	2.84	8 (42%)	25,31,34	1.91	6 (24%)
42	PSU	2	1194	42	18,21,22	4.37	8 (44%)	21,30,33	2.15	5 (23%)
44	OMG	7	75	44	23,26,27	2.32	9 (39%)	32,38,41	2.42	13 (40%)
42	OMG	2	1360	42	23,26,27	2.35	9 (39%)	32,38,41	2.44	12 (37%)
42	PSU	2	1361	42	18,21,22	4.55	7 (38%)	21,30,33	2.09	5 (23%)
41	PSU	1	1011	42,41	18,21,22	4.58	7 (38%)	21,30,33	2.07	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	OMU	1	845	41	19,22,23	2.86	7 (36%)	25,31,34	1.87	5 (20%)
20	PSU	S1	1192	20	18,21,22	4.53	7 (38%)	21,30,33	1.76	4 (19%)
42	PSU	2	78	42	18,21,22	4.40	9 (50%)	21,30,33	1.89	5 (23%)
42	PSU	2	1413	42	18,21,22	4.34	8 (44%)	21,30,33	1.91	4 (19%)
41	OMC	1	1552	41	19,22,23	2.82	8 (42%)	25,31,34	0.78	0
20	OMC	S1	2140	20	19,22,23	2.98	8 (42%)	25,31,34	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OMU	S1	2048	20	-	0/9/27/28	0/2/2/2
44	PSU	7	74	44	-	0/7/25/26	0/2/2/2
20	G7M	S1	1995	20	-	0/7/25/26	0/3/3/3
42	OMC	2	1159	42	-	0/9/27/28	0/2/2/2
41	PSU	1	239	41	-	2/7/25/26	0/2/2/2
41	OMU	1	1371	41	-	4/9/27/28	0/2/2/2
42	PSU	2	1403	42	-	1/7/25/26	0/2/2/2
42	OMG	2	1078	42	-	0/9/27/28	0/3/3/3
20	OMG	S1	1647	20	-	0/9/27/28	0/3/3/3
41	A2M	1	437	41	-	1/9/27/28	0/3/3/3
20	OMU	S1	8	20	-	6/9/27/28	0/2/2/2
20	A2M	S1	2021	20	-	3/9/27/28	0/3/3/3
42	A2M	2	95	42	-	1/9/27/28	0/3/3/3
42	PSU	2	1265	42	-	2/7/25/26	0/2/2/2
20	PSU	S1	1156	20	-	0/7/25/26	0/2/2/2
20	PSU	S1	33	20	-	2/7/25/26	0/2/2/2
20	OMU	S1	661	20	-	0/9/27/28	0/2/2/2
20	OMU	S1	1621	20	-	0/9/27/28	0/2/2/2
41	PSU	1	1533	42,41	-	0/7/25/26	0/2/2/2
42	A2M	2	1384	42	-	1/9/27/28	0/3/3/3
20	OMC	S1	1866	20	-	0/9/27/28	0/2/2/2
42	PSU	2	506	42	-	1/7/25/26	0/2/2/2
42	OMC	2	1397	42	-	0/9/27/28	0/2/2/2
41	A2M	1	955	41	-	0/9/27/28	0/3/3/3
41	PSU	1	870	41,84	-	0/7/25/26	0/2/2/2
42	OMG	2	1046	42	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PSU	S1	607	20	-	6/7/25/26	0/2/2/2
42	OMG	2	1231	42	-	0/9/27/28	0/3/3/3
20	5MC	S1	2061	20	-	0/7/25/26	0/2/2/2
20	OMG	S1	1550	20	-	2/9/27/28	0/3/3/3
42	PSU	2	662	42,84	-	0/7/25/26	0/2/2/2
20	PSU	S1	1539	20	-	1/7/25/26	0/2/2/2
20	C4J	S1	1543	20	-	3/16/34/35	0/2/2/2
42	PSU	2	1058	42	-	0/7/25/26	0/2/2/2
20	5MC	S1	1544	20	-	0/7/25/26	0/2/2/2
41	OMC	1	695	41	-	0/9/27/28	0/2/2/2
44	A2M	7	43	44	-	0/9/27/28	0/3/3/3
41	A2M	1	678	42,41	-	0/9/27/28	0/3/3/3
42	A2M	2	570	42,41	-	4/9/27/28	0/3/3/3
42	OMG	2	71	42	-	0/9/27/28	0/3/3/3
41	PSU	1	672	41,84	-	0/7/25/26	0/2/2/2
41	A2M	1	1539	42,41,87,84	-	0/9/27/28	0/3/3/3
42	5MC	2	524	42,84	-	0/7/25/26	0/2/2/2
20	OMC	S1	38	20	-	0/9/27/28	0/2/2/2
20	A2M	S1	28	20	-	0/9/27/28	0/3/3/3
20	OMG	S1	1623	20	-	0/9/27/28	0/3/3/3
42	OMU	2	1419	42	-	1/9/27/28	0/2/2/2
20	PSU	S1	1657	20	-	1/7/25/26	0/2/2/2
42	OMG	2	1229	42	-	0/9/27/28	0/3/3/3
42	A2M	2	527	42	-	2/9/27/28	0/3/3/3
42	OMC	2	359	42	-	0/9/27/28	0/2/2/2
20	OMG	S1	600	20	-	2/9/27/28	0/3/3/3
41	PSU	1	1171	41	-	2/7/25/26	0/2/2/2
20	PSU	S1	104	20	-	0/7/25/26	0/2/2/2
42	A2M	2	665	42	-	3/9/27/28	0/3/3/3
20	OMG	S1	2151	20	-	0/9/27/28	0/3/3/3
41	PSU	1	1664	41	-	0/7/25/26	0/2/2/2
42	A2M	2	628	42	-	2/9/27/28	0/3/3/3
41	OMG	1	1626	41	-	0/9/27/28	0/3/3/3
42	PSU	2	1354	42	-	0/7/25/26	0/2/2/2
42	PSU	2	510	42	-	0/7/25/26	0/2/2/2
20	A2M	S1	479	20	-	1/9/27/28	0/3/3/3
20	OMG	S1	1478	20	-	1/9/27/28	0/3/3/3
42	A2M	2	1372	42	-	0/9/27/28	0/3/3/3
42	PSU	2	626	42	-	0/7/25/26	0/2/2/2
42	PSU	2	437	42	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PSU	1	940	41	-	0/7/25/26	0/2/2/2
42	OMU	2	667	42	-	0/9/27/28	0/2/2/2
42	OMU	2	1077	42	-	0/9/27/28	0/2/2/2
20	MA6	S1	2185	20	-	1/11/29/30	0/3/3/3
42	OMC	2	1248	42	-	1/9/27/28	0/2/2/2
42	OMC	2	443	42	-	4/9/27/28	0/2/2/2
41	A2M	1	681	41	-	3/9/27/28	0/3/3/3
20	A2M	S1	668	20	-	5/9/27/28	0/3/3/3
42	OMC	2	1317	42	-	0/9/27/28	0/2/2/2
42	OMG	2	534	42	-	2/9/27/28	0/3/3/3
20	MA6	S1	2184	20	-	0/11/29/30	0/3/3/3
42	PSU	2	1318	42	-	0/7/25/26	0/2/2/2
42	OMU	2	560	42	-	1/9/27/28	0/2/2/2
44	A2M	7	162	44,41	-	1/9/27/28	0/3/3/3
42	PSU	2	1382	42	-	0/7/25/26	0/2/2/2
41	A2M	1	697	41	-	1/9/27/28	0/3/3/3
42	OMU	2	73	42	-	0/9/27/28	0/2/2/2
42	OMG	2	641	42	-	0/9/27/28	0/3/3/3
42	A2M	2	1185	42	-	3/9/27/28	0/3/3/3
20	PSU	S1	2202	20	-	1/7/25/26	0/2/2/2
41	OMU	1	847	41	-	0/9/27/28	0/2/2/2
42	A2M	2	572	42	-	0/9/27/28	0/3/3/3
81	OMU	3	13	81	-	0/9/27/28	0/2/2/2
42	PSU	2	472	42	-	0/7/25/26	0/2/2/2
42	PSU	2	500	42	-	3/7/25/26	0/2/2/2
20	A2M	S1	512	20	-	3/9/27/28	0/3/3/3
44	PSU	7	69	44	-	2/7/25/26	0/2/2/2
41	OMG	1	1190	41	-	0/9/27/28	0/3/3/3
42	PSU	2	1144	42	-	0/7/25/26	0/2/2/2
41	PSU	1	422	41	-	0/7/25/26	0/2/2/2
20	PSU	S1	1533	20	-	2/7/25/26	0/2/2/2
41	PSU	1	1017	41	-	0/7/25/26	0/2/2/2
20	PSU	S1	2046	20	-	0/7/25/26	0/2/2/2
42	OMU	2	1359	42	-	1/9/27/28	0/2/2/2
41	PSU	1	1402	41	-	1/7/25/26	0/2/2/2
42	PSU	2	1060	42	-	1/7/25/26	0/2/2/2
41	OMG	1	856	41	-	0/9/27/28	0/3/3/3
42	OMG	2	655	42	-	1/9/27/28	0/3/3/3
41	1MA	1	677	41,84	-	0/7/25/26	0/3/3/3
42	5MC	2	1308	42	-	6/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	A2M	S1	98	20	-	1/9/27/28	0/3/3/3
42	A2M	2	591	42	-	0/9/27/28	0/3/3/3
20	PSU	S1	12	20	-	0/7/25/26	0/2/2/2
42	PSU	2	1264	42	-	0/7/25/26	0/2/2/2
41	PSU	1	1528	41	-	0/7/25/26	0/2/2/2
42	OMG	2	1253	42	-	0/9/27/28	0/3/3/3
20	OMU	S1	1833	20	-	3/9/27/28	0/2/2/2
43	OMG	4	74	43	-	0/9/27/28	0/3/3/3
20	A2M	S1	897	20	-	2/9/27/28	0/3/3/3
41	PSU	1	1181	41	-	3/7/25/26	0/2/2/2
41	A2M	1	858	41	-	0/9/27/28	0/3/3/3
20	OMU	S1	1979	20	-	3/9/27/28	0/2/2/2
42	A2M	2	604	42,41	-	1/9/27/28	0/3/3/3
20	PSU	S1	1566	20	-	0/7/25/26	0/2/2/2
42	A2M	2	382	42	-	1/9/27/28	0/3/3/3
20	OMU	S1	29	20	-	0/9/27/28	0/2/2/2
20	PSU	S1	609	20	-	0/7/25/26	0/2/2/2
20	OMC	S1	18	20	-	0/9/27/28	0/2/2/2
20	OMG	S1	1829	20	-	2/9/27/28	0/3/3/3
41	OMC	1	1527	41	-	0/9/27/28	0/2/2/2
41	OMG	1	1540	42,41	-	2/9/27/28	0/3/3/3
20	PSU	S1	1841	20	-	1/7/25/26	0/2/2/2
41	OMG	1	1524	41	-	1/9/27/28	0/3/3/3
41	OMU	1	1659	41	-	0/9/27/28	0/2/2/2
20	OMU	S1	1777	20	-	0/9/27/28	0/2/2/2
41	OMG	1	959	41	-	2/9/27/28	0/3/3/3
20	OMG	S1	1865	20	-	0/9/27/28	0/3/3/3
42	PSU	2	504	42	-	3/7/25/26	0/2/2/2
20	PSU	S1	1246	20	-	2/7/25/26	0/2/2/2
42	PSU	2	597	42	-	0/7/25/26	0/2/2/2
20	PSU	S1	455	20	-	0/7/25/26	0/2/2/2
42	PSU	2	1303	42	-	2/7/25/26	0/2/2/2
42	OMC	2	583	42	-	0/9/27/28	0/2/2/2
42	PSU	2	593	42	-	0/7/25/26	0/2/2/2
41	OMU	1	1107	41	-	0/9/27/28	0/2/2/2
42	PSU	2	1194	42	-	0/7/25/26	0/2/2/2
44	OMG	7	75	44	-	0/9/27/28	0/3/3/3
42	OMG	2	1360	42	-	0/9/27/28	0/3/3/3
42	PSU	2	1361	42	-	2/7/25/26	0/2/2/2
41	PSU	1	1011	42,41	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	OMU	1	845	41	-	0/9/27/28	0/2/2/2
20	PSU	S1	1192	20	-	2/7/25/26	0/2/2/2
42	PSU	2	78	42	-	2/7/25/26	0/2/2/2
42	PSU	2	1413	42	-	0/7/25/26	0/2/2/2
41	OMC	1	1552	41	-	0/9/27/28	0/2/2/2
20	OMC	S1	2140	20	-	2/9/27/28	0/2/2/2

All (1200) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	607	PSU	C6-C5	12.67	1.49	1.35
20	S1	33	PSU	C6-C5	12.30	1.48	1.35
20	S1	1156	PSU	C6-C5	12.28	1.48	1.35
20	S1	1246	PSU	C6-C5	12.25	1.48	1.35
41	1	1011	PSU	C6-C5	12.25	1.48	1.35
42	2	1303	PSU	C6-C5	12.24	1.48	1.35
42	2	1264	PSU	C6-C5	12.22	1.48	1.35
42	2	1265	PSU	C6-C5	12.19	1.48	1.35
20	S1	455	PSU	C6-C5	12.16	1.48	1.35
20	S1	2202	PSU	C6-C5	12.11	1.48	1.35
42	2	1058	PSU	C6-C5	12.02	1.48	1.35
20	S1	1192	PSU	C6-C5	12.02	1.48	1.35
20	S1	609	PSU	C6-C5	11.99	1.48	1.35
20	S1	104	PSU	C6-C5	11.95	1.48	1.35
42	2	1361	PSU	C6-C5	11.92	1.48	1.35
44	7	74	PSU	C6-C5	11.91	1.48	1.35
42	2	1060	PSU	C6-C5	11.91	1.48	1.35
20	S1	1841	PSU	C6-C5	11.88	1.48	1.35
42	2	472	PSU	C6-C5	11.83	1.48	1.35
20	S1	2046	PSU	C6-C5	11.83	1.48	1.35
42	2	1144	PSU	C6-C5	11.81	1.48	1.35
44	7	69	PSU	C6-C5	11.81	1.48	1.35
41	1	1528	PSU	C6-C5	11.80	1.48	1.35
42	2	626	PSU	C6-C5	11.80	1.48	1.35
41	1	239	PSU	C6-C5	11.80	1.48	1.35
20	S1	1539	PSU	C6-C5	11.77	1.48	1.35
42	2	78	PSU	C6-C5	11.76	1.48	1.35
41	1	870	PSU	C6-C5	11.75	1.48	1.35
42	2	1318	PSU	C6-C5	11.75	1.48	1.35
41	1	422	PSU	C6-C5	11.72	1.48	1.35
20	S1	12	PSU	C6-C5	11.70	1.48	1.35
42	2	1354	PSU	C6-C5	11.69	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	1181	PSU	C6-C5	11.65	1.48	1.35
20	S1	1533	PSU	C6-C5	11.62	1.48	1.35
42	2	662	PSU	C6-C5	11.62	1.48	1.35
42	2	1413	PSU	C6-C5	11.61	1.48	1.35
41	1	672	PSU	C6-C5	11.54	1.48	1.35
41	1	1017	PSU	C6-C5	11.54	1.48	1.35
41	1	1664	PSU	C6-C5	11.53	1.48	1.35
42	2	1403	PSU	C6-C5	11.50	1.48	1.35
41	1	940	PSU	C6-C5	11.50	1.48	1.35
42	2	1194	PSU	C6-C5	11.48	1.48	1.35
20	S1	1657	PSU	C6-C5	11.46	1.48	1.35
42	2	593	PSU	C6-C5	11.45	1.48	1.35
42	2	1382	PSU	C6-C5	11.36	1.47	1.35
41	1	1402	PSU	C6-C5	11.36	1.47	1.35
42	2	597	PSU	C6-C5	11.33	1.47	1.35
42	2	437	PSU	C6-C5	11.24	1.47	1.35
41	1	1171	PSU	C6-C5	11.18	1.47	1.35
41	1	1533	PSU	C6-C5	11.03	1.47	1.35
20	S1	1995	G7M	C8-N7	10.77	1.51	1.33
20	S1	1156	PSU	C2-N1	10.02	1.49	1.36
42	2	1264	PSU	C2-N1	10.02	1.49	1.36
42	2	1265	PSU	C2-N1	10.01	1.49	1.36
20	S1	33	PSU	C2-N1	9.99	1.49	1.36
20	S1	455	PSU	C2-N1	9.97	1.49	1.36
20	S1	609	PSU	C2-N1	9.94	1.49	1.36
20	S1	104	PSU	C2-N1	9.93	1.49	1.36
20	S1	607	PSU	C2-N1	9.92	1.49	1.36
42	2	1303	PSU	C2-N1	9.91	1.49	1.36
20	S1	12	PSU	C2-N1	9.81	1.49	1.36
20	S1	2202	PSU	C2-N1	9.79	1.49	1.36
42	2	1361	PSU	C2-N1	9.72	1.49	1.36
20	S1	1841	PSU	C2-N1	9.72	1.49	1.36
42	2	472	PSU	C2-N1	9.72	1.49	1.36
20	S1	1192	PSU	C2-N1	9.71	1.49	1.36
42	2	1144	PSU	C2-N1	9.71	1.49	1.36
41	1	1011	PSU	C2-N1	9.69	1.49	1.36
41	1	239	PSU	C2-N1	9.66	1.49	1.36
20	S1	2046	PSU	C2-N1	9.59	1.49	1.36
20	S1	1543	C4J	C6-C5	9.58	1.48	1.35
20	S1	1246	PSU	C2-N1	9.57	1.49	1.36
42	2	1060	PSU	C2-N1	9.54	1.49	1.36
42	2	1058	PSU	C2-N1	9.54	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	7	69	PSU	C2-N1	9.52	1.49	1.36
42	2	1308	5MC	C6-C5	9.50	1.50	1.34
20	S1	1533	PSU	C2-N1	9.48	1.49	1.36
41	1	422	PSU	C2-N1	9.48	1.49	1.36
41	1	1181	PSU	C2-N1	9.47	1.49	1.36
42	2	1354	PSU	C2-N1	9.46	1.49	1.36
20	S1	1657	PSU	C2-N1	9.44	1.49	1.36
41	1	940	PSU	C2-N1	9.43	1.49	1.36
44	7	74	PSU	C2-N1	9.40	1.48	1.36
20	S1	1539	PSU	C2-N1	9.32	1.48	1.36
41	1	1533	PSU	C2-N1	9.29	1.48	1.36
42	2	1194	PSU	C2-N1	9.27	1.48	1.36
42	2	597	PSU	C2-N1	9.26	1.48	1.36
41	1	1664	PSU	C2-N1	9.25	1.48	1.36
41	1	870	PSU	C2-N1	9.24	1.48	1.36
20	S1	897	A2M	C3'-C4'	-9.23	1.29	1.53
42	2	593	PSU	C2-N1	9.20	1.48	1.36
42	2	1403	PSU	C2-N1	9.19	1.48	1.36
42	2	662	PSU	C2-N1	9.19	1.48	1.36
42	2	1382	PSU	C2-N1	9.18	1.48	1.36
42	2	437	PSU	C2-N1	9.18	1.48	1.36
41	1	672	PSU	C2-N1	9.14	1.48	1.36
41	1	1528	PSU	C2-N1	9.13	1.48	1.36
42	2	78	PSU	C2-N1	9.05	1.48	1.36
42	2	626	PSU	C2-N1	9.03	1.48	1.36
20	S1	1544	5MC	C6-C5	9.01	1.49	1.34
42	2	1318	PSU	C2-N1	9.01	1.48	1.36
41	1	1171	PSU	C2-N1	9.00	1.48	1.36
41	1	1017	PSU	C2-N1	8.99	1.48	1.36
42	2	665	A2M	C3'-C4'	-8.99	1.30	1.53
42	2	1372	A2M	C3'-C4'	-8.98	1.30	1.53
44	7	162	A2M	C3'-C4'	-8.96	1.30	1.53
42	2	628	A2M	C3'-C4'	-8.92	1.30	1.53
42	2	1413	PSU	C2-N1	8.90	1.48	1.36
41	1	678	A2M	C3'-C4'	-8.85	1.30	1.53
42	2	95	A2M	C3'-C4'	-8.83	1.30	1.53
42	2	1384	A2M	C3'-C4'	-8.83	1.30	1.53
20	S1	2021	A2M	C3'-C4'	-8.81	1.30	1.53
42	2	570	A2M	C3'-C4'	-8.79	1.30	1.53
44	7	43	A2M	C3'-C4'	-8.77	1.30	1.53
42	2	591	A2M	C3'-C4'	-8.76	1.30	1.53
20	S1	28	A2M	C3'-C4'	-8.75	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	668	A2M	C3'-C4'	-8.75	1.30	1.53
41	1	858	A2M	C3'-C4'	-8.74	1.30	1.53
42	2	524	5MC	C6-C5	8.70	1.48	1.34
41	1	955	A2M	C3'-C4'	-8.69	1.30	1.53
41	1	1402	PSU	C2-N1	8.67	1.48	1.36
42	2	604	A2M	C3'-C4'	-8.65	1.31	1.53
42	2	382	A2M	C3'-C4'	-8.61	1.31	1.53
20	S1	98	A2M	C3'-C4'	-8.61	1.31	1.53
20	S1	479	A2M	C3'-C4'	-8.60	1.31	1.53
41	1	437	A2M	C3'-C4'	-8.59	1.31	1.53
41	1	697	A2M	C3'-C4'	-8.59	1.31	1.53
42	2	1185	A2M	C3'-C4'	-8.59	1.31	1.53
41	1	681	A2M	C3'-C4'	-8.58	1.31	1.53
41	1	1539	A2M	C3'-C4'	-8.50	1.31	1.53
42	2	527	A2M	C3'-C4'	-8.50	1.31	1.53
42	2	572	A2M	C3'-C4'	-8.48	1.31	1.53
42	2	572	A2M	O4'-C4'	7.94	1.62	1.45
42	2	591	A2M	O4'-C4'	7.88	1.62	1.45
42	2	382	A2M	O4'-C4'	7.82	1.62	1.45
20	S1	607	PSU	C2-N3	7.82	1.50	1.37
20	S1	98	A2M	O4'-C4'	7.79	1.62	1.45
42	2	527	A2M	O4'-C4'	7.77	1.62	1.45
20	S1	897	A2M	O4'-C4'	7.76	1.62	1.45
41	1	681	A2M	O4'-C4'	7.76	1.62	1.45
44	7	43	A2M	O4'-C4'	7.76	1.62	1.45
41	1	678	A2M	O4'-C4'	7.76	1.62	1.45
20	S1	1246	PSU	C2-N3	7.75	1.50	1.37
20	S1	2046	PSU	C2-N3	7.73	1.50	1.37
20	S1	455	PSU	C2-N3	7.73	1.50	1.37
20	S1	33	PSU	C2-N3	7.73	1.50	1.37
20	S1	609	PSU	C2-N3	7.72	1.50	1.37
20	S1	2202	PSU	C2-N3	7.72	1.50	1.37
20	S1	479	A2M	O4'-C4'	7.72	1.62	1.45
42	2	570	A2M	O4'-C4'	7.71	1.62	1.45
42	2	628	A2M	O4'-C4'	7.71	1.62	1.45
42	2	604	A2M	O4'-C4'	7.69	1.62	1.45
41	1	955	A2M	O4'-C4'	7.67	1.62	1.45
41	1	697	A2M	O4'-C4'	7.67	1.62	1.45
20	S1	1156	PSU	C2-N3	7.67	1.50	1.37
42	2	1265	PSU	C2-N3	7.67	1.50	1.37
42	2	1303	PSU	C2-N3	7.66	1.50	1.37
20	S1	28	A2M	O4'-C4'	7.66	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	104	PSU	C2-N3	7.64	1.50	1.37
42	2	1361	PSU	C2-N3	7.64	1.50	1.37
41	1	437	A2M	O4'-C4'	7.63	1.62	1.45
20	S1	2021	A2M	O4'-C4'	7.62	1.61	1.45
20	S1	1841	PSU	C2-N3	7.61	1.50	1.37
20	S1	1657	PSU	C2-N3	7.58	1.50	1.37
42	2	1264	PSU	C2-N3	7.55	1.49	1.37
42	2	1384	A2M	O4'-C4'	7.55	1.61	1.45
41	1	1539	A2M	O4'-C4'	7.54	1.61	1.45
42	2	665	A2M	O4'-C4'	7.54	1.61	1.45
41	1	1011	PSU	C2-N3	7.54	1.49	1.37
42	2	95	A2M	O4'-C4'	7.52	1.61	1.45
42	2	1372	A2M	O4'-C4'	7.50	1.61	1.45
20	S1	1192	PSU	C2-N3	7.50	1.49	1.37
41	1	1181	PSU	C2-N3	7.48	1.49	1.37
44	7	162	A2M	O4'-C4'	7.47	1.61	1.45
20	S1	668	A2M	O4'-C4'	7.45	1.61	1.45
20	S1	1539	PSU	C2-N3	7.45	1.49	1.37
41	1	239	PSU	C2-N3	7.44	1.49	1.37
41	1	422	PSU	C2-N3	7.43	1.49	1.37
42	2	1185	A2M	O4'-C4'	7.41	1.61	1.45
20	S1	1533	PSU	C2-N3	7.35	1.49	1.37
42	2	472	PSU	C2-N3	7.34	1.49	1.37
44	7	74	PSU	C2-N3	7.33	1.49	1.37
41	1	1533	PSU	C2-N3	7.31	1.49	1.37
20	S1	1833	OMU	C2-N1	7.31	1.49	1.38
41	1	1402	PSU	C2-N3	7.28	1.49	1.37
41	1	1371	OMU	C2-N1	7.27	1.49	1.38
20	S1	12	PSU	C2-N3	7.25	1.49	1.37
41	1	1528	PSU	C2-N3	7.25	1.49	1.37
42	2	1382	PSU	C2-N3	7.24	1.49	1.37
42	2	1354	PSU	C2-N3	7.24	1.49	1.37
42	2	1403	PSU	C2-N3	7.23	1.49	1.37
42	2	1060	PSU	C2-N3	7.21	1.49	1.37
41	1	858	A2M	O4'-C4'	7.19	1.61	1.45
42	2	1194	PSU	C2-N3	7.17	1.49	1.37
20	S1	29	OMU	C2-N1	7.15	1.49	1.38
41	1	940	PSU	C2-N3	7.15	1.49	1.37
42	2	1318	PSU	C2-N3	7.12	1.49	1.37
41	1	1171	PSU	C2-N3	7.12	1.49	1.37
42	2	1413	PSU	C2-N3	7.11	1.49	1.37
41	1	672	PSU	C2-N3	7.10	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	437	PSU	C2-N3	7.04	1.49	1.37
42	2	1058	PSU	C2-N3	7.02	1.49	1.37
20	S1	8	OMU	C2-N1	6.98	1.49	1.38
44	7	69	PSU	C2-N3	6.94	1.48	1.37
42	2	560	OMU	C2-N1	6.94	1.49	1.38
20	S1	661	OMU	C2-N1	6.94	1.49	1.38
20	S1	1777	OMU	C2-N1	6.93	1.49	1.38
42	2	1144	PSU	C2-N3	6.91	1.48	1.37
41	1	870	PSU	C2-N3	6.90	1.48	1.37
20	S1	1833	OMU	C2-N3	6.88	1.49	1.38
41	1	1017	PSU	C2-N3	6.87	1.48	1.37
42	2	78	PSU	C2-N3	6.86	1.48	1.37
42	2	662	PSU	C2-N3	6.85	1.48	1.37
42	2	1077	OMU	C2-N1	6.81	1.49	1.38
41	1	1664	PSU	C2-N3	6.81	1.48	1.37
20	S1	2048	OMU	C2-N1	6.80	1.49	1.38
20	S1	29	OMU	C2-N3	6.79	1.49	1.38
20	S1	1979	OMU	C2-N1	6.74	1.49	1.38
20	S1	1621	OMU	C2-N3	6.72	1.49	1.38
42	2	593	PSU	C2-N3	6.71	1.48	1.37
42	2	597	PSU	C2-N3	6.70	1.48	1.37
20	S1	8	OMU	C2-N3	6.70	1.49	1.38
20	S1	1777	OMU	C2-N3	6.67	1.49	1.38
81	3	13	OMU	C2-N1	6.64	1.48	1.38
42	2	1419	OMU	C2-N1	6.64	1.48	1.38
20	S1	661	OMU	C2-N3	6.64	1.49	1.38
20	S1	1621	OMU	C2-N1	6.64	1.48	1.38
20	S1	2048	OMU	C2-N3	6.60	1.49	1.38
42	2	626	PSU	C2-N3	6.60	1.48	1.37
20	S1	2151	OMG	C4-N3	6.58	1.49	1.34
41	1	845	OMU	C2-N1	6.49	1.48	1.38
20	S1	600	OMG	C4-N3	6.47	1.49	1.34
42	2	667	OMU	C2-N1	6.45	1.48	1.38
42	2	1077	OMU	C2-N3	6.45	1.49	1.38
41	1	1107	OMU	C2-N3	6.43	1.49	1.38
42	2	1359	OMU	C2-N1	6.43	1.48	1.38
20	S1	1979	OMU	C2-N3	6.42	1.49	1.38
42	2	560	OMU	C2-N3	6.41	1.49	1.38
42	2	667	OMU	C2-N3	6.39	1.49	1.38
41	1	1659	OMU	C2-N1	6.39	1.48	1.38
42	2	1359	OMU	C2-N3	6.37	1.49	1.38
20	S1	1544	5MC	C4-N3	6.35	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	2140	OMC	C2-N3	6.35	1.48	1.36
20	S1	1623	OMG	C4-N3	6.32	1.48	1.34
41	1	1371	OMU	C2-N3	6.31	1.49	1.38
42	2	1419	OMU	C2-N3	6.31	1.49	1.38
42	2	73	OMU	C2-N1	6.31	1.48	1.38
81	3	13	OMU	C2-N3	6.30	1.48	1.38
42	2	359	OMC	C2-N3	6.27	1.48	1.36
41	1	847	OMU	C2-N1	6.27	1.48	1.38
42	2	73	OMU	C2-N3	6.26	1.48	1.38
20	S1	1550	OMG	C4-N3	6.24	1.48	1.34
41	1	845	OMU	C2-N3	6.22	1.48	1.38
20	S1	38	OMC	C2-N3	6.22	1.48	1.36
42	2	1046	OMG	C4-N3	6.20	1.48	1.34
20	S1	1478	OMG	C4-N3	6.19	1.48	1.34
20	S1	18	OMC	C2-N3	6.19	1.48	1.36
41	1	1107	OMU	C2-N1	6.18	1.48	1.38
20	S1	1829	OMG	C4-N3	6.17	1.48	1.34
41	1	847	OMU	C2-N3	6.14	1.48	1.38
20	S1	1995	G7M	C2-N3	6.13	1.48	1.33
41	1	959	OMG	C4-N3	6.13	1.48	1.34
42	2	1231	OMG	C4-N3	6.12	1.48	1.34
20	S1	1865	OMG	C4-N3	6.11	1.48	1.34
42	2	655	OMG	C4-N3	6.10	1.48	1.34
20	S1	1647	OMG	C4-N3	6.08	1.48	1.34
41	1	1659	OMU	C2-N3	6.02	1.48	1.38
41	1	1190	OMG	C4-N3	6.02	1.48	1.34
44	7	75	OMG	C4-N3	6.01	1.48	1.34
42	2	1308	5MC	C5-C4	6.01	1.48	1.44
42	2	1360	OMG	C4-N3	6.00	1.48	1.34
41	1	1524	OMG	C4-N3	6.00	1.48	1.34
42	2	534	OMG	C4-N3	5.98	1.47	1.34
20	S1	1995	G7M	C5-N7	5.98	1.46	1.39
42	2	1159	OMC	C2-N3	5.96	1.48	1.36
42	2	1248	OMC	C6-C5	5.95	1.48	1.35
42	2	1253	OMG	C4-N3	5.95	1.47	1.34
42	2	1229	OMG	C4-N3	5.94	1.47	1.34
20	S1	1544	5MC	C2-N3	5.94	1.48	1.36
20	S1	1866	OMC	C2-N3	5.94	1.48	1.36
42	2	641	OMG	C4-N3	5.94	1.47	1.34
20	S1	1995	G7M	C8-N9	5.91	1.51	1.35
20	S1	2061	5MC	C5-C4	5.90	1.48	1.44
41	1	1552	OMC	C2-N3	5.90	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	1543	C4J	C2-N3	5.89	1.49	1.38
41	1	1552	OMC	C6-C5	5.87	1.48	1.35
41	1	1626	OMG	C4-N3	5.83	1.47	1.34
41	1	1540	OMG	C4-N3	5.83	1.47	1.34
42	2	1248	OMC	C2-N3	5.82	1.47	1.36
42	2	1317	OMC	C2-N3	5.82	1.47	1.36
42	2	1078	OMG	C4-N3	5.82	1.47	1.34
20	S1	38	OMC	C6-C5	5.81	1.48	1.35
41	1	856	OMG	C4-N3	5.81	1.47	1.34
20	S1	18	OMC	C6-C5	5.79	1.48	1.35
20	S1	2140	OMC	C6-C5	5.78	1.48	1.35
42	2	71	OMG	C4-N3	5.78	1.47	1.34
20	S1	1866	OMC	C6-C5	5.75	1.48	1.35
42	2	359	OMC	C6-C5	5.74	1.48	1.35
42	2	524	5MC	C4-N3	5.73	1.43	1.34
43	4	74	OMG	C4-N3	5.72	1.47	1.34
42	2	1308	5MC	C4-N3	5.72	1.43	1.34
42	2	1159	OMC	C6-C5	5.69	1.48	1.35
42	2	1397	OMC	C2-N3	5.67	1.47	1.36
42	2	1317	OMC	C6-C5	5.66	1.48	1.35
41	1	695	OMC	C2-N3	5.64	1.47	1.36
42	2	1308	5MC	C2-N3	5.63	1.47	1.36
20	S1	1833	OMU	C6-C5	5.60	1.48	1.35
42	2	524	5MC	C2-N3	5.60	1.47	1.36
20	S1	8	OMU	C6-C5	5.60	1.48	1.35
20	S1	29	OMU	C6-C5	5.59	1.48	1.35
42	2	524	5MC	C5-C4	5.56	1.48	1.44
20	S1	1621	OMU	C6-C5	5.56	1.48	1.35
42	2	1077	OMU	C6-C5	5.55	1.47	1.35
42	2	583	OMC	C6-C5	5.54	1.47	1.35
41	1	695	OMC	C6-C5	5.54	1.47	1.35
42	2	1359	OMU	C6-C5	5.53	1.47	1.35
42	2	527	A2M	O4'-C1'	-5.52	1.29	1.42
20	S1	1777	OMU	C6-C5	5.52	1.47	1.35
20	S1	661	OMU	C6-C5	5.49	1.47	1.35
41	1	1527	OMC	C2-N3	5.48	1.47	1.36
41	1	1527	OMC	C6-C5	5.48	1.47	1.35
42	2	1397	OMC	C6-C5	5.47	1.47	1.35
81	3	13	OMU	C6-C5	5.47	1.47	1.35
20	S1	1995	G7M	C4-N3	5.45	1.46	1.34
42	2	583	OMC	C2-N3	5.42	1.47	1.36
20	S1	1544	5MC	C5-C4	5.40	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1419	OMU	C6-C5	5.39	1.47	1.35
41	1	847	OMU	C6-C5	5.39	1.47	1.35
20	S1	607	PSU	C6-N1	5.38	1.45	1.36
20	S1	1156	PSU	C6-N1	5.38	1.45	1.36
42	2	667	OMU	C6-C5	5.34	1.47	1.35
20	S1	2048	OMU	C6-C5	5.34	1.47	1.35
42	2	560	OMU	C6-C5	5.34	1.47	1.35
20	S1	609	PSU	C6-N1	5.34	1.45	1.36
42	2	1264	PSU	C6-N1	5.33	1.45	1.36
42	2	73	OMU	C6-C5	5.33	1.47	1.35
42	2	1265	PSU	C6-N1	5.32	1.45	1.36
41	1	1107	OMU	C6-C5	5.31	1.47	1.35
20	S1	1657	PSU	C6-N1	5.31	1.45	1.36
20	S1	1979	OMU	C6-C5	5.30	1.47	1.35
20	S1	104	PSU	C6-N1	5.28	1.44	1.36
20	S1	455	PSU	C6-N1	5.26	1.44	1.36
20	S1	33	PSU	C6-N1	5.25	1.44	1.36
20	S1	2151	OMG	C2-N3	5.24	1.45	1.33
20	S1	2140	OMC	C4-N3	5.24	1.44	1.34
41	1	1371	OMU	C6-C5	5.23	1.47	1.35
20	S1	2202	PSU	C6-N1	5.21	1.44	1.36
41	1	1659	OMU	C6-C5	5.19	1.47	1.35
41	1	959	OMG	C2-N3	5.19	1.45	1.33
42	2	1303	PSU	C6-N1	5.17	1.44	1.36
41	1	239	PSU	C6-N1	5.17	1.44	1.36
20	S1	1246	PSU	C6-N1	5.17	1.44	1.36
44	7	69	PSU	C6-N1	5.16	1.44	1.36
20	S1	600	OMG	C2-N3	5.14	1.45	1.33
41	1	858	A2M	O4'-C1'	-5.13	1.30	1.42
41	1	845	OMU	C6-C5	5.13	1.47	1.35
41	1	697	A2M	O4'-C1'	-5.13	1.30	1.42
41	1	422	PSU	C6-N1	5.11	1.44	1.36
41	1	1181	PSU	C6-N1	5.10	1.44	1.36
42	2	1058	PSU	C6-N1	5.08	1.44	1.36
44	7	43	A2M	O4'-C1'	-5.08	1.30	1.42
20	S1	38	OMC	C4-N3	5.07	1.44	1.34
42	2	1060	PSU	C6-N1	5.06	1.44	1.36
20	S1	1550	OMG	C2-N3	5.05	1.45	1.33
20	S1	1533	PSU	C6-N1	5.03	1.44	1.36
42	2	472	PSU	C6-N1	5.03	1.44	1.36
20	S1	12	PSU	C6-N1	5.02	1.44	1.36
41	1	1539	A2M	O4'-C1'	-5.02	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1361	PSU	C6-N1	5.01	1.44	1.36
20	S1	1192	PSU	C6-N1	5.01	1.44	1.36
20	S1	1539	PSU	C6-N1	5.01	1.44	1.36
42	2	1372	A2M	O4'-C1'	-5.01	1.30	1.42
20	S1	2046	PSU	C6-N1	5.00	1.44	1.36
42	2	1185	A2M	O4'-C1'	-5.00	1.30	1.42
42	2	570	A2M	O4'-C1'	-4.99	1.30	1.42
20	S1	1841	PSU	C6-N1	4.99	1.44	1.36
42	2	572	A2M	O4'-C1'	-4.98	1.30	1.42
42	2	1046	OMG	C2-N3	4.98	1.45	1.33
41	1	437	A2M	O4'-C1'	-4.98	1.30	1.42
20	S1	1623	OMG	C2-N3	4.96	1.45	1.33
20	S1	668	A2M	O4'-C1'	-4.95	1.30	1.42
20	S1	2021	A2M	O4'-C1'	-4.95	1.30	1.42
20	S1	479	A2M	O4'-C1'	-4.93	1.30	1.42
42	2	1308	5MC	C6-N1	4.91	1.46	1.38
42	2	1354	PSU	C6-N1	4.91	1.44	1.36
44	7	162	A2M	O4'-C1'	-4.91	1.30	1.42
42	2	1384	A2M	O4'-C1'	-4.89	1.30	1.42
41	1	681	A2M	O4'-C1'	-4.89	1.30	1.42
20	S1	18	OMC	C4-N3	4.88	1.44	1.34
42	2	1382	PSU	C6-N1	4.88	1.44	1.36
41	1	1011	PSU	C6-N1	4.88	1.44	1.36
44	7	74	PSU	C6-N1	4.87	1.44	1.36
41	1	1524	OMG	C2-N3	4.86	1.45	1.33
42	2	604	A2M	O4'-C1'	-4.85	1.30	1.42
20	S1	1866	OMC	C4-N3	4.84	1.44	1.34
41	1	678	A2M	O4'-C1'	-4.83	1.30	1.42
42	2	359	OMC	C4-N3	4.83	1.44	1.34
41	1	672	PSU	C6-N1	4.83	1.44	1.36
41	1	1552	OMC	C4-N3	4.82	1.44	1.34
20	S1	1478	OMG	C2-N3	4.81	1.44	1.33
41	1	1190	OMG	C2-N3	4.81	1.44	1.33
42	2	662	PSU	C6-N1	4.81	1.44	1.36
20	S1	1829	OMG	C2-N3	4.81	1.44	1.33
42	2	628	A2M	O4'-C1'	-4.81	1.30	1.42
41	1	1528	PSU	C6-N1	4.81	1.44	1.36
42	2	382	A2M	O4'-C1'	-4.81	1.30	1.42
41	1	940	PSU	C6-N1	4.80	1.44	1.36
42	2	437	PSU	C6-N1	4.79	1.44	1.36
42	2	78	PSU	C6-N1	4.79	1.44	1.36
42	2	95	A2M	O4'-C1'	-4.79	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1403	PSU	C6-N1	4.78	1.44	1.36
42	2	1144	PSU	C6-N1	4.76	1.44	1.36
42	2	1318	PSU	C6-N1	4.75	1.44	1.36
41	1	955	A2M	O4'-C1'	-4.74	1.31	1.42
42	2	591	A2M	O4'-C1'	-4.74	1.31	1.42
42	2	1229	OMG	C2-N3	4.73	1.44	1.33
41	1	940	PSU	C1'-C5	-4.73	1.39	1.50
41	1	870	PSU	C6-N1	4.72	1.44	1.36
42	2	626	PSU	C6-N1	4.71	1.44	1.36
20	S1	98	A2M	O4'-C1'	-4.71	1.31	1.42
42	2	665	A2M	O4'-C1'	-4.71	1.31	1.42
42	2	655	OMG	C2-N3	4.71	1.44	1.33
20	S1	28	A2M	O4'-C1'	-4.70	1.31	1.42
20	S1	12	PSU	C1'-C5	-4.69	1.39	1.50
41	1	1011	PSU	C1'-C5	-4.69	1.39	1.50
42	2	534	OMG	C2-N3	4.69	1.44	1.33
41	1	1664	PSU	C6-N1	4.68	1.44	1.36
42	2	1413	PSU	C6-N1	4.68	1.44	1.36
42	2	1159	OMC	C4-N3	4.68	1.43	1.34
42	2	1046	OMG	C2-N2	4.67	1.45	1.34
42	2	597	PSU	C6-N1	4.67	1.43	1.36
42	2	1360	OMG	C2-N3	4.66	1.44	1.33
42	2	593	PSU	C6-N1	4.65	1.43	1.36
44	7	75	OMG	C2-N3	4.63	1.44	1.33
20	S1	600	OMG	C2-N2	4.63	1.45	1.34
42	2	1354	PSU	C1'-C5	-4.63	1.39	1.50
20	S1	1533	PSU	C1'-C5	-4.63	1.39	1.50
41	1	1533	PSU	C1'-C5	-4.63	1.39	1.50
42	2	593	PSU	C1'-C5	-4.62	1.39	1.50
20	S1	1550	OMG	C2-N2	4.62	1.45	1.34
20	S1	1623	OMG	C2-N2	4.62	1.45	1.34
20	S1	1544	5MC	C6-N1	4.61	1.45	1.38
42	2	1231	OMG	C2-N3	4.61	1.44	1.33
42	2	359	OMC	C4-N4	4.60	1.45	1.33
20	S1	2151	OMG	C2-N2	4.60	1.44	1.34
20	S1	897	A2M	O4'-C1'	-4.60	1.31	1.42
20	S1	2140	OMC	C4-N4	4.59	1.45	1.33
41	1	959	OMG	C2-N2	4.59	1.44	1.34
20	S1	18	OMC	C4-N4	4.58	1.45	1.33
20	S1	1865	OMG	C2-N3	4.58	1.44	1.33
41	1	856	OMG	C2-N3	4.58	1.44	1.33
42	2	662	PSU	C1'-C5	-4.57	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	1171	PSU	C6-N1	4.57	1.43	1.36
42	2	1382	PSU	C1'-C5	-4.56	1.40	1.50
20	S1	1865	OMG	C2-N2	4.56	1.44	1.34
20	S1	2140	OMC	C2-N1	4.56	1.49	1.40
20	S1	38	OMC	C4-N4	4.55	1.44	1.33
41	1	672	PSU	C1'-C5	-4.54	1.40	1.50
42	2	1194	PSU	C6-N1	4.54	1.43	1.36
42	2	1397	OMC	C4-N3	4.53	1.43	1.34
42	2	1058	PSU	C1'-C5	-4.53	1.40	1.50
20	S1	1841	PSU	C1'-C5	-4.52	1.40	1.50
20	S1	2046	PSU	C1'-C5	-4.51	1.40	1.50
41	1	1402	PSU	C6-N1	4.51	1.43	1.36
20	S1	1829	OMG	C2-N2	4.50	1.44	1.34
42	2	1194	PSU	C1'-C5	-4.49	1.40	1.50
42	2	641	OMG	C2-N3	4.48	1.44	1.33
20	S1	1647	OMG	C2-N3	4.47	1.44	1.33
20	S1	455	PSU	C1'-C5	-4.47	1.40	1.50
20	S1	512	A2M	C5-C4	4.47	1.47	1.39
20	S1	1478	OMG	C2-N2	4.47	1.44	1.34
20	S1	33	PSU	C1'-C5	-4.47	1.40	1.50
41	1	1190	OMG	C2-N2	4.46	1.44	1.34
42	2	472	PSU	C1'-C5	-4.46	1.40	1.50
42	2	1144	PSU	C1'-C5	-4.45	1.40	1.50
44	7	74	PSU	C1'-C5	-4.45	1.40	1.50
42	2	1264	PSU	C1'-C5	-4.45	1.40	1.50
41	1	1527	OMC	C4-N3	4.44	1.43	1.34
42	2	1229	OMG	C2-N2	4.43	1.44	1.34
41	1	239	PSU	C1'-C5	-4.43	1.40	1.50
42	2	1078	OMG	C2-N3	4.43	1.43	1.33
41	1	1626	OMG	C2-N3	4.43	1.43	1.33
41	1	870	PSU	C1'-C5	-4.43	1.40	1.50
41	1	695	OMC	C4-N3	4.43	1.43	1.34
42	2	1303	PSU	C1'-C5	-4.42	1.40	1.50
42	2	1253	OMG	C2-N3	4.42	1.43	1.33
42	2	583	OMC	C4-N3	4.42	1.43	1.34
20	S1	609	PSU	C1'-C5	-4.41	1.40	1.50
41	1	422	PSU	C1'-C5	-4.41	1.40	1.50
41	1	1017	PSU	C1'-C5	-4.41	1.40	1.50
42	2	1159	OMC	C4-N4	4.41	1.44	1.33
41	1	1533	PSU	C6-N1	4.40	1.43	1.36
41	1	1402	PSU	C1'-C5	-4.39	1.40	1.50
42	2	1361	PSU	C1'-C5	-4.39	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	104	PSU	C1'-C5	-4.39	1.40	1.50
42	2	71	OMG	C2-N3	4.38	1.43	1.33
41	1	1664	PSU	C1'-C5	-4.38	1.40	1.50
42	2	1360	OMG	C2-N2	4.38	1.44	1.34
42	2	1413	PSU	C1'-C5	-4.38	1.40	1.50
20	S1	38	OMC	C2-N1	4.37	1.49	1.40
44	7	75	OMG	C2-N2	4.37	1.44	1.34
42	2	1317	OMC	C4-N4	4.36	1.44	1.33
42	2	1078	OMG	C2-N2	4.36	1.44	1.34
20	S1	607	PSU	C1'-C5	-4.35	1.40	1.50
20	S1	1647	OMG	C2-N2	4.35	1.44	1.34
42	2	1248	OMC	C4-N3	4.35	1.43	1.34
42	2	1253	OMG	C2-N2	4.34	1.44	1.34
41	1	1552	OMC	C4-N4	4.34	1.44	1.33
42	2	626	PSU	C1'-C5	-4.32	1.40	1.50
41	1	1528	PSU	C1'-C5	-4.32	1.40	1.50
20	S1	1544	5MC	C4-N4	4.31	1.45	1.34
41	1	1017	PSU	C6-N1	4.30	1.43	1.36
41	1	1626	OMG	C2-N2	4.30	1.44	1.34
20	S1	479	A2M	C6-N6	4.30	1.45	1.34
20	S1	1156	PSU	C1'-C5	-4.29	1.40	1.50
42	2	437	PSU	C1'-C5	-4.29	1.40	1.50
42	2	1060	PSU	C1'-C5	-4.29	1.40	1.50
20	S1	897	A2M	C6-N6	4.28	1.45	1.34
41	1	1540	OMG	C2-N2	4.28	1.44	1.34
42	2	534	OMG	C2-N2	4.26	1.44	1.34
20	S1	28	A2M	C6-N6	4.26	1.45	1.34
42	2	71	OMG	C2-N2	4.26	1.44	1.34
41	1	1540	OMG	C2-N3	4.26	1.43	1.33
41	1	856	OMG	C2-N2	4.26	1.44	1.34
20	S1	1866	OMC	C4-N4	4.26	1.44	1.33
41	1	1524	OMG	C2-N2	4.25	1.44	1.34
41	1	1171	PSU	C1'-C5	-4.25	1.40	1.50
42	2	1265	PSU	C1'-C5	-4.25	1.40	1.50
42	2	95	A2M	C6-N6	4.24	1.45	1.34
42	2	1248	OMC	C2-N1	4.24	1.49	1.40
44	7	69	PSU	C1'-C5	-4.24	1.40	1.50
43	4	74	OMG	C2-N3	4.23	1.43	1.33
20	S1	668	A2M	C6-N6	4.23	1.45	1.34
20	S1	2202	PSU	C1'-C5	-4.22	1.40	1.50
42	2	1317	OMC	C4-N3	4.22	1.42	1.34
41	1	1181	PSU	C1'-C5	-4.22	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	1539	PSU	C1'-C5	-4.21	1.40	1.50
42	2	1248	OMC	C4-N4	4.21	1.44	1.33
42	2	597	PSU	C1'-C5	-4.20	1.40	1.50
42	2	1231	OMG	C2-N2	4.20	1.44	1.34
20	S1	1192	PSU	C1'-C5	-4.19	1.40	1.50
20	S1	1657	PSU	C1'-C5	-4.19	1.40	1.50
42	2	1397	OMC	C4-N4	4.19	1.44	1.33
20	S1	98	A2M	C6-N6	4.19	1.44	1.34
20	S1	18	OMC	C2-N1	4.19	1.48	1.40
42	2	1318	PSU	C1'-C5	-4.18	1.40	1.50
20	S1	1621	OMU	C4-N3	4.18	1.45	1.38
42	2	583	OMC	C4-N4	4.18	1.44	1.33
42	2	1308	5MC	C2-N1	4.16	1.48	1.40
42	2	1308	5MC	C4-N4	4.16	1.44	1.34
42	2	1372	A2M	C6-N6	4.14	1.44	1.34
41	1	681	A2M	C6-N6	4.13	1.44	1.34
20	S1	29	OMU	C4-N3	4.13	1.45	1.38
20	S1	1544	5MC	C2-N1	4.11	1.48	1.40
41	1	858	A2M	C6-N6	4.10	1.44	1.34
20	S1	2021	A2M	C6-N6	4.10	1.44	1.34
42	2	1185	A2M	C6-N6	4.09	1.44	1.34
42	2	524	5MC	C6-N1	4.09	1.45	1.38
42	2	641	OMG	C2-N2	4.07	1.43	1.34
42	2	655	OMG	C2-N2	4.06	1.43	1.34
20	S1	1833	OMU	C4-N3	4.06	1.45	1.38
42	2	604	A2M	C6-N6	4.06	1.44	1.34
42	2	78	PSU	C1'-C5	-4.05	1.41	1.50
44	7	43	A2M	C6-N6	4.05	1.44	1.34
43	4	74	OMG	C2-N2	4.03	1.43	1.34
41	1	695	OMC	C2-N1	4.02	1.48	1.40
20	S1	1777	OMU	C4-N3	4.01	1.45	1.38
41	1	437	A2M	C6-N6	4.00	1.44	1.34
42	2	570	A2M	C6-N6	4.00	1.44	1.34
42	2	1159	OMC	C2-N1	3.99	1.48	1.40
42	2	591	A2M	C6-N6	3.97	1.44	1.34
42	2	527	A2M	C6-N6	3.97	1.44	1.34
42	2	628	A2M	C6-N6	3.95	1.44	1.34
41	1	1527	OMC	C2-N1	3.95	1.48	1.40
44	7	162	A2M	C6-N6	3.95	1.44	1.34
20	S1	1543	C4J	C6-N1	3.95	1.46	1.36
41	1	955	A2M	C6-N6	3.94	1.44	1.34
41	1	678	A2M	C6-N6	3.94	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1384	A2M	C6-N6	3.94	1.44	1.34
20	S1	2048	OMU	C4-N3	3.94	1.45	1.38
41	1	1527	OMC	C4-N4	3.94	1.43	1.33
42	2	665	A2M	C6-N6	3.93	1.44	1.34
20	S1	1866	OMC	C2-N1	3.93	1.48	1.40
41	1	1552	OMC	C2-N1	3.92	1.48	1.40
41	1	697	A2M	C6-N6	3.92	1.44	1.34
20	S1	661	OMU	C4-N3	3.92	1.45	1.38
42	2	382	A2M	C6-N6	3.91	1.44	1.34
41	1	695	OMC	C4-N4	3.91	1.43	1.33
41	1	1539	A2M	C6-N6	3.90	1.44	1.34
20	S1	1246	PSU	C1'-C5	-3.90	1.41	1.50
42	2	1317	OMC	C2-N1	3.90	1.48	1.40
42	2	1403	PSU	C1'-C5	-3.90	1.41	1.50
20	S1	2185	MA6	C6-N6	3.89	1.47	1.36
42	2	1397	OMC	C2-N1	3.89	1.48	1.40
41	1	845	OMU	O4-C4	-3.88	1.16	1.24
42	2	78	PSU	O4-C4	-3.88	1.16	1.23
42	2	1265	PSU	C4-N3	3.87	1.46	1.38
20	S1	2184	MA6	C6-N6	3.86	1.47	1.36
20	S1	8	OMU	C4-N3	3.85	1.45	1.38
42	2	583	OMC	C2-N1	3.85	1.48	1.40
42	2	524	5MC	C4-N4	3.85	1.43	1.34
42	2	359	OMC	C2-N1	3.84	1.48	1.40
81	3	13	OMU	C4-N3	3.83	1.45	1.38
20	S1	1246	PSU	C4-N3	3.81	1.46	1.38
42	2	572	A2M	C6-N6	3.78	1.43	1.34
20	S1	607	PSU	C4-N3	3.78	1.45	1.38
42	2	95	A2M	C5-C4	-3.77	1.32	1.39
20	S1	609	PSU	C4-N3	3.77	1.45	1.38
20	S1	33	PSU	C4-N3	3.77	1.45	1.38
20	S1	1156	PSU	C4-N3	3.76	1.45	1.38
42	2	560	OMU	O4-C4	-3.75	1.17	1.24
42	2	1359	OMU	O4-C4	-3.73	1.17	1.24
20	S1	104	PSU	C4-N3	3.73	1.45	1.38
20	S1	1979	OMU	C4-N3	3.72	1.45	1.38
41	1	847	OMU	O4-C4	-3.72	1.17	1.24
20	S1	2202	PSU	C4-N3	3.71	1.45	1.38
20	S1	1657	PSU	C4-N3	3.71	1.45	1.38
42	2	572	A2M	C5-C4	-3.70	1.32	1.39
42	2	1359	OMU	C4-N3	3.69	1.44	1.38
20	S1	455	PSU	C4-N3	3.68	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	695	OMC	O2-C2	-3.68	1.16	1.23
42	2	524	5MC	C2-N1	3.68	1.47	1.40
42	2	1419	OMU	O4-C4	-3.67	1.17	1.24
20	S1	1192	PSU	C4-N3	3.67	1.45	1.38
42	2	1372	A2M	C5-C4	-3.67	1.32	1.39
42	2	583	OMC	O2-C2	-3.66	1.16	1.23
41	1	955	A2M	C5-C4	-3.65	1.32	1.39
42	2	1264	PSU	C4-N3	3.64	1.45	1.38
41	1	870	PSU	O4-C4	-3.64	1.16	1.23
42	2	667	OMU	O4-C4	-3.64	1.17	1.24
42	2	73	OMU	O4-C4	-3.64	1.17	1.24
42	2	1303	PSU	C4-N3	3.63	1.45	1.38
44	7	43	A2M	C5-C4	-3.62	1.32	1.39
41	1	697	A2M	C5-C4	-3.61	1.32	1.39
41	1	1107	OMU	O4-C4	-3.61	1.17	1.24
41	1	437	A2M	C5-C4	-3.60	1.32	1.39
41	1	1659	OMU	O4-C4	-3.60	1.17	1.24
41	1	681	A2M	C5-C4	-3.59	1.32	1.39
20	S1	1539	PSU	C4-N3	3.59	1.45	1.38
42	2	570	A2M	C5-C4	-3.58	1.32	1.39
41	1	239	PSU	C4-N3	3.58	1.45	1.38
42	2	527	A2M	C5-C4	-3.57	1.32	1.39
42	2	1382	PSU	O4-C4	-3.57	1.16	1.23
41	1	1527	OMC	O2-C2	-3.57	1.17	1.23
41	1	1664	PSU	O4-C4	-3.56	1.16	1.23
20	S1	2046	PSU	C4-N3	3.56	1.45	1.38
42	2	1077	OMU	C4-N3	3.56	1.44	1.38
42	2	1419	OMU	C4-N3	3.56	1.44	1.38
41	1	1371	OMU	O4-C4	-3.55	1.17	1.24
20	S1	1841	PSU	C4-N3	3.55	1.45	1.38
42	2	1361	PSU	C4-N3	3.55	1.45	1.38
41	1	678	A2M	C5-C4	-3.53	1.32	1.39
42	2	597	PSU	O4-C4	-3.53	1.16	1.23
41	1	1659	OMU	C4-N3	3.52	1.44	1.38
44	7	162	A2M	C5-C4	-3.52	1.32	1.39
42	2	665	A2M	C5-C4	-3.50	1.32	1.39
41	1	1011	PSU	C4-N3	3.50	1.45	1.38
81	3	13	OMU	O4-C4	-3.49	1.17	1.24
42	2	1397	OMC	O2-C2	-3.49	1.17	1.23
20	S1	1543	C4J	C4-N3	3.47	1.46	1.40
42	2	472	PSU	C4-N3	3.47	1.45	1.38
42	2	662	PSU	O4-C4	-3.46	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1318	PSU	C4-N3	3.45	1.45	1.38
42	2	1403	PSU	C4-N3	3.45	1.45	1.38
20	S1	2021	A2M	C5-C4	-3.45	1.32	1.39
42	2	1317	OMC	O2-C2	-3.44	1.17	1.23
42	2	382	A2M	C5-C4	-3.43	1.33	1.39
41	1	1107	OMU	C4-N3	3.43	1.44	1.38
41	1	845	OMU	C4-N3	3.43	1.44	1.38
42	2	1185	A2M	C5-C4	-3.43	1.33	1.39
43	4	74	OMG	O6-C6	-3.42	1.17	1.23
41	1	1171	PSU	O4-C4	-3.40	1.17	1.23
20	S1	1533	PSU	C4-N3	3.39	1.45	1.38
20	S1	1979	OMU	O4-C4	-3.39	1.17	1.24
41	1	1181	PSU	C4-N3	3.38	1.45	1.38
20	S1	1995	G7M	O6-C6	-3.37	1.17	1.23
42	2	1413	PSU	C4-N3	3.37	1.45	1.38
42	2	1159	OMC	O2-C2	-3.36	1.17	1.23
42	2	604	A2M	C5-C4	-3.36	1.33	1.39
41	1	1402	PSU	O4-C4	-3.36	1.17	1.23
41	1	1533	PSU	C4-N3	3.36	1.45	1.38
42	2	437	PSU	C4-N3	3.36	1.45	1.38
42	2	560	OMU	C4-N3	3.36	1.44	1.38
42	2	73	OMU	C4-N3	3.36	1.44	1.38
20	S1	2048	OMU	O4-C4	-3.35	1.18	1.24
41	1	1539	A2M	C5-C4	-3.35	1.33	1.39
42	2	382	A2M	C5-N7	-3.35	1.33	1.39
20	S1	1995	G7M	C6-N1	3.35	1.45	1.38
44	7	74	PSU	C4-N3	3.34	1.45	1.38
42	2	593	PSU	O4-C4	-3.34	1.17	1.23
42	2	71	OMG	O6-C6	-3.34	1.17	1.23
41	1	847	OMU	O2-C2	-3.34	1.17	1.23
42	2	667	OMU	C4-N3	3.33	1.44	1.38
42	2	73	OMU	O2-C2	-3.33	1.17	1.23
42	2	665	A2M	C5-N7	-3.33	1.33	1.39
42	2	95	A2M	C8-N9	-3.33	1.31	1.37
20	S1	1566	PSU	C6-C5	3.32	1.39	1.35
41	1	422	PSU	C4-N3	3.32	1.45	1.38
42	2	591	A2M	C5-C4	-3.32	1.33	1.39
20	S1	1995	G7M	C2-N1	3.32	1.45	1.37
20	S1	8	OMU	O4-C4	-3.32	1.18	1.24
41	1	955	A2M	C5-N7	-3.32	1.33	1.39
42	2	1318	PSU	O4-C4	-3.32	1.17	1.23
42	2	1384	A2M	C5-C4	-3.31	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	71	OMG	C4-N9	-3.31	1.29	1.38
42	2	591	A2M	C5-N7	-3.31	1.33	1.39
41	1	1528	PSU	O4-C4	-3.31	1.17	1.23
42	2	95	A2M	C5-N7	-3.30	1.33	1.39
42	2	1248	OMC	O2-C2	-3.30	1.17	1.23
42	2	527	A2M	C8-N9	-3.30	1.31	1.37
41	1	1371	OMU	C4-N3	3.29	1.44	1.38
41	1	1659	OMU	O2-C2	-3.29	1.17	1.23
20	S1	12	PSU	C4-N3	3.29	1.45	1.38
42	2	641	OMG	C4-N9	-3.28	1.29	1.38
42	2	570	A2M	C8-N9	-3.27	1.32	1.37
41	1	1539	A2M	C8-N9	-3.27	1.32	1.37
42	2	1372	A2M	C8-N9	-3.26	1.32	1.37
41	1	845	OMU	O2-C2	-3.26	1.17	1.23
42	2	628	A2M	C5-N7	-3.26	1.33	1.39
42	2	1077	OMU	O4-C4	-3.26	1.18	1.24
42	2	382	A2M	C8-N9	-3.26	1.32	1.37
42	2	626	PSU	O4-C4	-3.26	1.17	1.23
20	S1	1478	OMG	O6-C6	-3.26	1.17	1.23
41	1	1402	PSU	C4-N3	3.26	1.44	1.38
41	1	955	A2M	C8-N9	-3.25	1.32	1.37
41	1	1524	OMG	C5-N7	-3.25	1.32	1.39
42	2	665	A2M	C8-N9	-3.25	1.32	1.37
41	1	940	PSU	O4-C4	-3.25	1.17	1.23
41	1	1540	OMG	O6-C6	-3.24	1.17	1.23
42	2	1058	PSU	C4-N3	3.24	1.44	1.38
41	1	856	OMG	O6-C6	-3.23	1.17	1.23
20	S1	661	OMU	O4-C4	-3.23	1.18	1.24
42	2	628	A2M	C4-N9	-3.23	1.31	1.37
44	7	69	PSU	C4-N3	3.23	1.44	1.38
41	1	697	A2M	C5-N7	-3.23	1.33	1.39
42	2	591	A2M	C8-N9	-3.23	1.32	1.37
42	2	71	OMG	C5-N7	-3.22	1.32	1.39
20	S1	1621	OMU	O4-C4	-3.22	1.18	1.24
20	S1	98	A2M	C5-C4	-3.22	1.33	1.39
42	2	1194	PSU	C4-N3	3.22	1.44	1.38
20	S1	668	A2M	C5-C4	-3.22	1.33	1.39
42	2	1253	OMG	O6-C6	-3.22	1.17	1.23
42	2	1253	OMG	C5-N7	-3.22	1.32	1.39
42	2	1185	A2M	C8-N9	-3.21	1.32	1.37
42	2	1413	PSU	O4-C4	-3.21	1.17	1.23
41	1	672	PSU	O4-C4	-3.21	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1354	PSU	C4-N3	3.21	1.44	1.38
41	1	1540	OMG	C4-N9	-3.21	1.29	1.38
42	2	504	PSU	C6-C5	3.20	1.38	1.35
42	2	437	PSU	O4-C4	-3.20	1.17	1.23
20	S1	2184	MA6	C5-C4	-3.20	1.33	1.39
20	S1	1777	OMU	O4-C4	-3.20	1.18	1.24
20	S1	1995	G7M	C2-N2	3.20	1.41	1.34
42	2	1194	PSU	O4-C4	-3.20	1.17	1.23
42	2	641	OMG	O6-C6	-3.20	1.17	1.23
42	2	1384	A2M	C8-N9	-3.20	1.32	1.37
42	2	667	OMU	O2-C2	-3.19	1.17	1.23
41	1	1626	OMG	O6-C6	-3.19	1.17	1.23
20	S1	28	A2M	C5-C4	-3.19	1.33	1.39
42	2	1078	OMG	O6-C6	-3.19	1.17	1.23
42	2	524	5MC	O2-C2	-3.18	1.17	1.23
42	2	510	PSU	C6-C5	3.18	1.38	1.35
20	S1	2140	OMC	C6-N1	3.18	1.45	1.38
41	1	1539	A2M	C5-N7	-3.18	1.33	1.39
42	2	1229	OMG	O6-C6	-3.18	1.17	1.23
42	2	534	OMG	O6-C6	-3.18	1.17	1.23
20	S1	1866	OMC	O2-C2	-3.17	1.17	1.23
41	1	1017	PSU	O4-C4	-3.17	1.17	1.23
41	1	940	PSU	C4-N3	3.17	1.44	1.38
43	4	74	OMG	C4-N9	-3.17	1.30	1.38
42	2	1360	OMG	C5-N7	-3.17	1.32	1.39
42	2	628	A2M	O2'-C2'	-3.17	1.34	1.42
42	2	1060	PSU	C4-N3	3.17	1.44	1.38
41	1	1371	OMU	O2-C2	-3.16	1.17	1.23
20	S1	1543	C4J	O4-C4	-3.16	1.16	1.23
41	1	437	A2M	C8-N9	-3.15	1.32	1.37
42	2	359	OMC	C6-N1	3.15	1.45	1.38
20	S1	1647	OMG	O6-C6	-3.15	1.17	1.23
41	1	1626	OMG	C4-N9	-3.14	1.30	1.38
42	2	1231	OMG	O6-C6	-3.14	1.17	1.23
20	S1	2021	A2M	C8-N9	-3.13	1.32	1.37
41	1	672	PSU	C4-N3	3.13	1.44	1.38
42	2	655	OMG	O6-C6	-3.13	1.17	1.23
20	S1	29	OMU	O4-C4	-3.13	1.18	1.24
44	7	43	A2M	C5-N7	-3.12	1.33	1.39
42	2	1354	PSU	O4-C4	-3.12	1.17	1.23
20	S1	2185	MA6	C5-C4	-3.12	1.33	1.39
20	S1	18	OMC	O2-C2	-3.12	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1361	PSU	O4-C4	-3.11	1.17	1.23
41	1	697	A2M	C8-N9	-3.11	1.32	1.37
41	1	1171	PSU	C4-N3	3.11	1.44	1.38
42	2	597	PSU	C4-N3	3.11	1.44	1.38
20	S1	479	A2M	C5-C4	-3.11	1.33	1.39
41	1	1528	PSU	C4-N3	3.11	1.44	1.38
20	S1	38	OMC	C6-N1	3.10	1.45	1.38
20	S1	1647	OMG	C5-N7	-3.10	1.32	1.39
42	2	359	OMC	O2-C2	-3.10	1.17	1.23
42	2	527	A2M	O3'-C3'	3.10	1.50	1.43
42	2	1403	PSU	O4-C4	-3.09	1.17	1.23
20	S1	1833	OMU	O4-C4	-3.09	1.18	1.24
20	S1	1995	G7M	C5-C6	3.09	1.51	1.43
44	7	69	PSU	O4-C4	-3.09	1.17	1.23
20	S1	1995	G7M	C4-N9	3.09	1.45	1.38
41	1	681	A2M	C5-N7	-3.09	1.33	1.39
42	2	1144	PSU	O4-C4	-3.08	1.17	1.23
20	S1	1478	OMG	C5-N7	-3.08	1.32	1.39
42	2	570	A2M	C5-N7	-3.08	1.33	1.39
42	2	1253	OMG	C4-N9	-3.07	1.30	1.38
20	S1	1543	C4J	O4'-C1'	-3.07	1.39	1.43
42	2	506	PSU	C6-C5	3.07	1.38	1.35
20	S1	1865	OMG	C5-N7	-3.07	1.32	1.39
42	2	500	PSU	C6-C5	3.07	1.38	1.35
42	2	572	A2M	O3'-C3'	3.06	1.50	1.43
42	2	1384	A2M	C5-N7	-3.06	1.33	1.39
41	1	437	A2M	O2'-C2'	-3.06	1.35	1.42
20	S1	18	OMC	C6-N1	3.06	1.45	1.38
42	2	1382	PSU	C4-N3	3.06	1.44	1.38
41	1	870	PSU	C4-N3	3.06	1.44	1.38
41	1	1540	OMG	C5-N7	-3.06	1.32	1.39
41	1	1664	PSU	C4-N3	3.05	1.44	1.38
42	2	1308	5MC	O2-C2	-3.05	1.18	1.23
20	S1	668	A2M	O3'-C3'	3.05	1.50	1.43
20	S1	897	A2M	C5-C4	-3.05	1.33	1.39
41	1	959	OMG	C5-N7	-3.05	1.32	1.39
41	1	1533	PSU	O4-C4	-3.05	1.17	1.23
41	1	1552	OMC	O2-C2	-3.05	1.18	1.23
42	2	572	A2M	C8-N9	-3.05	1.32	1.37
41	1	437	A2M	C5-N7	-3.05	1.33	1.39
41	1	858	A2M	C5-C4	-3.05	1.33	1.39
41	1	422	PSU	O4-C4	-3.04	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1317	OMC	C6-N1	3.04	1.45	1.38
41	1	681	A2M	C8-N9	-3.04	1.32	1.37
20	S1	479	A2M	O3'-C3'	3.04	1.50	1.43
42	2	665	A2M	O2'-C2'	-3.04	1.35	1.42
42	2	572	A2M	C5-N7	-3.04	1.33	1.39
44	7	74	PSU	O4-C4	-3.03	1.17	1.23
43	4	74	OMG	C5-N7	-3.02	1.33	1.39
42	2	1060	PSU	O4-C4	-3.02	1.17	1.23
42	2	1144	PSU	C4-N3	3.02	1.44	1.38
42	2	1360	OMG	O6-C6	-3.01	1.17	1.23
41	1	678	A2M	C8-N9	-3.01	1.32	1.37
42	2	1229	OMG	C4-N9	-3.01	1.30	1.38
41	1	856	OMG	C5-N7	-3.01	1.33	1.39
20	S1	1543	C4J	C2-N1	3.01	1.47	1.39
41	1	678	A2M	C5-N7	-3.01	1.33	1.39
20	S1	1865	OMG	O6-C6	-3.00	1.17	1.23
41	1	1539	A2M	O2'-C2'	-3.00	1.35	1.42
42	2	78	PSU	C4-N3	3.00	1.44	1.38
20	S1	1533	PSU	O4-C4	-3.00	1.17	1.23
44	7	43	A2M	C8-N9	-2.99	1.32	1.37
41	1	1011	PSU	O4-C4	-2.99	1.17	1.23
41	1	695	OMC	C6-N1	2.99	1.45	1.38
42	2	527	A2M	C5-N7	-2.99	1.33	1.39
42	2	1419	OMU	O2-C2	-2.99	1.17	1.23
42	2	641	OMG	C5-N7	-2.98	1.33	1.39
41	1	1017	PSU	C4-N3	2.97	1.44	1.38
44	7	162	A2M	C8-N9	-2.97	1.32	1.37
20	S1	1647	OMG	C4-N9	-2.97	1.30	1.38
81	3	13	OMU	O2-C2	-2.97	1.17	1.23
20	S1	1623	OMG	C5-N7	-2.97	1.33	1.39
20	S1	1539	PSU	O4-C4	-2.96	1.17	1.23
41	1	239	PSU	O4-C4	-2.96	1.18	1.23
41	1	697	A2M	O2'-C2'	-2.96	1.35	1.42
42	2	534	OMG	C5-N7	-2.96	1.33	1.39
42	2	626	PSU	C4-N3	2.95	1.44	1.38
42	2	1231	OMG	C4-N9	-2.95	1.30	1.38
42	2	1229	OMG	C5-N7	-2.95	1.33	1.39
41	1	678	A2M	O2'-C2'	-2.95	1.35	1.42
41	1	1527	OMC	C6-N1	2.95	1.45	1.38
42	2	1078	OMG	C4-N9	-2.95	1.30	1.38
20	S1	2021	A2M	C5-N7	-2.95	1.33	1.39
20	S1	38	OMC	O2-C2	-2.95	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1248	OMC	C6-N1	2.94	1.45	1.38
44	7	162	A2M	O2'-C2'	-2.93	1.35	1.42
42	2	572	A2M	O2'-C2'	-2.93	1.35	1.42
41	1	1190	OMG	O6-C6	-2.93	1.18	1.23
41	1	847	OMU	C4-N3	2.93	1.43	1.38
41	1	1552	OMC	C6-N1	2.93	1.45	1.38
20	S1	1657	PSU	O4-C4	-2.92	1.18	1.23
20	S1	2048	OMU	O2-C2	-2.92	1.17	1.23
41	1	1626	OMG	C5-N7	-2.92	1.33	1.39
41	1	856	OMG	C4-N9	-2.92	1.30	1.38
20	S1	1866	OMC	C6-N1	2.91	1.45	1.38
42	2	1360	OMG	C4-N9	-2.91	1.30	1.38
41	1	955	A2M	O2'-C2'	-2.91	1.35	1.42
20	S1	668	A2M	C8-N9	-2.91	1.32	1.37
42	2	1185	A2M	C5-N7	-2.91	1.33	1.39
42	2	506	PSU	C4-N3	-2.91	1.33	1.38
20	S1	1550	OMG	C5-N7	-2.91	1.33	1.39
42	2	1185	A2M	O2'-C2'	-2.91	1.35	1.42
20	S1	1621	OMU	O2-C2	-2.90	1.17	1.23
41	1	959	OMG	O6-C6	-2.90	1.18	1.23
42	2	655	OMG	C5-N7	-2.90	1.33	1.39
42	2	583	OMC	C6-N1	2.90	1.45	1.38
42	2	1372	A2M	O3'-C3'	2.90	1.50	1.43
42	2	1372	A2M	C5-N7	-2.89	1.33	1.39
42	2	604	A2M	O2'-C2'	-2.89	1.35	1.42
42	2	662	PSU	C4-N3	2.89	1.44	1.38
20	S1	1841	PSU	O4-C4	-2.89	1.18	1.23
42	2	1384	A2M	O2'-C2'	-2.88	1.35	1.42
20	S1	1550	OMG	O6-C6	-2.88	1.18	1.23
42	2	560	OMU	O2-C2	-2.88	1.18	1.23
20	S1	1544	5MC	O2-C2	-2.88	1.18	1.23
44	7	43	A2M	O2'-C2'	-2.88	1.35	1.42
41	1	858	A2M	O3'-C3'	2.87	1.50	1.43
42	2	1359	OMU	C6-N1	2.87	1.44	1.38
42	2	1359	OMU	O2-C2	-2.87	1.18	1.23
42	2	593	PSU	C4-N3	2.87	1.44	1.38
20	S1	1623	OMG	O6-C6	-2.86	1.18	1.23
41	1	437	A2M	O3'-C3'	2.86	1.50	1.43
42	2	1185	A2M	O3'-C3'	2.86	1.50	1.43
42	2	1231	OMG	C5-N7	-2.86	1.33	1.39
42	2	604	A2M	C8-N9	-2.86	1.32	1.37
42	2	510	PSU	C4-N3	-2.85	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	1829	OMG	C5-N7	-2.85	1.33	1.39
42	2	591	A2M	O2'-C2'	-2.85	1.35	1.42
42	2	1046	OMG	C5-N7	-2.84	1.33	1.39
20	S1	1478	OMG	C4-N9	-2.84	1.30	1.38
42	2	1159	OMC	C6-N1	2.84	1.44	1.38
44	7	75	OMG	C5-N7	-2.84	1.33	1.39
44	7	75	OMG	O6-C6	-2.84	1.18	1.23
20	S1	897	A2M	O2'-C2'	-2.83	1.35	1.42
20	S1	12	PSU	O4-C4	-2.83	1.18	1.23
42	2	1264	PSU	O4-C4	-2.83	1.18	1.23
42	2	1372	A2M	O2'-C2'	-2.83	1.35	1.42
41	1	1539	A2M	O3'-C3'	2.82	1.49	1.43
20	S1	98	A2M	C8-N9	-2.82	1.32	1.37
20	S1	661	OMU	C6-N1	2.82	1.44	1.38
42	2	472	PSU	O4-C4	-2.82	1.18	1.23
41	1	1190	OMG	C5-N7	-2.81	1.33	1.39
42	2	500	PSU	C4-N3	-2.81	1.33	1.38
42	2	1303	PSU	O4-C4	-2.81	1.18	1.23
41	1	1190	OMG	C4-N9	-2.81	1.30	1.38
20	S1	29	OMU	C6-N1	2.81	1.44	1.38
20	S1	1979	OMU	O2-C2	-2.81	1.18	1.23
20	S1	1833	OMU	C6-N1	2.80	1.44	1.38
42	2	1078	OMG	C5-N7	-2.80	1.33	1.39
20	S1	98	A2M	O2'-C2'	-2.80	1.35	1.42
42	2	570	A2M	O3'-C3'	2.80	1.49	1.43
41	1	858	A2M	O2'-C2'	-2.79	1.35	1.42
20	S1	1192	PSU	O4-C4	-2.79	1.18	1.23
41	1	1181	PSU	O4-C4	-2.79	1.18	1.23
44	7	75	OMG	C4-N9	-2.79	1.31	1.38
20	S1	2021	A2M	O2'-C2'	-2.79	1.35	1.42
42	2	95	A2M	O2'-C2'	-2.79	1.35	1.42
20	S1	600	OMG	C5-N7	-2.79	1.33	1.39
41	1	1524	OMG	O6-C6	-2.78	1.18	1.23
20	S1	600	OMG	O6-C6	-2.78	1.18	1.23
42	2	1397	OMC	C6-N1	2.78	1.44	1.38
42	2	534	OMG	C4-N9	-2.78	1.31	1.38
42	2	604	A2M	C5-N7	-2.78	1.34	1.39
41	1	858	A2M	C5-N7	-2.78	1.34	1.39
20	S1	1829	OMG	O6-C6	-2.77	1.18	1.23
20	S1	1543	C4J	O2-C2	-2.77	1.17	1.22
44	7	162	A2M	C5-N7	-2.77	1.34	1.39
41	1	697	A2M	O3'-C3'	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	628	A2M	C5-C4	-2.77	1.34	1.39
20	S1	8	OMU	C6-N1	2.77	1.44	1.38
20	S1	897	A2M	C8-N9	-2.77	1.32	1.37
20	S1	2151	OMG	C5-N7	-2.77	1.33	1.39
42	2	1077	OMU	O2-C2	-2.77	1.18	1.23
20	S1	1246	PSU	O4-C4	-2.76	1.18	1.23
20	S1	479	A2M	C8-N9	-2.76	1.32	1.37
20	S1	2140	OMC	O2-C2	-2.76	1.18	1.23
20	S1	1777	OMU	C6-N1	2.76	1.44	1.38
20	S1	661	OMU	O2-C2	-2.75	1.18	1.23
20	S1	98	A2M	C5-N7	-2.75	1.34	1.39
20	S1	28	A2M	O2'-C2'	-2.75	1.35	1.42
42	2	382	A2M	O3'-C3'	2.75	1.49	1.43
41	1	681	A2M	O3'-C3'	2.75	1.49	1.43
42	2	1046	OMG	C2-N1	2.74	1.44	1.37
42	2	628	A2M	O3'-C3'	2.74	1.49	1.43
20	S1	98	A2M	O3'-C3'	2.73	1.49	1.43
20	S1	455	PSU	O4-C4	-2.72	1.18	1.23
41	1	681	A2M	O2'-C2'	-2.72	1.35	1.42
42	2	1419	OMU	C6-N1	2.72	1.44	1.38
20	S1	479	A2M	C5-N7	-2.72	1.34	1.39
20	S1	2021	A2M	O3'-C3'	2.72	1.49	1.43
20	S1	1550	OMG	C4-N9	-2.72	1.31	1.38
42	2	1058	PSU	O4-C4	-2.71	1.18	1.23
42	2	667	OMU	C6-N1	2.71	1.44	1.38
20	S1	1566	PSU	C4-N3	-2.71	1.33	1.38
20	S1	2184	MA6	C5-N7	-2.71	1.34	1.39
41	1	678	A2M	O3'-C3'	2.71	1.49	1.43
42	2	527	A2M	O2'-C2'	-2.71	1.36	1.42
42	2	604	A2M	O3'-C3'	2.71	1.49	1.43
20	S1	28	A2M	C8-N9	-2.71	1.32	1.37
41	1	1107	OMU	O2-C2	-2.71	1.18	1.23
20	S1	1156	PSU	O4-C4	-2.70	1.18	1.23
42	2	504	PSU	C4-N3	-2.70	1.33	1.38
20	S1	2185	MA6	C5-N7	-2.70	1.34	1.39
20	S1	1621	OMU	C6-N1	2.70	1.44	1.38
42	2	1077	OMU	C6-N1	2.69	1.44	1.38
20	S1	609	PSU	O4-C4	-2.69	1.18	1.23
41	1	1190	OMG	C2-N1	2.69	1.44	1.37
20	S1	2046	PSU	O4-C4	-2.69	1.18	1.23
20	S1	1777	OMU	O2-C2	-2.68	1.18	1.23
42	2	382	A2M	O2'-C2'	-2.68	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	2151	OMG	C2-N1	2.68	1.44	1.37
20	S1	2202	PSU	O4-C4	-2.68	1.18	1.23
20	S1	8	OMU	O2-C2	-2.68	1.18	1.23
20	S1	1865	OMG	C2-N1	2.68	1.44	1.37
41	1	959	OMG	C2-N1	2.67	1.44	1.37
41	1	1371	OMU	C6-N1	2.67	1.44	1.38
20	S1	1550	OMG	C2-N1	2.67	1.44	1.37
20	S1	28	A2M	O3'-C3'	2.66	1.49	1.43
42	2	1046	OMG	O6-C6	-2.66	1.18	1.23
20	S1	600	OMG	C2-N1	2.65	1.44	1.37
20	S1	479	A2M	O2'-C2'	-2.65	1.36	1.42
20	S1	1865	OMG	C4-N9	-2.65	1.31	1.38
20	S1	512	A2M	C5-C6	2.64	1.48	1.41
42	2	665	A2M	O3'-C3'	2.64	1.49	1.43
20	S1	1829	OMG	C2-N1	2.63	1.44	1.37
42	2	655	OMG	C4-N9	-2.63	1.31	1.38
20	S1	33	PSU	O4-C4	-2.62	1.18	1.23
20	S1	897	A2M	C5-N7	-2.62	1.34	1.39
20	S1	668	A2M	O2'-C2'	-2.62	1.36	1.42
20	S1	2151	OMG	O6-C6	-2.61	1.18	1.23
20	S1	607	PSU	O4-C4	-2.61	1.18	1.23
42	2	597	PSU	O2-C2	-2.61	1.17	1.23
20	S1	29	OMU	O2-C2	-2.61	1.18	1.23
20	S1	1829	OMG	C4-N9	-2.61	1.31	1.38
20	S1	104	PSU	O4-C4	-2.60	1.18	1.23
42	2	591	A2M	O3'-C3'	2.60	1.49	1.43
42	2	1046	OMG	C4-N9	-2.60	1.31	1.38
41	1	1659	OMU	C6-N1	2.58	1.44	1.38
20	S1	1647	OMG	C2-N1	2.58	1.43	1.37
20	S1	2185	MA6	C4-N9	-2.58	1.32	1.37
41	1	858	A2M	C8-N9	-2.58	1.33	1.37
41	1	1107	OMU	C6-N1	2.57	1.44	1.38
42	2	1265	PSU	O4-C4	-2.57	1.18	1.23
81	3	13	OMU	C6-N1	2.57	1.44	1.38
20	S1	897	A2M	O3'-C3'	2.57	1.49	1.43
42	2	95	A2M	O3'-C3'	2.56	1.49	1.43
44	7	162	A2M	C4-N9	-2.56	1.32	1.37
20	S1	2048	OMU	C6-N1	2.56	1.44	1.38
20	S1	1833	OMU	O2-C2	-2.55	1.18	1.23
20	S1	2184	MA6	C4-N9	-2.54	1.32	1.37
20	S1	668	A2M	C5-N7	-2.54	1.34	1.39
44	7	43	A2M	O3'-C3'	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	1979	OMU	C6-N1	2.54	1.44	1.38
41	1	1540	OMG	C2-N1	2.54	1.43	1.37
42	2	1046	OMG	C5-C6	2.53	1.53	1.44
42	2	73	OMU	C6-N1	2.53	1.44	1.38
41	1	1524	OMG	C4-N9	-2.52	1.31	1.38
41	1	845	OMU	C6-N1	2.52	1.44	1.38
42	2	1360	OMG	C2-N1	2.51	1.43	1.37
20	S1	1623	OMG	C2-N1	2.51	1.43	1.37
42	2	78	PSU	O4'-C1'	-2.51	1.40	1.43
20	S1	28	A2M	C5-N7	-2.50	1.34	1.39
41	1	1524	OMG	C5-C6	2.49	1.53	1.44
42	2	1253	OMG	C5-C6	2.49	1.53	1.44
20	S1	2061	5MC	C6-N1	-2.48	1.33	1.38
44	7	75	OMG	C2-N1	2.48	1.43	1.37
42	2	655	OMG	C5-C6	2.48	1.53	1.44
42	2	1078	OMG	C5-C6	2.47	1.53	1.44
41	1	847	OMU	C6-N1	2.47	1.44	1.38
41	1	1171	PSU	O2-C2	-2.47	1.18	1.23
42	2	1384	A2M	O3'-C3'	2.46	1.49	1.43
42	2	626	PSU	O2-C2	-2.45	1.18	1.23
42	2	641	OMG	C5-C6	2.45	1.53	1.44
41	1	1190	OMG	C5-C6	2.45	1.53	1.44
20	S1	2151	OMG	C5-C6	2.44	1.53	1.44
42	2	1231	OMG	C2-N1	2.44	1.43	1.37
20	S1	600	OMG	C5-C6	2.44	1.53	1.44
42	2	1403	PSU	O4'-C1'	-2.43	1.40	1.43
41	1	1017	PSU	O2-C2	-2.43	1.18	1.23
44	7	75	OMG	C5-C6	2.43	1.53	1.44
42	2	560	OMU	C6-N1	2.43	1.43	1.38
42	2	534	OMG	C2-N1	2.42	1.43	1.37
41	1	856	OMG	C5-C6	2.42	1.53	1.44
41	1	1626	OMG	C5-C6	2.42	1.53	1.44
42	2	1194	PSU	O2-C2	-2.41	1.18	1.23
41	1	1524	OMG	C2-N1	2.41	1.43	1.37
42	2	78	PSU	O2-C2	-2.39	1.18	1.23
42	2	655	OMG	C2-N1	2.39	1.43	1.37
41	1	856	OMG	C2-N1	2.39	1.43	1.37
42	2	570	A2M	O2'-C2'	-2.39	1.36	1.42
42	2	1046	OMG	C6-N1	2.39	1.43	1.38
20	S1	1829	OMG	C5-C6	2.38	1.53	1.44
42	2	662	PSU	O2-C2	-2.38	1.18	1.23
20	S1	600	OMG	C4-N9	-2.38	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	1540	OMG	C5-C6	2.38	1.53	1.44
42	2	593	PSU	O2-C2	-2.37	1.18	1.23
42	2	1360	OMG	C5-C6	2.37	1.53	1.44
41	1	1626	OMG	C2-N1	2.37	1.43	1.37
42	2	1372	A2M	C4-N9	-2.37	1.32	1.37
42	2	1078	OMG	C2-N1	2.36	1.43	1.37
44	7	162	A2M	O3'-C3'	2.36	1.48	1.43
42	2	641	OMG	C2-N1	2.36	1.43	1.37
20	S1	1550	OMG	C5-C6	2.35	1.53	1.44
20	S1	38	OMC	C5-C4	2.35	1.48	1.42
20	S1	2061	5MC	C6-C5	2.35	1.38	1.34
41	1	870	PSU	O2-C2	-2.35	1.18	1.23
20	S1	2140	OMC	C5-C4	2.34	1.48	1.42
42	2	1077	OMU	C5-C4	2.34	1.48	1.43
20	S1	1543	C4J	C31-C3	2.34	1.59	1.52
42	2	534	OMG	C5-C6	2.33	1.53	1.44
42	2	1229	OMG	C5-C6	2.33	1.53	1.44
41	1	1664	PSU	O2-C2	-2.33	1.18	1.23
20	S1	1623	OMG	C5-C6	2.33	1.53	1.44
20	S1	1478	OMG	C2-N1	2.33	1.43	1.37
42	2	95	A2M	C4-N9	-2.31	1.32	1.37
42	2	1382	PSU	O2-C2	-2.31	1.18	1.23
41	1	697	A2M	C4-N9	-2.31	1.32	1.37
20	S1	512	A2M	C5-N7	-2.30	1.34	1.39
20	S1	1478	OMG	C5-C6	2.30	1.53	1.44
42	2	1413	PSU	O2-C2	-2.30	1.18	1.23
20	S1	1623	OMG	C4-N9	-2.30	1.32	1.38
44	7	75	OMG	C6-N1	2.30	1.43	1.38
41	1	955	A2M	O3'-C3'	2.30	1.48	1.43
20	S1	29	OMU	C5-C4	2.30	1.48	1.43
42	2	527	A2M	C4-N9	-2.29	1.32	1.37
42	2	71	OMG	C5-C6	2.29	1.53	1.44
20	S1	8	OMU	C5-C4	2.28	1.48	1.43
20	S1	512	A2M	C8-N7	2.28	1.36	1.31
20	S1	2151	OMG	C6-N1	2.28	1.43	1.38
43	4	74	OMG	C2-N1	2.27	1.43	1.37
42	2	71	OMG	C2-N1	2.27	1.43	1.37
20	S1	600	OMG	C6-N1	2.27	1.43	1.38
20	S1	1833	OMU	C5-C4	2.26	1.48	1.43
42	2	604	A2M	C4-N9	-2.26	1.33	1.37
42	2	1229	OMG	C2-N1	2.26	1.43	1.37
42	2	1231	OMG	C5-C6	2.26	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	359	OMC	C5-C4	2.25	1.48	1.42
41	1	959	OMG	C5-C6	2.25	1.52	1.44
20	S1	1865	OMG	C5-C6	2.24	1.52	1.44
41	1	959	OMG	C4-N9	-2.24	1.32	1.38
42	2	1253	OMG	C2-N1	2.24	1.43	1.37
41	1	1371	OMU	C5-C4	2.24	1.48	1.43
42	2	572	A2M	C4-N9	-2.23	1.33	1.37
41	1	1190	OMG	C6-N1	2.23	1.43	1.38
20	S1	18	OMC	C5-C4	2.23	1.48	1.42
44	7	43	A2M	C4-N9	-2.23	1.33	1.37
42	2	1058	PSU	O2-C2	-2.23	1.18	1.23
42	2	437	PSU	O2-C2	-2.23	1.18	1.23
20	S1	2151	OMG	C4-N9	-2.22	1.32	1.38
20	S1	1777	OMU	C5-C4	2.22	1.48	1.43
41	1	1528	PSU	O2-C2	-2.22	1.18	1.23
20	S1	1246	PSU	O4'-C1'	-2.20	1.40	1.43
42	2	1144	PSU	O2-C2	-2.20	1.18	1.23
20	S1	1550	OMG	C6-N1	2.20	1.43	1.38
42	2	1318	PSU	O2-C2	-2.20	1.18	1.23
41	1	437	A2M	C4-N9	-2.20	1.33	1.37
41	1	672	PSU	O2-C2	-2.19	1.18	1.23
20	S1	1647	OMG	C5-C6	2.19	1.52	1.44
20	S1	1621	OMU	C5-C4	2.18	1.48	1.43
41	1	1171	PSU	O4'-C1'	-2.18	1.40	1.43
41	1	1533	PSU	O2-C2	-2.17	1.18	1.23
43	4	74	OMG	C5-C6	2.17	1.52	1.44
42	2	1248	OMC	C5-C4	2.15	1.47	1.42
20	S1	661	OMU	C5-C4	2.15	1.48	1.43
42	2	1359	OMU	C5-C4	2.15	1.48	1.43
42	2	628	A2M	C8-N9	-2.15	1.33	1.37
41	1	959	OMG	C6-N1	2.14	1.42	1.38
42	2	382	A2M	C4-N9	-2.14	1.33	1.37
41	1	1552	OMC	C5-C4	2.14	1.47	1.42
42	2	570	A2M	C4-N9	-2.14	1.33	1.37
42	2	667	OMU	C5-C4	2.13	1.48	1.43
41	1	1107	OMU	C5-C4	2.13	1.48	1.43
42	2	1382	PSU	O4'-C1'	-2.13	1.40	1.43
42	2	1403	PSU	O2-C2	-2.12	1.18	1.23
42	2	593	PSU	O4'-C1'	-2.11	1.40	1.43
42	2	1060	PSU	O2-C2	-2.10	1.18	1.23
41	1	1402	PSU	O4'-C1'	-2.10	1.40	1.43
20	S1	1866	OMC	C5-C4	2.10	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1419	OMU	C5-C4	2.10	1.48	1.43
20	S1	2184	MA6	C8-N9	-2.10	1.34	1.37
41	1	422	PSU	O2-C2	-2.10	1.18	1.23
20	S1	1647	OMG	C6-N1	2.09	1.42	1.38
41	1	940	PSU	O2-C2	-2.08	1.18	1.23
41	1	1402	PSU	O2-C2	-2.08	1.18	1.23
41	1	856	OMG	C6-N1	2.08	1.42	1.38
42	2	1384	A2M	C4-N9	-2.07	1.33	1.37
44	7	69	PSU	O4'-C1'	-2.07	1.41	1.43
42	2	510	PSU	C2-N3	-2.07	1.34	1.37
42	2	591	A2M	C4-N9	-2.07	1.33	1.37
42	2	1317	OMC	C5-C4	2.07	1.47	1.42
20	S1	2185	MA6	C10-N6	2.06	1.50	1.45
20	S1	1829	OMG	C6-N1	2.06	1.42	1.38
20	S1	1979	OMU	C5-C4	2.05	1.48	1.43
41	1	695	OMC	C5-C4	2.04	1.47	1.42
42	2	506	PSU	C2-N3	-2.04	1.34	1.37
44	7	74	PSU	O2-C2	-2.04	1.19	1.23
42	2	1360	OMG	C6-N1	2.03	1.42	1.38
41	1	1539	A2M	C4-N9	-2.03	1.33	1.37
20	S1	479	A2M	C4-N9	-2.03	1.33	1.37
41	1	681	A2M	C4-N9	-2.02	1.33	1.37
42	2	500	PSU	C2-N3	-2.02	1.34	1.37
20	S1	1566	PSU	C2-N3	-2.02	1.34	1.37
41	1	1540	OMG	C6-N1	2.02	1.42	1.38
20	S1	2184	MA6	C10-N6	2.02	1.50	1.45
41	1	955	A2M	C4-N9	-2.01	1.33	1.37
42	2	665	A2M	C4-N9	-2.01	1.33	1.37
42	2	641	OMG	C6-N1	2.01	1.42	1.38
42	2	628	A2M	C5-C6	-2.01	1.35	1.41
20	S1	1865	OMG	C6-N1	2.01	1.42	1.38
42	2	1397	OMC	C5-C4	2.01	1.47	1.42
42	2	1229	OMG	C6-N1	2.00	1.42	1.38
42	2	1303	PSU	C4-C5	2.00	1.49	1.44

All (1070) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	2185	MA6	N1-C6-N6	-10.25	104.36	116.86
20	S1	2184	MA6	N1-C6-N6	-9.80	104.91	116.86
41	1	959	OMG	C1'-N9-C8	-7.91	104.27	126.73
20	S1	2151	OMG	C1'-N9-C8	-7.71	104.83	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1623	OMG	C1'-N9-C8	-7.70	104.85	126.73
20	S1	600	OMG	C1'-N9-C8	-7.52	105.37	126.73
41	1	858	A2M	N6-C6-N1	-7.42	101.86	118.38
20	S1	1829	OMG	C1'-N9-C8	-7.41	105.67	126.73
42	2	534	OMG	C1'-N9-C8	-7.27	106.08	126.73
20	S1	1550	OMG	C1'-N9-C8	-7.25	106.12	126.73
42	2	1046	OMG	C1'-N9-C8	-7.10	106.56	126.73
41	1	959	OMG	C1'-N9-C4	7.09	147.44	126.49
41	1	697	A2M	N6-C6-N1	-7.08	102.60	118.38
20	S1	1865	OMG	C1'-N9-C8	-6.99	106.89	126.73
42	2	572	A2M	N6-C6-N1	-6.90	103.02	118.38
20	S1	1478	OMG	C1'-N9-C8	-6.82	107.37	126.73
42	2	506	PSU	N1-C2-N3	6.78	122.33	115.17
41	1	1524	OMG	C1'-N9-C8	-6.78	107.46	126.73
41	1	437	A2M	N6-C6-N1	-6.78	103.27	118.38
42	2	604	A2M	N6-C6-N1	-6.76	103.33	118.38
42	2	1360	OMG	C1'-N9-C8	-6.75	107.54	126.73
42	2	1372	A2M	N6-C6-N1	-6.64	103.58	118.38
20	S1	2021	A2M	N6-C6-N1	-6.64	103.58	118.38
42	2	500	PSU	N1-C2-N3	6.63	122.16	115.17
20	S1	1623	OMG	C1'-N9-C4	6.62	146.04	126.49
42	2	591	A2M	N6-C6-N1	-6.62	103.63	118.38
20	S1	1647	OMG	C1'-N9-C8	-6.62	107.94	126.73
20	S1	28	A2M	N6-C6-N1	-6.59	103.69	118.38
44	7	162	A2M	N6-C6-N1	-6.59	103.70	118.38
41	1	1371	OMU	C4-N3-C2	-6.59	118.43	126.61
42	2	1185	A2M	N6-C6-N1	-6.58	103.72	118.38
20	S1	2185	MA6	C5-C6-N6	6.57	135.73	125.33
41	1	1190	OMG	C1'-N9-C8	-6.57	108.08	126.73
44	7	43	A2M	N6-C6-N1	-6.56	103.76	118.38
20	S1	479	A2M	N6-C6-N1	-6.55	103.79	118.38
42	2	1231	OMG	C1'-N9-C8	-6.55	108.13	126.73
20	S1	668	A2M	N6-C6-N1	-6.53	103.83	118.38
44	7	75	OMG	C1'-N9-C8	-6.50	108.26	126.73
41	1	678	A2M	N6-C6-N1	-6.49	103.92	118.38
42	2	510	PSU	N1-C2-N3	6.45	121.97	115.17
20	S1	2184	MA6	C5-C6-N6	6.45	135.54	125.33
20	S1	2151	OMG	C1'-N9-C4	6.40	145.38	126.49
20	S1	897	A2M	N6-C6-N1	-6.38	104.18	118.38
20	S1	600	OMG	C1'-N9-C4	6.37	145.30	126.49
42	2	527	A2M	N6-C6-N1	-6.37	104.20	118.38
42	2	628	A2M	O4'-C1'-N9	6.36	120.31	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	382	A2M	N6-C6-N1	-6.36	104.21	118.38
42	2	655	OMG	C1'-N9-C8	-6.35	108.68	126.73
42	2	504	PSU	N1-C2-N3	6.35	121.87	115.17
41	1	856	OMG	C1'-N9-C8	-6.32	108.77	126.73
41	1	955	A2M	N6-C6-N1	-6.32	104.30	118.38
20	S1	1566	PSU	N1-C2-N3	6.32	121.83	115.17
42	2	1229	OMG	C1'-N9-C8	-6.30	108.83	126.73
42	2	527	A2M	C2'-C1'-N9	-6.30	103.39	113.75
41	1	1626	OMG	C1'-N9-C8	-6.30	108.85	126.73
42	2	628	A2M	N6-C6-N1	-6.28	104.40	118.38
42	2	1253	OMG	C1'-N9-C8	-6.27	108.92	126.73
20	S1	1829	OMG	C1'-N9-C4	6.26	144.98	126.49
42	2	1078	OMG	C1'-N9-C8	-6.25	108.97	126.73
41	1	1539	A2M	N6-C6-N1	-6.25	104.45	118.38
44	7	162	A2M	C4-N9-C1'	-6.22	112.08	126.63
20	S1	98	A2M	N6-C6-N1	-6.22	104.52	118.38
42	2	95	A2M	N6-C6-N1	-6.18	104.62	118.38
42	2	1384	A2M	N6-C6-N1	-6.16	104.65	118.38
20	S1	1550	OMG	C1'-N9-C4	6.15	144.64	126.49
43	4	74	OMG	C1'-N9-C8	-6.14	109.29	126.73
41	1	681	A2M	N6-C6-N1	-6.10	104.78	118.38
41	1	1540	OMG	C1'-N9-C8	-6.10	109.41	126.73
42	2	1046	OMG	C1'-N9-C4	6.09	144.47	126.49
41	1	1659	OMU	C4-N3-C2	-6.08	119.06	126.61
42	2	534	OMG	C1'-N9-C4	6.07	144.42	126.49
42	2	665	A2M	N6-C6-N1	-6.05	104.90	118.38
81	3	13	OMU	C4-N3-C2	-6.05	119.10	126.61
42	2	527	A2M	N3-C2-N1	-6.04	119.44	128.58
44	7	162	A2M	N3-C2-N1	-6.03	119.45	128.58
42	2	1077	OMU	C4-N3-C2	-6.02	119.13	126.61
42	2	1359	OMU	C4-N3-C2	-6.01	119.15	126.61
42	2	572	A2M	N3-C2-N1	-5.99	119.52	128.58
20	S1	1979	OMU	C4-N3-C2	-5.97	119.20	126.61
20	S1	1865	OMG	C1'-N9-C4	5.94	144.05	126.49
42	2	570	A2M	N6-C6-N1	-5.94	105.14	118.38
41	1	847	OMU	C4-N3-C2	-5.92	119.26	126.61
41	1	681	A2M	N9-C8-N7	-5.92	105.54	113.94
42	2	71	OMG	C1'-N9-C8	-5.92	109.91	126.73
44	7	162	A2M	N9-C8-N7	-5.90	105.56	113.94
41	1	1524	OMG	C1'-N9-C4	5.89	143.87	126.49
20	S1	1621	OMU	C4-N3-C2	-5.87	119.32	126.61
42	2	1372	A2M	N9-C8-N7	-5.87	105.61	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	7	43	A2M	N3-C2-N1	-5.84	119.74	128.58
42	2	667	OMU	C4-N3-C2	-5.84	119.37	126.61
41	1	1107	OMU	C4-N3-C2	-5.83	119.38	126.61
41	1	858	A2M	N3-C2-N1	-5.81	119.78	128.58
42	2	1185	A2M	N9-C8-N7	-5.81	105.69	113.94
41	1	858	A2M	C5-C6-N6	5.81	137.67	123.29
44	7	43	A2M	N9-C8-N7	-5.81	105.70	113.94
42	2	628	A2M	C5-C6-N6	5.80	137.65	123.29
41	1	1539	A2M	N3-C2-N1	-5.79	119.82	128.58
20	S1	2048	OMU	C4-N3-C2	-5.79	119.43	126.61
41	1	678	A2M	N3-C2-N1	-5.78	119.83	128.58
20	S1	668	A2M	N9-C8-N7	-5.77	105.75	113.94
42	2	570	A2M	N3-C2-N1	-5.76	119.86	128.58
20	S1	28	A2M	N9-C8-N7	-5.76	105.77	113.94
42	2	560	OMU	C4-N3-C2	-5.75	119.47	126.61
20	S1	2184	MA6	N1-C2-N3	-5.75	119.88	128.58
42	2	382	A2M	N3-C2-N1	-5.74	119.89	128.58
20	S1	1777	OMU	C4-N3-C2	-5.74	119.49	126.61
20	S1	28	A2M	N3-C2-N1	-5.73	119.90	128.58
20	S1	512	A2M	C5-C4-N3	-5.72	118.84	126.72
42	2	604	A2M	N9-C8-N7	-5.71	105.83	113.94
41	1	697	A2M	C5-C6-N6	5.71	137.42	123.29
42	2	527	A2M	N9-C8-N7	-5.69	105.86	113.94
20	S1	8	OMU	C4-N3-C2	-5.69	119.55	126.61
20	S1	2021	A2M	N3-C2-N1	-5.68	119.98	128.58
42	2	1372	A2M	N3-C2-N1	-5.68	119.98	128.58
42	2	1419	OMU	C4-N3-C2	-5.68	119.56	126.61
20	S1	98	A2M	N9-C8-N7	-5.67	105.89	113.94
42	2	665	A2M	N3-C2-N1	-5.67	120.00	128.58
20	S1	668	A2M	N3-C2-N1	-5.65	120.03	128.58
42	2	1372	A2M	C4-N9-C1'	-5.65	113.42	126.63
20	S1	1478	OMG	C1'-N9-C4	5.65	143.18	126.49
42	2	604	A2M	N3-C2-N1	-5.65	120.03	128.58
20	S1	2185	MA6	N1-C2-N3	-5.64	120.04	128.58
20	S1	28	A2M	C4-N9-C1'	-5.64	113.45	126.63
41	1	845	OMU	C4-N3-C2	-5.63	119.62	126.61
20	S1	661	OMU	C4-N3-C2	-5.63	119.62	126.61
42	2	1360	OMG	C1'-N9-C4	5.63	143.11	126.49
42	2	572	A2M	N9-C8-N7	-5.62	105.96	113.94
41	1	437	A2M	N3-C2-N1	-5.61	120.09	128.58
20	S1	479	A2M	C4-N9-C1'	-5.61	113.52	126.63
20	S1	668	A2M	C4-N9-C1'	-5.61	113.52	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	897	A2M	N9-C8-N7	-5.61	105.98	113.94
41	1	437	A2M	N9-C8-N7	-5.60	105.99	113.94
41	1	955	A2M	N9-C8-N7	-5.60	105.99	113.94
41	1	437	A2M	C4-N9-C1'	-5.60	113.55	126.63
20	S1	29	OMU	C4-N3-C2	-5.60	119.67	126.61
42	2	1185	A2M	N3-C2-N1	-5.59	120.12	128.58
41	1	697	A2M	N9-C8-N7	-5.59	106.01	113.94
20	S1	479	A2M	N9-C8-N7	-5.57	106.03	113.94
42	2	591	A2M	N3-C2-N1	-5.57	120.15	128.58
41	1	678	A2M	N9-C8-N7	-5.57	106.03	113.94
41	1	697	A2M	N3-C2-N1	-5.57	120.15	128.58
20	S1	479	A2M	N3-C2-N1	-5.55	120.18	128.58
42	2	570	A2M	C2'-C1'-N9	-5.55	104.62	113.75
42	2	604	A2M	C4-N9-C1'	-5.55	113.65	126.63
41	1	955	A2M	N3-C2-N1	-5.54	120.20	128.58
41	1	681	A2M	N3-C2-N1	-5.50	120.25	128.58
20	S1	897	A2M	N3-C2-N1	-5.50	120.25	128.58
42	2	1253	OMG	C1'-N9-C4	5.49	142.69	126.49
41	1	697	A2M	C4-N9-C1'	-5.49	113.80	126.63
42	2	1384	A2M	N3-C2-N1	-5.44	120.34	128.58
42	2	73	OMU	C4-N3-C2	-5.43	119.87	126.61
42	2	604	A2M	C5-C6-N6	5.42	136.70	123.29
42	2	665	A2M	N9-C8-N7	-5.42	106.25	113.94
42	2	665	A2M	C5-C4-N3	-5.41	119.26	126.72
44	7	43	A2M	C4-N9-C8	5.41	111.42	105.74
20	S1	1833	OMU	C4-N3-C2	-5.40	119.90	126.61
20	S1	98	A2M	N3-C2-N1	-5.40	120.40	128.58
41	1	681	A2M	C4-N9-C8	5.40	111.41	105.74
42	2	655	OMG	C1'-N9-C4	5.38	142.39	126.49
42	2	1372	A2M	C4-N9-C8	5.38	111.38	105.74
20	S1	1647	OMG	C1'-N9-C4	5.37	142.35	126.49
42	2	641	OMG	C1'-N9-C8	-5.37	111.48	126.73
42	2	1185	A2M	C4-N9-C1'	-5.36	114.10	126.63
41	1	678	A2M	C5-C4-N3	-5.36	119.34	126.72
42	2	95	A2M	N9-C8-N7	-5.36	106.34	113.94
44	7	75	OMG	C1'-N9-C4	5.36	142.31	126.49
42	2	597	PSU	C4-N3-C2	-5.35	119.00	126.37
41	1	1539	A2M	C4-N9-C1'	-5.35	114.13	126.63
42	2	591	A2M	C5-C6-N6	5.34	136.52	123.29
42	2	1384	A2M	N9-C8-N7	-5.34	106.36	113.94
42	2	570	A2M	N9-C8-N7	-5.34	106.36	113.94
41	1	437	A2M	C5-C6-N6	5.32	136.46	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	593	PSU	N1-C2-N3	5.32	120.78	115.17
41	1	1539	A2M	N9-C8-N7	-5.32	106.39	113.94
41	1	1190	OMG	C1'-N9-C4	5.31	142.18	126.49
20	S1	2021	A2M	N9-C8-N7	-5.31	106.40	113.94
42	2	1231	OMG	C1'-N9-C4	5.31	142.18	126.49
42	2	572	A2M	C5-C6-N6	5.31	136.43	123.29
42	2	527	A2M	C4-N9-C8	5.30	111.30	105.74
42	2	527	A2M	C4-N9-C1'	-5.29	114.27	126.63
44	7	162	A2M	C4-N9-C8	5.26	111.27	105.74
20	S1	2021	A2M	C5-C4-N3	-5.25	119.49	126.72
41	1	870	PSU	C4-N3-C2	-5.25	119.15	126.37
42	2	591	A2M	N9-C8-N7	-5.24	106.50	113.94
42	2	1185	A2M	C5-C6-N6	5.24	136.25	123.29
42	2	95	A2M	C5-C4-N3	-5.24	119.51	126.72
44	7	43	A2M	C5-C6-N6	5.23	136.25	123.29
42	2	382	A2M	N9-C8-N7	-5.23	106.51	113.94
20	S1	479	A2M	C5-C6-N6	5.23	136.24	123.29
44	7	162	A2M	C5-C6-N6	5.22	136.22	123.29
20	S1	98	A2M	C4-N9-C1'	-5.22	114.42	126.63
42	2	570	A2M	C5-C4-N3	-5.21	119.54	126.72
41	1	1533	PSU	N1-C2-N3	5.21	120.66	115.17
20	S1	897	A2M	C4-N9-C1'	-5.20	114.47	126.63
42	2	628	A2M	N3-C2-N1	-5.19	120.72	128.58
20	S1	28	A2M	C5-C6-N6	5.19	136.13	123.29
41	1	955	A2M	C5-C4-N3	-5.18	119.58	126.72
20	S1	2021	A2M	C5-C6-N6	5.18	136.11	123.29
41	1	1539	A2M	C5-C6-N6	5.18	136.10	123.29
42	2	437	PSU	C4-N3-C2	-5.17	119.24	126.37
42	2	1185	A2M	C4-N9-C8	5.17	111.17	105.74
20	S1	668	A2M	C5-C6-N6	5.17	136.08	123.29
42	2	1372	A2M	C5-C6-N6	5.17	136.08	123.29
43	4	74	OMG	C1'-N9-C4	5.16	141.74	126.49
42	2	1229	OMG	C1'-N9-C4	5.16	141.72	126.49
42	2	78	PSU	C4-N3-C2	-5.16	119.27	126.37
42	2	1144	PSU	C4-N3-C2	-5.15	119.28	126.37
42	2	591	A2M	C5-C4-N3	-5.15	119.63	126.72
42	2	1194	PSU	C4-N3-C2	-5.14	119.29	126.37
42	2	1382	PSU	C4-N3-C2	-5.14	119.29	126.37
42	2	572	A2M	C4-N9-C1'	-5.14	114.61	126.63
41	1	1626	OMG	C1'-N9-C4	5.14	141.68	126.49
41	1	681	A2M	C5-C4-N3	-5.14	119.64	126.72
41	1	1533	PSU	C4-N3-C2	-5.14	119.29	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	98	A2M	C4-N9-C8	5.14	111.13	105.74
42	2	95	A2M	N3-C2-N1	-5.12	120.83	128.58
41	1	856	OMG	C1'-N9-C4	5.12	141.62	126.49
42	2	1194	PSU	N1-C2-N3	5.10	120.55	115.17
41	1	1540	OMG	C1'-N9-C4	5.10	141.56	126.49
41	1	672	PSU	C4-N3-C2	-5.09	119.36	126.37
42	2	1078	OMG	C1'-N9-C4	5.08	141.50	126.49
42	2	597	PSU	N1-C2-N3	5.07	120.52	115.17
42	2	593	PSU	C4-N3-C2	-5.07	119.39	126.37
20	S1	28	A2M	C4-N9-C8	5.06	111.05	105.74
42	2	1144	PSU	N1-C2-N3	5.06	120.50	115.17
41	1	422	PSU	C4-N3-C2	-5.05	119.42	126.37
41	1	858	A2M	C5-C4-N3	-5.04	119.77	126.72
42	2	1384	A2M	C4-N9-C1'	-5.04	114.84	126.63
42	2	604	A2M	C4-N9-C8	5.04	111.03	105.74
20	S1	897	A2M	C5-C6-N6	5.04	135.76	123.29
20	S1	668	A2M	C4-N9-C8	5.04	111.03	105.74
42	2	1384	A2M	C5-C6-N6	5.02	135.72	123.29
42	2	382	A2M	C5-C6-N6	5.02	135.71	123.29
42	2	1354	PSU	C4-N3-C2	-5.02	119.46	126.37
42	2	1318	PSU	C4-N3-C2	-5.01	119.47	126.37
41	1	955	A2M	C5-C6-N6	5.01	135.69	123.29
41	1	858	A2M	N9-C8-N7	-5.01	106.83	113.94
42	2	572	A2M	C5-C4-N3	-5.01	119.82	126.72
44	7	74	PSU	C4-N3-C2	-5.00	119.48	126.37
44	7	43	A2M	C4-N9-C1'	-5.00	114.94	126.63
41	1	672	PSU	N1-C2-N3	4.99	120.43	115.17
20	S1	98	A2M	C5-C6-N6	4.99	135.64	123.29
42	2	1361	PSU	C4-N3-C2	-4.99	119.50	126.37
20	S1	897	A2M	C4-N9-C8	4.99	110.97	105.74
20	S1	1533	PSU	C4-N3-C2	-4.99	119.50	126.37
42	2	1384	A2M	C5-C4-N3	-4.98	119.86	126.72
20	S1	2046	PSU	C4-N3-C2	-4.97	119.52	126.37
20	S1	12	PSU	C4-N3-C2	-4.96	119.54	126.37
41	1	678	A2M	C5-C6-N6	4.96	135.57	123.29
42	2	1303	PSU	C4-N3-C2	-4.96	119.54	126.37
42	2	382	A2M	C5-C4-N3	-4.95	119.90	126.72
41	1	1011	PSU	C4-N3-C2	-4.95	119.56	126.37
20	S1	12	PSU	N1-C2-N3	4.93	120.37	115.17
42	2	1264	PSU	C4-N3-C2	-4.93	119.58	126.37
42	2	1384	A2M	C4-N9-C8	4.92	110.91	105.74
42	2	570	A2M	C4-N9-C8	4.91	110.90	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	527	A2M	C5-C6-N6	4.91	135.45	123.29
42	2	95	A2M	C5-C6-N6	4.91	135.45	123.29
20	S1	479	A2M	C4-N9-C8	4.91	110.89	105.74
41	1	1528	PSU	C4-N3-C2	-4.91	119.61	126.37
20	S1	2021	A2M	C4-N9-C1'	-4.90	115.17	126.63
41	1	959	OMG	C5-C4-N3	-4.90	120.59	128.39
42	2	1303	PSU	N1-C2-N3	4.90	120.33	115.17
42	2	1354	PSU	N1-C2-N3	4.89	120.33	115.17
44	7	69	PSU	C4-N3-C2	-4.89	119.63	126.37
20	S1	455	PSU	C4-N3-C2	-4.89	119.63	126.37
42	2	572	A2M	C4-N9-C8	4.87	110.86	105.74
41	1	1524	OMG	C5-C4-N3	-4.87	120.64	128.39
20	S1	1841	PSU	C4-N3-C2	-4.87	119.67	126.37
41	1	847	OMU	N3-C2-N1	4.86	121.22	114.89
20	S1	897	A2M	C5-C4-N3	-4.86	120.02	126.72
41	1	681	A2M	C4-N9-C1'	-4.86	115.26	126.63
42	2	1185	A2M	C5-C4-N3	-4.86	120.03	126.72
20	S1	98	A2M	C5-C4-N3	-4.85	120.04	126.72
41	1	437	A2M	C5-C4-N3	-4.85	120.04	126.72
42	2	1361	PSU	N1-C2-N3	4.84	120.28	115.17
41	1	678	A2M	C4-N9-C8	4.84	110.82	105.74
42	2	382	A2M	C4-N9-C1'	-4.84	115.32	126.63
20	S1	2046	PSU	N1-C2-N3	4.83	120.26	115.17
42	2	665	A2M	C5-C6-N6	4.83	135.24	123.29
20	S1	33	PSU	C4-N3-C2	-4.82	119.73	126.37
20	S1	609	PSU	C4-N3-C2	-4.82	119.73	126.37
41	1	955	A2M	C4-N9-C8	4.82	110.80	105.74
20	S1	104	PSU	C4-N3-C2	-4.82	119.73	126.37
41	1	422	PSU	N1-C2-N3	4.82	120.25	115.17
41	1	681	A2M	C5-C6-N6	4.81	135.20	123.29
44	7	43	A2M	C5-C4-N3	-4.81	120.10	126.72
20	S1	455	PSU	N1-C2-N3	4.81	120.24	115.17
41	1	940	PSU	C4-N3-C2	-4.80	119.75	126.37
42	2	1413	PSU	C4-N3-C2	-4.80	119.75	126.37
42	2	71	OMG	C1'-N9-C4	4.80	140.67	126.49
42	2	382	A2M	C4-N9-C8	4.80	110.77	105.74
42	2	1229	OMG	C2-N3-C4	4.79	120.54	112.30
20	S1	668	A2M	C5-C4-N3	-4.78	120.13	126.72
20	S1	479	A2M	C5-C4-N3	-4.77	120.15	126.72
42	2	95	A2M	C4-N9-C1'	-4.77	115.48	126.63
42	2	472	PSU	C4-N3-C2	-4.77	119.80	126.37
41	1	437	A2M	C4-N9-C8	4.77	110.74	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1657	PSU	C4-N3-C2	-4.77	119.81	126.37
42	2	437	PSU	N1-C2-N3	4.76	120.19	115.17
42	2	628	A2M	C4-N9-C1'	-4.76	115.50	126.63
42	2	626	PSU	C4-N3-C2	-4.76	119.82	126.37
41	1	239	PSU	C4-N3-C2	-4.75	119.82	126.37
42	2	591	A2M	C4-N9-C1'	-4.75	115.52	126.63
41	1	681	A2M	N3-C4-N9	4.75	135.24	127.17
41	1	678	A2M	N3-C4-N9	4.74	135.23	127.17
20	S1	1478	OMG	C2-N3-C4	4.74	120.46	112.30
41	1	1539	A2M	C5-C4-N3	-4.74	120.19	126.72
20	S1	28	A2M	C5-C4-N3	-4.73	120.20	126.72
20	S1	1156	PSU	C4-N3-C2	-4.73	119.86	126.37
42	2	527	A2M	C5-C4-N3	-4.72	120.21	126.72
42	2	665	A2M	N3-C4-N9	4.71	135.17	127.17
41	1	1181	PSU	C4-N3-C2	-4.70	119.89	126.37
42	2	570	A2M	N3-C4-N9	4.69	135.15	127.17
41	1	1371	OMU	N3-C2-N1	4.69	121.00	114.89
41	1	1402	PSU	N1-C2-N3	4.69	120.11	115.17
42	2	1372	A2M	C5-C4-N3	-4.68	120.27	126.72
41	1	697	A2M	C5-C4-N3	-4.68	120.27	126.72
42	2	626	PSU	N1-C2-N3	4.68	120.11	115.17
42	2	662	PSU	C4-N3-C2	-4.68	119.92	126.37
44	7	74	PSU	N1-C2-N3	4.68	120.10	115.17
42	2	604	A2M	C5-C4-N3	-4.68	120.28	126.72
41	1	1539	A2M	C4-N9-C8	4.67	110.64	105.74
42	2	665	A2M	C4-N9-C8	4.66	110.64	105.74
41	1	697	A2M	C4-N9-C8	4.66	110.63	105.74
20	S1	1623	OMG	C5-C4-N3	-4.66	120.98	128.39
41	1	1011	PSU	N1-C2-N3	4.65	120.08	115.17
20	S1	2202	PSU	C4-N3-C2	-4.65	119.97	126.37
20	S1	2151	OMG	C5-C4-N3	-4.64	121.00	128.39
41	1	1402	PSU	C4-N3-C2	-4.64	119.98	126.37
42	2	662	PSU	N1-C2-N3	4.64	120.06	115.17
42	2	1253	OMG	C2-N3-C4	4.64	120.29	112.30
42	2	1060	PSU	C4-N3-C2	-4.63	119.99	126.37
41	1	870	PSU	N1-C2-N3	4.63	120.05	115.17
42	2	1264	PSU	N1-C2-N3	4.62	120.05	115.17
41	1	1171	PSU	C4-N3-C2	-4.62	120.01	126.37
42	2	1231	OMG	C2-N3-C4	4.61	120.23	112.30
20	S1	1841	PSU	N1-C2-N3	4.60	120.02	115.17
20	S1	512	A2M	C2'-C1'-N9	-4.60	106.17	113.75
42	2	570	A2M	C5-C6-N6	4.60	134.68	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	1060	PSU	N1-C2-N3	4.60	120.02	115.17
41	1	1664	PSU	C4-N3-C2	-4.60	120.04	126.37
41	1	858	A2M	C4-N9-C1'	-4.60	115.88	126.63
20	S1	2021	A2M	C4-N9-C8	4.59	110.56	105.74
42	2	1403	PSU	C4-N3-C2	-4.59	120.05	126.37
20	S1	1533	PSU	N1-C2-N3	4.58	119.99	115.17
42	2	382	A2M	N3-C4-N9	4.57	134.94	127.17
41	1	856	OMG	C2-N3-C4	4.57	120.17	112.30
20	S1	1539	PSU	C4-N3-C2	-4.57	120.07	126.37
41	1	1181	PSU	N1-C2-N3	4.56	119.98	115.17
41	1	959	OMG	C2-N3-C4	4.56	120.15	112.30
42	2	1078	OMG	C2-N3-C4	4.56	120.15	112.30
20	S1	2202	PSU	N1-C2-N3	4.55	119.97	115.17
44	7	43	A2M	N3-C4-N9	4.55	134.91	127.17
20	S1	2184	MA6	C5-C4-N3	-4.54	120.47	126.72
41	1	1540	OMG	C2-N3-C4	4.54	120.11	112.30
20	S1	512	A2M	N3-C4-N9	4.54	134.88	127.17
20	S1	1995	G7M	C2-N3-C4	4.54	120.11	112.30
41	1	1524	OMG	C2-N3-C4	4.53	120.11	112.30
41	1	955	A2M	N3-C4-N9	4.53	134.88	127.17
44	7	75	OMG	C2-N3-C4	4.53	120.10	112.30
41	1	678	A2M	C4-N9-C1'	-4.53	116.05	126.63
20	S1	600	OMG	C5-C4-N3	-4.52	121.20	128.39
42	2	95	A2M	C4-N9-C8	4.51	110.48	105.74
41	1	1190	OMG	C2-N3-C4	4.51	120.08	112.30
20	S1	33	PSU	N1-C2-N3	4.51	119.93	115.17
42	2	641	OMG	N9-C8-N7	-4.51	105.03	113.40
41	1	1017	PSU	C4-N3-C2	-4.51	120.16	126.37
20	S1	2185	MA6	C5-C4-N3	-4.51	120.51	126.72
20	S1	2151	OMG	C2-N3-C4	4.51	120.06	112.30
42	2	1265	PSU	C4-N3-C2	-4.50	120.17	126.37
20	S1	1539	PSU	N1-C2-N3	4.50	119.91	115.17
20	S1	609	PSU	N1-C2-N3	4.50	119.91	115.17
44	7	69	PSU	N1-C2-N3	4.49	119.90	115.17
42	2	1058	PSU	N1-C2-N3	4.48	119.89	115.17
42	2	1046	OMG	C2-N3-C4	4.48	120.02	112.30
42	2	641	OMG	C2-N3-C4	4.48	120.01	112.30
43	4	74	OMG	C2-N3-C4	4.47	120.00	112.30
42	2	1413	PSU	N1-C2-N3	4.47	119.88	115.17
42	2	1384	A2M	N3-C4-N9	4.47	134.77	127.17
20	S1	1246	PSU	C4-N3-C2	-4.47	120.22	126.37
41	1	1017	PSU	N1-C2-N3	4.46	119.88	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	955	A2M	C4-N9-C1'	-4.46	116.21	126.63
42	2	1058	PSU	C4-N3-C2	-4.46	120.23	126.37
42	2	472	PSU	N1-C2-N3	4.45	119.86	115.17
42	2	591	A2M	C4-N9-C8	4.44	110.40	105.74
41	1	940	PSU	N1-C2-N3	4.44	119.85	115.17
44	7	162	A2M	C5-C4-N3	-4.44	120.61	126.72
20	S1	1865	OMG	C2-N3-C4	4.44	119.94	112.30
41	1	1626	OMG	C2-N3-C4	4.43	119.93	112.30
20	S1	607	PSU	C4-N3-C2	-4.42	120.28	126.37
20	S1	607	PSU	N1-C2-N3	4.42	119.83	115.17
20	S1	2021	A2M	N3-C4-N9	4.42	134.69	127.17
20	S1	600	OMG	C2-N3-C4	4.39	119.86	112.30
20	S1	1623	OMG	C2-N3-C4	4.39	119.86	112.30
20	S1	1550	OMG	C2-N3-C4	4.39	119.86	112.30
20	S1	104	PSU	N1-C2-N3	4.38	119.79	115.17
42	2	1382	PSU	N1-C2-N3	4.38	119.78	115.17
42	2	1360	OMG	C2-N3-C4	4.37	119.82	112.30
42	2	655	OMG	C2-N3-C4	4.36	119.82	112.30
20	S1	2184	MA6	N9-C8-N7	-4.36	107.75	113.94
20	S1	1550	OMG	C5-C4-N3	-4.36	121.45	128.39
42	2	591	A2M	N3-C4-N9	4.36	134.58	127.17
20	S1	1156	PSU	N1-C2-N3	4.35	119.76	115.17
41	1	1171	PSU	N1-C2-N3	4.34	119.75	115.17
42	2	1318	PSU	N1-C2-N3	4.34	119.74	115.17
42	2	95	A2M	N3-C4-N9	4.31	134.49	127.17
42	2	78	PSU	N1-C2-N3	4.30	119.71	115.17
20	S1	98	A2M	N3-C4-N9	4.30	134.47	127.17
42	2	667	OMU	N3-C2-N1	4.30	120.48	114.89
20	S1	1543	C4J	C4-N3-C2	-4.30	120.33	125.62
42	2	534	OMG	C2-N3-C4	4.29	119.69	112.30
20	S1	2185	MA6	N9-C8-N7	-4.28	107.86	113.94
20	S1	1566	PSU	C4-N3-C2	-4.28	120.48	126.37
42	2	1046	OMG	C5-C4-N3	-4.28	121.58	128.39
41	1	1528	PSU	N1-C2-N3	4.28	119.68	115.17
20	S1	1192	PSU	C4-N3-C2	-4.27	120.48	126.37
42	2	572	A2M	N3-C4-N9	4.26	134.41	127.17
44	7	162	A2M	C1'-N9-C8	4.26	136.54	127.09
42	2	1403	PSU	N1-C2-N3	4.26	119.66	115.17
42	2	665	A2M	C4-N9-C1'	-4.25	116.68	126.63
42	2	1359	OMU	N3-C2-N1	4.25	120.42	114.89
20	S1	1478	OMG	C5-C4-N3	-4.25	121.63	128.39
20	S1	1246	PSU	N1-C2-N3	4.24	119.64	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1995	G7M	C5-C4-N3	-4.24	120.14	128.15
42	2	527	A2M	N3-C4-N9	4.24	134.37	127.17
20	S1	1647	OMG	C2-N3-C4	4.23	119.58	112.30
42	2	506	PSU	C4-N3-C2	-4.23	120.55	126.37
42	2	1265	PSU	N1-C2-N3	4.23	119.62	115.17
20	S1	1865	OMG	C5-C4-N3	-4.22	121.67	128.39
41	1	1664	PSU	N1-C2-N3	4.21	119.61	115.17
41	1	239	PSU	N1-C2-N3	4.20	119.60	115.17
42	2	1185	A2M	N3-C4-N9	4.20	134.31	127.17
42	2	1077	OMU	N3-C2-N1	4.19	120.35	114.89
81	3	13	OMU	C5-C4-N3	4.19	120.67	114.80
20	S1	897	A2M	N3-C4-N9	4.18	134.28	127.17
41	1	1659	OMU	C5-C4-N3	4.17	120.64	114.80
20	S1	1829	OMG	C2-N3-C4	4.16	119.47	112.30
42	2	73	OMU	N3-C2-N1	4.15	120.30	114.89
41	1	1371	OMU	C5-C4-N3	4.15	120.62	114.80
41	1	1190	OMG	C5-C4-N3	-4.15	121.78	128.39
20	S1	1829	OMG	C5-C4-N3	-4.15	121.78	128.39
41	1	1539	A2M	N3-C4-N9	4.13	134.18	127.17
42	2	71	OMG	C2-N3-C4	4.11	119.38	112.30
20	S1	29	OMU	N3-C2-N1	4.10	120.23	114.89
42	2	655	OMG	C5-C4-N3	-4.10	121.86	128.39
42	2	1360	OMG	C5-C4-N3	-4.09	121.88	128.39
20	S1	1657	PSU	N1-C2-N3	4.07	119.46	115.17
42	2	504	PSU	C4-N3-C2	-4.07	120.77	126.37
42	2	534	OMG	C5-C4-N3	-4.07	121.92	128.39
20	S1	1192	PSU	N1-C2-N3	4.07	119.46	115.17
41	1	1107	OMU	C5-C4-N3	4.06	120.49	114.80
42	2	510	PSU	C4-N3-C2	-4.05	120.79	126.37
42	2	1359	OMU	C5-C4-N3	4.05	120.47	114.80
42	2	560	OMU	N3-C2-N1	4.05	120.16	114.89
42	2	570	A2M	C4-N9-C1'	-4.05	117.17	126.63
42	2	1078	OMG	N9-C8-N7	-4.04	105.91	113.40
41	1	856	OMG	C5-C4-N3	-4.04	121.96	128.39
42	2	504	PSU	C3'-C2'-C1'	4.03	106.45	101.69
41	1	858	A2M	C4-N9-C8	4.03	109.97	105.74
42	2	1372	A2M	N3-C4-N9	4.03	134.02	127.17
20	S1	479	A2M	N3-C4-N9	4.03	134.01	127.17
20	S1	1777	OMU	N3-C2-N1	4.02	120.12	114.89
41	1	1659	OMU	N3-C2-N1	4.01	120.11	114.89
42	2	500	PSU	C4-N3-C2	-4.00	120.86	126.37
41	1	437	A2M	N3-C4-N9	3.98	133.94	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1979	OMU	N3-C2-N1	3.98	120.08	114.89
44	7	75	OMG	C5-C4-N3	-3.98	122.06	128.39
20	S1	668	A2M	N3-C4-N9	3.98	133.93	127.17
42	2	1253	OMG	C5-C4-N3	-3.97	122.08	128.39
41	1	858	A2M	N3-C4-N9	3.96	133.91	127.17
42	2	1229	OMG	C5-C4-N3	-3.96	122.08	128.39
42	2	504	PSU	O2-C2-N1	-3.96	118.71	122.79
42	2	641	OMG	C1'-N9-C4	3.96	138.18	126.49
20	S1	1995	G7M	C5-C6-N1	3.95	120.00	111.84
42	2	1419	OMU	N3-C2-N1	3.95	120.03	114.89
42	2	1419	OMU	C5-C4-N3	3.94	120.33	114.80
42	2	604	A2M	N3-C4-N9	3.94	133.87	127.17
20	S1	1647	OMG	N9-C8-N7	-3.94	106.09	113.40
41	1	845	OMU	N3-C2-N1	3.94	120.02	114.89
20	S1	1979	OMU	C5-C4-N3	3.94	120.31	114.80
20	S1	1621	OMU	N3-C2-N1	3.94	120.01	114.89
20	S1	8	OMU	N3-C2-N1	3.93	120.00	114.89
81	3	13	OMU	N3-C2-N1	3.92	119.99	114.89
41	1	1402	PSU	C6-N1-C2	-3.92	119.06	122.69
20	S1	28	A2M	N3-C4-N9	3.91	133.81	127.17
20	S1	2184	MA6	C4-C5-C6	3.91	119.95	115.91
44	7	75	OMG	N9-C8-N7	-3.90	106.16	113.40
42	2	667	OMU	C5-C4-N3	3.90	120.27	114.80
20	S1	1833	OMU	N3-C2-N1	3.90	119.97	114.89
41	1	856	OMG	N9-C8-N7	-3.90	106.17	113.40
41	1	845	OMU	C5-C4-N3	3.89	120.25	114.80
41	1	1190	OMG	N9-C8-N7	-3.89	106.18	113.40
41	1	1540	OMG	C5-C4-N3	-3.89	122.20	128.39
20	S1	661	OMU	N3-C2-N1	3.89	119.95	114.89
41	1	437	A2M	C1'-N9-C8	3.88	135.70	127.09
41	1	1533	PSU	C6-N1-C2	-3.87	119.10	122.69
20	S1	2048	OMU	N3-C2-N1	3.87	119.92	114.89
20	S1	2048	OMU	C5-C4-N3	3.86	120.20	114.80
41	1	697	A2M	N3-C4-N9	3.85	133.72	127.17
42	2	1078	OMG	C5-C4-N3	-3.85	122.26	128.39
20	S1	1647	OMG	C5-C4-N3	-3.85	122.26	128.39
42	2	1231	OMG	C5-C4-N3	-3.85	122.27	128.39
42	2	1077	OMU	C5-C4-N3	3.85	120.19	114.80
41	1	1626	OMG	C5-C4-N3	-3.84	122.28	128.39
20	S1	1621	OMU	C5-C4-N3	3.84	120.18	114.80
41	1	1540	OMG	N9-C8-N7	-3.83	106.29	113.40
20	S1	479	A2M	C1'-N9-C8	3.83	135.59	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1626	OMG	N9-C8-N7	-3.83	106.31	113.40
41	1	697	A2M	C1'-N9-C8	3.81	135.56	127.09
42	2	1361	PSU	C6-N1-C2	-3.81	119.16	122.69
42	2	628	A2M	C4-N9-C8	3.81	109.73	105.74
42	2	1229	OMG	N9-C8-N7	-3.80	106.34	113.40
42	2	71	OMG	N9-C8-N7	-3.79	106.37	113.40
20	S1	28	A2M	C1'-N9-C8	3.78	135.48	127.09
42	2	655	OMG	N9-C8-N7	-3.77	106.41	113.40
20	S1	668	A2M	C1'-N9-C8	3.76	135.45	127.09
41	1	1533	PSU	O2-C2-N1	-3.76	118.91	122.79
42	2	1060	PSU	C6-N1-C2	-3.76	119.20	122.69
20	S1	1777	OMU	C5-C4-N3	3.76	120.06	114.80
41	1	1402	PSU	O2-C2-N1	-3.74	118.93	122.79
20	S1	512	A2M	C2-N3-C4	3.74	120.98	111.83
42	2	628	A2M	N9-C8-N7	-3.74	108.63	113.94
20	S1	8	OMU	C5-C4-N3	3.73	120.03	114.80
20	S1	12	PSU	C6-C5-C4	3.73	120.69	118.17
20	S1	661	OMU	C5-C4-N3	3.73	120.02	114.80
20	S1	2151	OMG	N9-C8-N7	-3.73	106.49	113.40
42	2	1231	OMG	N9-C8-N7	-3.72	106.49	113.40
20	S1	1478	OMG	N9-C8-N7	-3.72	106.50	113.40
43	4	74	OMG	C5-C4-N3	-3.72	122.47	128.39
42	2	524	5MC	C5-C6-N1	-3.70	119.30	123.31
42	2	604	A2M	C1'-N9-C8	3.70	135.30	127.09
41	1	1171	PSU	C6-N1-C2	-3.69	119.26	122.69
42	2	1360	OMG	N9-C8-N7	-3.69	106.56	113.40
42	2	506	PSU	O2-C2-N1	-3.68	118.99	122.79
42	2	593	PSU	C6-N1-C2	-3.67	119.28	122.69
41	1	1107	OMU	N3-C2-N1	3.67	119.67	114.89
20	S1	1246	PSU	C6-N1-C2	-3.66	119.30	122.69
42	2	641	OMG	C5-C4-N3	-3.65	122.57	128.39
41	1	858	A2M	C2-N3-C4	3.65	120.75	111.83
42	2	1372	A2M	C1'-N9-C8	3.65	135.19	127.09
20	S1	1829	OMG	N9-C8-N7	-3.63	106.66	113.40
20	S1	607	PSU	C6-N1-C2	-3.62	119.33	122.69
44	7	162	A2M	N3-C4-N9	3.61	133.31	127.17
41	1	1539	A2M	C1'-N9-C8	3.60	135.08	127.09
20	S1	600	OMG	N9-C8-N7	-3.59	106.74	113.40
42	2	1046	OMG	N9-C8-N7	-3.59	106.75	113.40
42	2	534	OMG	N9-C8-N7	-3.58	106.76	113.40
42	2	570	A2M	C2-N3-C4	3.57	120.56	111.83
42	2	1185	A2M	C5-N7-C8	3.57	109.06	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	4	74	OMG	N9-C8-N7	-3.56	106.80	113.40
20	S1	2046	PSU	C6-N1-C2	-3.55	119.39	122.69
42	2	572	A2M	C2-N3-C4	3.55	120.50	111.83
20	S1	668	A2M	C5-N7-C8	3.55	109.03	103.45
41	1	1524	OMG	N9-C8-N7	-3.54	106.83	113.40
20	S1	29	OMU	C5-C4-N3	3.53	119.75	114.80
20	S1	1865	OMG	N9-C8-N7	-3.53	106.86	113.40
42	2	500	PSU	O2-C2-N1	-3.52	119.15	122.79
20	S1	512	A2M	C4-C5-N7	-3.52	106.55	110.58
20	S1	2185	MA6	C4-C5-C6	3.52	119.55	115.91
20	S1	1539	PSU	C6-N1-C2	-3.52	119.42	122.69
42	2	662	PSU	C6-N1-C2	-3.52	119.42	122.69
42	2	560	OMU	C5-C4-N3	3.52	119.73	114.80
42	2	527	A2M	O4'-C1'-N9	3.52	114.84	108.09
20	S1	2061	5MC	C5-C6-N1	-3.51	119.50	123.31
20	S1	2184	MA6	C2-N1-C6	3.51	120.40	111.83
42	2	527	A2M	C2-N3-C4	3.51	120.40	111.83
42	2	665	A2M	C2-N3-C4	3.51	120.39	111.83
20	S1	1544	5MC	C5-C6-N1	-3.51	119.51	123.31
41	1	678	A2M	C2-N3-C4	3.50	120.39	111.83
41	1	697	A2M	C5-N7-C8	3.50	108.95	103.45
42	2	500	PSU	C3'-C2'-C1'	3.50	105.82	101.69
20	S1	1623	OMG	N9-C8-N7	-3.50	106.91	113.40
41	1	422	PSU	C6-N1-C2	-3.50	119.44	122.69
20	S1	2021	A2M	C2-N3-C4	3.50	120.37	111.83
42	2	1058	PSU	C6-N1-C2	-3.49	119.46	122.69
41	1	681	A2M	C5-N7-C8	3.48	108.92	103.45
20	S1	1550	OMG	N9-C8-N7	-3.47	106.96	113.40
42	2	506	PSU	C3'-C2'-C1'	3.47	105.79	101.69
42	2	1194	PSU	C6-N1-C2	-3.46	119.48	122.69
42	2	1354	PSU	C6-N1-C2	-3.46	119.48	122.69
41	1	955	A2M	C5-N7-C8	3.46	108.89	103.45
42	2	510	PSU	O2-C2-N1	-3.46	119.22	122.79
42	2	628	A2M	C1'-N9-C8	3.45	134.76	127.09
42	2	604	A2M	C5-N7-C8	3.45	108.87	103.45
20	S1	455	PSU	C6-N1-C2	-3.45	119.49	122.69
20	S1	1833	OMU	C5-C4-N3	3.44	119.62	114.80
42	2	1185	A2M	C1'-N9-C8	3.44	134.73	127.09
41	1	955	A2M	C2-N3-C4	3.43	120.21	111.83
42	2	1403	PSU	C6-N1-C2	-3.42	119.51	122.69
42	2	570	A2M	O2'-C2'-C1'	3.42	115.48	108.99
41	1	437	A2M	C5-N7-C8	3.41	108.81	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1566	PSU	O2-C2-N1	-3.41	119.27	122.79
20	S1	28	A2M	C5-N7-C8	3.41	108.81	103.45
20	S1	2202	PSU	C6-N1-C2	-3.40	119.53	122.69
20	S1	1192	PSU	C6-N1-C2	-3.40	119.54	122.69
42	2	665	A2M	C5-N7-C8	3.40	108.79	103.45
41	1	847	OMU	C5-C4-N3	3.40	119.56	114.80
20	S1	897	A2M	C5-N7-C8	3.39	108.78	103.45
20	S1	28	A2M	C2-N3-C4	3.39	120.12	111.83
20	S1	1841	PSU	C6-N1-C2	-3.39	119.54	122.69
20	S1	512	A2M	N3-C2-N1	-3.39	123.45	128.58
20	S1	2185	MA6	C2-N1-C6	3.38	120.09	111.83
42	2	1253	OMG	N9-C8-N7	-3.38	107.13	113.40
20	S1	668	A2M	C2-N3-C4	3.38	120.08	111.83
44	7	162	A2M	C2-N3-C4	3.38	120.08	111.83
41	1	681	A2M	C2-N3-C4	3.38	120.08	111.83
42	2	1372	A2M	C5-N7-C8	3.37	108.75	103.45
20	S1	98	A2M	C5-N7-C8	3.37	108.75	103.45
44	7	162	A2M	C5-N7-C8	3.36	108.74	103.45
20	S1	897	A2M	C1'-N9-C8	3.36	134.55	127.09
42	2	73	OMU	C5-C4-N3	3.36	119.50	114.80
42	2	1372	A2M	C2-N3-C4	3.36	120.03	111.83
42	2	572	A2M	C1'-N9-C8	3.35	134.54	127.09
42	2	382	A2M	C2-N3-C4	3.35	120.02	111.83
44	7	43	A2M	C5-N7-C8	3.34	108.71	103.45
41	1	678	A2M	C5-N7-C8	3.34	108.70	103.45
42	2	1265	PSU	C6-N1-C2	-3.34	119.59	122.69
42	2	572	A2M	C5-N7-C8	3.34	108.70	103.45
42	2	591	A2M	C5-N7-C8	3.34	108.70	103.45
20	S1	1566	PSU	C3'-C2'-C1'	3.34	105.63	101.69
20	S1	479	A2M	C5-N7-C8	3.33	108.69	103.45
42	2	71	OMG	C5-C4-N3	-3.32	123.10	128.39
42	2	591	A2M	C2-N3-C4	3.32	119.94	111.83
20	S1	12	PSU	C6-N1-C2	-3.32	119.61	122.69
20	S1	98	A2M	C1'-N9-C8	3.31	134.45	127.09
42	2	527	A2M	C5-N7-C8	3.31	108.66	103.45
44	7	43	A2M	C2-N3-C4	3.31	119.91	111.83
20	S1	2185	MA6	C2-N3-C4	3.31	119.91	111.83
41	1	1181	PSU	C6-N1-C2	-3.31	119.62	122.69
20	S1	609	PSU	C6-N1-C2	-3.30	119.62	122.69
41	1	1539	A2M	C5-N7-C8	3.30	108.64	103.45
41	1	1017	PSU	C6-N1-C2	-3.30	119.63	122.69
41	1	437	A2M	C2-N3-C4	3.30	119.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	1361	PSU	O2-C2-N1	-3.30	119.39	122.79
42	2	1144	PSU	C6-N1-C2	-3.29	119.64	122.69
41	1	1524	OMG	C2-N1-C6	-3.28	119.16	125.11
20	S1	2048	OMU	O4-C4-C5	-3.28	119.51	125.16
42	2	1185	A2M	C2-N3-C4	3.27	119.83	111.83
42	2	1303	PSU	C6-N1-C2	-3.27	119.66	122.69
20	S1	1995	G7M	O6-C6-C5	-3.27	120.72	128.01
20	S1	897	A2M	C2-N3-C4	3.26	119.80	111.83
20	S1	479	A2M	C2-N3-C4	3.26	119.80	111.83
41	1	1664	PSU	C6-N1-C2	-3.26	119.67	122.69
42	2	604	A2M	C2-N3-C4	3.25	119.78	111.83
42	2	597	PSU	C6-N1-C2	-3.25	119.68	122.69
20	S1	2184	MA6	C2-N3-C4	3.24	119.75	111.83
20	S1	1657	PSU	C6-N1-C2	-3.24	119.68	122.69
42	2	472	PSU	C6-N1-C2	-3.24	119.69	122.69
41	1	1011	PSU	C6-C5-C4	3.23	120.36	118.17
42	2	1264	PSU	C6-N1-C2	-3.23	119.69	122.69
20	S1	33	PSU	C6-N1-C2	-3.23	119.69	122.69
42	2	527	A2M	C1'-N9-C8	3.23	134.25	127.09
42	2	1384	A2M	C1'-N9-C8	3.22	134.25	127.09
41	1	1371	OMU	C1'-N1-C2	3.22	123.38	117.59
41	1	672	PSU	C6-N1-C2	-3.22	119.70	122.69
20	S1	2021	A2M	C1'-N9-C8	3.21	134.23	127.09
41	1	697	A2M	C2-N3-C4	3.21	119.67	111.83
42	2	1194	PSU	O2-C2-N1	-3.21	119.48	122.79
41	1	1011	PSU	C6-N1-C2	-3.20	119.72	122.69
42	2	1384	A2M	C2-N3-C4	3.20	119.65	111.83
20	S1	98	A2M	C2-N3-C4	3.20	119.64	111.83
20	S1	2021	A2M	C5-N7-C8	3.19	108.47	103.45
42	2	95	A2M	C5-N7-C8	3.19	108.46	103.45
42	2	95	A2M	C2-N3-C4	3.18	119.60	111.83
41	1	858	A2M	C1'-N9-C8	3.17	134.12	127.09
42	2	626	PSU	C6-N1-C2	-3.16	119.75	122.69
41	1	1539	A2M	C2-N3-C4	3.16	119.56	111.83
42	2	1384	A2M	C5-N7-C8	3.15	108.39	103.45
42	2	570	A2M	C5-N7-C8	3.14	108.39	103.45
42	2	591	A2M	C1'-N9-C8	3.13	134.04	127.09
42	2	437	PSU	C6-N1-C2	-3.13	119.79	122.69
42	2	95	A2M	C1'-N9-C8	3.11	133.99	127.09
42	2	382	A2M	C5-N7-C8	3.11	108.33	103.45
41	1	940	PSU	C6-N1-C2	-3.10	119.82	122.69
81	3	13	OMU	O4-C4-C5	-3.09	119.83	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1995	G7M	C2-N1-C6	-3.09	119.51	125.11
41	1	1659	OMU	O4-C4-C5	-3.09	119.84	125.16
41	1	1533	PSU	C6-C5-C4	3.09	120.26	118.17
41	1	959	OMG	C2-N1-C6	-3.08	119.52	125.11
42	2	1413	PSU	C6-N1-C2	-3.08	119.83	122.69
41	1	1190	OMG	C2-N1-C6	-3.08	119.53	125.11
42	2	641	OMG	C2'-C1'-N9	-3.08	108.40	114.24
41	1	845	OMU	O4-C4-C5	-3.08	119.86	125.16
20	S1	1156	PSU	C6-N1-C2	-3.07	119.84	122.69
44	7	74	PSU	C6-N1-C2	-3.06	119.85	122.69
42	2	382	A2M	C1'-N9-C8	3.05	133.87	127.09
41	1	858	A2M	C5-N7-C8	3.03	108.22	103.45
20	S1	1550	OMG	C2-N1-C6	-3.03	119.62	125.11
42	2	1308	5MC	C5-C6-N1	-3.02	120.04	123.31
20	S1	1979	OMU	O4-C4-C5	-3.01	119.96	125.16
20	S1	1478	OMG	C5-C6-N1	3.01	120.91	113.25
20	S1	1533	PSU	C6-N1-C2	-3.01	119.90	122.69
42	2	1078	OMG	C2-N1-C6	-3.00	119.67	125.11
42	2	1360	OMG	C2-N1-C6	-3.00	119.67	125.11
20	S1	1777	OMU	O4-C4-C5	-2.99	120.00	125.16
41	1	847	OMU	O2-C2-N1	-2.99	118.90	122.80
42	2	1229	OMG	C5-C6-N1	2.99	120.86	113.25
20	S1	1623	OMG	C2-N1-C6	-2.97	119.72	125.11
20	S1	104	PSU	C6-N1-C2	-2.97	119.94	122.69
42	2	628	A2M	O4'-C4'-C3'	-2.97	99.27	105.15
20	S1	455	PSU	C6-C5-C4	2.96	120.17	118.17
42	2	1078	OMG	C6-C5-N7	2.95	135.66	130.29
44	7	43	A2M	C1'-N9-C8	2.95	133.64	127.09
20	S1	29	OMU	O4-C4-C5	-2.95	120.07	125.16
42	2	534	OMG	C2-N1-C6	-2.95	119.76	125.11
20	S1	1647	OMG	C2-N1-C6	-2.95	119.77	125.11
20	S1	1865	OMG	C2-N1-C6	-2.94	119.78	125.11
20	S1	1621	OMU	O4-C4-C5	-2.93	120.11	125.16
41	1	1540	OMG	N2-C2-N1	2.92	122.93	116.76
20	S1	1543	C4J	N3-C2-N1	2.92	120.28	116.72
42	2	641	OMG	C8-N7-C5	2.92	109.46	104.26
42	2	1194	PSU	C6-C5-C4	2.91	120.14	118.17
42	2	1413	PSU	O2-C2-N1	-2.91	119.79	122.79
42	2	1078	OMG	C5-C6-N1	2.91	120.66	113.25
41	1	1371	OMU	O4-C4-C5	-2.91	120.15	125.16
20	S1	600	OMG	C2-N1-C6	-2.90	119.85	125.11
41	1	1528	PSU	O2-C2-N1	-2.89	119.81	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	628	A2M	N3-C4-N9	2.89	132.08	127.17
42	2	1303	PSU	O2-C2-N1	-2.88	119.82	122.79
41	1	239	PSU	C6-N1-C2	-2.88	120.02	122.69
44	7	69	PSU	C6-N1-C2	-2.88	120.02	122.69
20	S1	1246	PSU	O2-C2-N1	-2.86	119.84	122.79
41	1	959	OMG	N9-C8-N7	-2.86	108.10	113.40
42	2	1382	PSU	C6-N1-C2	-2.86	120.04	122.69
43	4	74	OMG	C5-C6-N1	2.86	120.53	113.25
20	S1	8	OMU	O4-C4-C5	-2.86	120.23	125.16
20	S1	2046	PSU	C6-C5-C4	2.86	120.10	118.17
42	2	641	OMG	C6-C5-N7	2.86	135.49	130.29
20	S1	512	A2M	C4-N9-C8	2.85	108.73	105.74
20	S1	1833	OMU	O4-C4-C5	-2.85	120.25	125.16
43	4	74	OMG	C2-N1-C6	-2.85	119.95	125.11
20	S1	2202	PSU	O2-C2-N1	-2.84	119.86	122.79
20	S1	2151	OMG	N9-C4-N3	2.84	131.63	125.95
20	S1	2151	OMG	C2-N1-C6	-2.84	119.96	125.11
41	1	959	OMG	N9-C4-N3	2.83	131.62	125.95
42	2	1046	OMG	C2-N1-C6	-2.83	119.97	125.11
20	S1	661	OMU	O4-C4-C5	-2.83	120.28	125.16
42	2	1231	OMG	C5-C6-N1	2.83	120.45	113.25
42	2	628	A2M	C5-C4-N3	-2.82	122.83	126.72
20	S1	1550	OMG	C5-C6-N1	2.82	120.43	113.25
41	1	1190	OMG	C5-C6-N1	2.82	120.43	113.25
41	1	1540	OMG	C2-N1-C6	-2.82	120.00	125.11
20	S1	1841	PSU	O2-C2-N1	-2.82	119.88	122.79
20	S1	1478	OMG	C2-N1-C6	-2.82	120.00	125.11
42	2	78	PSU	C6-N1-C2	-2.82	120.08	122.69
42	2	1144	PSU	C6-C5-C4	2.81	120.07	118.17
42	2	1303	PSU	C6-C5-C4	2.81	120.07	118.17
42	2	1253	OMG	C5-C6-N1	2.81	120.41	113.25
41	1	856	OMG	C2-N1-C6	-2.81	120.02	125.11
44	7	75	OMG	C2-N1-C6	-2.80	120.03	125.11
20	S1	1829	OMG	C2-N1-C6	-2.80	120.03	125.11
20	S1	2046	PSU	O2-C2-N1	-2.80	119.90	122.79
41	1	681	A2M	C1'-N9-C8	2.80	133.30	127.09
42	2	641	OMG	C5-C6-N1	2.78	120.34	113.25
20	S1	2185	MA6	C5-N7-C8	2.78	107.82	103.45
42	2	73	OMU	O4-C4-C5	-2.78	120.37	125.16
44	7	74	PSU	O2-C2-N1	-2.78	119.93	122.79
42	2	534	OMG	C5-C6-N1	2.77	120.31	113.25
41	1	1626	OMG	C2-N1-C6	-2.77	120.08	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	641	OMG	C2-N1-C6	-2.77	120.09	125.11
20	S1	2151	OMG	C5-C6-N1	2.77	120.30	113.25
20	S1	1865	OMG	C5-C6-N1	2.77	120.29	113.25
20	S1	1623	OMG	C5-C6-N1	2.76	120.28	113.25
42	2	1360	OMG	C5-C6-N1	2.76	120.28	113.25
20	S1	1647	OMG	C5-C6-N1	2.76	120.28	113.25
41	1	672	PSU	O2-C2-N1	-2.76	119.94	122.79
42	2	1185	A2M	C2'-C1'-N9	-2.76	109.21	113.75
41	1	1107	OMU	O4-C4-C5	-2.76	120.41	125.16
20	S1	1539	PSU	O2-C2-N1	-2.75	119.95	122.79
42	2	655	OMG	C2-N1-C6	-2.74	120.14	125.11
20	S1	2184	MA6	C5-N7-C8	2.74	107.75	103.45
42	2	71	OMG	C2'-C1'-N9	-2.74	109.04	114.24
42	2	1229	OMG	C6-C5-N7	2.74	135.27	130.29
41	1	1171	PSU	O2-C2-N1	-2.74	119.97	122.79
41	1	959	OMG	C5-C6-N1	2.73	120.21	113.25
41	1	1626	OMG	C5-C6-N1	2.73	120.21	113.25
20	S1	609	PSU	C6-C5-C4	2.73	120.02	118.17
20	S1	600	OMG	C5-C6-N1	2.73	120.19	113.25
20	S1	1533	PSU	O2-C2-N1	-2.72	119.98	122.79
41	1	1524	OMG	C5-C6-N1	2.72	120.17	113.25
42	2	527	A2M	O4'-C1'-C2'	-2.71	101.92	106.59
20	S1	2184	MA6	N3-C4-N9	2.71	131.77	127.17
20	S1	1543	C4J	C31-C3-N3	-2.71	107.43	112.16
42	2	95	A2M	C6-C5-C4	2.70	120.87	117.18
41	1	1528	PSU	C6-N1-C2	-2.70	120.18	122.69
20	S1	607	PSU	O2-C2-N1	-2.70	120.00	122.79
41	1	856	OMG	C5-C6-N1	2.70	120.12	113.25
42	2	1253	OMG	C6-C5-N7	2.70	135.20	130.29
44	7	75	OMG	C5-C6-N1	2.70	120.11	113.25
41	1	1540	OMG	C5-C6-N1	2.70	120.11	113.25
41	1	678	A2M	C1'-N9-C8	2.70	133.08	127.09
42	2	437	PSU	O2-C2-N1	-2.69	120.01	122.79
41	1	847	OMU	O4-C4-C5	-2.69	120.52	125.16
20	S1	2184	MA6	C4-N9-C8	2.69	108.56	105.74
42	2	71	OMG	N2-C2-N1	2.69	122.44	116.76
42	2	1359	OMU	O4-C4-C5	-2.69	120.52	125.16
42	2	628	A2M	C4'-O4'-C1'	-2.69	103.53	109.47
41	1	1107	OMU	O2-C2-N1	-2.69	119.30	122.80
42	2	1229	OMG	C2-N1-C6	-2.69	120.24	125.11
42	2	655	OMG	C5-C6-N1	2.69	120.09	113.25
41	1	422	PSU	O2-C2-N1	-2.68	120.03	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	572	A2M	O4'-C1'-C2'	-2.68	101.98	106.59
20	S1	1833	OMU	C1'-N1-C2	2.67	122.39	117.59
20	S1	1623	OMG	N9-C4-N3	2.67	131.28	125.95
42	2	1078	OMG	C8-N7-C5	2.66	109.01	104.26
20	S1	1647	OMG	N2-C2-N1	2.66	122.38	116.76
42	2	667	OMU	O4-C4-C5	-2.66	120.57	125.16
41	1	1540	OMG	C6-C5-N7	2.65	135.11	130.29
42	2	641	OMG	N2-C2-N1	2.65	122.35	116.76
42	2	71	OMG	C5-C6-N1	2.64	119.98	113.25
41	1	955	A2M	C1'-N9-C8	2.64	132.95	127.09
42	2	1253	OMG	C2-N1-C6	-2.63	120.33	125.11
42	2	1231	OMG	C2'-C1'-N9	-2.63	109.25	114.24
20	S1	1865	OMG	O6-C6-C5	-2.63	119.58	126.53
42	2	1046	OMG	C5-C6-N1	2.63	119.95	113.25
41	1	856	OMG	C2'-C1'-N9	-2.63	109.25	114.24
42	2	1253	OMG	N2-C2-N1	2.62	122.30	116.76
20	S1	1533	PSU	C6-C5-C4	2.62	119.94	118.17
41	1	1626	OMG	N2-C2-N1	2.61	122.28	116.76
41	1	959	OMG	O6-C6-C5	-2.61	119.64	126.53
41	1	856	OMG	C8-N7-C5	2.61	108.91	104.26
42	2	655	OMG	C8-N7-C5	2.61	108.90	104.26
20	S1	1543	C4J	C3-N3-C4	2.60	120.86	117.18
41	1	940	PSU	O2-C2-N1	-2.60	120.10	122.79
20	S1	512	A2M	C5-N7-C8	2.60	107.54	103.45
20	S1	455	PSU	O2-C2-N1	-2.60	120.11	122.79
43	4	74	OMG	C6-C5-N7	2.60	135.01	130.29
20	S1	1829	OMG	C5-C6-N1	2.59	119.85	113.25
20	S1	1841	PSU	C6-C5-C4	2.59	119.92	118.17
42	2	1419	OMU	O4-C4-C5	-2.59	120.70	125.16
20	S1	609	PSU	O2-C2-N1	-2.59	120.12	122.79
42	2	597	PSU	O2-C2-N1	-2.59	120.12	122.79
20	S1	1865	OMG	N2-C2-N1	2.57	122.19	116.76
20	S1	600	OMG	N9-C4-N3	2.57	131.10	125.95
42	2	73	OMU	O2-C2-N1	-2.57	119.45	122.80
42	2	71	OMG	C2-N1-C6	-2.57	120.45	125.11
42	2	593	PSU	C6-C5-C4	2.57	119.91	118.17
41	1	940	PSU	C6-C5-C4	2.57	119.91	118.17
41	1	1524	OMG	C8-N7-C5	2.56	108.82	104.26
41	1	1540	OMG	C8-N7-C5	2.56	108.82	104.26
42	2	71	OMG	C6-C5-N7	2.55	134.94	130.29
42	2	1384	A2M	C2'-C1'-N9	-2.55	109.55	113.75
42	2	1077	OMU	O4-C4-C5	-2.55	120.77	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	1231	OMG	N1-C2-N3	-2.54	118.67	123.32
20	S1	1550	OMG	O6-C6-C5	-2.54	119.82	126.53
42	2	1354	PSU	O2-C2-N1	-2.54	120.17	122.79
42	2	1078	OMG	N2-C2-N1	2.54	122.12	116.76
42	2	593	PSU	O2-C2-N1	-2.54	120.17	122.79
41	1	1664	PSU	O2-C2-N1	-2.53	120.18	122.79
42	2	472	PSU	O2-C2-N1	-2.52	120.19	122.79
41	1	1626	OMG	C6-C5-N7	2.52	134.88	130.29
20	S1	33	PSU	O2-C2-N1	-2.52	120.19	122.79
42	2	665	A2M	C6-C5-C4	2.51	120.61	117.18
42	2	1078	OMG	C4-C5-N7	-2.51	106.69	110.67
20	S1	33	PSU	C6-C5-C4	2.51	119.87	118.17
20	S1	104	PSU	C6-C5-C4	2.51	119.87	118.17
42	2	665	A2M	C1'-N9-C8	2.51	132.67	127.09
20	S1	1621	OMU	O2-C2-N1	-2.51	119.53	122.80
20	S1	1657	PSU	O2-C2-N1	-2.50	120.21	122.79
42	2	1264	PSU	C6-C5-C4	2.50	119.86	118.17
42	2	1265	PSU	O2-C2-N1	-2.49	120.22	122.79
42	2	1231	OMG	C2-N1-C6	-2.49	120.59	125.11
43	4	74	OMG	N2-C2-N1	2.49	122.02	116.76
44	7	75	OMG	C8-N7-C5	2.49	108.69	104.26
41	1	672	PSU	C6-C5-C4	2.49	119.85	118.17
42	2	1229	OMG	N1-C2-N3	-2.48	118.77	123.32
42	2	1403	PSU	O2-C2-N1	-2.48	120.23	122.79
41	1	1539	A2M	C2'-C1'-N9	2.48	117.83	113.75
41	1	1190	OMG	C8-N7-C5	2.48	108.67	104.26
41	1	1017	PSU	O2-C2-N1	-2.47	120.24	122.79
42	2	641	OMG	C4-C5-N7	-2.47	106.75	110.67
42	2	655	OMG	C6-C5-N7	2.47	134.79	130.29
42	2	1248	OMC	O2-C2-N3	-2.45	118.47	122.33
41	1	1190	OMG	N2-C2-N1	2.45	121.92	116.76
20	S1	1192	PSU	O2-C2-N1	-2.45	120.27	122.79
44	7	75	OMG	N2-C2-N1	2.45	121.92	116.76
42	2	667	OMU	O2-C2-N1	-2.44	119.62	122.80
41	1	1540	OMG	C4-C5-N7	-2.44	106.80	110.67
42	2	1384	A2M	C6-C5-C4	2.44	120.51	117.18
20	S1	1156	PSU	C6-C5-C4	2.44	119.82	118.17
42	2	655	OMG	C4-C5-N7	-2.44	106.81	110.67
20	S1	1647	OMG	C8-N7-C5	2.44	108.60	104.26
20	S1	2151	OMG	C8-N7-C5	2.44	108.60	104.26
41	1	1107	OMU	C2'-C1'-N1	-2.43	109.62	114.24
20	S1	2061	5MC	C5-C4-N3	-2.43	119.26	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1190	OMG	C2'-C1'-N9	-2.42	109.64	114.24
42	2	1318	PSU	C6-N1-C2	-2.42	120.44	122.69
42	2	1229	OMG	C8-N7-C5	2.42	108.57	104.26
20	S1	1647	OMG	O6-C6-C5	-2.41	120.16	126.53
42	2	1360	OMG	N2-C2-N1	2.41	121.86	116.76
20	S1	104	PSU	O2-C2-N1	-2.41	120.31	122.79
42	2	534	OMG	O6-C6-C5	-2.41	120.18	126.53
20	S1	12	PSU	O2-C2-N1	-2.40	120.31	122.79
42	2	1046	OMG	C8-N7-C5	2.40	108.54	104.26
42	2	1308	5MC	O2-C2-N3	-2.40	118.55	122.33
41	1	681	A2M	C6-C5-C4	2.40	120.45	117.18
41	1	1524	OMG	C4-C5-N7	-2.39	106.88	110.67
41	1	1524	OMG	N2-C2-N1	2.39	121.81	116.76
41	1	856	OMG	N2-C2-N1	2.39	121.80	116.76
20	S1	1478	OMG	N1-C2-N3	-2.38	118.96	123.32
20	S1	600	OMG	C8-N7-C5	2.38	108.51	104.26
42	2	1360	OMG	O6-C6-C5	-2.38	120.24	126.53
42	2	655	OMG	N2-C2-N1	2.38	121.78	116.76
20	S1	2185	MA6	N3-C4-N9	2.38	131.21	127.17
41	1	955	A2M	C6-C5-C4	2.38	120.42	117.18
20	S1	607	PSU	C6-C5-C4	2.37	119.78	118.17
43	4	74	OMG	O6-C6-C5	-2.37	120.27	126.53
42	2	1317	OMC	O2-C2-N3	-2.37	118.59	122.33
41	1	1190	OMG	O6-C6-C5	-2.37	120.27	126.53
41	1	422	PSU	C6-C5-C4	2.37	119.78	118.17
41	1	856	OMG	C6-C5-N7	2.37	134.61	130.29
42	2	1359	OMU	O2-C2-N1	-2.37	119.71	122.80
20	S1	1478	OMG	C8-N7-C5	2.37	108.48	104.26
20	S1	2151	OMG	O6-C6-C5	-2.37	120.29	126.53
20	S1	1623	OMG	O6-C6-C5	-2.35	120.32	126.53
42	2	78	PSU	C5-C4-N3	2.35	121.71	116.55
42	2	1058	PSU	C6-C5-C4	2.34	119.75	118.17
42	2	1308	5MC	C5-C4-N3	-2.34	119.36	121.75
42	2	71	OMG	C8-N7-C5	2.34	108.42	104.26
41	1	1626	OMG	C8-N7-C5	2.33	108.41	104.26
20	S1	1566	PSU	C5-C6-N1	-2.33	118.91	122.14
20	S1	1550	OMG	N9-C4-N3	2.33	130.61	125.95
20	S1	1623	OMG	C8-N7-C5	2.33	108.40	104.26
20	S1	1829	OMG	C8-N7-C5	2.32	108.39	104.26
44	7	74	PSU	C6-C5-C4	2.31	119.73	118.17
42	2	510	PSU	C3'-C2'-C1'	2.31	104.41	101.69
42	2	472	PSU	C6-C5-C4	2.31	119.73	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	1360	OMG	C8-N7-C5	2.31	108.37	104.26
41	1	678	A2M	C6-C5-C4	2.30	120.32	117.18
42	2	560	OMU	O4-C4-C5	-2.30	121.19	125.16
20	S1	2185	MA6	C4-C5-N7	-2.30	107.95	110.58
41	1	1371	OMU	O2-C2-N3	-2.30	117.25	121.49
41	1	1011	PSU	O2-C2-N1	-2.30	120.42	122.79
42	2	1361	PSU	C6-C5-C4	2.30	119.72	118.17
41	1	1524	OMG	N9-C4-N3	2.29	130.53	125.95
42	2	1229	OMG	C2'-C1'-N9	-2.28	109.91	114.24
20	S1	8	OMU	O2-C2-N1	-2.28	119.83	122.80
20	S1	1156	PSU	O2-C2-N1	-2.28	120.44	122.79
41	1	239	PSU	O2-C2-N1	-2.28	120.44	122.79
42	2	591	A2M	C6-C5-C4	2.28	120.29	117.18
20	S1	1478	OMG	N2-C2-N1	2.28	121.56	116.76
42	2	1264	PSU	O2-C2-N1	-2.27	120.44	122.79
42	2	1318	PSU	O2-C2-N1	-2.27	120.44	122.79
44	7	75	OMG	C6-C5-N7	2.27	134.43	130.29
20	S1	1865	OMG	C8-N7-C5	2.27	108.30	104.26
20	S1	2185	MA6	C5-C4-N9	2.27	108.28	105.81
20	S1	2202	PSU	C6-C5-C4	2.27	119.70	118.17
20	S1	1478	OMG	C2'-C1'-N9	-2.27	109.94	114.24
42	2	510	PSU	C5-C6-N1	-2.26	119.00	122.14
41	1	1524	OMG	O6-C6-C5	-2.26	120.56	126.53
42	2	1231	OMG	O6-C6-C5	-2.26	120.56	126.53
42	2	1046	OMG	O6-C6-C5	-2.26	120.56	126.53
41	1	678	A2M	C2'-C1'-N9	2.26	117.47	113.75
20	S1	1550	OMG	N2-C2-N1	2.26	121.52	116.76
42	2	78	PSU	O2-C2-N1	-2.25	120.47	122.79
20	S1	600	OMG	O6-C6-C5	-2.25	120.59	126.53
20	S1	512	A2M	C6-C5-N7	2.25	136.42	132.09
42	2	1382	PSU	O2-C2-N1	-2.24	120.47	122.79
20	S1	1647	OMG	C6-C5-N7	2.24	134.37	130.29
20	S1	98	A2M	C6-C5-C4	2.24	120.24	117.18
42	2	1253	OMG	N1-C2-N3	-2.24	119.22	123.32
42	2	641	OMG	N1-C2-N3	-2.24	119.22	123.32
41	1	1540	OMG	O6-C6-C5	-2.24	120.62	126.53
20	S1	1829	OMG	O6-C6-C5	-2.24	120.63	126.53
41	1	870	PSU	C6-N1-C2	-2.24	120.62	122.69
20	S1	1647	OMG	C2'-C1'-N9	-2.23	110.00	114.24
41	1	856	OMG	C4-C5-N7	-2.23	107.13	110.67
42	2	1060	PSU	O2-C2-N1	-2.23	120.48	122.79
20	S1	2185	MA6	C4-N9-C8	2.23	108.08	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	1253	OMG	C4-C5-N7	-2.23	107.13	110.67
41	1	1181	PSU	O2-C2-N1	-2.23	120.49	122.79
20	S1	1478	OMG	C6-C5-N7	2.23	134.35	130.29
42	2	1354	PSU	C6-C5-C4	2.22	119.67	118.17
42	2	628	A2M	C2-N3-C4	2.22	117.25	111.83
41	1	1539	A2M	O4'-C1'-C2'	-2.22	102.77	106.59
41	1	870	PSU	C6-C5-C4	2.22	119.67	118.17
20	S1	1478	OMG	N9-C4-N3	2.21	130.37	125.95
41	1	1190	OMG	C6-C5-N7	2.21	134.31	130.29
81	3	13	OMU	O2-C2-N1	-2.21	119.92	122.80
41	1	1626	OMG	C4-C5-N7	-2.21	107.17	110.67
42	2	506	PSU	C5-C6-N1	-2.20	119.08	122.14
42	2	641	OMG	C8-N9-C4	2.20	110.15	106.03
44	7	75	OMG	O6-C6-C5	-2.20	120.74	126.53
42	2	534	OMG	N9-C4-N3	2.19	130.34	125.95
42	2	1229	OMG	N2-C2-N1	2.19	121.39	116.76
41	1	1190	OMG	C4-C5-N7	-2.19	107.19	110.67
44	7	69	PSU	O4'-C1'-C2'	2.19	108.19	105.15
42	2	1046	OMG	N2-C2-N1	2.19	121.38	116.76
42	2	1265	PSU	C6-C5-C4	2.19	119.65	118.17
20	S1	2021	A2M	C6-C5-C4	2.19	120.16	117.18
20	S1	1777	OMU	O2-C2-N1	-2.19	119.95	122.80
41	1	1017	PSU	C6-C5-C4	2.18	119.65	118.17
42	2	1253	OMG	C8-N7-C5	2.18	108.15	104.26
41	1	1539	A2M	C6-C5-C4	2.18	120.16	117.18
20	S1	1478	OMG	O6-C6-C5	-2.18	120.78	126.53
42	2	437	PSU	C6-C5-C4	2.18	119.64	118.17
42	2	1231	OMG	C6-C5-N7	2.18	134.25	130.29
42	2	570	A2M	C1'-N9-C8	2.18	131.93	127.09
20	S1	1543	C4J	C5-C4-N3	2.18	120.10	116.15
42	2	570	A2M	C6-C5-C4	2.17	120.14	117.18
20	S1	1550	OMG	C8-N7-C5	2.17	108.13	104.26
42	2	662	PSU	O2-C2-N1	-2.17	120.55	122.79
42	2	1303	PSU	O4'-C1'-C2'	2.17	108.16	105.15
20	S1	98	A2M	C2'-C1'-N9	-2.17	110.18	113.75
42	2	1229	OMG	C4-C5-N7	-2.17	107.23	110.67
43	4	74	OMG	C8-N7-C5	2.17	108.12	104.26
42	2	1231	OMG	C8-N7-C5	2.17	108.12	104.26
20	S1	1647	OMG	C4-C5-N7	-2.16	107.25	110.67
20	S1	1995	G7M	N9-C8-N7	-2.16	107.24	112.48
42	2	71	OMG	N1-C2-N3	-2.15	119.39	123.32
20	S1	512	A2M	N9-C8-N7	-2.15	110.89	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	7	75	OMG	N1-C2-N3	-2.13	119.42	123.32
41	1	239	PSU	C6-C5-C4	2.13	119.61	118.17
44	7	75	OMG	C4-C5-N7	-2.13	107.29	110.67
42	2	641	OMG	O6-C6-C5	-2.13	120.91	126.53
43	4	74	OMG	N1-C2-N3	-2.13	119.42	123.32
42	2	534	OMG	C8-N7-C5	2.13	108.05	104.26
20	S1	1865	OMG	N9-C4-N3	2.13	130.21	125.95
20	S1	29	OMU	O2-C2-N1	-2.12	120.03	122.80
41	1	856	OMG	O6-C6-C5	-2.12	120.92	126.53
41	1	1181	PSU	C6-C5-C4	2.12	119.61	118.17
20	S1	1829	OMG	N9-C4-N3	2.12	130.19	125.95
20	S1	1829	OMG	N2-C2-N1	2.12	121.22	116.76
42	2	71	OMG	O6-C6-C5	-2.11	120.95	126.53
41	1	1171	PSU	O4'-C1'-C2'	2.11	108.07	105.15
41	1	856	OMG	N1-C2-N3	-2.11	119.46	123.32
20	S1	897	A2M	C5'-C4'-C3'	-2.11	107.62	115.21
42	2	1185	A2M	C6-C5-C4	2.11	120.06	117.18
20	S1	2184	MA6	C4-C5-N7	-2.11	108.17	110.58
43	4	74	OMG	C2'-C1'-N9	-2.10	110.25	114.24
42	2	1382	PSU	O4'-C1'-C2'	2.10	108.06	105.15
41	1	1659	OMU	O2-C2-N1	-2.10	120.06	122.80
41	1	1540	OMG	N1-C2-N3	-2.10	119.48	123.32
42	2	524	5MC	CM5-C5-C6	-2.10	120.01	122.85
43	4	74	OMG	C4-C5-N7	-2.09	107.36	110.67
42	2	71	OMG	C4-C5-N7	-2.09	107.36	110.67
42	2	662	PSU	O4'-C1'-C2'	2.08	108.03	105.15
41	1	1626	OMG	O6-C6-C5	-2.08	121.05	126.53
20	S1	897	A2M	C6-C5-C4	2.07	120.01	117.18
20	S1	2048	OMU	C1'-N1-C2	2.07	121.30	117.59
41	1	1626	OMG	N1-C2-N3	-2.07	119.54	123.32
42	2	1046	OMG	N9-C4-N3	2.06	130.08	125.95
20	S1	1995	G7M	C5-C4-N9	2.06	110.28	105.88
42	2	504	PSU	C5-C6-N1	-2.06	119.28	122.14
41	1	858	A2M	C4'-O4'-C1'	-2.06	104.92	109.47
42	2	1046	OMG	C4-C5-N7	-2.05	107.42	110.67
42	2	1360	OMG	C2'-C1'-N9	-2.05	110.35	114.24
41	1	870	PSU	O2-C2-N1	-2.05	120.68	122.79
41	1	1626	OMG	C2'-C1'-N9	-2.05	110.36	114.24
42	2	1231	OMG	N2-C2-N1	2.04	121.08	116.76
42	2	1078	OMG	O6-C6-C5	-2.04	121.14	126.53
42	2	1360	OMG	N9-C4-N3	2.04	130.04	125.95
42	2	626	PSU	O2-C2-N1	-2.04	120.68	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1979	OMU	O2-C2-N1	-2.04	120.14	122.80
42	2	382	A2M	C6-C5-C4	2.04	119.96	117.18
20	S1	512	A2M	O4'-C1'-N9	2.04	112.00	108.09
41	1	677	1MA	N1-C6-N6	2.04	124.83	119.71
20	S1	668	A2M	C4-C5-N7	-2.03	108.26	110.58
41	1	845	OMU	O2-C2-N1	-2.03	120.15	122.80
20	S1	2151	OMG	N1-C2-N3	-2.03	119.61	123.32
20	S1	12	PSU	O4'-C1'-C2'	2.03	107.96	105.15
42	2	1078	OMG	N1-C2-N3	-2.03	119.61	123.32
42	2	1382	PSU	C5-C4-N3	2.02	121.00	116.55
42	2	583	OMC	O2-C2-N3	-2.02	119.15	122.33
20	S1	479	A2M	C6-C5-C4	2.01	119.93	117.18
20	S1	1550	OMG	C2'-C1'-N9	-2.01	110.42	114.24
41	1	1533	PSU	O4'-C1'-C2'	2.01	107.93	105.15
20	S1	1865	OMG	N1-C2-N3	-2.01	119.64	123.32
42	2	1046	OMG	N1-C2-N3	-2.00	119.66	123.32

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	7	69	PSU	O4'-C1'-C5-C4
44	7	69	PSU	O4'-C1'-C5-C6
44	7	162	A2M	C1'-C2'-O2'-CM'
20	S1	33	PSU	C3'-C4'-C5'-O5'
20	S1	33	PSU	O4'-C4'-C5'-O5'
20	S1	479	A2M	C1'-C2'-O2'-CM'
20	S1	512	A2M	C1'-C2'-O2'-CM'
20	S1	607	PSU	C2'-C1'-C5-C4
20	S1	607	PSU	O4'-C1'-C5-C4
20	S1	607	PSU	C2'-C1'-C5-C6
20	S1	607	PSU	O4'-C1'-C5-C6
20	S1	668	A2M	O4'-C4'-C5'-O5'
20	S1	668	A2M	C3'-C4'-C5'-O5'
20	S1	668	A2M	C1'-C2'-O2'-CM'
20	S1	897	A2M	O4'-C4'-C5'-O5'
20	S1	897	A2M	C3'-C4'-C5'-O5'
20	S1	1192	PSU	O4'-C4'-C5'-O5'
20	S1	1833	OMU	O4'-C1'-N1-C2
20	S1	1833	OMU	O4'-C1'-N1-C6
20	S1	1979	OMU	O4'-C4'-C5'-O5'
41	1	239	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
41	1	437	A2M	C1'-C2'-O2'-CM'
41	1	959	OMG	C1'-C2'-O2'-CM2
41	1	1371	OMU	O4'-C1'-N1-C2
41	1	1371	OMU	O4'-C1'-N1-C6
41	1	1540	OMG	O4'-C4'-C5'-O5'
42	2	95	A2M	C1'-C2'-O2'-CM'
42	2	382	A2M	C1'-C2'-O2'-CM'
42	2	500	PSU	C2'-C1'-C5-C4
42	2	500	PSU	O4'-C1'-C5-C4
42	2	500	PSU	O4'-C1'-C5-C6
42	2	504	PSU	C4'-C5'-O5'-P
42	2	534	OMG	O4'-C4'-C5'-O5'
42	2	570	A2M	C1'-C2'-O2'-CM'
42	2	628	A2M	O4'-C1'-N9-C8
42	2	628	A2M	O4'-C1'-N9-C4
42	2	1046	OMG	O4'-C4'-C5'-O5'
42	2	1265	PSU	O4'-C4'-C5'-O5'
42	2	1303	PSU	O4'-C4'-C5'-O5'
42	2	1308	5MC	C3'-C4'-C5'-O5'
42	2	1384	A2M	C1'-C2'-O2'-CM'
42	2	1419	OMU	C1'-C2'-O2'-CM2
20	S1	512	A2M	O4'-C4'-C5'-O5'
20	S1	600	OMG	O4'-C4'-C5'-O5'
20	S1	607	PSU	C3'-C4'-C5'-O5'
20	S1	1192	PSU	C3'-C4'-C5'-O5'
20	S1	1246	PSU	C3'-C4'-C5'-O5'
20	S1	1979	OMU	C3'-C4'-C5'-O5'
41	1	239	PSU	C3'-C4'-C5'-O5'
41	1	681	A2M	O4'-C4'-C5'-O5'
41	1	1371	OMU	C3'-C4'-C5'-O5'
42	2	78	PSU	C3'-C4'-C5'-O5'
42	2	534	OMG	C3'-C4'-C5'-O5'
42	2	1265	PSU	C3'-C4'-C5'-O5'
42	2	1303	PSU	C3'-C4'-C5'-O5'
20	S1	1550	OMG	C3'-C4'-C5'-O5'
20	S1	2140	OMC	C3'-C4'-C5'-O5'
20	S1	2140	OMC	O4'-C4'-C5'-O5'
41	1	1371	OMU	O4'-C4'-C5'-O5'
42	2	78	PSU	O4'-C4'-C5'-O5'
42	2	527	A2M	O4'-C4'-C5'-O5'
42	2	665	A2M	O4'-C4'-C5'-O5'
42	2	1046	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
42	2	1308	5MC	O4'-C4'-C5'-O5'
42	2	443	OMC	C2'-C1'-N1-C6
41	1	681	A2M	C3'-C4'-C5'-O5'
41	1	1540	OMG	C3'-C4'-C5'-O5'
20	S1	8	OMU	C2'-C1'-N1-C6
20	S1	1246	PSU	O4'-C4'-C5'-O5'
41	1	959	OMG	O4'-C4'-C5'-O5'
42	2	527	A2M	C3'-C4'-C5'-O5'
42	2	443	OMC	C2'-C1'-N1-C2
20	S1	512	A2M	C3'-C4'-C5'-O5'
20	S1	600	OMG	C3'-C4'-C5'-O5'
20	S1	607	PSU	O4'-C4'-C5'-O5'
20	S1	1533	PSU	C3'-C4'-C5'-O5'
20	S1	1550	OMG	O4'-C4'-C5'-O5'
41	1	1181	PSU	C3'-C4'-C5'-O5'
20	S1	1543	C4J	C4'-C5'-O5'-P
42	2	1308	5MC	C2'-C1'-N1-C6
42	2	570	A2M	C2'-C1'-N9-C8
20	S1	2021	A2M	C3'-C4'-C5'-O5'
42	2	1185	A2M	C3'-C4'-C5'-O5'
42	2	665	A2M	C3'-C4'-C5'-O5'
20	S1	2021	A2M	O4'-C4'-C5'-O5'
42	2	604	A2M	C1'-C2'-O2'-CM'
42	2	504	PSU	O4'-C4'-C5'-O5'
20	S1	1829	OMG	O4'-C4'-C5'-O5'
20	S1	668	A2M	C2'-C1'-N9-C8
42	2	1308	5MC	O4'-C1'-N1-C6
20	S1	8	OMU	O4'-C1'-N1-C6
42	2	443	OMC	O4'-C1'-N1-C6
42	2	443	OMC	O4'-C1'-N1-C2
20	S1	1533	PSU	O4'-C4'-C5'-O5'
41	1	1181	PSU	O4'-C4'-C5'-O5'
42	2	1185	A2M	O4'-C4'-C5'-O5'
42	2	1308	5MC	O4'-C1'-N1-C2
42	2	655	OMG	C3'-C2'-O2'-CM2
41	1	681	A2M	C4'-C5'-O5'-P
42	2	506	PSU	C4'-C5'-O5'-P
42	2	560	OMU	C4'-C5'-O5'-P
42	2	1361	PSU	C4'-C5'-O5'-P
41	1	1171	PSU	O4'-C1'-C5-C4
42	2	1361	PSU	O4'-C1'-C5-C4
42	2	570	A2M	C2'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
42	2	1060	PSU	C3'-C4'-C5'-O5'
20	S1	1543	C4J	N33-C32-C34-O36
20	S1	1478	OMG	C4'-C5'-O5'-P
41	1	1181	PSU	C4'-C5'-O5'-P
42	2	1248	OMC	C4'-C5'-O5'-P
41	1	1402	PSU	O4'-C4'-C5'-O5'
42	2	1403	PSU	C3'-C4'-C5'-O5'
20	S1	8	OMU	O4'-C1'-N1-C2
20	S1	8	OMU	C2'-C1'-N1-C2
20	S1	1833	OMU	C4'-C5'-O5'-P
20	S1	98	A2M	O4'-C4'-C5'-O5'
20	S1	2021	A2M	C1'-C2'-O2'-CM'
41	1	697	A2M	C1'-C2'-O2'-CM'
42	2	665	A2M	C1'-C2'-O2'-CM'
20	S1	1829	OMG	C4'-C5'-O5'-P
20	S1	8	OMU	O4'-C4'-C5'-O5'
42	2	504	PSU	C3'-C4'-C5'-O5'
20	S1	2202	PSU	O4'-C1'-C5-C6
41	1	1011	PSU	O4'-C1'-C5-C6
41	1	1171	PSU	O4'-C1'-C5-C6
42	2	1359	OMU	C3'-C2'-O2'-CM2
42	2	1308	5MC	C2'-C1'-N1-C2
42	2	570	A2M	O4'-C1'-N9-C8
20	S1	2185	MA6	C4'-C5'-O5'-P
20	S1	1979	OMU	C2'-C1'-N1-C2
20	S1	8	OMU	C3'-C2'-O2'-CM2
41	1	1524	OMG	C3'-C2'-O2'-CM2
20	S1	1539	PSU	C3'-C4'-C5'-O5'
20	S1	1841	PSU	O4'-C4'-C5'-O5'
20	S1	668	A2M	O4'-C1'-N9-C8
20	S1	1543	C4J	N3-C3-C31-C32
20	S1	1657	PSU	C4'-C5'-O5'-P
42	2	1185	A2M	C4'-C5'-O5'-P

There are no ring outliers.

48 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	S1	2048	OMU	1	0
20	S1	1995	G7M	1	0
42	2	1403	PSU	2	0
41	1	437	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	2	95	A2M	1	0
20	S1	1621	OMU	1	0
42	2	506	PSU	2	0
42	2	1046	OMG	1	0
20	S1	2061	5MC	2	0
41	1	695	OMC	1	0
42	2	1419	OMU	1	0
20	S1	1657	PSU	2	0
42	2	665	A2M	2	0
42	2	628	A2M	1	0
42	2	510	PSU	2	0
20	S1	479	A2M	1	0
42	2	626	PSU	1	0
20	S1	2185	MA6	1	0
42	2	443	OMC	1	0
20	S1	2184	MA6	1	0
42	2	1318	PSU	1	0
42	2	560	OMU	1	0
44	7	162	A2M	1	0
42	2	1382	PSU	1	0
41	1	697	A2M	2	0
20	S1	2202	PSU	1	0
41	1	847	OMU	1	0
81	3	13	OMU	1	0
42	2	500	PSU	1	0
20	S1	512	A2M	1	0
42	2	1308	5MC	2	0
20	S1	98	A2M	1	0
42	2	591	A2M	2	0
20	S1	1833	OMU	1	0
42	2	604	A2M	1	0
20	S1	1566	PSU	1	0
42	2	382	A2M	3	0
20	S1	18	OMC	1	0
20	S1	1829	OMG	2	0
41	1	1659	OMU	1	0
41	1	959	OMG	2	0
42	2	504	PSU	2	0
20	S1	1246	PSU	1	0
44	7	75	OMG	1	0
41	1	1011	PSU	2	0
41	1	845	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	2	78	PSU	1	0
42	2	1413	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 144 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	1	2
15	S4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S4	7:A	O3'	65:G	P	19.26
1	1	1097:A	O3'	1100:C	P	10.20
1	1	552:G	O3'	554:A	P	4.04

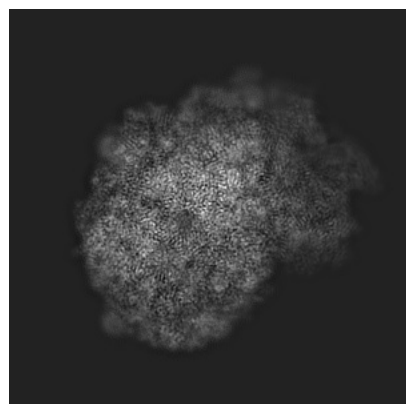
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15272. These allow visual inspection of the internal detail of the map and identification of artifacts.

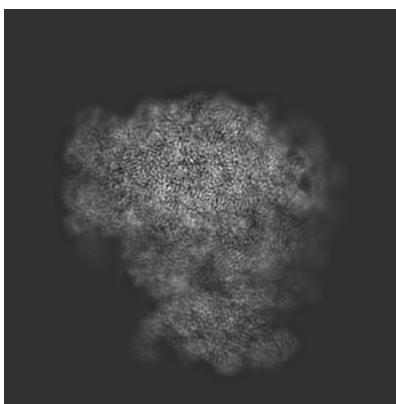
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

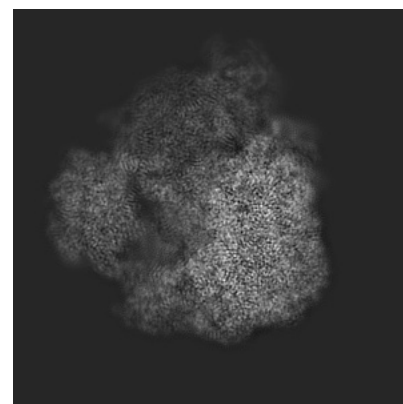
6.1.1 Primary map



X

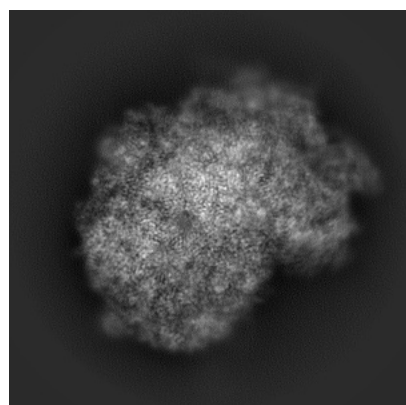


Y

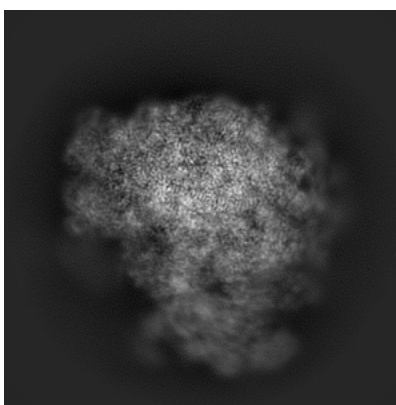


Z

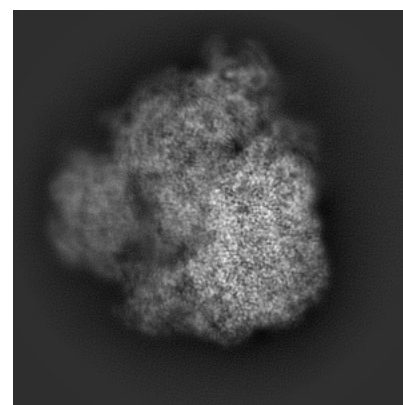
6.1.2 Raw map



X



Y

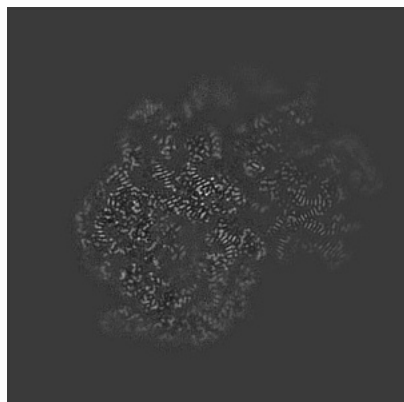


Z

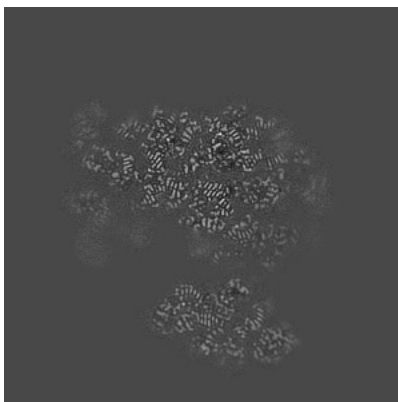
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

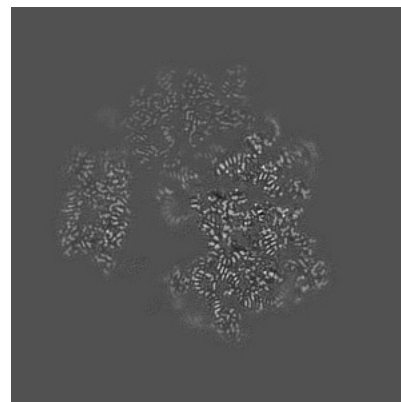
6.2.1 Primary map



X Index: 220

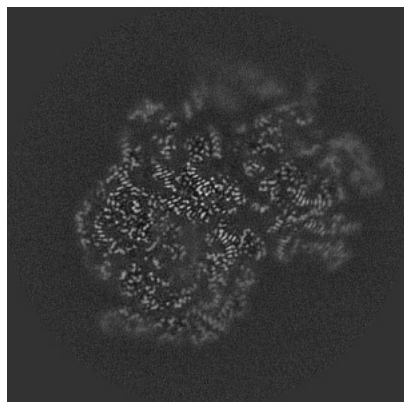


Y Index: 220

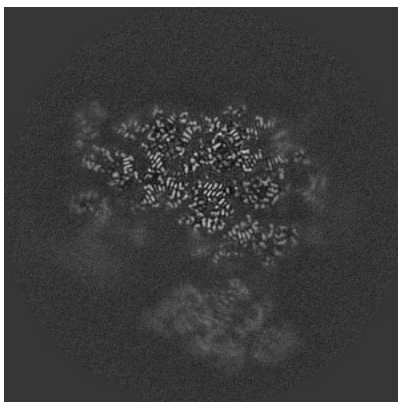


Z Index: 220

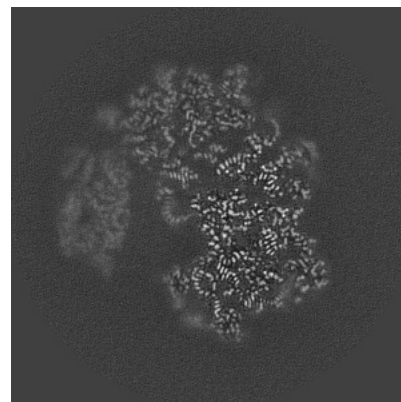
6.2.2 Raw map



X Index: 220



Y Index: 220

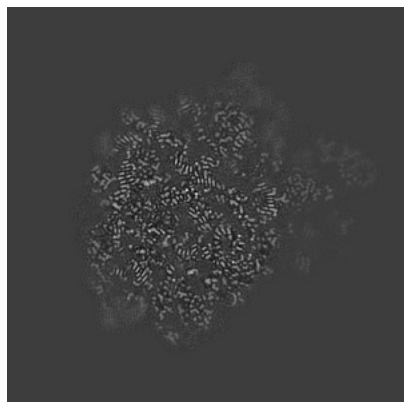


Z Index: 220

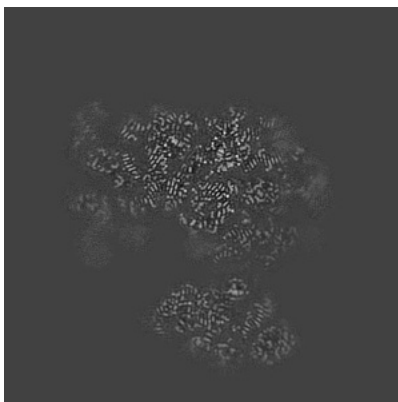
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

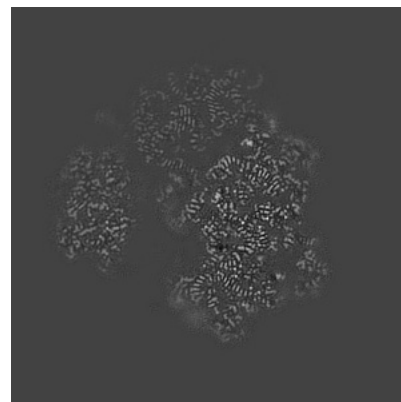
6.3.1 Primary map



X Index: 265

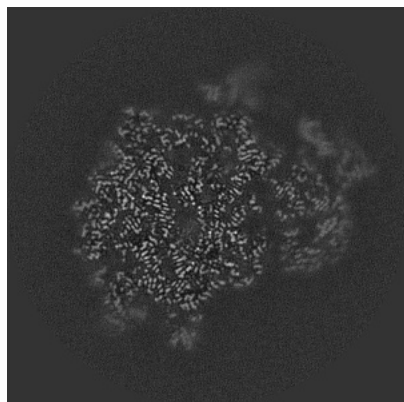


Y Index: 222

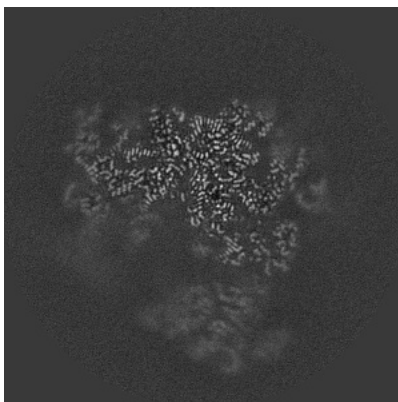


Z Index: 226

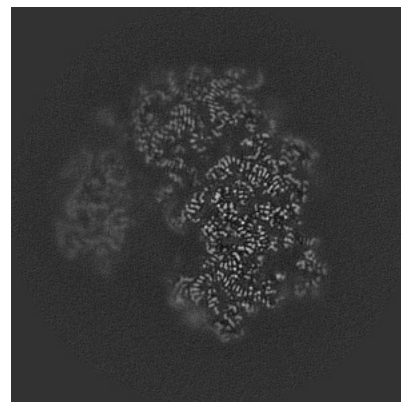
6.3.2 Raw map



X Index: 249



Y Index: 212

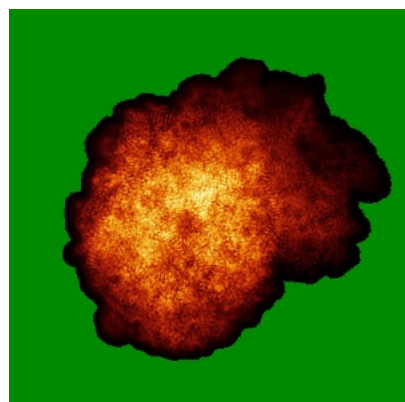


Z Index: 226

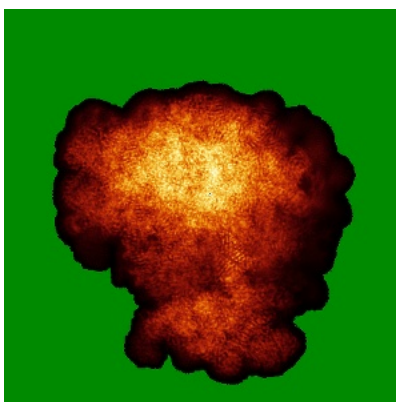
The images above show the largest variance slices of the map in three orthogonal directions.

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

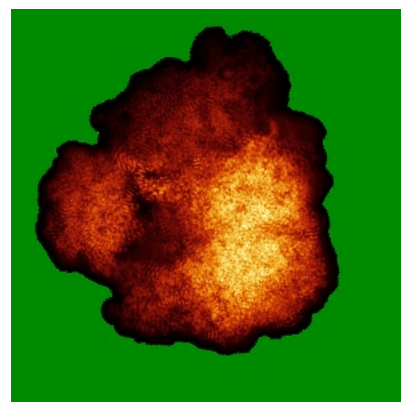
6.4.1 Primary map



X

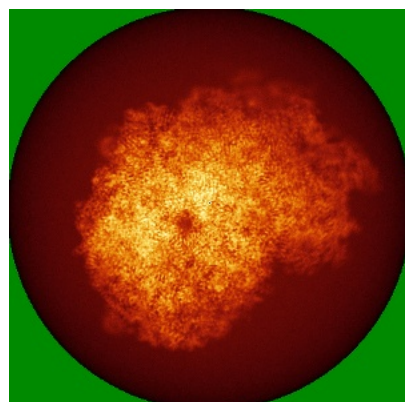


Y

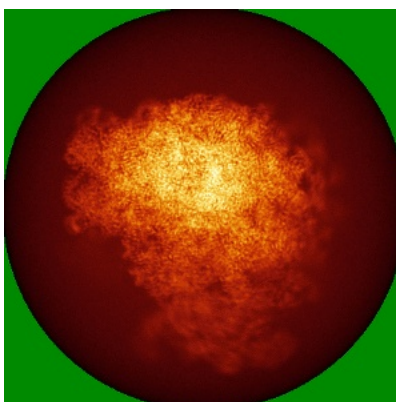


Z

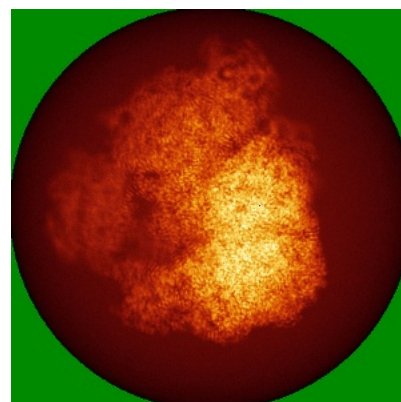
6.4.2 Raw map



X



Y

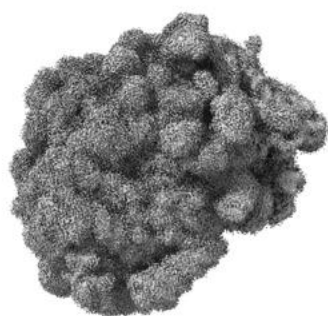


Z

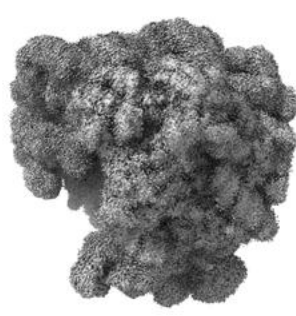
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

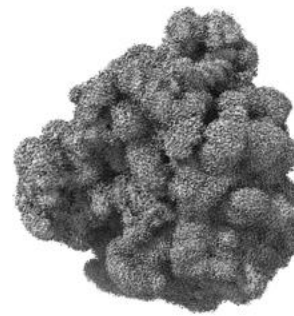
6.5.1 Primary map



X



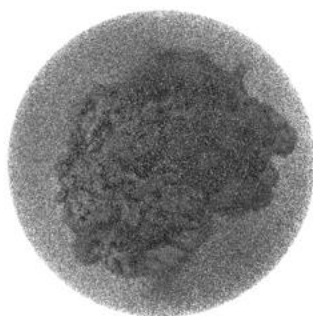
Y



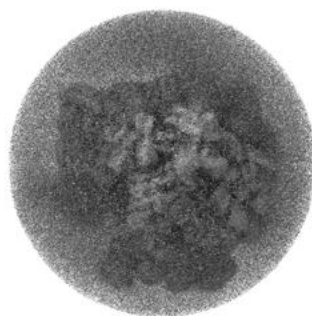
Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

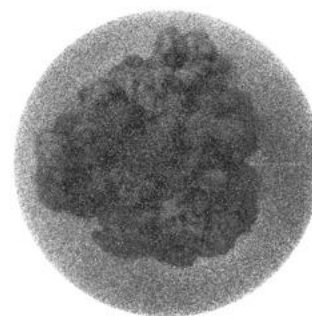
6.5.2 Raw map



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.

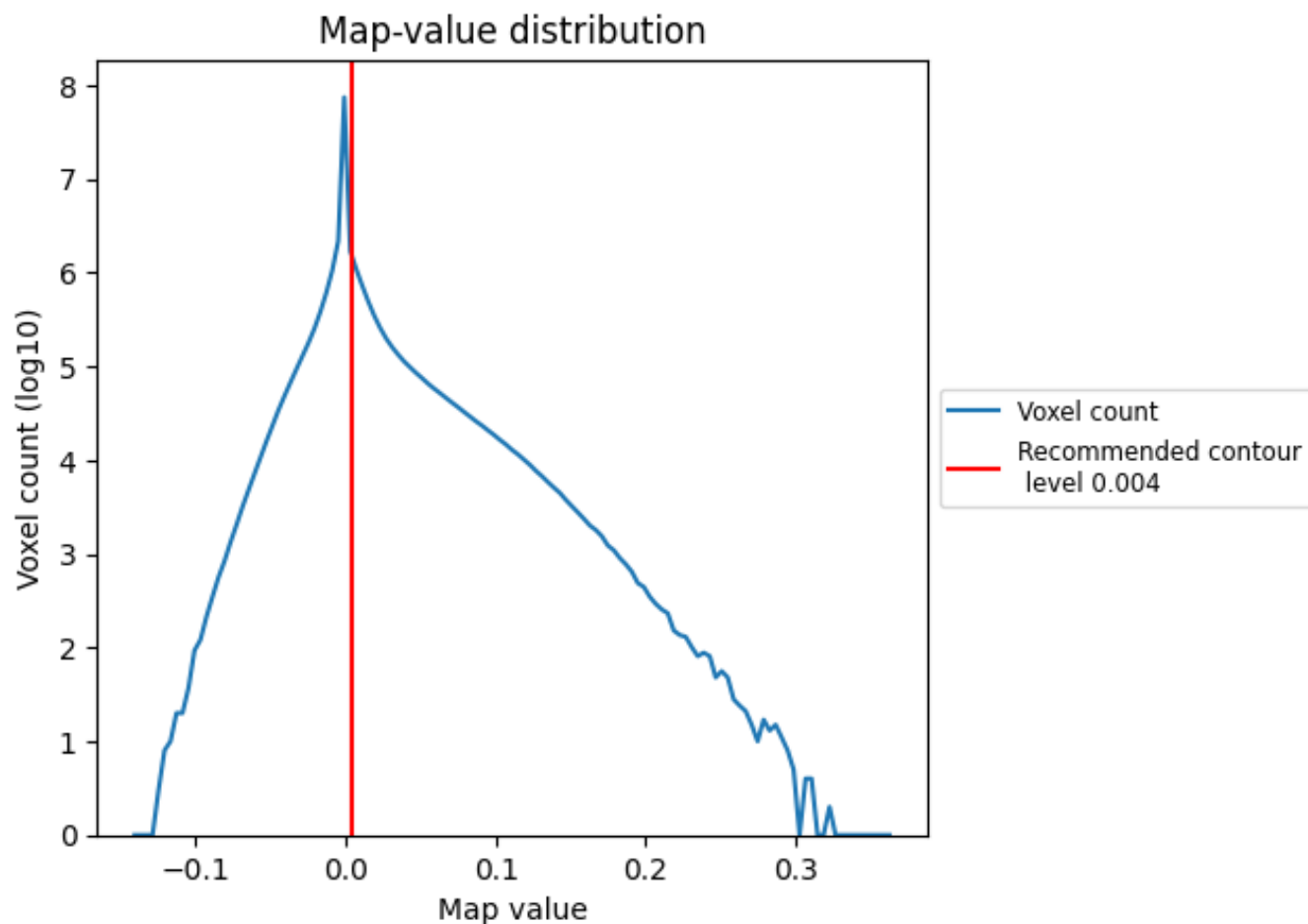
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

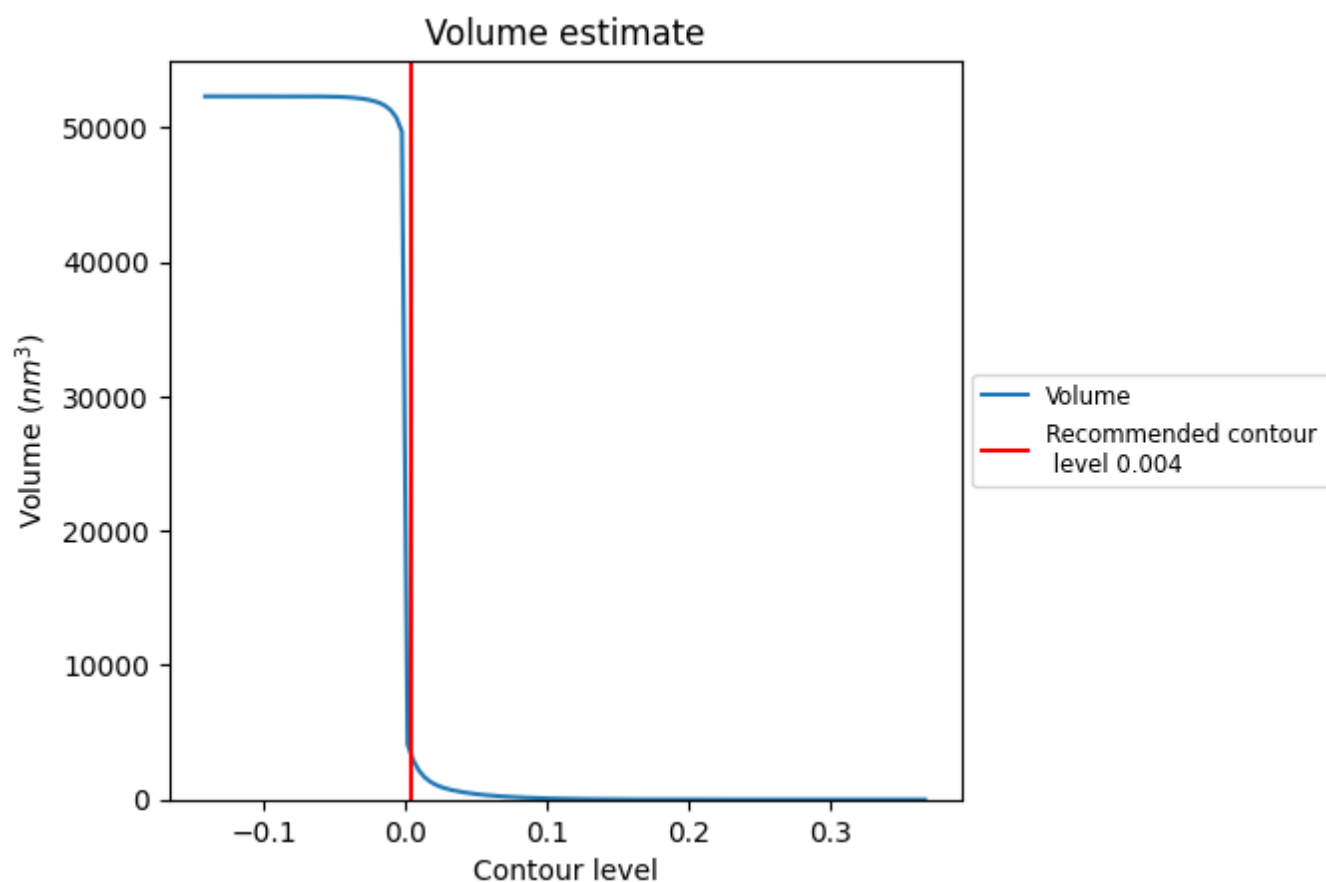
This section contains the results of statistical analysis of the map.

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.

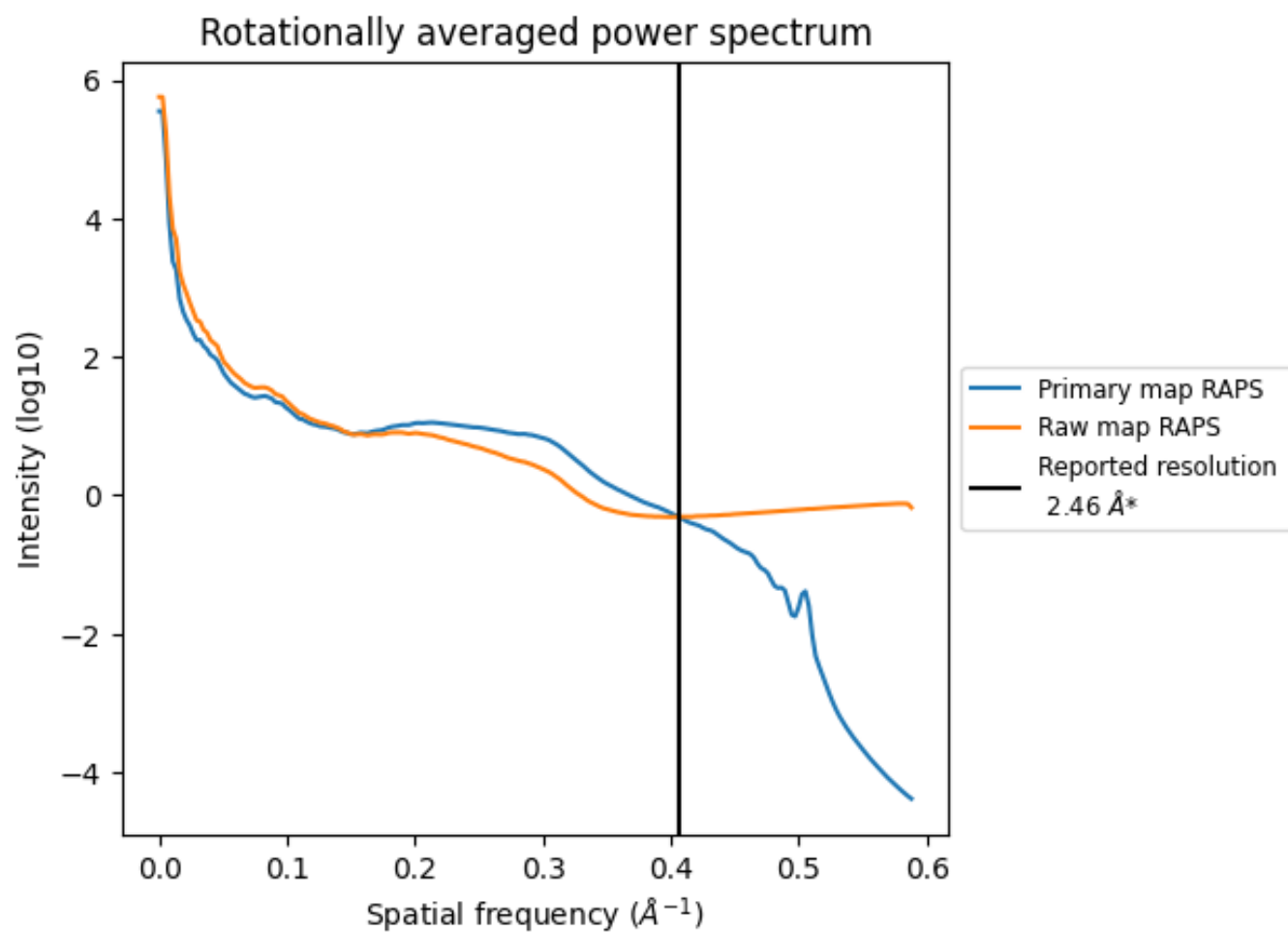
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3475 nm³; this corresponds to an approximate mass of 3139 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 ⓘ

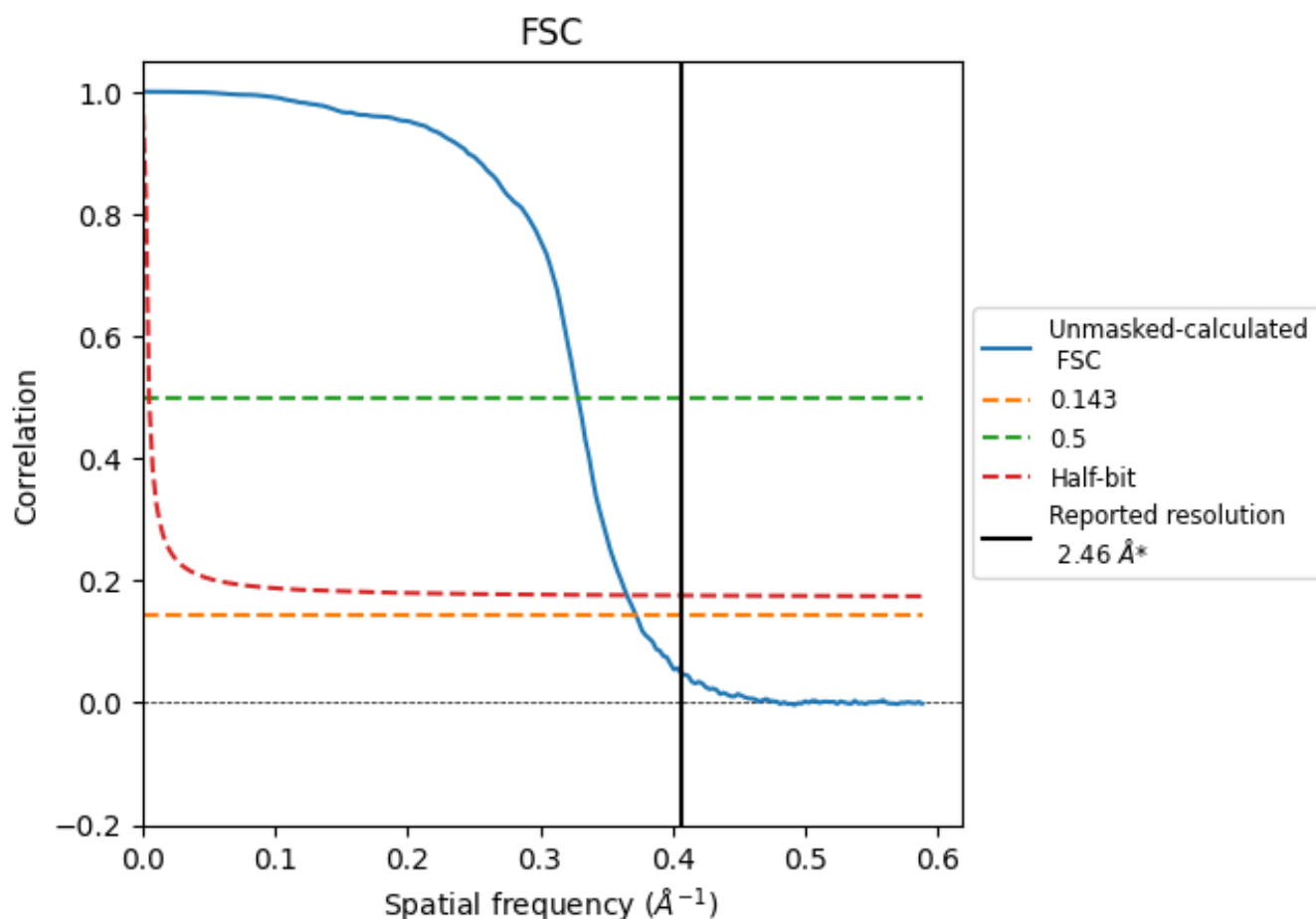


*Reported resolution corresponds to spatial frequency of 0.407 Å⁻¹

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 0.407 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

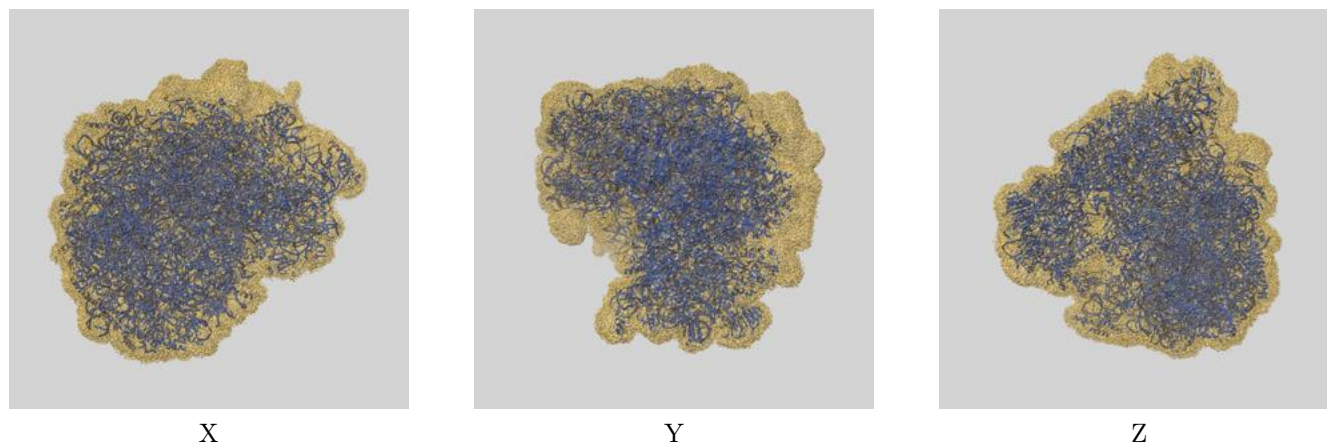
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.69	3.04	2.74

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

9 Map-model fit [i](#)

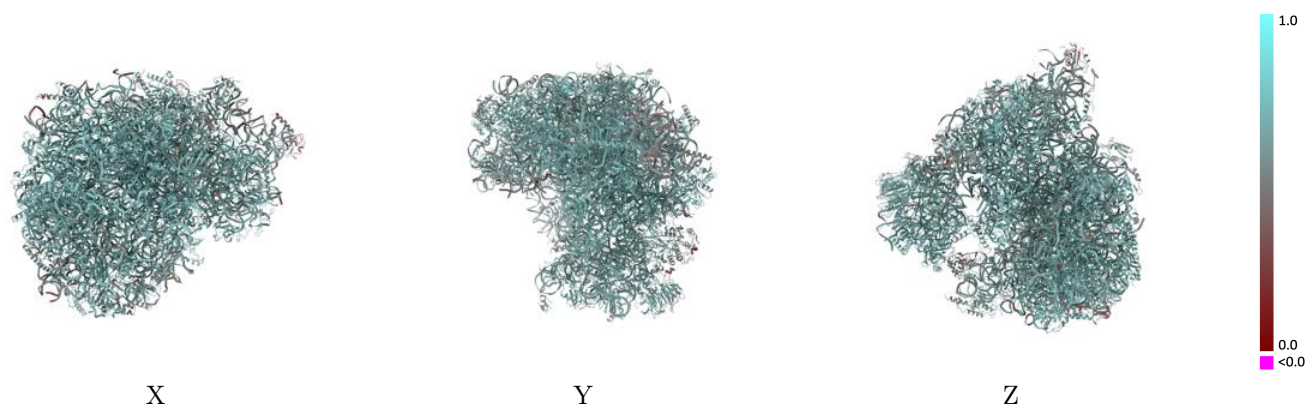
This section contains information regarding the fit between EMDB map EMD-15272 and PDB model 8A98. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



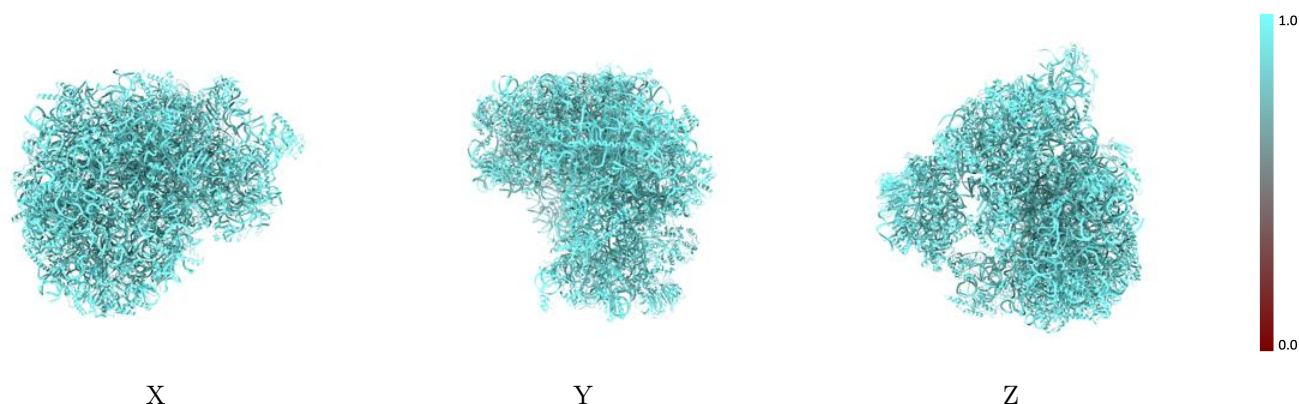
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



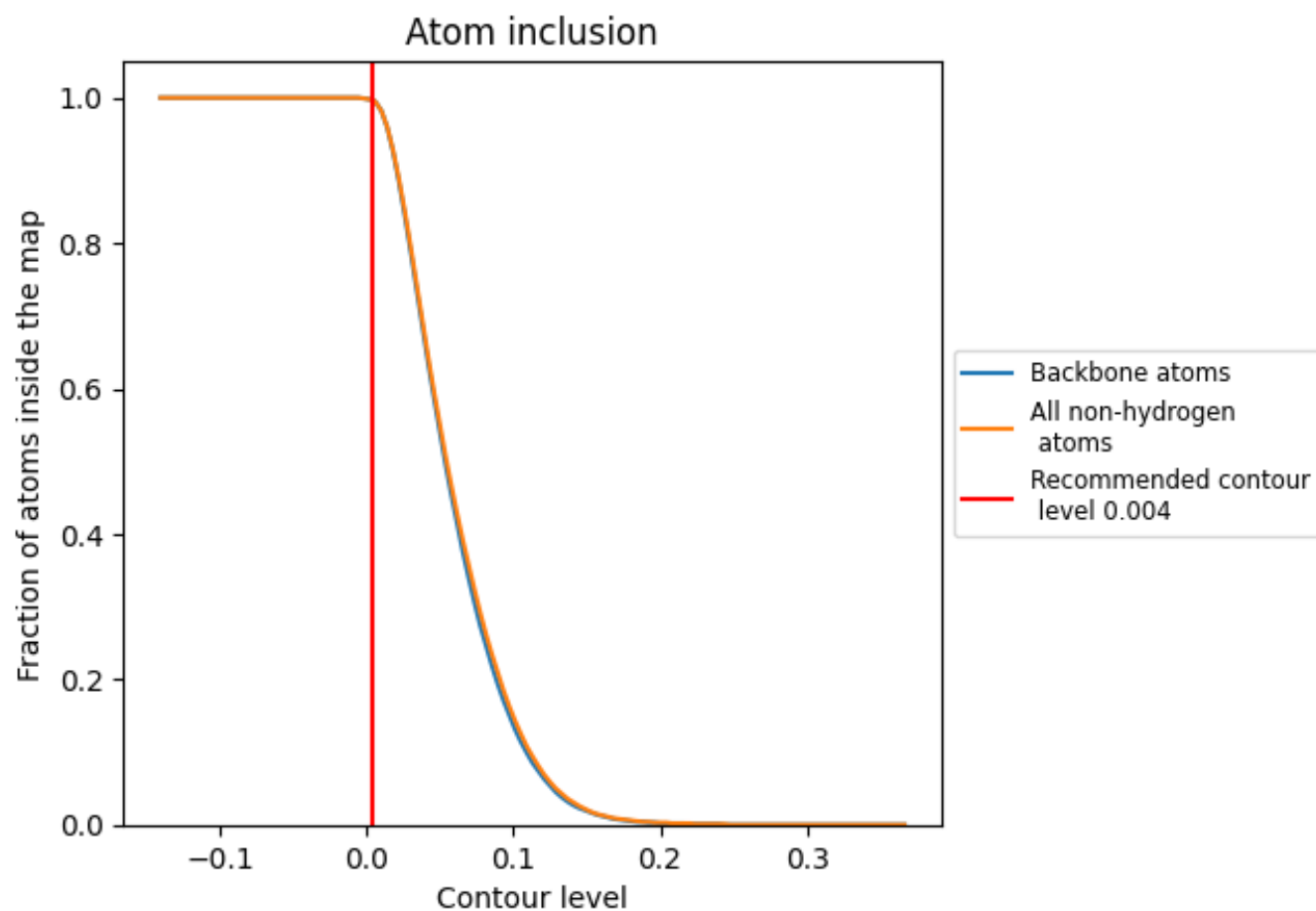
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9970	 0.6530
1	 0.9990	 0.6610
2	 0.9980	 0.6570
3	 0.9960	 0.6410
4	 0.9980	 0.6440
5	 0.9990	 0.6550
6	 0.9980	 0.6150
7	 1.0000	 0.6800
8	 0.9990	 0.6120
A	 1.0000	 0.7100
B	 0.9990	 0.6990
C	 0.9990	 0.6740
D	 0.9980	 0.5280
E	 0.9990	 0.5910
F	 0.9980	 0.6430
G	 0.9970	 0.6500
H	 0.9990	 0.6910
I	 0.9980	 0.6740
J	 0.9990	 0.6930
K	 0.9990	 0.6320
L	 0.9990	 0.7010
M	 0.9990	 0.7190
O	 1.0000	 0.6070
P	 0.9990	 0.6960
Q	 0.9980	 0.6590
R	 0.9970	 0.6680
S	 1.0000	 0.6660
S1	 0.9960	 0.6450
S4	 0.9950	 0.5650
SA	 0.9950	 0.6520
SB	 0.9890	 0.5470
SC	 1.0000	 0.6260
SD	 0.9850	 0.6420
SE	 0.9940	 0.6700
SF	 0.9910	 0.6410



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Chain	Atom inclusion	Q-score
SG	 0.9940	 0.6410
SH	 0.9980	 0.6630
SI	 0.9920	 0.6410
SJ	 0.9980	 0.6960
SK	 0.9940	 0.6700
SL	 0.9980	 0.6680
SM	 0.9970	 0.6400
SN	 0.9990	 0.6230
SO	 0.9930	 0.6650
SP	 0.9910	 0.6780
SQ	 0.9940	 0.5380
SR	 0.9990	 0.6660
SS	 0.9950	 0.6510
ST	 0.9930	 0.6780
SU	 0.9970	 0.6860
SV	 0.9640	 0.5630
SW	 1.0000	 0.6660
SX	 0.9990	 0.6700
SY	 0.9730	 0.5840
SZ	 0.9950	 0.6460
Sa	 0.9920	 0.6290
Sb	 1.0000	 0.6550
Sc	 0.9790	 0.5890
Sd	 0.9960	 0.6170
Se	 0.9800	 0.6070
Sg	 0.9950	 0.6100
Sh	 0.9560	 0.4460
T	 0.9990	 0.7110
U	 1.0000	 0.5860
V	 0.9980	 0.6810
W	 0.9990	 0.6710
X	 1.0000	 0.6860
Y	 0.9980	 0.6370
Z	 0.9990	 0.6500
a	 1.0000	 0.6700
b	 1.0000	 0.6880
c	 1.0000	 0.6850
d	 1.0000	 0.6370
e	 0.9940	 0.6450
f	 0.9990	 0.7060
g	 0.9990	 0.6780
h	 0.9990	 0.6630

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Chain	Atom inclusion	Q-score
i	 0.9970	 0.6380
j	 0.9980	 0.7250
k	 0.9960	 0.6300
l	 1.0000	 0.7140
n	 0.9880	 0.6180
o	 0.9960	 0.6780
p	 0.9960	 0.6280