



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:03 AM UTC

PDB ID : 8OVE / pdb_00008ove
EMDB ID : EMD-17212
Title : CRYO-EM STRUCTURE OF TRYPANOSOMA BRUCEI PROCYCLIC
FORM 80S RIBOSOME : TB11CS6H1 snoRNA mutant
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2023-04-25
Resolution : 2.60 Å (reported)
Based on initial models : 8A3W, 4V8M

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:

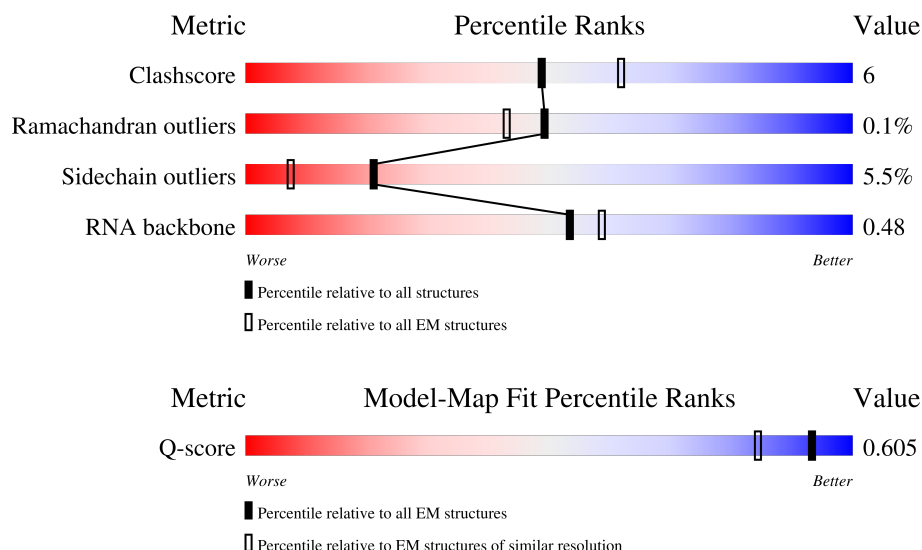
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.60 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.



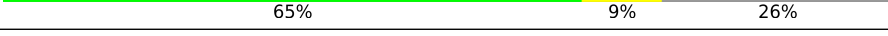
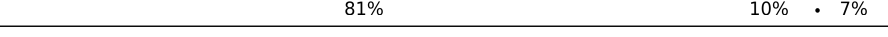
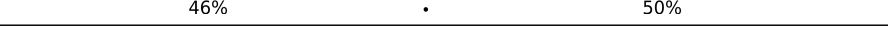
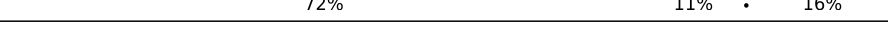
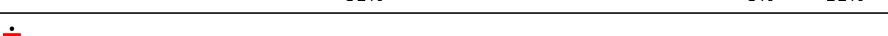
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	AA	2280	
2	AB	19	
3	BA	1920	

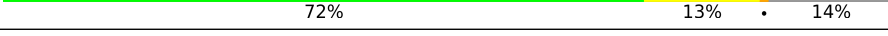
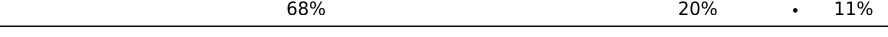
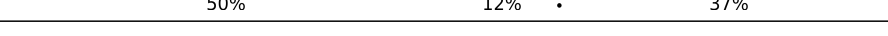
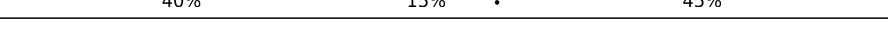
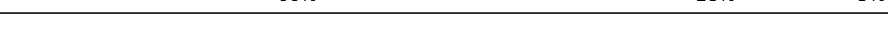
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Mol	Chain	Length	Quality of chain
4	BB	1536	
5	BC	209	
6	BD	119	
7	BE	216	
8	BP	189	
9	BQ	221	
10	BR	166	
11	BS	179	
12	BT	260	
13	BU	159	
14	BW	139	
15	BY	125	
16	BX	164	
17	BZ	143	
18	Bp	82	
19	Bq	51	
20	Br	374	
21	Bt	106	
22	Bw	257	
23	Bx	276	
24	Bl	149	
25	Bu	308	
26	By	189	
27	A0	256	
28	A2	190	

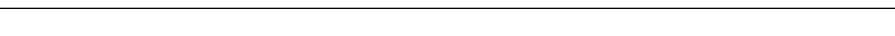
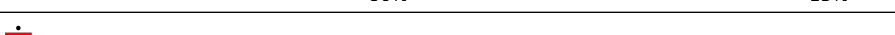
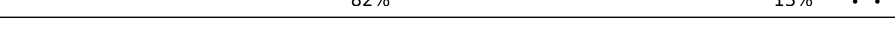
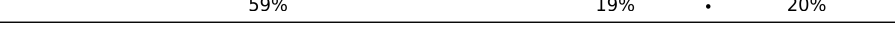
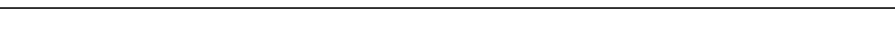
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Mol	Chain	Length	Quality of chain
29	A5	220	
30	AD	172	
31	A8	57	
32	AE	174	
33	AG	151	
34	AI	152	
35	AH	144	
36	AJ	130	
37	AL	142	
38	AM	153	
39	AO	167	
40	AP	266	
41	AS	143	
42	AU	113	
43	AX	214	
44	AZ	103	
45	A3	250	
46	AT	137	
47	A1	273	
48	AC	277	
49	Bc	146	
50	Bz	34	
51	Bo	93	
52	Bn	84	
53	Bm	109	

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Mol	Chain	Length	Quality of chain
54	Bk	127	
55	Bj	170	
56	Bi	132	
57	Bg	105	
58	Bd	71	
59	Bb	145	
60	Ba	133	
61	BO	222	
62	BN	218	
63	BL	194	
64	BK	213	
65	BI	193	
66	Be	260	
67	AK	149	
68	A6	190	
69	Bf	429	
70	AY	66	
71	Bv	192	
72	Bh	188	
73	BF	78	
74	BG	183	
75	BH	136	
76	Bs	128	
77	BV	130	
78	Az	279	

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Mol	Chain	Length	Quality of chain
79	AQ	117	
80	AR	194	
81	AV	111	
82	AW	86	
83	A4	202	
84	A7	318	
85	A	4	

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 203289 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 RNA chain called SSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1836	Total	C	N	O	P	0	0
			39217	17534	7038	12809	1836		

- Molecule 2 is a RNA chain called E-SITE TRNA.

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

- Molecule 3 is a RNA chain called LUS_alpha rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BA	1579	Total	C	N	O	P	1	0
			33850	15122	6138	11010	1580		

- Molecule 4 is a RNA chain called LSUB rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BB	1109	Total	C	N	O	P	0	0
			23703	10602	4238	7754	1109		

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BC	160	Total	C	N	O	P	0	0
			3407	1527	605	1116	159		

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BD	119	Total	C	N	O	P	0	0
			2533	1131	449	835	118		

- Molecule 7 is a RNA chain called SrRNA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BE	166	Total	C	N	O	P	0	0
			3526	1575	620	1165	166		

- Molecule 8 is a protein called 40S ribosomal protein L14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BP	154	Total	C	N	O	S	0	0
			1252	793	242	213	4		

- Molecule 9 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BQ	203	Total	C	N	O	S	0	0
			1716	1077	370	264	5		

- Molecule 10 is a protein called 60S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BR	150	Total	C	N	O	S	0	0
			1209	761	239	201	8		

- Molecule 11 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BS	178	Total	C	N	O	S	0	0
			1465	926	289	243	7		

- Molecule 12 is a protein called 60S ribosomal protein L19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BT	192	Total	C	N	O	S	0	0
			1570	962	345	255	8		

- Molecule 13 is a protein called 60S ribosomal protein L21E, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BU	151	Total	C	N	O	S	0	0
			1197	757	238	196	6		

- Molecule 14 is a protein called 60S ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BW	129	Total	C	N	O	S	0	0
			979	621	185	168	5		

- Molecule 15 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BY	62	Total	C	N	O	S	0	0
			531	347	103	77	4		

- Molecule 16 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BX	117	Total	C	N	O	S	0	0
			955	608	178	167	2		

- Molecule 17 is a protein called 60S ribosomal protein L26, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BZ	120	Total	C	N	O	S	0	0
			971	601	204	161	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Bp	75	Total	C	N	O	S	0	0
			609	383	121	101	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
19	Bq	50	Total	C	N	O	0	0
			457	297	98	62		

- Molecule 20 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Br	366	Total	C	N	O	S	0	0
			2871	1796	571	487	17		

- Molecule 21 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Bt	97	Total	C	N	O	S	0	0
			801	507	159	130	5		

- Molecule 22 is a protein called 60S ribosomal protein L7, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Bw	230	Total	C	N	O	S	0	0
			1872	1190	362	312	8		

- Molecule 23 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Bx	232	Total	C	N	O	S	0	0
			1847	1160	363	318	6		

- Molecule 24 is a protein called 60S ribosomal protein L35A, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Bl	144	Total	C	N	O	S	0	0
			1163	728	239	193	3		

- Molecule 25 is a protein called 60S ribosomal protein L5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Bu	240	Total	C	N	O	S	0	0
			1910	1203	366	336	5		

- Molecule 26 is a protein called 60S ribosomal protein L9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	By	180	Total	C	N	O	S	0	0
			1473	934	274	261	4		

- Molecule 27 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A0	218	Total	C	N	O	S	0	0
			1775	1121	334	312	8		

- Molecule 28 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A2	183	Total	C	N	O	S	0	0
			1464	915	282	262	5		

- Molecule 29 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A5	186	Total	C	N	O	S	0	0
			1457	920	287	248	2		

- Molecule 30 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AD	87	Total	C	N	O	S	0	0
			720	472	124	120	4		

- Molecule 31 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A8	53	Total	C	N	O	S	0	0
			439	270	92	72	5		

- Molecule 32 is a protein called 40S ribosomal proteins S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AE	152	Total	C	N	O	S	0	0
			1234	772	251	206	5		

- Molecule 33 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AG	141	Total	C	N	O	S	0	0
			1148	724	227	190	7		

- Molecule 34 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AI	106	Total	C	N	O	S	0	0
			856	548	161	144	3		

- Molecule 35 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AH	135	Total	C	N	O	S	0	0
			1004	616	194	185	9		

- Molecule 36 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AJ	129	Total	C	N	O	S	0	0
			1018	645	191	174	8		

- Molecule 37 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AL	122	Total	C	N	O	S	0	0
			945	600	184	156	5		

- Molecule 38 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	AM	133	Total	C	N	O	S	0	0
			1081	679	211	187	4		

- Molecule 39 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AO	149	Total	C	N	O	S	0	0
			1186	750	235	193	8		

- Molecule 40 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AP	220	Total	C	N	O	S	0	0
			1703	1086	303	305	9		

- Molecule 41 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AS	140	Total	C	N	O	S	0	0
			1096	696	213	185	2		

- Molecule 42 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AU	71	Total	C	N	O	S	0	1
			551	351	100	95	5		

- Molecule 43 is a protein called 40S ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AX	208	Total	C	N	O	S	0	0
			1652	1036	310	294	12		

- Molecule 44 is a protein called 40S ribosomal protein S33, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AZ	57	Total	C	N	O	S	0	0
			438	265	90	79	4		

- Molecule 45 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	A3	230	Total	C	N	O	S	0	0
			1808	1125	367	312	4		

- Molecule 46 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AT	122	Total	C	N	O	S	0	0
			980	623	192	162	3		

- Molecule 47 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	A1	260	Total	C	N	O	S	0	0
			2048	1298	386	355	9		

- Molecule 48 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AC	208	Total	C	N	O	S	0	0
			1648	1049	297	291	11		

- Molecule 49 is a protein called 60S ribosomal protein L28, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bc	144	Total	C	N	O	S	0	0
			1162	723	234	197	8		

- Molecule 50 is a protein called Ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bz	33	Total	C	N	O	S	0	0
			294	178	76	38	2		

- Molecule 51 is a protein called 60S ribosomal protein L37a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bo	89	Total	C	N	O	S	0	0
			699	434	144	115	6		

- Molecule 52 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bn	80	Total	C	N	O	S	0	0
			676	410	157	103	6		

- Molecule 53 is a protein called Ribosomal protein L36, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Bm	98	Total	C	N	O	S	0	0
			786	493	164	127	2		

- Molecule 54 is a protein called 60S ribosomal protein L35, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bk	123	Total	C	N	O	S	0	0
			1018	639	218	158	3		

- Molecule 55 is a protein called 60S ribosomal protein L34, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Bj	116	Total	C	N	O	S	0	0
			959	593	214	148	4		

- Molecule 56 is a protein called 60S ribosomal protein L32, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bi	131	Total	C	N	O	S	0	0
			1075	678	217	176	4		

- Molecule 57 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Bg	92	Total	C	N	O	S	0	0
			708	441	128	134	5		

- Molecule 58 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bd	69	Total	C	N	O	S	0	0
			561	343	126	91	1		

- Molecule 59 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bb	144	Total	C	N	O	S	0	0
			1137	717	228	186	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Ba	130	Total	C	N	O	S	0	0
			1077	684	220	170	3		

- Molecule 61 is a protein called 60S ribosomal protein L13a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BO	221	Total	C	N	O	S	0	0
			1801	1141	364	289	7		

- Molecule 62 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BN	210	Total	C	N	O	S	0	0
			1722	1074	358	284	6		

- Molecule 63 is a protein called 60S ribosomal protein L11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BL	156	Total	C	N	O	S	0	0
			1246	785	231	223	7		

- Molecule 64 is a protein called 60S ribosomal protein L10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BK	194	Total	C	N	O	S	0	0
			1584	1000	314	259	11		

- Molecule 65 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BI	191	Total	C	N	O	S	0	0
			1517	950	313	246	8		

- Molecule 66 is a protein called 60S ribosomal protein L2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Be	254	Total	C	N	O	S	1	0
			1902	1185	390	314	13		

- Molecule 67 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AK	142	Total	C	N	O	S	0	0
			1143	731	215	194	3		

- Molecule 68 is a protein called Probable 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	A6	178	Total	C	N	O	S	0	0
			1460	920	290	242	8		

- Molecule 69 is a protein called Ribosomal protein L3, mitochondrial, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bf	400	Total	C	N	O	S	0	0
			3211	2023	633	542	13		

- Molecule 70 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AY	59	Total	C	N	O	S	0	0
			471	296	97	77	1		

- Molecule 71 is a protein called 60S ribosomal protein L6, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bv	143	Total	C	N	O	S	0	0
			1101	699	202	197	3		

- Molecule 72 is a protein called 60S ribosomal subunit protein L31, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bh	147	Total	C	N	O	S	0	0
			1188	749	242	193	4		

- Molecule 73 is a RNA chain called SrRNA 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	BF	69	Total	C	N	O	P	0	0
			1444	646	239	490	69		

- Molecule 74 is a RNA chain called SrRNA 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	BG	183	Total	C	N	O	P	0	0
			3919	1746	708	1282	183		

- Molecule 75 is a RNA chain called SrRNA 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	BH	118	Total	C	N	O	P	0	0
			2520	1123	453	826	118		

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bs	50	Total	C	N	O	S	0	0
			394	247	80	60	7		

- Molecule 77 is a protein called 60S ribosomal protein L22, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	BV	122	Total	C	N	O	S	0	0
			973	626	176	168	3		

- Molecule 78 is a protein called RNA-binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	Az	43	Total	C	N	O	0	0
			340	210	68	62		

- Molecule 79 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AQ	100	Total	C	N	O	S	0	0
			800	501	152	144	3		

- Molecule 80 is a protein called 40S ribosomal protein S21, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AR	88	Total	C	N	O	S	0	0
			656	408	117	128	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	88	LYS	GLY	conflict	UNP Q385B8

- Molecule 81 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AV	103	Total	C	N	O	S	0	0
			830	512	175	135	8		

- Molecule 82 is a protein called 40S ribosomal protein S27, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	AW	85	Total	C	N	O	S	0	0
			660	411	124	116	9		

- Molecule 83 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	A4	198	Total	C	N	O	S	0	0
			1596	1020	305	266	5		

- Molecule 84 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	A7	303	Total	C	N	O	S	0	0
			2326	1457	412	445	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A7	28	THR	ALA	conflict	UNP P69103
A7	283	SER	LYS	conflict	UNP P69103

- Molecule 85 is a protein called HIS-THR-CYS-THR.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	A	4	Total	C	N	O	S	0	0
			30	17	6	6	1		

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	AA	52	Total	Mg	0
			52	52	
86	BA	47	Total	Mg	0
			47	47	
86	BB	39	Total	Mg	0
			39	39	
86	BE	3	Total	Mg	0
			3	3	
86	BR	1	Total	Mg	0
			1	1	
86	BW	1	Total	Mg	0
			1	1	
86	A0	1	Total	Mg	0
			1	1	
86	A5	1	Total	Mg	0
			1	1	
86	A3	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
86	Bf	1	Total 1	Mg 1	0
86	BG	2	Total 2	Mg 2	0

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

Mol	Chain	Residues	Atoms		AltConf
87	AA	26	Total 26	K 26	0
87	BA	2	Total 2	K 2	0
87	BB	8	Total 8	K 8	0
87	AG	1	Total 1	K 1	0
87	AP	1	Total 1	K 1	0
87	Be	1	Total 1	K 1	0
87	BG	1	Total 1	K 1	0
87	AV	1	Total 1	K 1	0

- Molecule 88 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
88	AA	26	Total 26	Na 26	0
88	BA	11	Total 11	Na 11	0
88	BB	10	Total 10	Na 10	0
88	BC	1	Total 1	Na 1	0
88	BD	1	Total 1	Na 1	0
88	Bi	1	Total 1	Na 1	0
88	Be	1	Total 1	Na 1	0

- Molecule 89 is water.

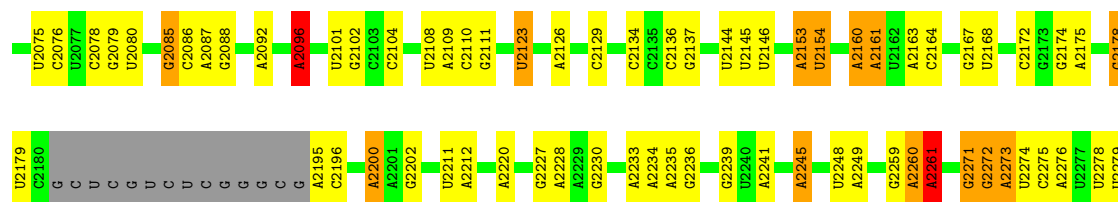
Mol	Chain	Residues	Atoms		AltConf
89	AA	92	Total 92	O 92	0
89	BA	78	Total 78	O 78	0
89	BB	100	Total 100	O 100	0
89	BC	3	Total 3	O 3	0
89	BE	3	Total 3	O 3	0
89	BQ	2	Total 2	O 2	0
89	BT	1	Total 1	O 1	0
89	Br	1	Total 1	O 1	0
89	A0	1	Total 1	O 1	0
89	A8	1	Total 1	O 1	0
89	AH	1	Total 1	O 1	0
89	AO	1	Total 1	O 1	0
89	AS	1	Total 1	O 1	0
89	A1	1	Total 1	O 1	0
89	Bz	2	Total 2	O 2	0
89	Bo	1	Total 1	O 1	0
89	Bn	3	Total 3	O 3	0
89	Bj	2	Total 2	O 2	0
89	Bd	1	Total 1	O 1	0
89	Bb	2	Total 2	O 2	0
89	BN	1	Total 1	O 1	0

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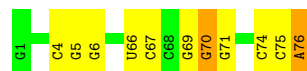
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Mol	Chain	Residues	Atoms		AltConf
89	BK	1	Total 1	O 1	0
89	BI	1	Total 1	O 1	0
89	Be	10	Total 10	O 10	0
89	BG	5	Total 5	O 5	0
89	BH	2	Total 2	O 2	0
89	AV	6	Total 6	O 6	0

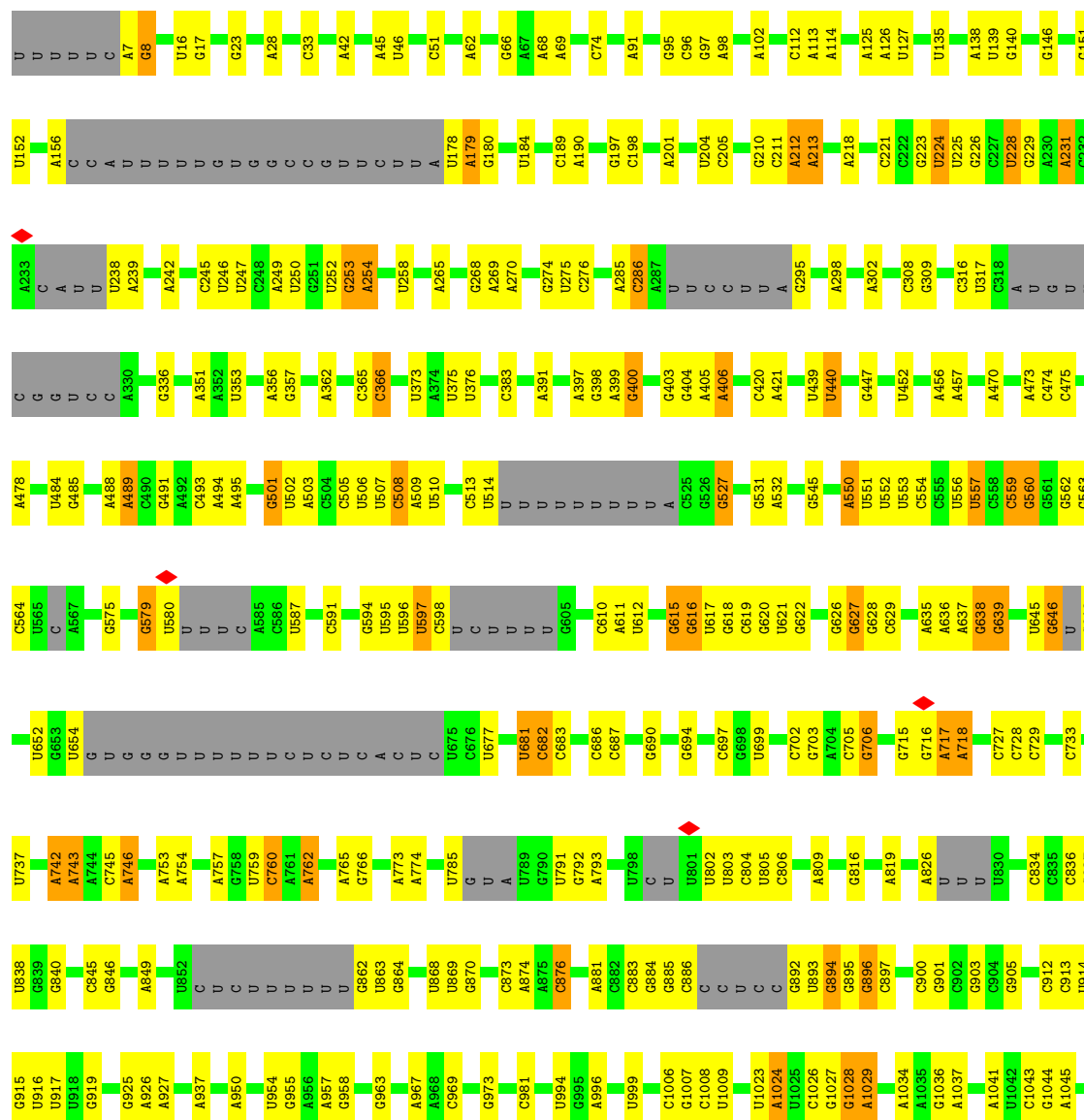
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A2000	A1927	A	A1773	A1661	G1590	U1472	U	U	C1236	C	U	U1006	G938	C
G2001	C1928	C	G1774	U1662	U1591	U1473	C	G	U1237	A	G	U1007	U941	A
C2002	G1931	G	G1775	C1663	U1592	U1474	A	G	U1238	G	U	U1008	U942	A
G2005	G1936	G	A1776	G1668	C1595	C1477	C	G	U1239	G1133	G	A1009	G943	A
A2008	A1937	C	C1777	A1669	B881936	U1478	C	G	C1240	A1135	C	A1011	U871	G870
A2009	A1938	C	C1780	G1676	A1599	U1479	C	C	U1241	A1139	G	A1012	C872	U878
C2010	G1941	A	A	G1696	C1600	U1482	G	C	U1242	G1144	A	G1013	A948	C879
A2012	U1946	U	U	C1697	A1601	U1483	U	U	A1243	G1145	A	U1014	U947	U874
G2014	G1947	C	C	U1698	G1604	A1484	C	U	U1244	U1146	C	U1015	C949	A
G2015	A1948	C	C	G1699	G1605	C1485	C	G	A1245	A1147	C	G1016	A950	A
A2016	G1949	U	U	G1700	G1606	G1496	C	U	U1246	G1148	C	U1017	A951	A
A2017	A1950	C	C	U1706	A1607	U1501	U	C	U1265	G1149	A	U1018	U952	A
U2018	A1951	C	C	U1711	G1617	U1502	U	C	U1266	U1150	C	U1019	G953	A
C2019	C1952	G	G	U1712	A1618	A1503	U	G	C1267	G1151	C	U1020	G954	A
A2020	A1953	C	C	G1713	U1619	C1504	U	U	A1268	U1149	A	G1021	A955	A
U2023	A1954	U	U	G1714	G1622	G1506	U	C	U1275	U1152	C	U1022	U956	A
A2024	G1955	G	G	U1719	G1623	U1512	U	C	U1276	G1153	C	U1023	G957	A
G2025	U1956	G	G	U1720	A1624	G1513	U	C	A1282	U1158	C	U1024	G958	A
A2026	G1957	C	C	G1723	C1625	G1516	U	C	U1291	G1159	C	U1025	G959	A
G2027	U1958	A	A	U1726	A1626	U1517	U	G	C1298	A1160	C	U1026	G960	A
C2028	C	U	U	A1727	G1627	G1518	U	C	C1301	G1161	C	U1027	G961	A
G2033	G1961	U	U	U1730	G1628	A1519	U	C	A1302	U1162	C	U1028	U962	A
G2034	A1962	C	C	G1731	G1629	G1519	U	C	A1303	U1163	C	U1029	U963	A
G2035	G	U	U	C1732	U1630	G1520	U	C	A1304	U1164	C	U1030	C964	A
C2036	C	U	U	U1743	G1631	G1521	U	C	C1305	G1165	C	U1031	U965	A
U2043	G1963	C	C	G1744	G1632	G1531	U	C	A1316	A1183	C	U1032	U966	A
A2044	A1964	C	C	U1745	G1633	U1536	U	C	U1317	A1184	C	U1033	U967	A
U2045	U	U	U	G1746	A1634	A1537	U	C	G1318	U1185	C	U1034	U968	A
A2046	C	U	U	C1747	U1635	U1538	U	C	U1322	U1186	C	U1035	U969	A
G2047	G1983	C	C	U1748	U1636	G1539	U	C	G1323	A1192	C	U1036	U970	A
C2048	A1984	C	C	G1750	U1637	U1540	U	C	G1324	C1198	C	U1037	U971	A
A2049	U1985	U	U	U1751	G1638	U1541	U	C	G1325	U1199	C	U1038	U972	A
U2051	G1986	C	C	A1752	U1639	A1543	U	C	G1326	A1201	C	U1039	U973	A
U2052	C	U	U	G1753	A1641	G1555	U	C	A1327	G1202	C	U1040	U974	A
A2053	G1987	U	U	U1754	U1642	A1556	U	C	A	A1207	C	U1041	U975	A
U2054	G1988	C	C	G1755	G1643	A1557	U	C	A	A1210	C	U1042	U976	A
G2057	U1989	C	C	U1756	U1644	G1560	U	C	U1328	A1211	C	U1043	U977	A
U2058	C1989	C	C	G1757	G1645	C1561	U	C	U1329	A1212	C	U1044	U978	A
C2059	G1990	U	U	C1758	U1646	U1562	U	C	G1330	G1213	C	U1045	U979	A
G2063	G1991	C	C	U1759	A1647	C1563	U	C	U1331	U1214	C	U1046	U980	A
A2064	C	U	U	U1760	G	C1564	U	C	A	A1215	C	U1047	U981	A
A2065	U1992	C	C	G1761	U	A1565	U	C	U1332	A1216	C	U1048	U982	A
G2069	C1993	C	C	U1762	G1650	A1566	U	C	U1333	A1217	C	U1049	U983	A
G2070	A1994	U	U	A1763	U1651	A1567	U	C	G1334	U1218	C	U1050	U984	A
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				U1765	U1653	G1569	U	C	G1336	U1220	C	U1052	U986	A
				U1766	U1654	U1570	U	C	U1337	U1221	C	U1053	U987	A
				U1767	U1655	G1571	U	C	A	U1222	C	U1054	U988	A
				U1768	U1656	U1572	U	C	U1338	C1223	C	U1055	U989	A
				U1769	U1657	A1573	U	C	U1339	A1224	C	U1056	U990	A
					U1658	A1574	U	C	U1401	A1225	C	U1057	U991	A
					U1659	A1575	U	C	A	A1226	C	U1058	U992	A
						A1576	U	C	U1402	A1227	C	U1059	U993	A
							U	C	U1403	A1228	C	U1060	U994	A
								C	U1404	A1229	C	U1061	U995	A
								U	U1405	A1230	C	U1062	U996	A
									U1406	A1231	C	U1063	U997	A
									U1407	A1232	C	U1064	U998	A
									U1408	A1233	C	U1065	U999	A
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									U1410	A1235	C	U1067	U1001	A
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									U1412	A1237	C	U1069	U1003	A
									U1413	A1238	C	U1070	U1004	A
									U1414	A1239	C	U1071	U1005	A
									U1415	A1240	C	U1072	U1006	A
									U1416	A1241	C	U1073	U1007	A
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									U1418	A1243	C	U1075	U1009	A
									U1419	A1244	C	U1076	U1010	A
									U1420	A1245	C	U1077	U1011	A
									U1421	A1246	C	U1078	U1012	A
									U1422	A1247	C	U1079	U1013	A
									U1423	A1248	C	U1080	U1014	A
									U1424	A1249	C	U1081	U1015	A
									U1425	A1250	C	U1082	U1016	A
									U1426	A1251	C	U1083	U1017	A
									U1427	A1252	C	U1084	U1018	A
									U1428	A1253	C	U1085	U1019	A
									U1429	A1254	C	U1086	U1020	A
									U1430	A1255	C	U1087	U1021	A
									U1431	A1256	C	U1088	U1022	A
									U1432	A1257	C	U1089	U1023	A
									U1433	A1258	C	U1090	U1024	A
									U1434	A1259	C	U1091	U1025	A
									U1435	A1260	C	U1092	U1026	A
									U1436	A1261	C	U1093	U1027	A
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									U1438	A1263	C	U1095	U1029	A
									U1439	A1264	C	U1096	U1030	A
									U1440	A1265	C	U1097	U1031	A
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									U1442	A1267	C	U1099	U1033	A
									U1443	A1268	C	U1100	U1034	A
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									U1451	A1276	C	U1108	U1042	A
									U1452	A1277	C	U1109	U1043	A
									U1453	A1278	C	U1110	U1044	A
									U1454	A1279	C	U1111	U1045	A
									U1455	A1280	C	U1112	U1046	A
									U1456	A1281	C	U1113	U1047	A
									U1457	A1282	C	U1114	U1048	A
									U1458	A1283	C	U1115	U1049	A
									U1459	A1284	C	U1116	U1050	A
									U1460	A1285	C	U1117	U1051	A
									U1461	A1286	C	U1118	U1052	A
									U1462	A1287	C	U1119	U1053	A
									U1463	A1288	C	U1120	U1054	A
									U1464	A1289	C	U1121	U1055	A
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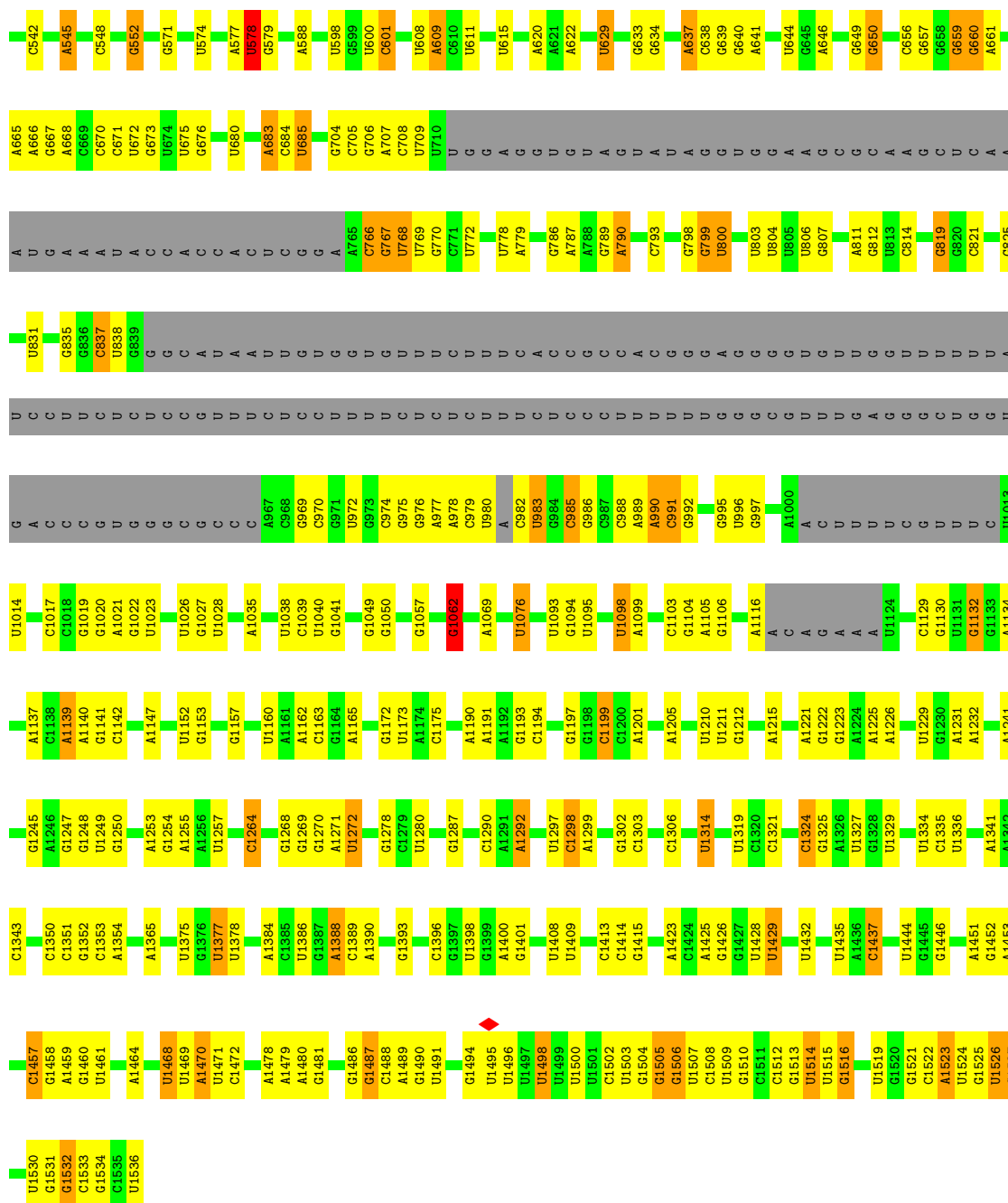


• Molecule 2: E-SITE TRNA



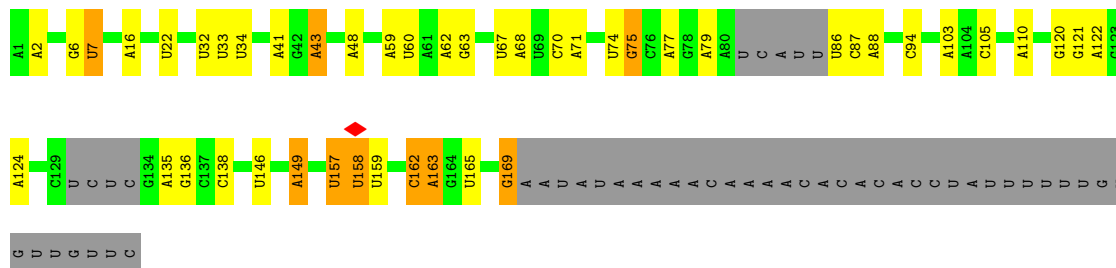
• Molecule 3: LUS_alpha rRNA





● Molecule 5: 5.8S rRNA

Chain BC:



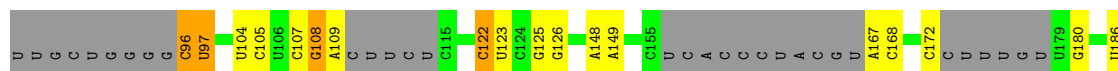
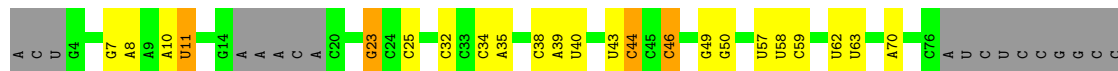
- Molecule 6: 5S rRNA

Chain BD: 



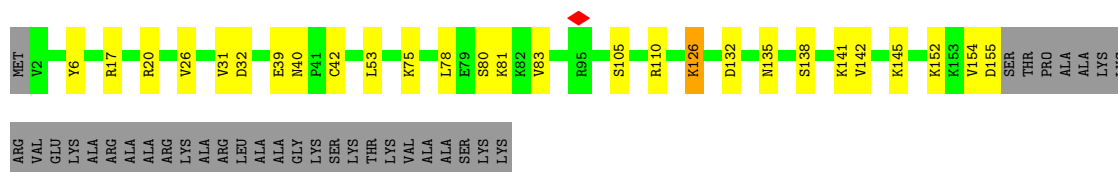
- Molecule 7: SrRNA 1

Chain BE: 



- Molecule 8: 40S ribosomal protein L14, putative

Chain BP: 



- Molecule 9: Ribosomal protein L15

Chain BQ: 



- Molecule 10: 60S ribosomal protein L17, putative

Chain BR: 



- Molecule 11: 60S ribosomal protein L18a

Chain BS: 

- Molecule 17: 60S ribosomal protein L26, putative

Chain BZ:  72% 11% 16%



- Molecule 18: 60S ribosomal protein L38, putative

Chain Bp:  70% 21% 9%



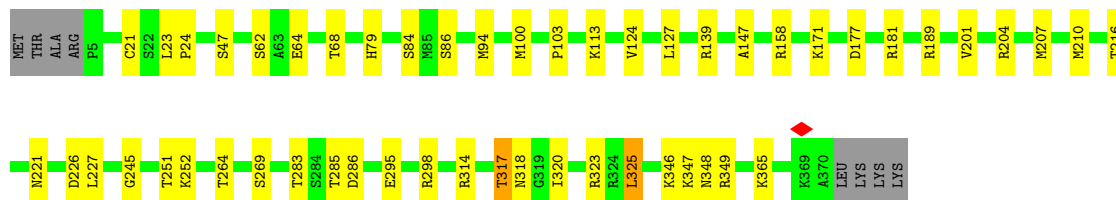
- Molecule 19: 60S ribosomal protein L39, putative

Chain Bq:  82% 12% 6%



- Molecule 20: 60S ribosomal protein L4

Chain Br:  84% 13% 3%



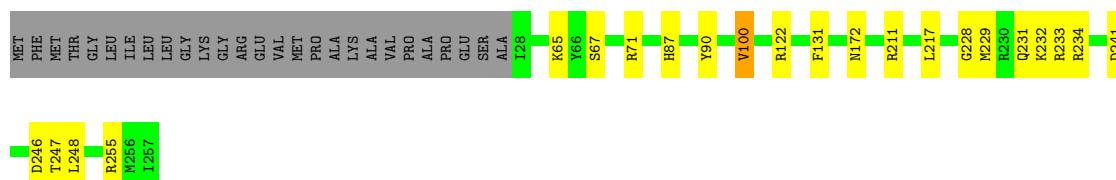
- Molecule 21: 60S ribosomal protein L44

Chain Bt:  74% 17% 9%

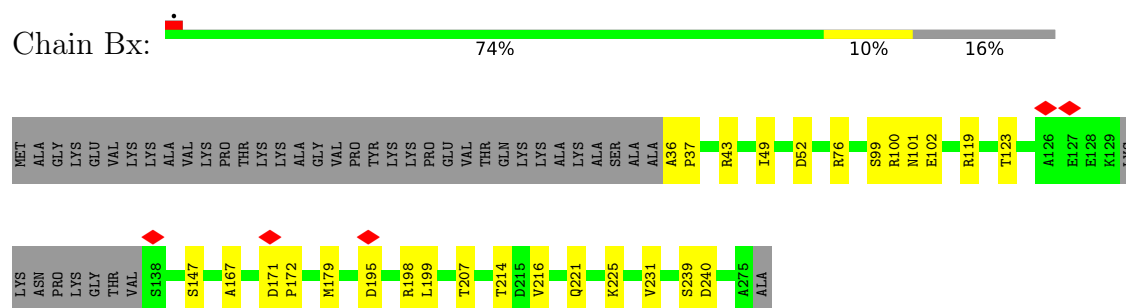


- Molecule 22: 60S ribosomal protein L7, putative

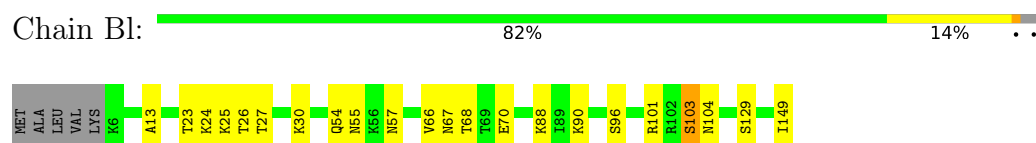
Chain Bw:  81% 8% 11%



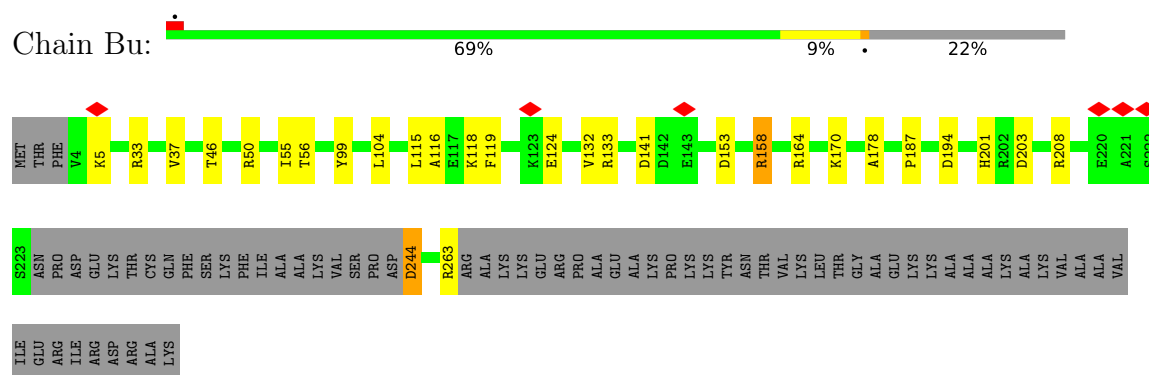
- Molecule 23: 60S ribosomal protein L7a



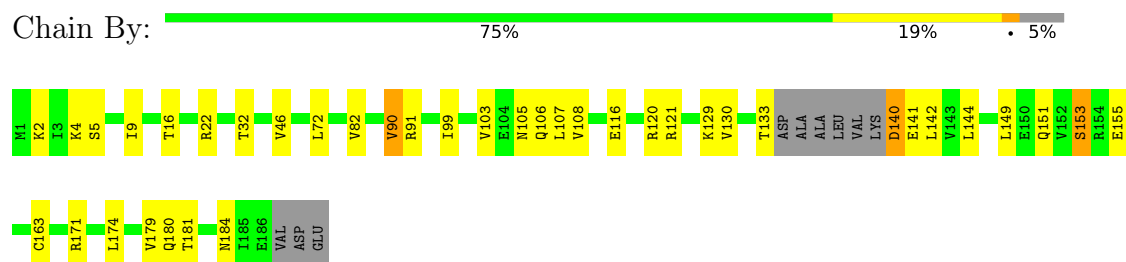
- Molecule 24: 60S ribosomal protein L35A, putative



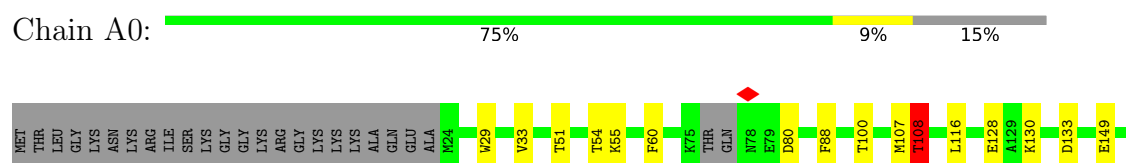
- Molecule 25: 60S ribosomal protein L5, putative



- Molecule 26: 60S ribosomal protein L9, putative



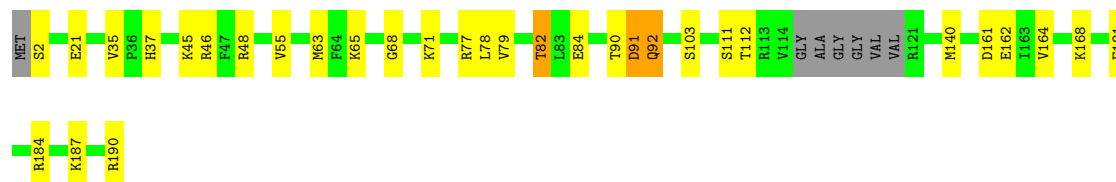
- Molecule 27: 40S ribosomal protein S3a





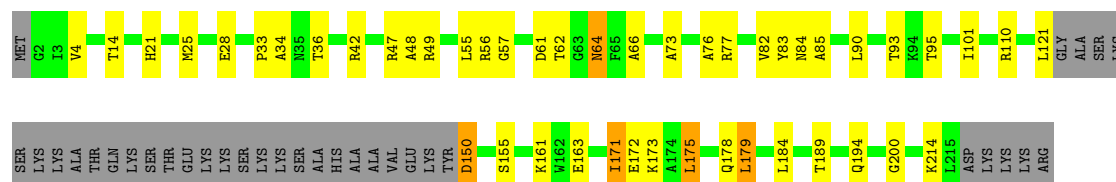
- Molecule 28: 40S ribosomal protein S5, putative

Chain A2: 79% 15% . .



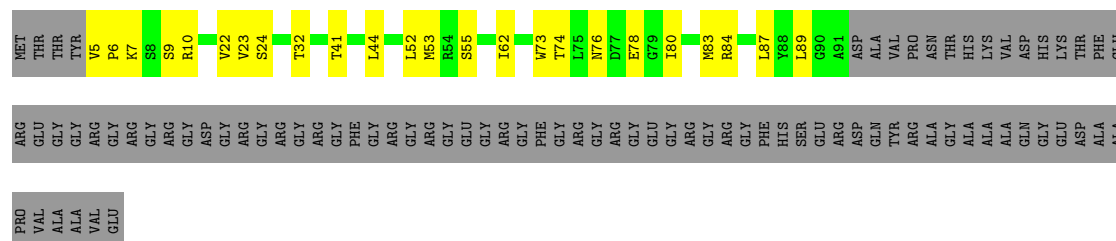
- Molecule 29: 40S ribosomal protein S8

Chain A5: 63% 19% . 15%



- Molecule 30: 40S ribosomal protein S10, putative

Chain AD: 37% 14% 49%



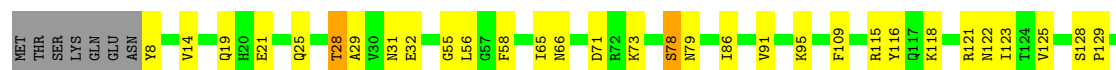
- Molecule 31: Putative ribosomal protein S29

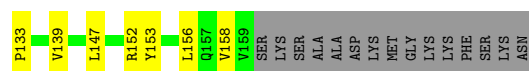
Chain A8: 74% 19% 7%



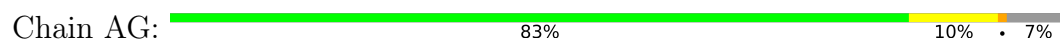
- Molecule 32: 40S ribosomal proteins S11, putative

Chain AE: 66% 21% . 13%





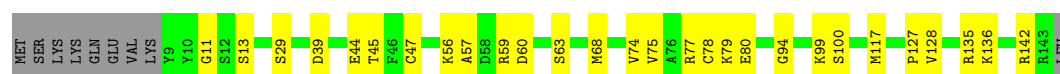
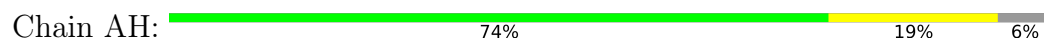
- Molecule 33: 40S ribosomal protein S13, putative



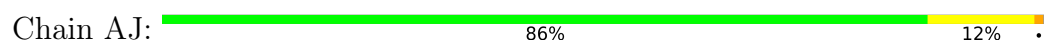
- Molecule 34: 40S ribosomal protein S15, putative



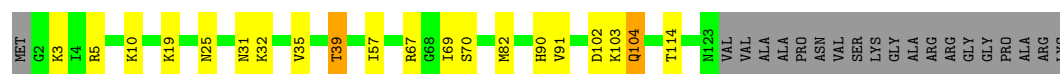
- Molecule 35: 40S ribosomal protein S14



- Molecule 36: 40S ribosomal protein S15a, putative



- Molecule 37: 40S ribosomal protein S17, putative



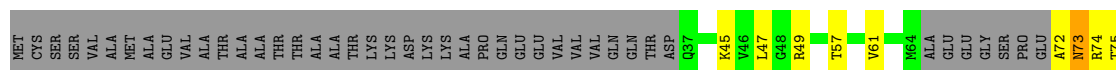
- Molecule 38: 40S ribosomal protein S18, putative





- Molecule 44: 40S ribosomal protein S33, putative

Chain AZ: 40% 15% 45%



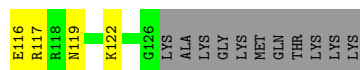
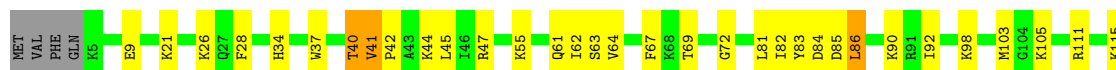
- Molecule 45: 40S ribosomal protein S6

Chain A3: 74% 17% 8%



- Molecule 46: 40S ribosomal protein S24

Chain AT: 62% 25% 11%



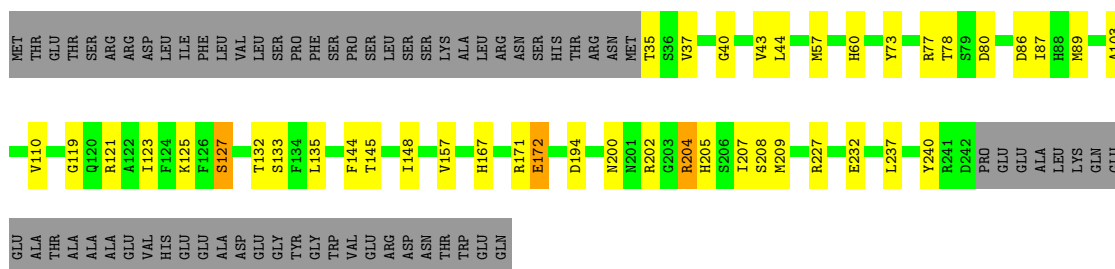
- Molecule 47: 40S ribosomal protein S4

Chain A1: 66% 28% 5%

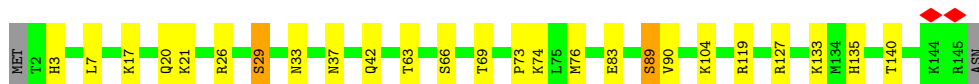
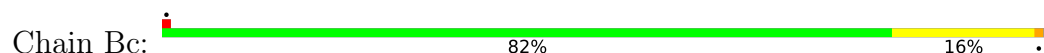


- Molecule 48: 40S ribosomal protein SA

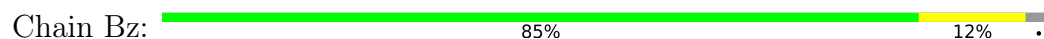
Chain AC: 60% 14% 25%



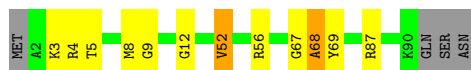
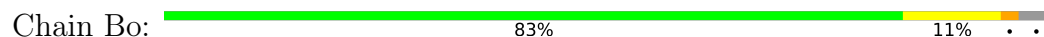
- Molecule 49: 60S ribosomal protein L28, putative



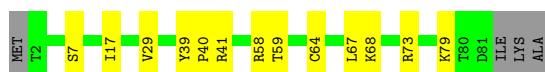
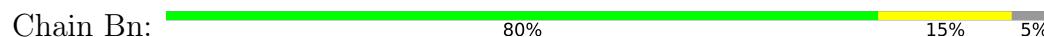
- Molecule 50: Ribosomal protein L41



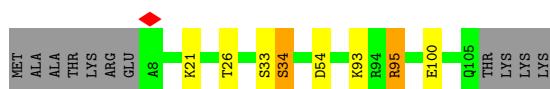
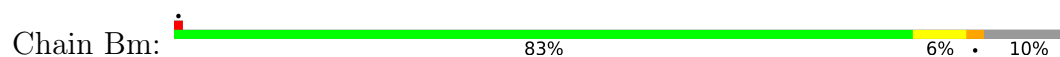
- Molecule 51: 60S ribosomal protein L37a, putative



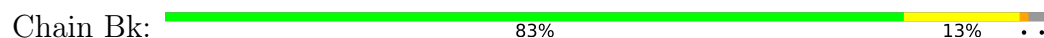
- Molecule 52: Ribosomal protein L37

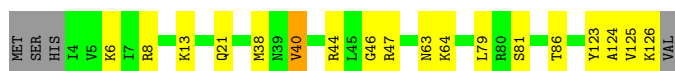


- Molecule 53: Ribosomal protein L36, putative

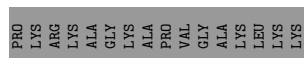
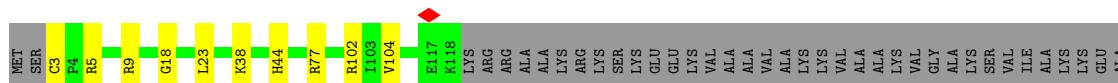


- Molecule 54: 60S ribosomal protein L35, putative

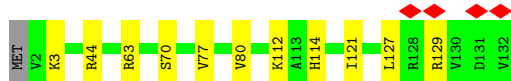




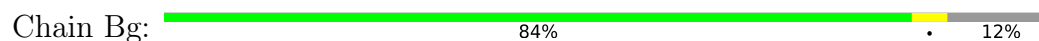
- Molecule 55: 60S ribosomal protein L34, putative



- Molecule 56: 60S ribosomal protein L32, putative



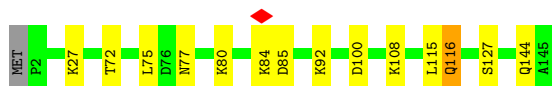
- Molecule 57: 60S ribosomal protein L30



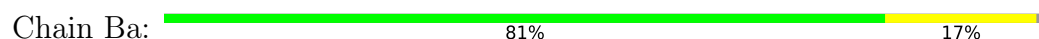
- Molecule 58: 60S ribosomal protein L29



- Molecule 59: 60S ribosomal protein L27a

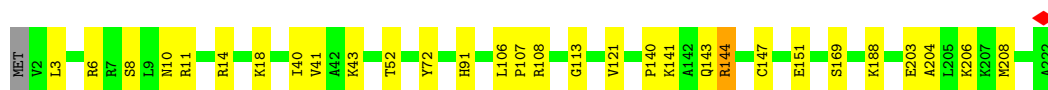


- Molecule 60: 60S ribosomal protein L27



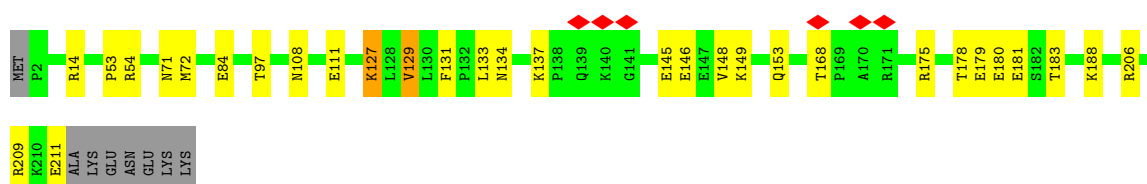
- Molecule 61: 60S ribosomal protein L13a, putative

Chain BO:  86% 13%



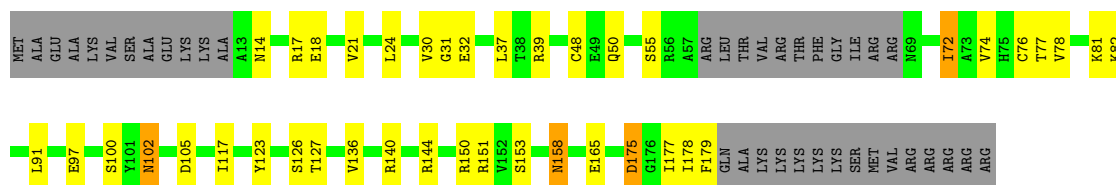
- Molecule 62: 60S ribosomal protein L13

Chain BN:  82% 13%



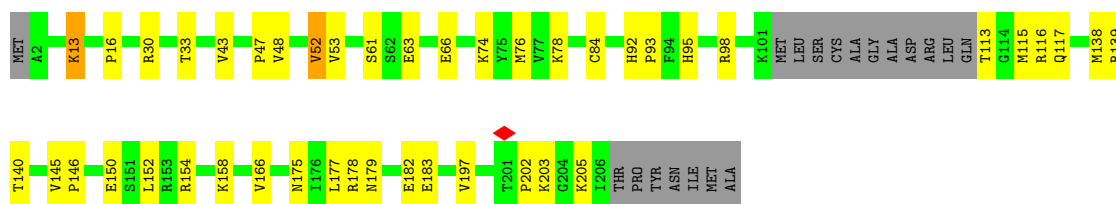
- Molecule 63: 60S ribosomal protein L11, putative

Chain BL:  59% 19% 20%



- Molecule 64: 60S ribosomal protein L10, putative

Chain BK:  70% 20% 9%



- Molecule 65: 60S ribosomal protein L18

Chain BI:  87% 11%



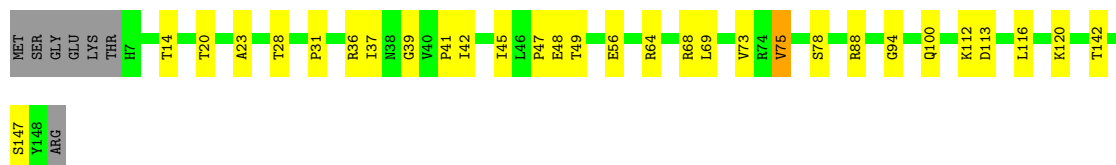
- Molecule 66: 60S ribosomal protein L2, putative

Chain Be:  88% 9%



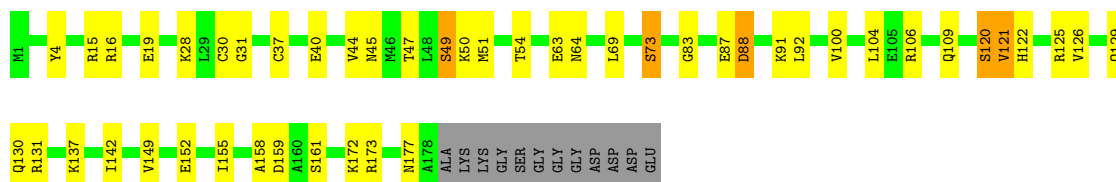
- Molecule 67: 40S ribosomal protein S16, putative

Chain AK: 75% 19% • 5%



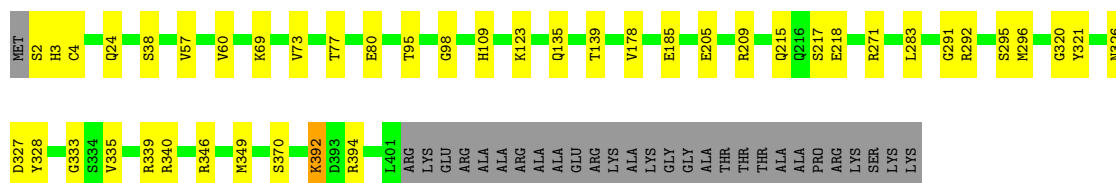
- Molecule 68: Probable 40S ribosomal protein S9

Chain A6: 68% 23% • 6%



- Molecule 69: Ribosomal protein L3, mitochondrial, putative

Chain Bf: 83% 10% 7%



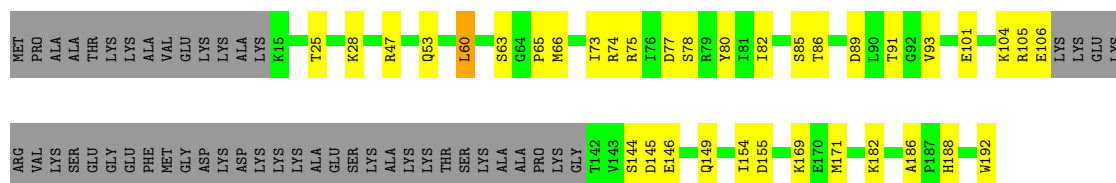
- Molecule 70: 40S ribosomal protein S30

Chain AY: 55% 35% 11%

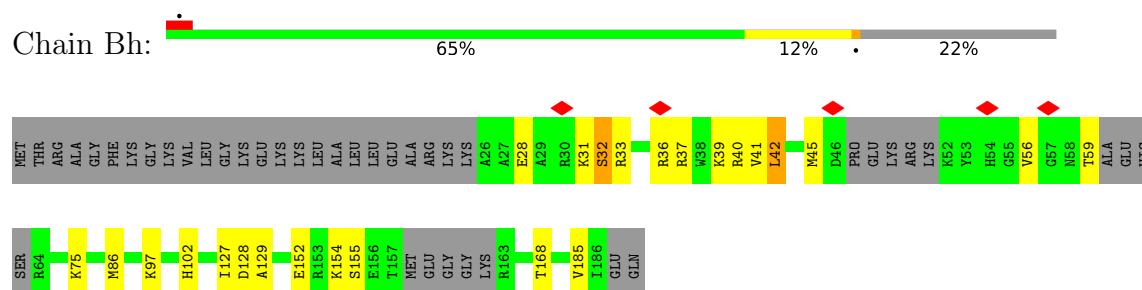


- Molecule 71: 60S ribosomal protein L6, putative

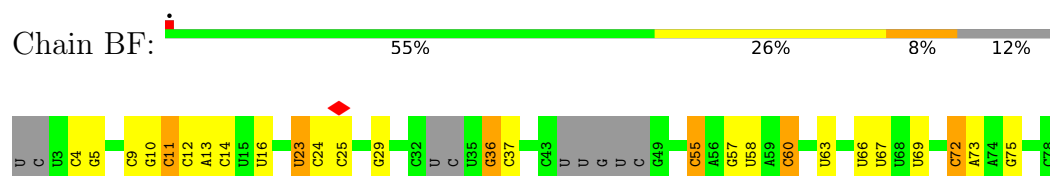
Chain Bv: 56% 18% • 26%



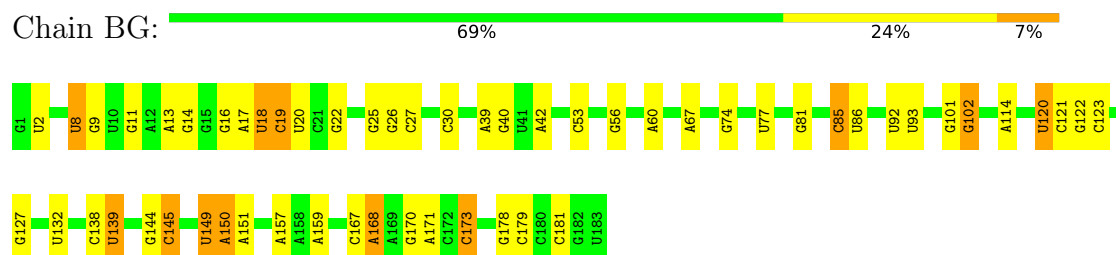
- Molecule 72: 60S ribosomal subunit protein L31, putative



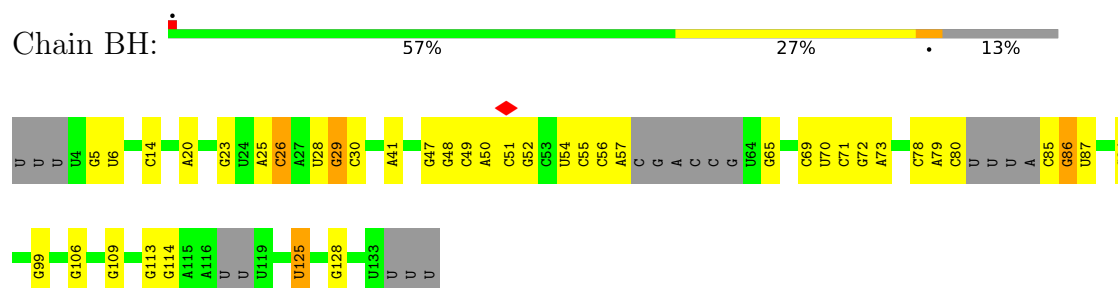
- Molecule 73: SrRNA 6



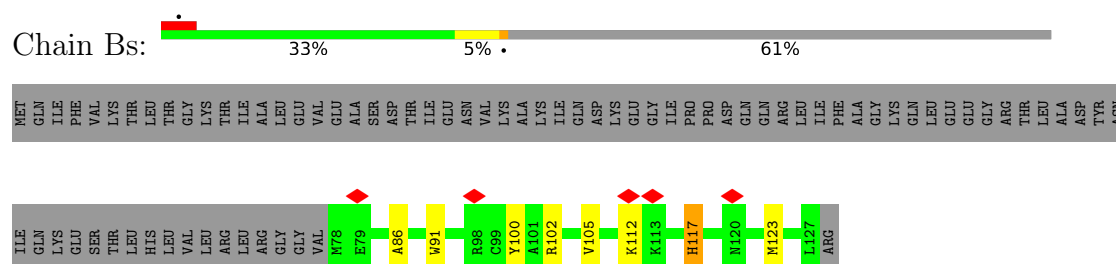
- Molecule 74: SrRNA 2



- Molecule 75: SrRNA 4



- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 77: 60S ribosomal protein L22, putative



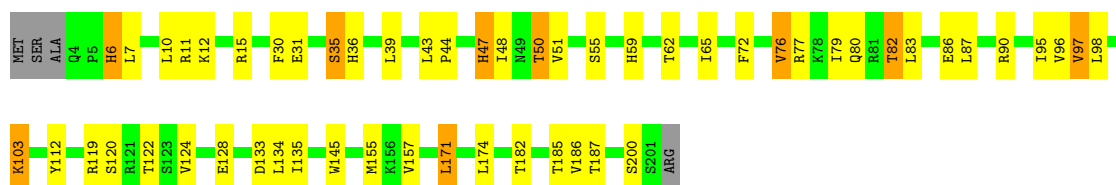
- Molecule 82: 40S ribosomal protein S27, putative

Chain AW: 79% 20%



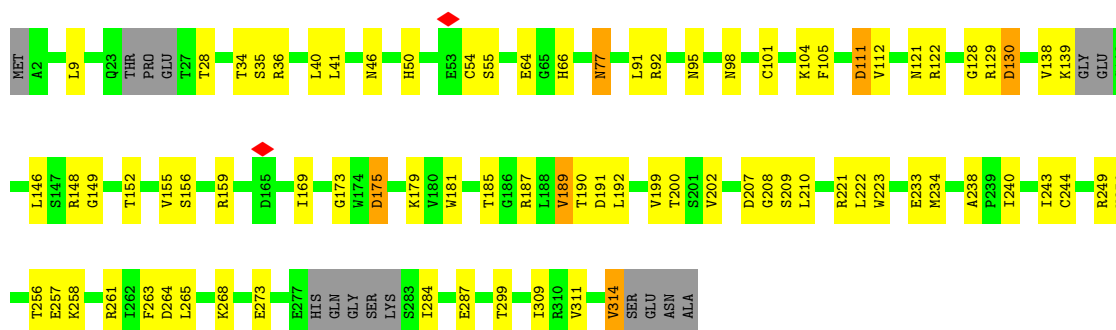
- Molecule 83: 40S ribosomal protein S7

Chain A4: 71% 23%



- Molecule 84: Guanine nucleotide-binding protein subunit beta-like protein

Chain A7: 70% 24% 5%



- Molecule 85: HIS-THR-CYS-THR

Chain A: 75% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	552813	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 ($e^-/\text{\AA}^2$)	1.16	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.301	Depositor
Minimum map value	-0.110	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, A2M, PSU, 1MA, OMU, K, MA6, NA, 5MC, MG, OMG, OMC, 7MG

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	AA	0.29	0/43029	0.35	0/67010
2	AB	0.16	0/450	0.31	0/698
3	BA	0.23	0/36963	0.32	0/57587
4	BB	0.26	0/25239	0.35	8/39334 (0.0%)
5	BC	0.24	0/3656	0.27	0/5690
6	BD	0.15	0/2830	0.25	0/4410
7	BE	0.20	0/3933	0.30	0/6113
8	BP	0.14	0/1271	0.35	0/1704
9	BQ	0.19	0/1755	0.32	0/2346
10	BR	0.17	0/1233	0.31	0/1654
11	BS	0.15	0/1500	0.35	0/2018
12	BT	0.17	0/1587	0.31	0/2102
13	BU	0.16	0/1221	0.30	0/1638
14	BW	0.18	0/996	0.33	0/1342
15	BY	0.17	0/551	0.32	0/742
16	BX	0.15	0/972	0.25	0/1308
17	BZ	0.15	0/984	0.29	0/1312
18	Bp	0.16	0/617	0.37	0/819
19	Bq	0.17	0/471	0.35	0/626
20	Br	0.16	0/2925	0.31	0/3926
21	Bt	0.18	0/815	0.29	0/1077
22	Bw	0.16	0/1907	0.28	0/2556
23	Bx	0.15	0/1873	0.26	0/2520
24	Bl	0.18	0/1187	0.33	0/1592
25	Bu	0.13	0/1944	0.32	0/2610
26	By	0.12	0/1493	0.28	0/2005
27	A0	0.26	0/1801	0.36	0/2421
28	A2	0.18	0/1486	0.32	0/1997
29	A5	0.20	0/1480	0.33	0/1986
30	AD	0.16	0/740	0.37	0/994
31	A8	0.16	0/445	0.28	0/588
32	AE	0.22	0/1258	0.34	0/1692

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AG	0.26	0/1170	0.35	0/1567
34	AI	0.18	0/871	0.33	0/1167
35	AH	0.27	0/1019	0.41	0/1367
36	AJ	0.27	0/1035	0.38	0/1386
37	AL	0.16	0/957	0.31	0/1282
38	AM	0.15	0/1098	0.33	0/1470
39	AO	0.15	0/1211	0.30	0/1621
40	AP	0.25	0/1738	0.38	0/2347
41	AS	0.25	0/1117	0.36	0/1495
42	AU	0.21	0/557	0.45	0/745
43	AX	0.15	0/1674	0.27	0/2236
44	AZ	0.22	0/437	0.45	0/581
45	A3	0.16	0/1828	0.33	0/2445
46	AT	0.18	0/995	0.33	0/1323
47	A1	0.19	0/2082	0.34	0/2799
48	AC	0.22	0/1682	0.34	0/2275
49	Bc	0.13	0/1179	0.29	0/1573
50	Bz	0.27	0/298	0.41	0/385
51	Bo	0.21	0/711	0.32	0/946
52	Bn	0.20	0/690	0.35	0/920
53	Bm	0.16	0/796	0.38	0/1057
54	Bk	0.16	0/1026	0.38	0/1355
55	Bj	0.16	0/977	0.28	0/1304
56	Bi	0.18	0/1097	0.28	0/1468
57	Bg	0.18	0/718	0.25	0/969
58	Bd	0.18	0/572	0.33	0/766
59	Bb	0.17	0/1165	0.30	0/1554
60	Ba	0.14	0/1096	0.25	0/1457
61	BO	0.16	0/1832	0.32	0/2446
62	BN	0.16	0/1753	0.32	0/2338
63	BL	0.11	0/1265	0.24	0/1689
64	BK	0.15	0/1616	0.33	0/2165
65	BI	0.16	0/1543	0.30	0/2059
66	Be	0.21	0/1943	0.31	0/2616
67	AK	0.17	0/1164	0.30	0/1565
68	A6	0.19	0/1490	0.34	0/2002
69	Bf	0.18	0/3281	0.31	0/4409
70	AY	0.18	0/477	0.32	0/630
71	Bv	0.13	0/1120	0.29	0/1511
72	Bh	0.15	0/1205	0.27	0/1603
73	BF	0.15	0/1604	0.31	0/2487
74	BG	0.19	0/4383	0.30	0/6835
75	BH	0.19	0/2813	0.30	0/4377

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Bs	0.09	0/400	0.25	0/531
77	BV	0.13	0/989	0.33	0/1322
78	Az	0.12	0/340	0.34	0/450
79	AQ	0.20	0/809	0.44	0/1091
80	AR	0.19	0/665	0.34	0/905
81	AV	0.32	0/846	0.36	0/1132
82	AW	0.23	0/674	0.36	0/904
83	A4	0.20	0/1628	0.37	0/2201
84	A7	0.15	0/2380	0.31	0/3242
85	A	0.09	0/30	0.36	0/40
All	All	0.23	0/214658	0.33	8/314827 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
40	AP	0	1
53	Bm	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	528	PSU	P-O3'-C3'	-8.20	107.91	120.20
4	BB	515	G	P-O3'-C3'	-7.38	109.12	120.20
4	BB	531	C	P-O3'-C3'	-7.14	109.49	120.20
4	BB	526	A	P-O3'-C3'	-7.14	109.50	120.20
4	BB	514	G	P-O3'-C3'	-6.88	109.87	120.20
4	BB	513	G	P-O3'-C3'	-6.19	110.92	120.20
4	BB	530	PSU	P-O3'-C3'	-5.65	111.73	120.20
4	BB	533	U	P-O3'-C3'	-5.58	111.83	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	AP	240	TRP	Peptide
53	Bm	21	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	39217	0	19840	537	0
2	AB	404	0	211	3	0
3	BA	33850	0	17102	244	0
4	BB	23703	0	12002	162	0
5	BC	3407	0	1735	20	0
6	BD	2533	0	1283	19	0
7	BE	3526	0	1791	23	0
8	BP	1252	0	1333	15	0
9	BQ	1716	0	1796	10	0
10	BR	1209	0	1271	7	0
11	BS	1465	0	1500	13	0
12	BT	1570	0	1642	16	0
13	BU	1197	0	1245	13	0
14	BW	979	0	1037	10	0
15	BY	531	0	533	3	0
16	BX	955	0	1017	5	0
17	BZ	971	0	1041	6	0
18	Bp	609	0	665	13	0
19	Bq	457	0	495	6	0
20	Br	2871	0	2999	30	0
21	Bt	801	0	863	11	0
22	Bw	1872	0	1966	12	0
23	Bx	1847	0	1974	12	0
24	Bl	1163	0	1221	16	0
25	Bu	1910	0	1949	19	0
26	By	1473	0	1541	16	0
27	A0	1775	0	1848	14	0
28	A2	1464	0	1524	26	0
29	A5	1457	0	1517	34	0
30	AD	720	0	729	11	0
31	A8	439	0	450	9	0
32	AE	1234	0	1283	24	0
33	AG	1148	0	1226	11	0
34	AI	856	0	895	15	0
35	AH	1004	0	1013	14	0
36	AJ	1018	0	1050	10	0
37	AL	945	0	996	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	AM	1081	0	1132	29	0
39	AO	1186	0	1250	26	0
40	AP	1703	0	1750	38	0
41	AS	1096	0	1151	19	0
42	AU	551	0	598	9	0
43	AX	1652	0	1721	22	0
44	AZ	438	0	470	11	0
45	A3	1808	0	1904	29	0
46	AT	980	0	1057	27	0
47	A1	2048	0	2167	57	0
48	AC	1648	0	1687	33	0
49	Bc	1162	0	1246	13	0
50	Bz	294	0	336	5	0
51	Bo	699	0	730	10	0
52	Bn	676	0	689	7	0
53	Bm	786	0	865	6	0
54	Bk	1018	0	1141	12	0
55	Bj	959	0	1026	6	0
56	Bi	1075	0	1135	12	0
57	Bg	708	0	726	2	0
58	Bd	561	0	583	7	0
59	Bb	1137	0	1174	7	0
60	Ba	1077	0	1152	13	0
61	BO	1801	0	1952	18	0
62	BN	1722	0	1828	17	0
63	BL	1246	0	1272	20	0
64	BK	1584	0	1650	27	0
65	BI	1517	0	1633	12	0
66	Be	1902	0	1952	15	0
67	AK	1143	0	1207	17	0
68	A6	1460	0	1509	31	0
69	Bf	3211	0	3336	23	0
70	AY	471	0	522	20	0
71	Bv	1101	0	1158	20	0
72	Bh	1188	0	1275	16	0
73	BF	1444	0	744	12	0
74	BG	3919	0	1975	31	0
75	BH	2520	0	1279	25	0
76	Bs	394	0	421	7	0
77	BV	973	0	991	9	0
78	Az	340	0	344	6	0
79	AQ	800	0	856	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	AR	656	0	651	16	0
81	AV	830	0	868	9	0
82	AW	660	0	666	10	0
83	A4	1596	0	1653	35	0
84	A7	2326	0	2243	49	0
85	A	30	0	25	1	0
86	A0	1	0	0	0	0
86	A3	1	0	0	0	0
86	A5	1	0	0	0	0
86	AA	52	0	0	0	0
86	BA	47	0	0	0	0
86	BB	39	0	0	0	0
86	BE	3	0	0	0	0
86	BG	2	0	0	0	0
86	BR	1	0	0	0	0
86	BW	1	0	0	0	0
86	Bf	1	0	0	0	0
87	AA	26	0	0	0	0
87	AG	1	0	0	0	0
87	AP	1	0	0	0	0
87	AV	1	0	0	0	0
87	BA	2	0	0	0	0
87	BB	8	0	0	0	0
87	BG	1	0	0	0	0
87	Be	1	0	0	0	0
88	AA	26	0	0	0	0
88	BA	11	0	0	0	0
88	BB	10	0	0	0	0
88	BC	1	0	0	0	0
88	BD	1	0	0	0	0
88	Be	1	0	0	0	0
88	Bi	1	0	0	0	0
89	A0	1	0	0	0	0
89	A1	1	0	0	1	0
89	A8	1	0	0	0	0
89	AA	92	0	0	3	0
89	AH	1	0	0	0	0
89	AO	1	0	0	0	0
89	AS	1	0	0	0	0
89	AV	6	0	0	1	0
89	BA	78	0	0	0	0
89	BB	100	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	BC	3	0	0	0	0
89	BE	3	0	0	0	0
89	BG	5	0	0	2	0
89	BH	2	0	0	0	0
89	BI	1	0	0	0	0
89	BK	1	0	0	0	0
89	BN	1	0	0	0	0
89	BQ	2	0	0	0	0
89	BT	1	0	0	0	0
89	Bb	2	0	0	0	0
89	Bd	1	0	0	0	0
89	Be	10	0	0	0	0
89	Bj	2	0	0	0	0
89	Bn	3	0	0	0	0
89	Bo	1	0	0	0	0
89	Br	1	0	0	0	0
89	Bz	2	0	0	1	0
All	All	203289	0	150283	1993	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 6.

All (1993) 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)
1:AA:158:G:H1	1:AA:169:A:N6	1.46	1.13
1:AA:1584:G:N2	1:AA:1927:A:H62	1.49	1.08
1:AA:1584:G:H21	1:AA:1927:A:N6	1.55	1.04
1:AA:224:U:H3	1:AA:271:G:H1	1.03	0.98
75:BH:79:A:C2	75:BH:86:G:N1	2.31	0.97
1:AA:769:G:H1	1:AA:781:U:H3	0.98	0.95
75:BH:79:A:H2	75:BH:86:G:N1	1.64	0.93
3:BA:1865:G:H1	4:BB:5:A:H61	1.20	0.90
75:BH:79:A:N1	75:BH:86:G:O6	2.06	0.89
1:AA:981:G:H1	1:AA:1014:U:H3	1.17	0.88
3:BA:23:G:H1	5:BC:149:A:H61	1.22	0.87
4:BB:1457:C:H5	73:BF:5:G:H1	1.19	0.87
3:BA:245:C:O2	74:BG:14:G:N2	2.09	0.85
1:AA:2172:C:O2	1:AA:2202:G:N2	2.08	0.84
3:BA:211:C:H42	3:BA:238:U:H3	1.20	0.82
3:BA:884:G:N2	3:BA:894:G:N7	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BB:620:A:H61	4:BB:1437:C:H5	1.28	0.81
5:BC:71:A:H62	5:BC:86:U:H3	1.28	0.81
28:A2:187:LYS:HZ2	28:A2:190:ARG:HH12	1.26	0.81
84:A7:192:LEU:HB3	84:A7:223:TRP:HZ3	1.45	0.81
1:AA:1124:G:H2'	1:AA:1125:G:C8	2.14	0.81
75:BH:57:A:C2	75:BH:65:G:N1	2.49	0.81
1:AA:158:G:N2	1:AA:169:A:N1	2.28	0.80
1:AA:281:C:H5	1:AA:357:G:H1	1.27	0.80
1:AA:158:G:H1	1:AA:169:A:H61	0.80	0.80
1:AA:844:A:H2	1:AA:889:G:H1	1.28	0.80
4:BB:793:C:H5	4:BB:1022:G:H1	1.28	0.79
4:BB:1514:U:O2	4:BB:1534:G:N2	2.15	0.79
75:BH:52:G:H1	75:BH:70:U:H3	1.28	0.79
28:A2:190:ARG:HD3	44:AZ:97:ARG:HH12	1.47	0.79
1:AA:394:A:OP1	47:A1:3:LYS:NZ	2.16	0.79
3:BA:885:G:N2	3:BA:892:G:O6	2.16	0.78
1:AA:121:G:H21	1:AA:519:G:H5'	1.47	0.78
1:AA:94:U:O2	45:A3:163:ARG:NH1	2.17	0.78
71:Bv:101:GLU:OE1	71:Bv:101:GLU:N	2.15	0.78
1:AA:953:G:N2	1:AA:954:C:N3	2.30	0.78
1:AA:287:A:OP1	32:AE:31:ASN:ND2	2.16	0.77
1:AA:159:C:H42	1:AA:168:C:H42	1.30	0.76
63:BL:81:LYS:H	63:BL:81:LYS:HZ3	1.32	0.76
1:AA:286:G:H1	1:AA:349:C:H5	1.31	0.76
1:AA:712:G:H1	1:AA:1513:G:H22	1.31	0.76
7:BE:43:U:HO2'	7:BE:44:C:H6	1.32	0.76
79:AQ:41:ARG:O	79:AQ:44:LYS:NZ	2.19	0.75
4:BB:709:U:O4	4:BB:766:C:N4	2.14	0.75
7:BE:191:G:O6	55:Bj:44:HIS:NE2	2.19	0.75
3:BA:245:C:N3	74:BG:14:G:N1	2.28	0.75
29:A5:34:ALA:HB2	29:A5:56:ARG:HD2	1.69	0.74
1:AA:1141:G:H1	1:AA:1242:C:H5	1.35	0.74
20:Br:100:MET:HE3	20:Br:103:PRO:HA	1.68	0.74
40:AP:82:ARG:O	40:AP:82:ARG:NH1	2.17	0.74
1:AA:118:A:H62	1:AA:489:G:H8	1.33	0.74
1:AA:225:C:N4	1:AA:270:G:O6	2.19	0.74
37:AL:102:ASP:OD1	37:AL:103:LYS:N	2.21	0.74
48:AC:144:PHE:HB2	48:AC:172:GLU:HG2	1.70	0.74
75:BH:79:A:H2	75:BH:86:G:H1	0.83	0.74
3:BA:1865:G:H1	4:BB:5:A:N6	1.84	0.73
29:A5:36:THR:OG1	29:A5:57:GLY:O	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:AP:171:LYS:NZ	40:AP:173:GLY:O	2.21	0.73
1:AA:1643:A:H3'	1:AA:1644:U:H5''	1.68	0.73
17:BZ:35:GLU:N	17:BZ:35:GLU:OE2	2.21	0.73
48:AC:232:GLU:N	48:AC:232:GLU:OE2	2.22	0.73
80:AR:21:LYS:NZ	80:AR:26:ASN:OD1	2.22	0.73
3:BA:884:G:N1	3:BA:894:G:O6	2.17	0.73
70:AY:58:ASN:OD1	70:AY:60:GLN:NE2	2.22	0.73
3:BA:513:C:H5	3:BA:715:G:H1	1.36	0.72
1:AA:786:C:H2'	1:AA:787:G:H8	1.54	0.72
63:BL:100:SER:HB3	63:BL:179:PHE:HA	1.71	0.72
3:BA:619[A]:C:O2'	3:BA:620:G:OP2	2.05	0.72
3:BA:1467:G:O2'	3:BA:1471:G:N2	2.21	0.72
3:BA:198:C:H5	3:BA:295:G:H1	1.38	0.72
3:BA:1316:U:OP1	61:BO:141:LYS:NZ	2.23	0.72
40:AP:160:GLU:OE2	40:AP:160:GLU:N	2.15	0.72
79:AQ:24:ARG:HD3	79:AQ:79:MET:HE3	1.72	0.72
40:AP:82:ARG:HG3	40:AP:84:GLY:H	1.53	0.72
7:BE:38:C:H5	7:BE:188:G:H1	1.37	0.72
35:AH:47:CYS:SG	35:AH:77:ARG:NE	2.63	0.72
19:Bq:13:TYR:OH	19:Bq:50:HIS:O	2.07	0.72
20:Br:285:THR:HG22	20:Br:286:ASP:H	1.55	0.71
1:AA:1318:G:H1	1:AA:1479:U:H3	1.39	0.71
3:BA:703:G:OP1	56:Bi:63:ARG:NH2	2.23	0.71
64:BK:16:PRO:O	64:BK:95:HIS:ND1	2.22	0.71
75:BH:79:A:N1	75:BH:86:G:C6	2.58	0.71
1:AA:1516:G:H1	1:AA:1539:C:H5	1.38	0.71
1:AA:867:C:N4	1:AA:879:G:O2'	2.24	0.70
3:BA:579:G:OP2	20:Br:365:LYS:NZ	2.23	0.70
3:BA:211:C:N4	3:BA:238:U:H3	1.89	0.70
3:BA:1498:C:H5	3:BA:1521:G:H1	1.37	0.70
38:AM:111:ASP:OD1	38:AM:114:ARG:NH2	2.23	0.70
14:BW:11:CYS:SG	89:BG:301:HOH:O	2.49	0.70
3:BA:1259:C:O2	3:BA:1267:OMG:N2	2.20	0.70
3:BA:873:C:O2'	58:Bd:29:MET:O	2.09	0.70
1:AA:332:G:N2	1:AA:335:G:OP1	2.24	0.69
1:AA:1569:G:H1	1:AA:2076:C:H5	1.40	0.69
4:BB:838:U:H3	4:BB:969:G:H1	1.40	0.69
1:AA:692:C:H2'	1:AA:693:A:H8	1.55	0.69
1:AA:1656:U:O2'	1:AA:1657:C:O2	2.08	0.69
73:BF:9:C:H5	73:BF:75:G:H1	1.40	0.69
83:A4:36:HIS:HB3	83:A4:39:LEU:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:493:A:H5'	29:A5:25:MET:HA	1.72	0.69
1:AA:2172:C:N3	1:AA:2202:G:N1	2.29	0.69
68:A6:87:GLU:OE1	68:A6:87:GLU:N	2.25	0.69
42:AU:49:ASP:OD2	42:AU:50:LYS:N	2.25	0.69
1:AA:168:C:H2'	1:AA:169:A:C8	2.28	0.69
4:BB:1469:U:H4'	4:BB:1470:A:H5''	1.74	0.69
30:AD:78:GLU:N	30:AD:78:GLU:OE2	2.26	0.69
32:AE:121:ARG:HH12	32:AE:123:ILE:HG13	1.57	0.69
63:BL:175:ASP:N	63:BL:175:ASP:OD1	2.23	0.69
3:BA:1346:G:H4'	76:Bs:117:HIS:HB2	1.73	0.69
1:AA:363:G:H1	1:AA:382:C:H5	1.40	0.69
1:AA:1145:G:H21	33:AG:52:MET:HE2	1.57	0.69
1:AA:765:A:H61	1:AA:786:C:H42	1.39	0.69
84:A7:111:ASP:OD1	84:A7:111:ASP:N	2.26	0.69
1:AA:430:G:H2'	1:AA:431:G:H5''	1.74	0.69
1:AA:323:U:O4	1:AA:1000:G:O2'	2.09	0.68
1:AA:209:A:H5'	1:AA:210:C:H5''	1.75	0.68
1:AA:393:G:HO2'	47:A1:2:ALA:N	1.92	0.68
3:BA:1671:G:O2'	3:BA:1673:G:OP2	2.10	0.68
25:Bu:124:GLU:OE1	25:Bu:124:GLU:N	2.23	0.68
1:AA:282:G:H1	1:AA:353:C:H5	1.41	0.68
1:AA:1743:C:H5	1:AA:1851:G:H1	1.39	0.68
10:BR:74:LYS:NZ	75:BH:20:A:OP1	2.27	0.68
70:AY:25:GLU:N	70:AY:25:GLU:OE2	2.26	0.68
75:BH:57:A:N1	75:BH:65:G:O6	2.27	0.68
1:AA:355:G:O2'	1:AA:357:G:OP2	2.10	0.68
3:BA:619[B]:C:N4	3:BA:622:G:N7	2.40	0.68
7:BE:11:U:OP2	55:Bj:77:ARG:NH2	2.20	0.68
62:BN:146:GLU:HA	62:BN:149:LYS:HG2	1.75	0.68
1:AA:1647:A:OP1	34:Al:66:ARG:NH1	2.26	0.68
7:BE:25:C:H5	7:BE:209:G:H1	1.39	0.68
7:BE:46:C:H5	7:BE:180:G:H1	1.41	0.68
52:Bn:73:ARG:NH2	52:Bn:79:LYS:O	2.27	0.68
1:AA:769:G:N2	1:AA:781:U:O2	2.23	0.67
1:AA:1584:G:H21	1:AA:1927:A:H62	0.74	0.67
3:BA:840:G:H22	3:BA:874:A:H2	1.42	0.67
29:A5:28:GLU:N	29:A5:28:GLU:OE2	2.24	0.67
1:AA:749:C:HO2'	1:AA:750:G:H8	1.41	0.67
42:AU:76:LYS:H	42:AU:76:LYS:HE2	1.58	0.67
1:AA:1625:C:H2'	1:AA:1626:A:H8	1.60	0.67
3:BA:223:G:H4'	3:BA:224:U:H5''	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BA:1642:U:H4'	3:BA:1643:U:H5'	1.77	0.67
1:AA:175:G:H2'	1:AA:176:G:C8	2.30	0.67
1:AA:1878:G:OP1	67:AK:120:LYS:NZ	2.28	0.67
3:BA:885:G:H21	3:BA:892:G:H1	1.43	0.67
4:BB:988:C:H5	7:BE:23:G:H1	1.42	0.67
49:Bc:119:ARG:NH1	56:Bi:114:HIS:O	2.28	0.67
69:Bf:320:GLY:O	69:Bf:340:ARG:NH1	2.27	0.67
48:AC:194:ASP:OD2	80:AR:64:ARG:NH1	2.27	0.67
1:AA:1028:U:H2'	1:AA:1029:G:C8	2.29	0.67
33:AG:83:GLU:OE2	33:AG:83:GLU:N	2.27	0.67
9:BQ:104:ALA:O	9:BQ:109:ARG:NH1	2.28	0.67
46:AT:116:GLU:OE1	46:AT:117:ARG:NH2	2.28	0.67
80:AR:44:VAL:HG12	80:AR:50:ILE:HA	1.77	0.67
3:BA:1817:A:OP2	16:BX:51:ARG:NH2	2.29	0.66
28:A2:187:LYS:NZ	44:AZ:94:GLU:OE1	2.28	0.66
4:BB:1523:A:H61	69:Bf:327:ASP:H	1.43	0.66
8:BP:42:CYS:SG	8:BP:75:LYS:NZ	2.68	0.66
22:Bw:228:GLY:O	22:Bw:255:ARG:NH2	2.28	0.66
60:Ba:87:ASP:OD1	60:Ba:118:ARG:NH2	2.29	0.66
1:AA:1178:G:N7	89:AA:2503:HOH:O	2.28	0.66
79:AQ:16:ARG:NH1	79:AQ:90:ALA:O	2.29	0.66
59:Bb:72:THR:HG22	59:Bb:108:LYS:HB3	1.77	0.66
1:AA:1998:A:O2'	1:AA:1999:G:O5'	2.14	0.66
1:AA:2174:G:O2'	1:AA:2200:A:N6	2.28	0.66
20:Br:317:THR:OG1	20:Br:318:ASN:N	2.29	0.66
80:AR:9:GLU:N	80:AR:9:GLU:OE2	2.29	0.66
84:A7:111:ASP:OD2	84:A7:129:ARG:NH1	2.28	0.66
1:AA:963:A:N7	83:A4:112:TYR:OH	2.26	0.66
1:AA:978:U:O4	1:AA:1017:U:N3	2.19	0.66
23:Bx:102:GLU:N	23:Bx:102:GLU:OE2	2.29	0.66
65:BI:16:ARG:NH2	65:BI:53:LEU:O	2.28	0.66
71:Bv:146:GLU:N	71:Bv:146:GLU:OE2	2.26	0.66
3:BA:1864:U:H2'	3:BA:1865:G:C8	2.31	0.65
5:BC:169:G:OP1	23:Bx:100:ARG:NH2	2.28	0.65
77:BV:16:GLN:HB3	77:BV:83:MET:HE3	1.76	0.65
27:A0:149:GLU:OE1	27:A0:149:GLU:N	2.18	0.65
83:A4:7:LEU:HB3	83:A4:15:ARG:HG2	1.78	0.65
4:BB:1140:A:H2'	4:BB:1141:G:C8	2.32	0.65
1:AA:541:G:H2'	1:AA:542:U:O2	1.97	0.65
4:BB:1489:A:H3'	4:BB:1490:G:H21	1.61	0.65
48:AC:43:VAL:HG13	48:AC:44:LEU:HG	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Bu:244:ASP:OD1	25:Bu:244:ASP:N	2.29	0.65
1:AA:425:G:OP2	29:A5:194:GLN:NE2	2.29	0.65
1:AA:1213:G:N7	81:AV:17:ARG:NH1	2.45	0.65
3:BA:1505:A:OP2	49:Bc:89:SER:OG	2.13	0.65
4:BB:992:G:O6	4:BB:1019:G:O6	2.15	0.65
65:BI:36:LEU:O	65:BI:40:THR:OG1	2.13	0.65
78:Az:184:ARG:NH1	78:Az:184:ARG:O	2.29	0.65
1:AA:60:U:OP1	41:AS:137:LYS:NZ	2.30	0.65
1:AA:765:A:N1	1:AA:787:G:C6	2.65	0.65
4:BB:1523:A:N1	69:Bf:326:ASN:ND2	2.44	0.65
20:Br:295:GLU:N	20:Br:295:GLU:OE2	2.30	0.65
24:Bl:55:ASN:ND2	24:Bl:57:ASN:OD1	2.30	0.65
48:AC:207:ILE:H	48:AC:207:ILE:HD12	1.61	0.65
32:AE:139:VAL:HG12	32:AE:158:VAL:HG23	1.78	0.65
43:AX:69:THR:HG22	43:AX:85:LEU:HG	1.79	0.65
1:AA:918:U:H3'	1:AA:919:G:H21	1.60	0.65
1:AA:118:A:N6	1:AA:489:G:H8	1.95	0.64
3:BA:551:U:OP1	11:BS:64:LYS:NZ	2.25	0.64
29:A5:62:THR:OG1	29:A5:76:ALA:O	2.14	0.64
75:BH:26:C:N3	75:BH:125:U:O2'	2.29	0.64
1:AA:930:A:OP2	1:AA:943:G:N2	2.30	0.64
1:AA:1637:U:H3	1:AA:1658:U:H3	1.45	0.64
24:Bl:101:ARG:NH2	73:BF:72:C:OP1	2.31	0.64
33:AG:87:ASP:OD1	33:AG:87:ASP:N	2.24	0.64
34:AI:95:GLU:N	34:AI:95:GLU:OE2	2.31	0.64
70:AY:42:GLN:O	70:AY:42:GLN:NE2	2.31	0.64
1:AA:650:G:H1	1:AA:692:C:H5	1.46	0.64
40:AP:116:ASP:OD1	40:AP:118:ASN:N	2.29	0.64
4:BB:997:G:H22	4:BB:1014:U:H3	1.43	0.64
79:AQ:96:LYS:O	79:AQ:100:SER:OG	2.16	0.64
14:BW:70:GLU:N	14:BW:70:GLU:OE2	2.31	0.64
38:AM:87:ARG:NH2	38:AM:111:ASP:OD2	2.29	0.64
1:AA:98:U:H2'	1:AA:99:G:H8	1.63	0.63
3:BA:629:C:H5	3:BA:694:G:H1	1.44	0.63
3:BA:1236:U:H5''	22:Bw:122:ARG:HD2	1.78	0.63
28:A2:35:VAL:HG13	28:A2:37:HIS:H	1.63	0.63
50:Bz:21:ARG:NH1	89:Bz:101:HOH:O	2.28	0.63
10:BR:78:GLN:NE2	10:BR:80:LYS:O	2.30	0.63
4:BB:477:A:H2'	4:BB:478:A:C8	2.33	0.63
84:A7:189:VAL:HG22	84:A7:190:THR:HG22	1.80	0.63
1:AA:2020:A:OP1	28:A2:77:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:AM:15:ARG:NH1	38:AM:20:ASN:OD1	2.31	0.63
47:A1:133:ILE:HG21	47:A1:145:ARG:HE	1.62	0.63
67:AK:56:GLU:OE2	67:AK:88:ARG:NH2	2.27	0.63
1:AA:550:A:O2'	1:AA:551:U:OP1	2.16	0.63
40:AP:81:ILE:HG22	40:AP:83:GLU:H	1.63	0.63
47:A1:197:ARG:NH1	47:A1:203:ASP:OD2	2.32	0.63
70:AY:47:LYS:O	70:AY:50:LYS:NZ	2.31	0.63
84:A7:148:ARG:HB3	84:A7:148:ARG:HH11	1.64	0.63
1:AA:659:G:H1	1:AA:689:C:H5	1.46	0.63
1:AA:2276:A:O2'	81:AV:99:ARG:O	2.14	0.63
46:AT:26:LYS:HG3	46:AT:82:ILE:HB	1.81	0.63
75:BH:57:A:N1	75:BH:65:G:C6	2.67	0.63
79:AQ:96:LYS:HE2	79:AQ:96:LYS:N	2.14	0.63
54:Bk:13:LYS:NZ	54:Bk:21:GLN:OE1	2.31	0.63
61:BO:11:ARG:HE	73:BF:4:C:H5	1.46	0.63
3:BA:1654:C:H5	10:BR:85:ARG:HH11	1.45	0.62
1:AA:1622:G:O6	31:A8:7:TRP:NE1	2.31	0.62
43:AX:131:LYS:HB2	43:AX:188:MET:HG2	1.81	0.62
60:Ba:2:LYS:NZ	60:Ba:29:ASP:OD2	2.32	0.62
1:AA:397:A:O3'	32:AE:152:ARG:NH1	2.32	0.62
32:AE:78:SER:OG	32:AE:79:ASN:N	2.26	0.62
54:Bk:40:VAL:HG12	54:Bk:44:ARG:HB3	1.82	0.62
13:BU:140:PRO:HG3	22:Bw:90:TYR:HE1	1.64	0.62
23:Bx:195:ASP:OD2	23:Bx:198:ARG:NH1	2.32	0.62
47:A1:32:PRO:HD2	47:A1:80:PRO:HG2	1.82	0.62
1:AA:1926:C:OP1	38:AM:125:ARG:NH2	2.30	0.62
3:BA:7:A:HO2'	3:BA:8:G:H8	1.48	0.62
63:BL:158:ASN:N	63:BL:158:ASN:OD1	2.33	0.62
64:BK:47:PRO:HB2	64:BK:178:ARG:HH21	1.64	0.62
1:AA:462:U:O2'	1:AA:463:A:OP1	2.17	0.62
45:A3:150:LEU:HD12	45:A3:154:ASP:HB3	1.82	0.62
1:AA:554:G:H2'	1:AA:555:A:C8	2.34	0.62
3:BA:703:G:P	56:Bi:63:ARG:HH22	2.22	0.62
59:Bb:100:ASP:OD1	59:Bb:144:GLN:NE2	2.32	0.62
83:A4:31:GLU:O	83:A4:35:SER:OG	2.13	0.62
1:AA:604:U:O2'	1:AA:605:U:O2	2.12	0.61
68:A6:88:ASP:N	68:A6:88:ASP:OD2	2.31	0.61
69:Bf:292:ARG:HG2	69:Bf:292:ARG:HH11	1.63	0.61
37:AL:35:VAL:O	37:AL:39:THR:OG1	2.14	0.61
4:BB:449:C:O2'	4:BB:578:OMU:OP2	2.18	0.61
1:AA:333:A:N7	45:A3:210:ARG:NH2	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BB:608:U:H2'	4:BB:609:A2M:H8	1.82	0.61
1:AA:2154:OMU:H5	1:AA:2220:A:N1	2.16	0.61
3:BA:1164:U:OP1	25:Bu:5:LYS:NZ	2.33	0.61
1:AA:581:G:N2	1:AA:604:U:O4'	2.33	0.61
3:BA:615:G:N3	3:BA:619[A]:C:N4	2.39	0.61
4:BB:1098:U:OP1	21:Bt:98:LYS:NZ	2.32	0.61
47:A1:3:LYS:H	47:A1:3:LYS:HD2	1.65	0.61
1:AA:605:U:H1'	1:AA:606:U:H5'	1.81	0.61
40:AP:228:LEU:O	40:AP:231:THR:OG1	2.19	0.61
46:AT:9:GLU:OE1	46:AT:9:GLU:N	2.33	0.61
67:AK:31:PRO:O	67:AK:68:ARG:NH1	2.31	0.61
1:AA:121:G:N2	1:AA:519:G:H5'	2.16	0.61
1:AA:867:C:H41	1:AA:879:G:H8	1.48	0.61
4:BB:1451:A:N6	74:BG:173:C:OP2	2.33	0.61
71:Bv:74:ARG:NH1	73:BF:66:U:OP1	2.34	0.61
47:A1:228:ASP:OD2	47:A1:229:MET:N	2.34	0.60
1:AA:53:C:O2	1:AA:568:A:O2'	2.17	0.60
1:AA:2137:G:H21	1:AA:2260:MA6:H8	1.65	0.60
7:BE:8:A:OP1	60:Ba:35:ARG:NH2	2.33	0.60
26:By:140:ASP:OD1	26:By:140:ASP:N	2.33	0.60
38:AM:103:MET:HE3	38:AM:107:ARG:HE	1.65	0.60
37:AL:82:MET:HE1	48:AC:121:ARG:HD3	1.83	0.60
1:AA:2179:U:H5	1:AA:2195:A:H62	1.48	0.60
48:AC:209:MET:HA	48:AC:209:MET:HE3	1.82	0.60
72:Bh:86:MET:HG2	72:Bh:185:VAL:HG22	1.83	0.60
79:AQ:15:GLN:HG2	79:AQ:114:PRO:HG2	1.83	0.60
1:AA:580:C:N4	1:AA:604:U:O4	2.35	0.60
1:AA:911:A:H2'	1:AA:912:A:O4'	2.01	0.60
3:BA:1026:C:O2'	3:BA:1029:A:N3	2.33	0.60
4:BB:979:C:H5'	55:Bj:102:ARG:HG2	1.83	0.60
43:AX:52:THR:HB	43:AX:93:ARG:HD2	1.82	0.60
47:A1:244:ILE:HD11	47:A1:249:GLU:HG2	1.82	0.60
1:AA:753:G:H2'	1:AA:754:U:C6	2.36	0.60
4:BB:656:C:O2'	69:Bf:271:ARG:NH2	2.32	0.60
4:BB:1039:C:H2'	4:BB:1040:U:O2	2.01	0.60
84:A7:46:ASN:ND2	84:A7:55:SER:OG	2.35	0.60
1:AA:1028:U:H2'	1:AA:1029:G:H8	1.65	0.60
1:AA:1503:A:OP1	40:AP:169:THR:OG1	2.19	0.60
1:AA:364:C:H5	1:AA:381:G:H1	1.50	0.60
83:A4:6:HIS:HA	83:A4:30:PHE:HD1	1.66	0.60
1:AA:338:U:O3'	47:A1:153:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1147:A:H2'	1:AA:1148:G:C8	2.36	0.59
1:AA:587:G:N2	1:AA:598:U:OP2	2.34	0.59
12:BT:187:ARG:HH12	12:BT:191:ASP:HB2	1.66	0.59
1:AA:1323:G:H1	1:AA:1474:U:H3	1.49	0.59
28:A2:2:SER:OG	67:AK:64:ARG:NH1	2.35	0.59
47:A1:97:ARG:NH2	47:A1:118:ILE:O	2.35	0.59
68:A6:45:ASN:O	68:A6:49:SER:OG	2.20	0.59
83:A4:77:ARG:NH2	83:A4:133:ASP:OD1	2.34	0.59
1:AA:827:G:O2'	1:AA:828:A:H5'	2.03	0.59
1:AA:1030:G:H2'	1:AA:1031:G:H8	1.67	0.59
1:AA:1162:G:H2'	1:AA:1163:U:C6	2.37	0.59
4:BB:649:G:O2'	4:BB:650:G:OP2	2.19	0.59
84:A7:91:LEU:HB2	84:A7:105:PHE:HB2	1.84	0.59
1:AA:174:U:OP1	45:A3:152:ARG:NH2	2.34	0.59
1:AA:623:A:O2'	1:AA:624:A:OP1	2.20	0.59
1:AA:1757:C:H41	1:AA:1837:G:H1	1.50	0.59
1:AA:2085:G:H1	1:AA:2101:U:H3	1.50	0.59
3:BA:869:U:H3	65:BI:147:ARG:HH21	1.48	0.59
1:AA:746:C:H2'	1:AA:747:C:H4'	1.84	0.59
1:AA:773:C:H3'	1:AA:774:G:H8	1.67	0.59
32:AE:73:LYS:HD3	32:AE:147:LEU:HD22	1.84	0.59
72:Bh:32:SER:O	72:Bh:32:SER:OG	2.21	0.59
3:BA:958:G:O2'	7:BE:122:C:O2'	2.14	0.59
46:AT:92:ILE:HG23	47:A1:60:MET:HE1	1.84	0.59
1:AA:186:C:O2'	45:A3:57:SER:OG	2.19	0.59
3:BA:612:U:O2	20:Br:314:ARG:NH2	2.35	0.59
1:AA:2043:U:OP1	38:AM:89:ARG:NH1	2.36	0.59
24:BI:66:VAL:HG23	24:BI:67:ASN:H	1.68	0.59
60:Ba:97:ASN:OD1	60:Ba:103:LYS:NZ	2.36	0.59
84:A7:192:LEU:HB3	84:A7:223:TRP:CZ3	2.34	0.59
3:BA:615:G:O2'	3:BA:618:G:N7	2.33	0.59
4:BB:814:C:H5	4:BB:819:G:H1	1.50	0.59
68:A6:106:ARG:NH2	68:A6:152:GLU:OE2	2.23	0.59
75:BH:78:C:H42	75:BH:87:U:H3	1.51	0.59
32:AE:19:GLN:NE2	32:AE:25:GLN:O	2.34	0.58
1:AA:835:A:H2'	1:AA:836:A:H8	1.67	0.58
29:A5:47:ARG:NH1	29:A5:48:ALA:O	2.36	0.58
46:AT:85:ASP:N	46:AT:85:ASP:OD1	2.36	0.58
47:A1:119:LYS:HE2	47:A1:121:MET:HE2	1.85	0.58
3:BA:1570:U:H2'	3:BA:1571:G:C8	2.38	0.58
74:BG:18:U:H2'	74:BG:19:C:C6	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:292:A:OP2	1:AA:842:G:N1	2.37	0.58
1:AA:2160:A:H2'	1:AA:2161:A:C8	2.39	0.58
21:Bt:35:LEU:HA	21:Bt:40:LYS:HG2	1.86	0.58
4:BB:1142:C:O2	13:BU:49:ARG:NH2	2.36	0.58
79:AQ:93:GLU:N	79:AQ:93:GLU:OE2	2.35	0.58
1:AA:56:A2M:H2'	1:AA:57:OMU:H6	1.86	0.58
6:BD:92:G:H2'	6:BD:93:G:C8	2.39	0.58
29:A5:61:ASP:OD1	29:A5:61:ASP:N	2.36	0.58
83:A4:36:HIS:HD2	83:A4:86:GLU:OE1	1.87	0.58
4:BB:1165:A:OP1	58:Bd:34:ARG:NH2	2.29	0.58
29:A5:64:ASN:OD1	29:A5:64:ASN:N	2.37	0.58
29:A5:84:ASN:OD1	29:A5:85:ALA:N	2.36	0.58
49:Bc:73:PRO:HA	49:Bc:76:MET:HG3	1.86	0.58
75:BH:47:G:H2'	75:BH:48:G:C8	2.38	0.58
1:AA:554:G:H2'	1:AA:555:A:H8	1.69	0.58
1:AA:1625:C:H2'	1:AA:1626:A:C8	2.39	0.58
30:AD:22:VAL:HG22	30:AD:74:THR:HG22	1.85	0.58
1:AA:301:C:O2'	1:AA:302:A:OP1	2.19	0.58
3:BA:302:A:H62	5:BC:32:U:H3	1.52	0.58
7:BE:109:A:H2	7:BE:126:G:H1	1.52	0.58
41:AS:127:SER:O	41:AS:127:SER:OG	2.19	0.58
45:A3:64:MET:HE2	45:A3:109:ILE:HD12	1.86	0.58
60:Ba:21:LYS:NZ	60:Ba:129:GLN:O	2.32	0.57
3:BA:881:A:H61	3:BA:897:C:H42	1.52	0.57
12:BT:171:ARG:NH1	12:BT:171:ARG:O	2.38	0.57
40:AP:182:ALA:HB3	40:AP:205:ASP:OD2	2.05	0.57
77:BV:105:ASP:OD1	77:BV:105:ASP:N	2.35	0.57
1:AA:2049:A:OP2	34:Al:54:ARG:NH1	2.37	0.57
47:A1:189:ILE:HD12	47:A1:241:GLY:HA3	1.85	0.57
3:BA:1342:A:H2'	3:BA:1343:A:C8	2.39	0.57
22:Bw:67:SER:OG	22:Bw:71:ARG:NH1	2.37	0.57
26:By:4:LYS:NZ	73:BF:36:G:OP1	2.36	0.57
83:A4:50:THR:OG1	83:A4:51:VAL:N	2.37	0.57
1:AA:1029:G:H2'	1:AA:1030:G:C8	2.39	0.57
1:AA:2230:G:N7	89:AA:2508:HOH:O	2.32	0.57
4:BB:835:G:H1	4:BB:972:U:H3	1.52	0.57
67:AK:48:GLU:OE2	67:AK:48:GLU:N	2.23	0.57
74:BG:92:U:H2'	74:BG:93:U:C6	2.40	0.57
3:BA:638:G:O2'	3:BA:639:G:O5'	2.20	0.57
3:BA:849:A:H2	3:BA:864:G:H22	1.52	0.57
60:Ba:53:VAL:HG22	60:Ba:56:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:761:C:O2'	1:AA:762:C:O2	2.18	0.57
1:AA:2273:A:OP2	81:AV:4:LYS:NZ	2.38	0.57
12:BT:105:LEU:HD23	12:BT:138:LEU:HD23	1.86	0.57
28:A2:21:GLU:HG3	28:A2:103:SER:HB3	1.85	0.57
39:AO:57:SER:HB2	39:AO:112:ALA:HA	1.86	0.57
69:Bf:123:LYS:HG3	75:BH:25:A:H5'	1.87	0.57
1:AA:301:C:H2'	1:AA:302:A:C8	2.40	0.57
3:BA:246:U:H3	74:BG:13:A:H62	1.52	0.57
28:A2:68:GLY:HA2	28:A2:71:LYS:HG3	1.87	0.57
41:AS:7:GLN:O	41:AS:8:HIS:ND1	2.35	0.57
43:AX:177:ARG:NH2	70:AY:63:GLY:O	2.38	0.57
65:BI:95:ASP:OD2	65:BI:96:ASP:N	2.37	0.57
1:AA:1034:C:H42	1:AA:1123:C:H42	1.52	0.56
1:AA:2160:A:H2'	1:AA:2161:A:H8	1.70	0.56
3:BA:1864:U:H2'	3:BA:1865:G:H8	1.68	0.56
81:AV:29:SER:O	81:AV:29:SER:OG	2.16	0.56
1:AA:747:C:O2	1:AA:801:G:N1	2.37	0.56
1:AA:2178:G:N3	1:AA:2196:C:N4	2.43	0.56
3:BA:826:A:O2'	3:BA:893:U:OP1	2.23	0.56
25:Bu:133:ARG:NH1	25:Bu:141:ASP:O	2.38	0.56
39:AO:52:GLU:OE1	39:AO:52:GLU:N	2.37	0.56
1:AA:1632:A:OP1	1:AA:1633:G:O2'	2.24	0.56
1:AA:2233:A:H2'	1:AA:2234:A:C8	2.40	0.56
3:BA:1442:A:O2'	3:BA:1443:A:O4'	2.12	0.56
4:BB:1140:A:H2'	4:BB:1141:G:H8	1.70	0.56
38:AM:82:GLU:HG2	38:AM:96:THR:HG21	1.87	0.56
73:BF:55:C:H42	73:BF:60:C:H5	1.53	0.56
1:AA:226:U:O2'	1:AA:227:U:O5'	2.24	0.56
1:AA:1032:G:H21	1:AA:1126:C:H42	1.53	0.56
3:BA:958:G:O6	51:Bo:4:ARG:NH2	2.39	0.56
1:AA:692:C:H2'	1:AA:693:A:C8	2.39	0.56
1:AA:765:A:O2'	48:AC:40:GLY:O	2.23	0.56
4:BB:1533:C:H2'	4:BB:1534:G:C8	2.40	0.56
1:AA:974:G:O6	1:AA:1021:G:O6	2.23	0.56
1:AA:1325:G:H1	1:AA:1472:U:H5	1.54	0.56
3:BA:254:A2M:H8	3:BA:254:A2M:O5'	2.06	0.56
11:BS:133:ASN:O	11:BS:134:HIS:ND1	2.38	0.56
12:BT:84:THR:HG22	12:BT:86:GLU:H	1.71	0.56
36:AJ:98:GLN:NE2	40:AP:153:TYR:O	2.39	0.56
46:AT:28:PHE:HE2	46:AT:82:ILE:HG13	1.71	0.56
53:Bm:33:SER:OG	53:Bm:34:SER:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1144:G:H1	1:AA:1237:U:H3	1.53	0.56
1:AA:1760:G:H1	1:AA:1828:U:H3	1.54	0.56
20:Br:295:GLU:H	20:Br:295:GLU:CD	2.13	0.56
30:AD:9:SER:HB3	30:AD:44:LEU:HD21	1.88	0.56
40:AP:134:ALA:O	40:AP:138:SER:OG	2.24	0.56
62:BN:84:GLU:HG3	62:BN:108:ASN:HD21	1.71	0.56
74:BG:120:U:O2'	74:BG:122:G:OP2	2.20	0.56
1:AA:1981:G:N2	1:AA:1981:G:OP2	2.37	0.56
13:BU:18:LYS:HB3	13:BU:21:LYS:HB2	1.87	0.56
79:AQ:38:GLU:OE1	79:AQ:39:HIS:ND1	2.39	0.56
1:AA:31:U:O2	68:A6:16:ARG:NH1	2.39	0.56
1:AA:1780:C:O2	39:AO:13:ARG:NH2	2.39	0.56
29:A5:150:ASP:OD1	29:A5:150:ASP:N	2.37	0.56
49:Bc:20:GLN:OE1	49:Bc:29:SER:OG	2.24	0.56
84:A7:77:ASN:OD1	84:A7:121:ASN:ND2	2.38	0.56
1:AA:754:U:H3	1:AA:794:G:H1	1.54	0.55
3:BA:201:A:OP1	17:BZ:121:ARG:NH1	2.37	0.55
81:AV:2:THR:N	89:AV:301:HOH:O	2.39	0.55
3:BA:627:G:O2'	20:Br:323:ARG:NH2	2.39	0.55
38:AM:61:SER:OG	38:AM:64:GLU:OE2	2.24	0.55
1:AA:755:G:H22	1:AA:793:U:H5	1.54	0.55
1:AA:981:G:N2	1:AA:1014:U:O2	2.35	0.55
29:A5:83:TYR:HB3	29:A5:101:ILE:HB	1.88	0.55
32:AE:56:LEU:O	32:AE:58:PHE:N	2.38	0.55
54:Bk:124:ALA:HB2	62:BN:53:PRO:HG2	1.89	0.55
69:Bf:95:THR:OG1	69:Bf:98:GLY:O	2.22	0.55
1:AA:339:U:O2'	1:AA:341:A:N7	2.38	0.55
1:AA:561:C:H2'	1:AA:562:A:C8	2.42	0.55
1:AA:1919:U:OP1	31:A8:10:ARG:NH2	2.40	0.55
1:AA:1991:G:H2'	1:AA:1998:A:H61	1.72	0.55
3:BA:873:C:H2'	3:BA:874:A:C8	2.41	0.55
61:BO:140:PRO:HA	61:BO:143:GLN:HG3	1.87	0.55
1:AA:393:G:OP1	47:A1:27:ARG:NH2	2.39	0.55
4:BB:1290:C:H5	4:BB:1306:C:H42	1.55	0.55
1:AA:2137:G:N2	1:AA:2260:MA6:H8	2.22	0.55
29:A5:189:THR:HG23	29:A5:200:GLY:HA2	1.88	0.55
46:AT:61:GLN:NE2	46:AT:83:TYR:O	2.40	0.55
47:A1:95:ARG:NH1	47:A1:113:GLU:OE2	2.39	0.55
82:AW:20:HIS:ND1	82:AW:21:LYS:O	2.40	0.55
3:BA:973:G:O6	51:Bo:3:LYS:NZ	2.40	0.55
3:BA:1318:G:OP1	8:BP:17:ARG:NH2	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BP:132:ASP:OD2	8:BP:138:SER:OG	2.22	0.55
18:Bp:54:ASP:O	18:Bp:58:ARG:HG3	2.06	0.55
20:Br:181:ARG:NH2	20:Br:204:ARG:O	2.39	0.55
34:AI:36:THR:HG23	34:AI:39:GLU:H	1.70	0.55
43:AX:202:ASP:OD2	43:AX:202:ASP:N	2.40	0.55
3:BA:563:G:H2'	3:BA:564:C:C6	2.42	0.55
6:BD:51:G:O2'	6:BD:52:U:OP1	2.24	0.55
17:BZ:8:ASN:HB3	17:BZ:11:LYS:HB2	1.89	0.55
72:Bh:75:LYS:HE2	72:Bh:75:LYS:HA	1.88	0.55
3:BA:1469:G:C2	11:BS:3:ARG:HG3	2.42	0.55
20:Br:21:CYS:SG	20:Br:252:LYS:NZ	2.80	0.55
23:Bx:171:ASP:HB3	23:Bx:172:PRO:HD3	1.88	0.55
47:A1:209:ASP:OD1	47:A1:210:ALA:N	2.38	0.55
3:BA:1518:A:OP1	49:Bc:37:ASN:ND2	2.36	0.55
8:BP:81:LYS:HB3	8:BP:83:VAL:HG23	1.88	0.55
40:AP:147:VAL:HG21	40:AP:229:ARG:HG2	1.87	0.55
64:BK:30:ARG:HG3	64:BK:63:GLU:HG3	1.89	0.55
1:AA:749:C:O2'	1:AA:750:G:H8	1.89	0.54
1:AA:961:U:O4	1:AA:962:A:N6	2.29	0.54
45:A3:39:GLY:O	45:A3:47:ARG:NH2	2.40	0.54
60:Ba:82:THR:HG22	60:Ba:84:TYR:H	1.71	0.54
1:AA:314:C:H3'	1:AA:315:G:H8	1.72	0.54
1:AA:967:A:H4'	1:AA:968:G:O5'	2.07	0.54
1:AA:1473:C:H2'	1:AA:1474:U:C6	2.42	0.54
46:AT:72:GLY:HA2	68:A6:131:ARG:HH22	1.70	0.54
52:Bn:17:ILE:HG12	52:Bn:29:VAL:HG22	1.90	0.54
3:BA:1832:A:O2'	3:BA:1857:U:O2	2.23	0.54
29:A5:90:LEU:HD22	29:A5:95:THR:HG21	1.89	0.54
36:AJ:54:ASP:HB2	83:A4:145:TRP:HZ3	1.73	0.54
75:BH:57:A:H2	75:BH:65:G:N1	2.04	0.54
1:AA:1463:C:H5	27:A0:169:ARG:HH22	1.56	0.54
29:A5:21:HIS:H	29:A5:21:HIS:CD2	2.25	0.54
40:AP:246:SER:OG	40:AP:247:ARG:N	2.39	0.54
41:AS:125:VAL:O	41:AS:128:VAL:HG12	2.07	0.54
53:Bm:26:THR:HB	62:BN:111:GLU:HG3	1.88	0.54
63:BL:31:GLY:HA2	63:BL:72:ILE:HG13	1.90	0.54
6:BD:2:G:O6	6:BD:118:C:N4	2.41	0.54
18:Bp:47:MET:HE1	18:Bp:52:LYS:HD2	1.88	0.54
39:AO:158:ARG:HH11	39:AO:158:ARG:HB2	1.73	0.54
62:BN:179:GLU:OE2	62:BN:179:GLU:N	2.40	0.54
1:AA:35:G:N7	40:AP:215:ARG:NH2	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BA:366:C:OP1	53:Bm:93:LYS:NZ	2.34	0.54
3:BA:501:G:H5'	24:Bl:129:SER:HB3	1.89	0.54
3:BA:639:G:OP1	22:Bw:71:ARG:NH2	2.41	0.54
5:BC:67:U:H2'	5:BC:68:A:C8	2.43	0.54
69:Bf:292:ARG:HG2	69:Bf:292:ARG:NH1	2.23	0.54
71:Bv:89:ASP:OD2	71:Bv:91:THR:OG1	2.22	0.54
1:AA:611:U:H2'	1:AA:612:G:C8	2.43	0.54
11:BS:79:ASP:OD2	11:BS:79:ASP:N	2.36	0.54
5:BC:71:A:N7	5:BC:86:U:O4	2.41	0.54
1:AA:220:G:O2'	1:AA:222:U:O2	2.18	0.54
1:AA:306:C:H2'	1:AA:307:C:C6	2.43	0.54
1:AA:1656:U:O2'	1:AA:1657:C:O5'	2.26	0.54
1:AA:1881:U:H3'	1:AA:1882:U:H5''	1.89	0.54
1:AA:1950:A:H4'	67:AK:78:SER:H	1.72	0.54
32:AE:21:GLU:N	32:AE:21:GLU:OE1	2.41	0.54
1:AA:924:C:C2	68:A6:142:ILE:HD13	2.43	0.54
1:AA:1916:U:H2'	1:AA:1917:U:C6	2.43	0.54
1:AA:2044:A:H2'	1:AA:2045:PSU:H6	1.73	0.54
3:BA:1816:A:H2'	3:BA:1817:A:C8	2.42	0.54
4:BB:1116:A:OP1	63:BL:102:ASN:ND2	2.40	0.54
7:BE:43:U:O2'	7:BE:44:C:H6	1.89	0.54
63:BL:39:ARG:HD2	63:BL:127:THR:HA	1.89	0.54
66:Be:246:ILE:HD13	66:Be:250:ARG:HG3	1.90	0.54
82:AW:43:ASN:ND2	82:AW:58:ASN:OD1	2.40	0.54
1:AA:93:A:OP1	45:A3:139:LYS:NZ	2.41	0.53
1:AA:300:C:H2'	1:AA:301:C:H6	1.73	0.53
1:AA:996:U:O2'	1:AA:997:U:O4'	2.26	0.53
3:BA:351:A:OP2	21:Bt:41:ARG:NH1	2.40	0.53
4:BB:812:G:H22	4:BB:821:C:H5	1.56	0.53
4:BB:1297:U:H5''	4:BB:1298:C:H5	1.71	0.53
13:BU:107:GLN:NE2	13:BU:107:GLN:O	2.41	0.53
63:BL:117:ILE:HD13	63:BL:123:TYR:HB2	1.90	0.53
1:AA:771:C:H42	1:AA:779:C:H42	1.57	0.53
4:BB:769:U:H2'	4:BB:770:G:C8	2.43	0.53
47:A1:228:ASP:OD2	47:A1:230:SER:N	2.38	0.53
67:AK:36:ARG:NH1	67:AK:39:GLY:O	2.41	0.53
1:AA:133:A:H2'	1:AA:134:G:C8	2.43	0.53
1:AA:1556:A:OP2	1:AA:2245:A:O2'	2.23	0.53
4:BB:496:A:H2'	4:BB:497:C:C6	2.43	0.53
27:A0:88:PHE:HB3	27:A0:100:THR:HB	1.90	0.53
39:AO:158:ARG:HB2	39:AO:158:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:AX:53:LYS:HB2	43:AX:56:GLU:HB2	1.89	0.53
47:A1:3:LYS:HD2	47:A1:3:LYS:N	2.23	0.53
74:BG:18:U:H2'	74:BG:19:C:H6	1.71	0.53
79:AQ:44:LYS:HE2	79:AQ:44:LYS:N	2.23	0.53
7:BE:203:A:H2'	7:BE:204:A:C8	2.43	0.53
34:AI:51:ARG:NH2	34:AI:89:ASP:OD1	2.42	0.53
45:A3:2:LYS:HB2	45:A3:111:VAL:HG22	1.89	0.53
1:AA:95:C:H5''	1:AA:97:C:H5	1.73	0.53
1:AA:773:C:H1'	1:AA:778:A:C6	2.42	0.53
1:AA:1565:A:H2'	1:AA:1566:C:H6	1.73	0.53
16:BX:153:ASP:HB3	16:BX:156:ASP:HB2	1.91	0.53
63:BL:150:ARG:HG2	63:BL:151:ARG:HG3	1.90	0.53
69:Bf:3:HIS:ND1	69:Bf:4:CYS:O	2.41	0.53
1:AA:1830:U:O2'	39:AO:139:ARG:NH2	2.41	0.53
4:BB:1510:G:H21	69:Bf:139:THR:HG22	1.74	0.53
32:AE:125:VAL:HG12	32:AE:153:TYR:HB2	1.90	0.53
3:BA:1502:U:HO2'	3:BA:1503:A:H8	1.57	0.53
4:BB:1487:G:H22	4:BB:1505:G:N2	2.06	0.53
11:BS:12:VAL:HG22	11:BS:28:LYS:HG2	1.91	0.53
17:BZ:54:ARG:NH1	17:BZ:64:GLU:OE2	2.42	0.53
47:A1:138:THR:HG22	47:A1:140:ASP:H	1.73	0.53
47:A1:229:MET:HE3	47:A1:229:MET:C	2.33	0.53
61:BO:52:THR:HG23	61:BO:121:VAL:HB	1.90	0.53
63:BL:140:ARG:NH2	63:BL:165:GLU:OE1	2.36	0.53
1:AA:769:G:O6	1:AA:781:U:O4	2.27	0.53
1:AA:1119:C:N4	1:AA:1120:G:O6	2.41	0.53
4:BB:29:C:OP1	4:BB:32:C:N4	2.40	0.53
4:BB:1040:U:H2'	4:BB:1041:G:C8	2.43	0.53
11:BS:79:ASP:HB3	11:BS:93:VAL:HG22	1.91	0.53
59:Bb:116:GLN:HE21	59:Bb:116:GLN:HA	1.73	0.53
1:AA:64:U:H2'	1:AA:65:U:H6	1.73	0.53
1:AA:71:A:O2'	1:AA:124:C:OP1	2.19	0.53
1:AA:2086:C:H2'	1:AA:2087:A:H8	1.74	0.53
3:BA:1608:OMC:HM22	20:Br:94:MET:HG3	1.91	0.53
26:By:149:LEU:O	26:By:153:SER:OG	2.24	0.53
39:AO:14:ARG:NH1	39:AO:17:LYS:O	2.42	0.53
74:BG:101:G:H2'	74:BG:102:G:O4'	2.09	0.53
1:AA:501:C:H2'	1:AA:502:C:H6	1.74	0.53
1:AA:517:C:O2'	1:AA:519:G:OP1	2.21	0.53
1:AA:612:G:H1	1:AA:645:C:H5	1.57	0.53
1:AA:1033:C:H2'	1:AA:1034:C:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1984:C:H5	1:AA:2005:G:H22	1.55	0.53
4:BB:473:U:H2'	4:BB:474:G:H8	1.74	0.53
4:BB:1504:G:H2'	4:BB:1505:G:C8	2.43	0.53
5:BC:121:G:H2'	5:BC:122:A:C8	2.44	0.53
41:AS:32:THR:HG23	41:AS:34:VAL:H	1.74	0.53
1:AA:331:A:H3'	1:AA:873:A:H2	1.74	0.52
1:AA:1984:C:H5	1:AA:2005:G:H1	1.57	0.52
3:BA:620:G:N2	3:BA:1514:U:OP2	2.39	0.52
48:AC:57:MET:HE2	48:AC:205:HIS:HB3	1.91	0.52
49:Bc:3:HIS:HB3	49:Bc:7:LEU:HD23	1.90	0.52
75:BH:5:G:H2'	75:BH:6:U:C6	2.44	0.52
84:A7:148:ARG:HB3	84:A7:148:ARG:NH1	2.24	0.52
1:AA:607:U:HO2'	1:AA:608:C:H6	1.56	0.52
1:AA:748:A:H2'	1:AA:749:C:C6	2.44	0.52
1:AA:1013:G:H2'	1:AA:1014:U:C6	2.43	0.52
1:AA:2167:G:H2'	1:AA:2168:U:C6	2.45	0.52
3:BA:1865:G:N2	4:BB:5:A:N1	2.51	0.52
26:By:103:VAL:HG22	26:By:108:VAL:HG22	1.90	0.52
42:AU:89:LEU:HD22	42:AU:94:LEU:HD12	1.91	0.52
61:BO:107:PRO:O	61:BO:113:GLY:HA3	2.09	0.52
72:Bh:41:VAL:HG13	72:Bh:45:MET:HE1	1.89	0.52
1:AA:788:U:O2'	1:AA:789:G:O5'	2.24	0.52
1:AA:920:C:H5	1:AA:928:G:H1	1.57	0.52
1:AA:950:A:H2'	1:AA:951:A:C8	2.44	0.52
3:BA:646:G:H2'	3:BA:648:G:H8	1.73	0.52
69:Bf:209:ARG:HH22	69:Bf:296:MET:HE1	1.73	0.52
3:BA:870:G:H21	3:BA:1096:U:H4'	1.73	0.52
3:BA:1189:C:H4'	3:BA:1190:A:H5''	1.90	0.52
75:BH:48:G:H1	75:BH:94:G:H22	1.56	0.52
79:AQ:48:ARG:HB2	79:AQ:87:ASP:HB3	1.91	0.52
84:A7:130:ASP:OD1	84:A7:130:ASP:N	2.42	0.52
1:AA:608:C:HO2'	1:AA:609:A:H8	1.57	0.52
3:BA:876:C:OP1	58:Bd:45:ARG:NH1	2.43	0.52
3:BA:1206:U:H2'	3:BA:1210:A:C2	2.44	0.52
40:AP:177:VAL:HG11	40:AP:224:THR:HG22	1.91	0.52
44:AZ:45:LYS:NZ	44:AZ:47:LEU:HB2	2.25	0.52
51:Bo:5:THR:HG21	51:Bo:9:GLY:H	1.73	0.52
1:AA:87:C:H42	1:AA:91:G:H1	1.56	0.52
1:AA:375:U:H5'	45:A3:185:SER:HB3	1.91	0.52
1:AA:481:G:H2'	1:AA:482:G:H8	1.75	0.52
1:AA:752:A:H2	1:AA:797:C:H42	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1201:A:H2'	1:AA:1202:G:C8	2.45	0.52
1:AA:2110:C:H2'	28:A2:46:ARG:HD2	1.91	0.52
3:BA:509:A:H2'	3:BA:510:U:C6	2.45	0.52
3:BA:1332:G:H2'	3:BA:1333:A:C8	2.45	0.52
3:BA:1568:G:O2'	3:BA:1570:U:OP1	2.24	0.52
12:BT:44:LEU:HD22	12:BT:49:LEU:HD12	1.91	0.52
80:AR:23:HIS:CE1	80:AR:58:CYS:HB2	2.45	0.52
1:AA:541:G:OP1	47:A1:26:PRO:HD3	2.10	0.52
3:BA:210:G:H21	3:BA:231:A:H2	1.58	0.52
3:BA:1336:C:H3'	3:BA:1337:G:H5''	1.91	0.52
4:BB:991:C:H5''	4:BB:992:G:N2	2.24	0.52
18:Bp:51:LYS:HD3	18:Bp:52:LYS:H	1.75	0.52
46:AT:90:LYS:HZ3	46:AT:103:MET:HG3	1.75	0.52
59:Bb:75:LEU:HD22	59:Bb:115:LEU:HD13	1.92	0.52
72:Bh:152:GLU:HG2	72:Bh:154:LYS:HE3	1.91	0.52
77:BV:90:PHE:O	77:BV:94:THR:OG1	2.26	0.52
1:AA:598:U:H1'	1:AA:599:G:C8	2.45	0.52
1:AA:613:G:N2	1:AA:639:G:H21	2.08	0.52
1:AA:712:G:H1	1:AA:1513:G:N2	2.04	0.52
3:BA:527:G:H1	56:Bi:3:LYS:NZ	2.07	0.52
4:BB:633:G:H2'	4:BB:634:G:C8	2.45	0.52
37:AL:19:LYS:HD3	43:AX:209:PRO:HD3	1.92	0.52
40:AP:153:TYR:OH	40:AP:159:GLY:O	2.27	0.52
74:BG:2:U:H5	74:BG:22:G:H1	1.58	0.52
3:BA:595:U:OP2	20:Br:323:ARG:NH1	2.41	0.52
3:BA:805:U:H2'	3:BA:806:C:C6	2.45	0.52
61:BO:144:ARG:HA	61:BO:147:CYS:HB2	1.92	0.52
1:AA:1216:A:OP1	33:AG:114:ARG:NH2	2.43	0.52
4:BB:1468:U:H5''	4:BB:1470:A:H62	1.75	0.52
14:BW:17:LEU:HD13	14:BW:53:ALA:HB3	1.91	0.52
18:Bp:51:LYS:C	18:Bp:53:ALA:H	2.18	0.52
42:AU:67:THR:HB	42:AU:70:ILE:HG13	1.91	0.52
65:BI:161:ALA:O	65:BI:167:SER:OG	2.26	0.52
68:A6:158:ALA:O	68:A6:161:SER:OG	2.28	0.52
1:AA:283:A:H2'	1:AA:284:A:H8	1.74	0.51
1:AA:2092:A:OP1	31:A8:20:ARG:NH2	2.43	0.51
3:BA:594:G:H21	3:BA:597:U:H6	1.56	0.51
47:A1:208:LYS:NZ	47:A1:214:GLU:OE2	2.43	0.51
72:Bh:31:LYS:HZ2	72:Bh:33:ARG:H	1.56	0.51
1:AA:682:A:O2'	1:AA:684:U:OP2	2.22	0.51
1:AA:757:G:N1	1:AA:793:U:O2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BA:286:C:O2'	3:BA:295:G:O4'	2.28	0.51
3:BA:531:G:H2'	3:BA:532:A:C8	2.45	0.51
43:AX:24:LEU:HD12	43:AX:28:LEU:HD23	1.91	0.51
78:Az:172:GLN:HE21	78:Az:216:ARG:HH21	1.58	0.51
84:A7:112:VAL:HA	84:A7:128:GLY:HA3	1.92	0.51
1:AA:583:C:O2	1:AA:603:G:N2	2.42	0.51
1:AA:839:A:H61	1:AA:892:C:H42	1.57	0.51
1:AA:1642:G:N1	1:AA:1654:U:O4	2.44	0.51
1:AA:2047:G:O6	34:Al:50:ARG:NH1	2.44	0.51
12:BT:28:GLU:HG3	12:BT:49:LEU:HD22	1.92	0.51
22:Bw:122:ARG:NH2	22:Bw:217:LEU:O	2.43	0.51
29:A5:178:GLN:HB3	29:A5:184:LEU:HD12	1.92	0.51
46:AT:90:LYS:HZ2	46:AT:98:LYS:HE2	1.75	0.51
48:AC:200:ASN:OD1	48:AC:202:ARG:NH2	2.42	0.51
1:AA:44:G:H2'	1:AA:45:C:C6	2.45	0.51
1:AA:520:C:H2'	1:AA:521:A:C8	2.45	0.51
1:AA:778:A:H2'	1:AA:779:C:O4'	2.09	0.51
28:A2:90:THR:HG22	28:A2:92:GLN:HB3	1.91	0.51
30:AD:10:ARG:HD3	30:AD:52:LEU:HD11	1.92	0.51
47:A1:19:LYS:HG3	47:A1:20:LEU:HD23	1.91	0.51
69:Bf:185:GLU:OE2	74:BG:30:C:O2'	2.27	0.51
84:A7:185:THR:HG23	84:A7:187:ARG:HG2	1.92	0.51
84:A7:222:LEU:C	84:A7:223:TRP:HD1	2.18	0.51
1:AA:788:U:H2'	1:AA:789:G:C5	2.45	0.51
1:AA:802:C:H2'	1:AA:803:C:C6	2.46	0.51
17:BZ:117:GLU:N	17:BZ:117:GLU:OE2	2.44	0.51
20:Br:318:ASN:O	20:Br:320:ILE:N	2.38	0.51
28:A2:161:ASP:OD1	28:A2:161:ASP:N	2.44	0.51
40:AP:237:PRO:HA	40:AP:240:TRP:NE1	2.24	0.51
47:A1:192:ILE:HA	47:A1:207:LEU:HD23	1.92	0.51
64:BK:202:PRO:HG2	64:BK:203:LYS:HE3	1.91	0.51
1:AA:599:G:H2'	1:AA:600:G:C2	2.46	0.51
1:AA:832:A:H3'	1:AA:834:G:H21	1.76	0.51
1:AA:1644:U:H2'	1:AA:1645:G:C8	2.45	0.51
1:AA:1652:OMU:H2'	1:AA:1653:C:C6	2.45	0.51
1:AA:2272:G:O2'	81:AV:5:ARG:NH2	2.43	0.51
3:BA:616:G:H5''	3:BA:706:G:H1'	1.93	0.51
1:AA:694:A:O2'	1:AA:695:A:H8	1.94	0.51
1:AA:908:A:H2'	1:AA:908:A:N3	2.26	0.51
3:BA:16:U:H2'	3:BA:17:G:H8	1.75	0.51
4:BB:790:A:OP1	66:Be:37:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Bu:187:PRO:HD2	25:Bu:201:HIS:CD2	2.46	0.51
45:A3:54:ARG:HG3	45:A3:115:THR:HG23	1.92	0.51
69:Bf:394:ARG:NH1	69:Bf:394:ARG:HB3	2.25	0.51
1:AA:928:G:OP1	47:A1:19:LYS:NZ	2.37	0.51
1:AA:1014:U:H2'	1:AA:1015:C:C6	2.45	0.51
1:AA:1954:A:H61	1:AA:2011:C:H5	1.58	0.51
4:BB:608:U:H2'	4:BB:609:A2M:C8	2.41	0.51
4:BB:1514:U:H3	4:BB:1534:G:H1	1.58	0.51
25:Bu:115:LEU:HD22	25:Bu:119:PHE:HE2	1.76	0.51
44:AZ:74:ARG:NH2	44:AZ:95:THR:O	2.40	0.51
67:AK:37:ILE:HD13	67:AK:42:ILE:HD13	1.92	0.51
1:AA:1576:A:O2'	1:AA:2065:A:N3	2.40	0.51
1:AA:1916:U:H2'	1:AA:1917:U:H6	1.75	0.51
5:BC:70:C:OP2	17:BZ:111:ARG:NH1	2.43	0.51
44:AZ:45:LYS:HD2	44:AZ:45:LYS:C	2.36	0.51
61:BO:106:LEU:O	61:BO:108:ARG:NH1	2.44	0.51
84:A7:155:VAL:HA	84:A7:173:GLY:HA2	1.92	0.51
3:BA:265:A:N3	20:Br:221:ASN:ND2	2.58	0.51
29:A5:77:ARG:NH2	75:BH:85:C:OP2	2.44	0.51
1:AA:156:U:O2'	1:AA:172:A:N1	2.39	0.50
1:AA:788:U:H2'	1:AA:789:G:C8	2.46	0.50
4:BB:424:G:H2'	4:BB:425:C:C6	2.46	0.50
4:BB:812:G:H1	4:BB:821:C:H5	1.59	0.50
4:BB:1423:A:N7	66:Be:215:ASN:ND2	2.59	0.50
19:Bq:16:LYS:HG3	19:Bq:49:LEU:HD11	1.93	0.50
35:AH:135:ARG:HH21	81:AV:29:SER:HB2	1.76	0.50
40:AP:92:LEU:HD22	40:AP:217:ARG:HB3	1.92	0.50
64:BK:182:GLU:OE1	64:BK:182:GLU:HA	2.11	0.50
74:BG:16:G:H2'	74:BG:17:A:C8	2.47	0.50
3:BA:1619:U:H2'	3:BA:1620:A2M:H8	1.92	0.50
4:BB:4:C:H2'	4:BB:5:A:C8	2.45	0.50
68:A6:159:ASP:OD1	68:A6:159:ASP:N	2.44	0.50
80:AR:17:TYR:CG	80:AR:17:TYR:O	2.65	0.50
1:AA:55:U:H2'	1:AA:56:A2M:H8	1.92	0.50
1:AA:343:U:N3	32:AE:28:THR:OG1	2.41	0.50
1:AA:955:A:N6	89:AA:2515:HOH:O	2.44	0.50
6:BD:62:A:O2'	64:BK:205:LYS:NZ	2.44	0.50
12:BT:179:LYS:O	12:BT:179:LYS:HG2	2.10	0.50
42:AU:50:LYS:HE2	42:AU:50:LYS:HA	1.93	0.50
52:Bn:64:CYS:O	52:Bn:68:LYS:HG3	2.11	0.50
1:AA:2060:G:OP1	38:AM:41:PHE:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BB:1516:G:OP2	72:Bh:36:ARG:NH1	2.40	0.50
6:BD:27:A:H2'	6:BD:28:C:C6	2.46	0.50
7:BE:38:C:H2'	7:BE:39:A:O4'	2.12	0.50
18:Bp:28:ASN:HB2	18:Bp:31:VAL:HG12	1.93	0.50
24:Bl:88:LYS:HE2	24:Bl:90:LYS:NZ	2.27	0.50
84:A7:92:ARG:HH21	84:A7:104:LYS:HE2	1.75	0.50
1:AA:2233:A:H2'	1:AA:2234:A:H8	1.76	0.50
3:BA:488:A:H2'	3:BA:489:A:O4'	2.11	0.50
45:A3:40:ALA:HA	45:A3:47:ARG:CZ	2.42	0.50
63:BL:30:VAL:HG13	63:BL:32:GLU:H	1.76	0.50
82:AW:22:ARG:HA	82:AW:27:GLN:HB3	1.93	0.50
1:AA:647:A:H61	1:AA:696:A:H5''	1.77	0.50
1:AA:759:U:H2'	1:AA:760:G:C8	2.47	0.50
1:AA:1021:G:H3'	83:A4:12:LYS:HE2	1.93	0.50
1:AA:1622:G:H1	31:A8:8:ARG:HH21	1.58	0.50
1:AA:1847:U:O2'	1:AA:1848:G:N7	2.40	0.50
1:AA:2092:A:OP2	31:A8:33:ARG:NH2	2.44	0.50
7:BE:8:A:C2	7:BE:104:U:H4'	2.46	0.50
39:AO:132:LYS:HA	39:AO:138:HIS:HA	1.93	0.50
3:BA:912:C:H2'	3:BA:913:C:C6	2.47	0.50
4:BB:361:U:H2'	4:BB:362:G:C8	2.47	0.50
4:BB:1488:C:H2'	4:BB:1489:A:H8	1.76	0.50
14:BW:98:GLU:HG3	15:BY:21:TYR:OH	2.12	0.50
28:A2:45:LYS:HG2	28:A2:48:ARG:HH21	1.77	0.50
54:Bk:46:GLY:O	54:Bk:47:ARG:HG2	2.11	0.50
1:AA:1032:G:N2	1:AA:1126:C:H42	2.08	0.50
1:AA:1034:C:N4	1:AA:1123:C:H42	2.10	0.50
1:AA:1853:A:H4'	1:AA:1854:U:O5'	2.12	0.50
4:BB:1526:U:O2'	4:BB:1527:G:H5''	2.12	0.50
29:A5:21:HIS:H	29:A5:21:HIS:HD2	1.60	0.50
74:BG:67:A:N3	89:BG:301:HOH:O	2.35	0.50
1:AA:1595:C:O2'	1:AA:1596:B8N:OP2	2.30	0.50
62:BN:54:ARG:O	62:BN:153:GLN:NE2	2.36	0.50
80:AR:85:ILE:HD11	82:AW:4:PHE:HD1	1.77	0.50
1:AA:209:A:H3'	1:AA:210:C:C5'	2.42	0.49
1:AA:393:G:O2'	47:A1:2:ALA:N	2.44	0.49
1:AA:1998:A:O2'	1:AA:1999:G:O4'	2.30	0.49
3:BA:1740:G:H2'	3:BA:1741:U:O2	2.11	0.49
33:AG:61:ALA:HB2	82:AW:33:PHE:HZ	1.76	0.49
38:AM:55:ARG:NH2	38:AM:59:THR:O	2.34	0.49
43:AX:95:LEU:HD13	43:AX:189:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:A1:29:ARG:NH2	47:A1:78:LYS:HE2	2.27	0.49
47:A1:244:ILE:CD1	47:A1:249:GLU:HG2	2.42	0.49
60:Ba:87:ASP:OD1	60:Ba:87:ASP:N	2.43	0.49
68:A6:120:SER:OG	68:A6:121:VAL:N	2.44	0.49
84:A7:191:ASP:OD1	84:A7:192:LEU:N	2.43	0.49
4:BB:997:G:H1	4:BB:1014:U:H3	1.59	0.49
5:BC:60:U:O4	54:Bk:63:ASN:ND2	2.40	0.49
21:Bt:14:ASP:HB3	21:Bt:17:CYS:SG	2.51	0.49
30:AD:87:LEU:HB3	30:AD:89:LEU:HG	1.93	0.49
46:AT:90:LYS:NZ	46:AT:98:LYS:HE2	2.28	0.49
63:BL:14:ASN:HB3	63:BL:17:ARG:HG3	1.94	0.49
68:A6:152:GLU:HA	68:A6:155:ILE:HD12	1.94	0.49
1:AA:797:C:H2'	1:AA:798:C:C6	2.47	0.49
1:AA:965:G:H2'	1:AA:966:A:C8	2.47	0.49
3:BA:1187:A:H2'	3:BA:1233:A:N7	2.27	0.49
4:BB:1165:A:H5'	58:Bd:34:ARG:HE	1.78	0.49
4:BB:1314:U:H5'	4:BB:1393:G:H5''	1.95	0.49
47:A1:61:ILE:HG23	47:A1:66:LEU:HD12	1.93	0.49
1:AA:225:C:H4'	78:Az:216:ARG:HH22	1.77	0.49
1:AA:1712:U:H3	1:AA:1723:G:H22	1.61	0.49
3:BA:1192:C:H2'	3:BA:1193:C:H6	1.77	0.49
4:BB:440:U:OP1	66:Be:54:ARG:NH2	2.38	0.49
4:BB:1451:A:H2'	4:BB:1451:A:N3	2.28	0.49
28:A2:63:MET:HB2	28:A2:68:GLY:O	2.13	0.49
32:AE:115:ARG:HG2	41:AS:7:GLN:HA	1.95	0.49
54:Bk:79:LEU:C	54:Bk:81:SER:H	2.21	0.49
1:AA:1767:C:H3'	1:AA:1768:C:H6	1.77	0.49
4:BB:989:A:H5'	4:BB:990:A:H5''	1.95	0.49
34:Al:74:VAL:HG21	34:Al:80:PRO:HA	1.95	0.49
47:A1:19:LYS:NZ	68:A6:4:TYR:O	2.45	0.49
66:Be:234:LYS:HG2	66:Be:238:ILE:HG12	1.95	0.49
67:AK:23:ALA:HB2	67:AK:75:VAL:HG13	1.94	0.49
3:BA:1515:G:O2'	3:BA:1516:A:H5''	2.13	0.49
28:A2:181:GLU:OE2	28:A2:184:ARG:NH1	2.46	0.49
36:Aj:54:ASP:HB2	83:A4:145:TRP:CZ3	2.48	0.49
48:AC:60:HIS:HB3	48:AC:87:ILE:HD11	1.93	0.49
69:Bf:57:VAL:HG22	69:Bf:73:VAL:HG22	1.94	0.49
1:AA:709:G:H5'	1:AA:715:G:N2	2.27	0.49
1:AA:1477:C:H2'	1:AA:1478:U:H5''	1.94	0.49
3:BA:213:A:OP2	49:Bc:140:THR:OG1	2.25	0.49
3:BA:1316:U:H5	3:BA:1457:A:N7	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BB:97:A:O2'	4:BB:384:C:O2	2.28	0.49
4:BB:1386:U:O2	4:BB:1388:A2M:H8	2.11	0.49
4:BB:1525:G:H1	72:Bh:39:LYS:HG3	1.77	0.49
26:By:22:ARG:NH1	73:BF:23:U:OP2	2.44	0.49
61:BO:203:GLU:O	61:BO:203:GLU:HG3	2.12	0.49
72:Bh:97:LYS:HE3	74:BG:85:C:H4'	1.93	0.49
1:AA:315:G:O2'	1:AA:316:G:H5'	2.13	0.49
1:AA:602:U:H2'	1:AA:603:G:C2	2.47	0.49
1:AA:762:C:H3'	1:AA:763:G:C8	2.48	0.49
1:AA:2087:A:H2'	1:AA:2088:G:H8	1.78	0.49
1:AA:2168:U:OP1	45:A3:95:ARG:NH1	2.43	0.49
3:BA:508:C:H2'	3:BA:509:A:H8	1.78	0.49
3:BA:1007:G:H2'	3:BA:1008:C:C6	2.48	0.49
3:BA:1239:G:N7	65:BI:13:ARG:NH2	2.61	0.49
4:BB:1105:A:H2'	4:BB:1106:G:C8	2.47	0.49
24:Bl:68:THR:HG22	24:Bl:70:GLU:H	1.78	0.49
61:BO:72:TYR:OH	61:BO:91:HIS:O	2.31	0.49
84:A7:261:ARG:HB2	84:A7:263:PHE:CZ	2.47	0.49
1:AA:300:C:H2'	1:AA:301:C:C6	2.48	0.49
1:AA:1566:C:C2	1:AA:1567:A:C8	3.01	0.49
3:BA:1315:C:H5'	3:BA:1316:U:H5'	1.94	0.49
4:BB:637:A:N3	4:BB:1278:G:O2'	2.38	0.49
6:BD:44:U:OP2	63:BL:144:ARG:NH1	2.41	0.49
47:A1:102:VAL:HG23	47:A1:241:GLY:HA2	1.94	0.49
77:BV:95:LYS:HD3	77:BV:104:ARG:NH2	2.28	0.49
1:AA:168:C:H2'	1:AA:169:A:H8	1.75	0.49
3:BA:16:U:H2'	3:BA:17:G:C8	2.48	0.49
4:BB:1514:U:O2	4:BB:1534:G:C2	2.65	0.49
20:Br:64:GLU:HG2	20:Br:79:HIS:NE2	2.27	0.49
27:A0:107:MET:O	27:A0:108:THR:HB	2.12	0.49
28:A2:91:ASP:OD1	42:AU:64:LYS:NZ	2.46	0.49
29:A5:163:GLU:H	29:A5:163:GLU:CD	2.18	0.49
38:AM:26:LYS:HA	38:AM:56:ARG:HA	1.95	0.49
46:AT:84:ASP:N	46:AT:84:ASP:OD2	2.46	0.49
48:AC:148:ILE:HD12	48:AC:148:ILE:O	2.12	0.49
69:Bf:69:LYS:NZ	69:Bf:69:LYS:HB2	2.27	0.49
1:AA:64:U:H2'	1:AA:65:U:C6	2.48	0.48
6:BD:46:G:OP1	25:Bu:164:ARG:HG3	2.13	0.48
18:Bp:52:LYS:HA	18:Bp:55:LYS:HB2	1.94	0.48
26:By:90:VAL:HG23	26:By:142:LEU:HB3	1.94	0.48
63:BL:105:ASP:OD2	63:BL:105:ASP:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Be:109:GLU:OE2	66:Be:109:GLU:N	2.38	0.48
1:AA:828:A:HO2'	1:AA:829:U:H6	1.61	0.48
1:AA:894:U:H3'	1:AA:895:G:H21	1.78	0.48
1:AA:1953:A:N6	1:AA:2012:A:H61	2.11	0.48
1:AA:2058:U:H2'	1:AA:2059:C:C6	2.48	0.48
4:BB:1292:A:H4'	64:BK:74:LYS:HG2	1.95	0.48
4:BB:1526:U:O2'	4:BB:1527:G:N2	2.45	0.48
9:BQ:138:VAL:HG21	9:BQ:148:GLU:HG3	1.95	0.48
35:AH:60:ASP:O	35:AH:63:SER:OG	2.28	0.48
84:A7:35:SER:OG	84:A7:36:ARG:N	2.46	0.48
1:AA:147:G:H1	1:AA:389:U:H5	1.61	0.48
1:AA:835:A:H2'	1:AA:836:A:C8	2.47	0.48
1:AA:959:G:N2	36:AJ:105:THR:O	2.46	0.48
30:AD:80:ILE:O	30:AD:84:ARG:HG2	2.13	0.48
40:AP:72:LYS:NZ	48:AC:145:THR:O	2.46	0.48
84:A7:234:MET:HE1	84:A7:263:PHE:CD2	2.48	0.48
1:AA:273:A:O2'	1:AA:274:C:OP1	2.30	0.48
1:AA:316:G:O2'	1:AA:317:A:O5'	2.29	0.48
1:AA:760:G:H2'	1:AA:761:C:O4'	2.14	0.48
1:AA:866:G:C6	1:AA:879:G:H2'	2.48	0.48
1:AA:1151:C:H2'	1:AA:1152:G:C8	2.48	0.48
13:BU:100:ARG:NE	13:BU:103:GLU:OE1	2.47	0.48
45:A3:96:ARG:HG3	45:A3:97:ARG:N	2.28	0.48
48:AC:127:SER:HB3	48:AC:132:THR:O	2.14	0.48
1:AA:623:A:H2'	1:AA:624:A:C8	2.49	0.48
1:AA:1636:U:H4'	1:AA:1663:C:H2'	1.95	0.48
1:AA:1936:A:H4'	1:AA:2035:G:H4'	1.94	0.48
3:BA:74:C:O2'	62:BN:71:ASN:OD1	2.25	0.48
3:BA:1459:C:O2'	11:BS:117:ARG:NH1	2.47	0.48
4:BB:982:C:O2'	4:BB:983:U:O5'	2.30	0.48
4:BB:1487:G:H22	4:BB:1505:G:H22	1.60	0.48
6:BD:7:G:OP1	25:Bu:33:ARG:NH1	2.46	0.48
34:AI:43:LEU:O	38:AM:89:ARG:NH2	2.45	0.48
39:AO:154:LYS:HG3	39:AO:158:ARG:NH1	2.29	0.48
62:BN:131:PHE:CE2	62:BN:148:VAL:HG13	2.49	0.48
1:AA:275:G:H2'	1:AA:276:U:C6	2.49	0.48
1:AA:359:G:O2'	1:AA:360:A:H5''	2.13	0.48
1:AA:801:G:H2'	1:AA:802:C:C6	2.49	0.48
3:BA:151:G:OP1	9:BQ:66:ARG:NH2	2.42	0.48
3:BA:502:U:H2'	3:BA:503:A:C8	2.49	0.48
4:BB:534:A:H2'	4:BB:535:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:A7:149:GLY:O	84:A7:179:LYS:NZ	2.35	0.48
1:AA:1185:U:H3'	1:AA:1186:U:H5''	1.95	0.48
3:BA:1315:C:H5'	3:BA:1316:U:C5'	2.42	0.48
4:BB:640:G:H2'	4:BB:641:A:C8	2.48	0.48
75:BH:86:G:H8	75:BH:86:G:OP2	1.95	0.48
1:AA:220:G:OP2	29:A5:155:SER:OG	2.25	0.48
1:AA:771:C:N4	1:AA:779:C:H42	2.11	0.48
30:AD:7:LYS:HA	30:AD:7:LYS:HE3	1.95	0.48
32:AE:32:GLU:OE2	32:AE:32:GLU:N	2.23	0.48
34:AI:61:PRO:HA	34:AI:64:LEU:HD12	1.94	0.48
38:AM:14:VAL:N	38:AM:21:VAL:O	2.47	0.48
49:Bc:33:ASN:OD1	49:Bc:42:GLN:HB3	2.14	0.48
67:AK:113:ASP:OD1	67:AK:113:ASP:N	2.45	0.48
83:A4:10:LEU:HD12	83:A4:11:ARG:H	1.77	0.48
83:A4:145:TRP:NE1	83:A4:155:MET:HG3	2.29	0.48
1:AA:608:C:O2'	1:AA:609:A:H8	1.96	0.48
1:AA:802:C:H2'	1:AA:803:C:H6	1.78	0.48
1:AA:1145:G:H2'	1:AA:1146:U:C6	2.49	0.48
2:AB:5:G:H2'	2:AB:6:G:C8	2.49	0.48
3:BA:1172:A:N3	4:BB:1076:PSU:O2'	2.46	0.48
3:BA:1643:U:H5''	10:BR:42:ARG:HG3	1.95	0.48
13:BU:33:ASN:O	13:BU:98:LYS:NZ	2.42	0.48
45:A3:43:GLY:O	45:A3:44:GLU:HG3	2.13	0.48
1:AA:693:A:O2'	1:AA:694:A:H5'	2.13	0.48
1:AA:1565:A:H2'	1:AA:1566:C:C6	2.49	0.48
54:Bk:123:TYR:O	62:BN:129:VAL:HG13	2.13	0.48
3:BA:69:A:O2'	3:BA:383:C:O2	2.32	0.47
16:BX:62:ARG:HH11	16:BX:62:ARG:HG3	1.78	0.47
19:Bq:28:ARG:NH2	19:Bq:36:LYS:O	2.47	0.47
69:Bf:109:HIS:HB2	69:Bf:205:GLU:CD	2.39	0.47
84:A7:234:MET:HE1	84:A7:263:PHE:CG	2.49	0.47
1:AA:122:C:H1'	1:AA:519:G:H5''	1.96	0.47
1:AA:607:U:O2'	1:AA:608:C:H5'	2.14	0.47
1:AA:1994:C:O2'	39:AO:50:CYS:SG	2.68	0.47
3:BA:505:C:P	24:Bl:88:LYS:NZ	2.87	0.47
3:BA:1193:C:H2'	3:BA:1194:C:H6	1.78	0.47
3:BA:1837:G:H2'	3:BA:1839:A:N7	2.30	0.47
3:BA:1863:G:H2'	3:BA:1864:U:C6	2.48	0.47
4:BB:1471:U:H4'	4:BB:1472:C:H5'	1.96	0.47
7:BE:104:U:H2'	7:BE:105:C:C6	2.49	0.47
11:BS:85:GLN:O	11:BS:86:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AS:24:ASP:OD1	41:AS:24:ASP:N	2.33	0.47
71:Bv:101:GLU:HA	71:Bv:104:LYS:HB3	1.95	0.47
79:AQ:18:LEU:HD22	79:AQ:85:LEU:HD11	1.96	0.47
1:AA:318:G:H2'	1:AA:319:G:C8	2.49	0.47
3:BA:97:G:H2'	3:BA:98:A:C8	2.49	0.47
3:BA:1342:A:H2'	3:BA:1343:A:H8	1.78	0.47
13:BU:36:VAL:HA	13:BU:64:VAL:HG22	1.94	0.47
26:By:9:ILE:HG23	26:By:72:LEU:HD13	1.96	0.47
28:A2:181:GLU:OE2	28:A2:181:GLU:HA	2.14	0.47
35:AH:13:SER:O	35:AH:13:SER:OG	2.31	0.47
48:AC:123:ILE:O	48:AC:127:SER:OG	2.32	0.47
48:AC:167:HIS:HE1	48:AC:171:ARG:HH21	1.61	0.47
80:AR:3:THR:O	80:AR:3:THR:OG1	2.23	0.47
84:A7:95:ASN:ND2	84:A7:98:ASN:OD1	2.47	0.47
1:AA:181:C:O2'	1:AA:182:U:H5'	2.14	0.47
1:AA:274:C:H2'	1:AA:275:G:H8	1.80	0.47
1:AA:1029:G:H2'	1:AA:1030:G:H8	1.77	0.47
6:BD:51:G:HO2'	6:BD:52:U:P	2.36	0.47
39:AO:98:SER:OG	39:AO:99:LYS:N	2.46	0.47
43:AX:6:LYS:O	43:AX:10:MET:HG2	2.15	0.47
45:A3:227:LYS:HB2	45:A3:227:LYS:NZ	2.28	0.47
51:Bo:52:VAL:HG23	51:Bo:68:ALA:HA	1.95	0.47
83:A4:83:LEU:HD12	83:A4:98:LEU:HD11	1.96	0.47
1:AA:1574:G:N1	1:AA:2070:7MG:OP2	2.41	0.47
1:AA:1762:A:O2'	1:AA:1763:U:H5'	2.13	0.47
39:AO:99:LYS:HG2	39:AO:107:GLU:HB3	1.95	0.47
47:A1:261:ARG:HE	47:A1:261:ARG:C	2.22	0.47
83:A4:6:HIS:HA	83:A4:30:PHE:CD1	2.48	0.47
1:AA:1986:C:H2'	1:AA:1987:G:H8	1.79	0.47
3:BA:615:G:H1'	3:BA:619[A]:C:N4	2.30	0.47
3:BA:1234:A:C2'	3:BA:1235:U:H5'	2.44	0.47
11:BS:168:PHE:HB2	11:BS:178:VAL:HB	1.96	0.47
15:BY:39:LYS:NZ	75:BH:41:A:OP2	2.47	0.47
23:Bx:225:LYS:HB3	23:Bx:225:LYS:HE3	1.68	0.47
29:A5:172:GLU:OE1	29:A5:172:GLU:N	2.42	0.47
35:AH:99:LYS:HE3	35:AH:128:VAL:HG22	1.95	0.47
38:AM:55:ARG:NH2	38:AM:59:THR:OG1	2.48	0.47
40:AP:88:ASP:C	40:AP:88:ASP:OD2	2.58	0.47
60:Ba:65:SER:O	60:Ba:116:GLN:NE2	2.43	0.47
66:Be:80:GLU:HG3	66:Be:170:ALA:HA	1.97	0.47
71:Bv:63:SER:HB2	71:Bv:73:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Bh:37:ARG:HA	72:Bh:40:ARG:HD3	1.97	0.47
1:AA:96:A:H5''	1:AA:97:C:H5''	1.97	0.47
1:AA:363:G:O2'	1:AA:364:C:O2	2.19	0.47
1:AA:1004:G:H2'	1:AA:1005:U:C6	2.49	0.47
1:AA:1140:G:H5'	82:AW:22:ARG:HH12	1.78	0.47
3:BA:681:U:O2'	3:BA:682:C:O5'	2.31	0.47
3:BA:896:G:H5''	58:Bd:38:LEU:HD21	1.97	0.47
3:BA:1023:U:H2'	3:BA:1024:A2M:H8	1.96	0.47
3:BA:1193:C:H2'	3:BA:1194:C:C6	2.50	0.47
3:BA:1337:G:H8	3:BA:1337:G:OP1	1.97	0.47
4:BB:367:C:HO2'	4:BB:368:U:H6	1.62	0.47
7:BE:96:C:O2'	7:BE:97:U:OP1	2.31	0.47
12:BT:92:LYS:O	12:BT:96:MET:HG3	2.15	0.47
26:By:107:LEU:HD21	26:By:121:ARG:HG2	1.97	0.47
34:AI:48:ALA:O	34:AI:52:MET:HG3	2.15	0.47
39:AO:23:LEU:HD23	39:AO:82:TYR:CD1	2.50	0.47
46:AT:55:LYS:HA	46:AT:55:LYS:HE3	1.96	0.47
47:A1:57:GLU:O	47:A1:61:ILE:HD12	2.15	0.47
47:A1:91:LYS:HB2	47:A1:91:LYS:HE3	1.71	0.47
63:BL:78:VAL:HG13	63:BL:82:LYS:HE2	1.95	0.47
76:Bs:112:LYS:HA	76:Bs:112:LYS:HD2	1.75	0.47
1:AA:547:A:H2'	1:AA:548:A:C8	2.50	0.47
3:BA:375:U:H2'	3:BA:376:U:C6	2.50	0.47
3:BA:876:C:H42	3:BA:903:G:H21	1.62	0.47
3:BA:957:A:OP2	51:Bo:4:ARG:NH1	2.42	0.47
3:BA:1481:U:H2'	3:BA:1482:A:H8	1.79	0.47
19:Bq:5:LYS:HE3	19:Bq:5:LYS:HB3	1.43	0.47
29:A5:83:TYR:CZ	29:A5:214:LYS:HD3	2.49	0.47
46:AT:34:HIS:HB2	46:AT:37:TRP:HB2	1.96	0.47
47:A1:133:ILE:HG21	47:A1:145:ARG:NE	2.29	0.47
64:BK:150:GLU:OE2	64:BK:154:ARG:NH1	2.48	0.47
84:A7:240:ILE:HG21	84:A7:243:ILE:HG23	1.96	0.47
3:BA:229:G:H5''	49:Bc:127:ARG:HD2	1.96	0.47
4:BB:991:C:H6	23:Bx:43:ARG:H	1.61	0.47
26:By:151:GLN:O	26:By:155:GLU:HG2	2.14	0.47
27:A0:133:ASP:OD2	27:A0:183:ILE:N	2.44	0.47
38:AM:135:GLN:HA	85:A:136:HIS:N	2.30	0.47
39:AO:49:ASN:OD1	39:AO:49:ASN:N	2.38	0.47
62:BN:175:ARG:NH2	62:BN:181:GLU:OE1	2.46	0.47
68:A6:122:HIS:CE1	70:AY:37:ARG:HD2	2.50	0.47
73:BF:66:U:H4'	73:BF:67:U:H3'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:157:U:H2'	1:AA:158:G:C8	2.50	0.47
4:BB:101:G:OP1	12:BT:85:ARG:NH2	2.48	0.47
4:BB:473:U:H2'	4:BB:474:G:C8	2.50	0.47
4:BB:799:G:O2'	4:BB:800:U:H6	1.98	0.47
7:BE:43:U:O2'	7:BE:44:C:O5'	2.32	0.47
47:A1:163:GLU:OE1	47:A1:165:LYS:HG2	2.15	0.47
84:A7:221:ARG:HB3	84:A7:223:TRP:HE1	1.79	0.47
1:AA:1216:A:H2'	1:AA:1217:A:C8	2.49	0.46
1:AA:1714:G:H1'	1:AA:1863:U:C4	2.50	0.46
1:AA:1745:G:H2'	1:AA:1746:C:C6	2.50	0.46
1:AA:2271:G:O2'	50:Bz:3:THR:HG23	2.13	0.46
28:A2:168:LYS:HE2	28:A2:168:LYS:HB2	1.60	0.46
29:A5:110:ARG:NH1	29:A5:179:LEU:O	2.48	0.46
47:A1:16:MET:HE1	47:A1:105:ARG:HD2	1.97	0.46
1:AA:1726:A:H4'	1:AA:1727:A:O5'	2.15	0.46
3:BA:478:A:C2	5:BC:16:A:H1'	2.49	0.46
3:BA:681:U:O2'	3:BA:682:C:H6	1.98	0.46
3:BA:765:A:H2'	3:BA:766:G:C8	2.49	0.46
4:BB:360:U:H2'	4:BB:361:U:C6	2.50	0.46
4:BB:1531:G:C2	4:BB:1532:G:C5	3.03	0.46
14:BW:18:ALA:HB2	14:BW:85:LYS:HB3	1.98	0.46
32:AE:133:PRO:HB3	32:AE:158:VAL:HG21	1.96	0.46
44:AZ:98:GLU:HA	44:AZ:98:GLU:OE2	2.14	0.46
68:A6:129:GLN:HG3	68:A6:130:GLN:HG3	1.96	0.46
1:AA:57:OMU:HM21	41:AS:123:VAL:HG11	1.98	0.46
3:BA:1191:A:H2'	3:BA:1192:C:C6	2.50	0.46
4:BB:974:C:O4'	4:BB:976:G:N2	2.49	0.46
18:Bp:55:LYS:HD3	18:Bp:55:LYS:HA	1.73	0.46
34:AI:95:GLU:H	34:AI:95:GLU:CD	2.23	0.46
45:A3:38:ASP:C	45:A3:38:ASP:OD2	2.58	0.46
45:A3:132:VAL:HG22	45:A3:133:PRO:HD2	1.98	0.46
47:A1:84:MET:HE2	47:A1:84:MET:HB2	1.72	0.46
51:Bo:56:ARG:HG3	51:Bo:56:ARG:HH11	1.79	0.46
68:A6:31:GLY:HA3	70:AY:40:TYR:CG	2.50	0.46
84:A7:249:ARG:HH22	84:A7:314:VAL:HG21	1.80	0.46
1:AA:273:A:H2'	1:AA:274:C:C6	2.50	0.46
1:AA:616:G:H1	1:AA:631:U:H3	1.63	0.46
1:AA:1696:G:C8	1:AA:1697:G:C8	3.03	0.46
1:AA:1853:A:H62	1:AA:1876:G:H21	1.64	0.46
20:Br:147:ALA:HB2	49:Bc:74:LYS:HE2	1.98	0.46
21:Bt:17:CYS:HB3	21:Bt:76:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A2:65:LYS:HD3	28:A2:65:LYS:HA	1.83	0.46
36:AJ:47:ILE:HG13	36:AJ:48:GLY:H	1.80	0.46
41:AS:6:GLY:O	41:AS:7:GLN:HB3	2.15	0.46
48:AC:57:MET:HE2	48:AC:205:HIS:CB	2.46	0.46
48:AC:232:GLU:H	48:AC:232:GLU:CD	2.19	0.46
71:Bv:105:ARG:NH2	71:Bv:106:GLU:O	2.49	0.46
1:AA:354:C:H5'	1:AA:356:U:O4	2.15	0.46
4:BB:1414:C:H2'	4:BB:1415:G:C8	2.51	0.46
25:Bu:55:ILE:HG21	25:Bu:164:ARG:HH21	1.81	0.46
38:AM:26:LYS:HE2	38:AM:54:GLU:HA	1.98	0.46
38:AM:87:ARG:HG3	38:AM:99:LEU:HD13	1.97	0.46
40:AP:172:CYS:O	40:AP:219:ASN:ND2	2.44	0.46
48:AC:204:ARG:NH2	48:AC:240:TYR:O	2.33	0.46
68:A6:69:LEU:O	68:A6:73:SER:OG	2.31	0.46
84:A7:233:GLU:OE2	84:A7:234:MET:N	2.49	0.46
1:AA:1776:A:H2'	1:AA:1777:C:C6	2.50	0.46
3:BA:863:U:H2'	3:BA:864:G:C8	2.50	0.46
4:BB:477:A:H2'	4:BB:478:A:H8	1.81	0.46
4:BB:1488:C:H2'	4:BB:1489:A:C8	2.50	0.46
9:BQ:145:LEU:HD22	9:BQ:147:TYR:CE2	2.51	0.46
20:Br:158:ARG:HD2	20:Br:210:MET:SD	2.56	0.46
21:Bt:28:TYR:HD1	21:Bt:71:LYS:HE2	1.80	0.46
45:A3:8:PRO:C	45:A3:10:ASN:H	2.24	0.46
45:A3:20:ASP:OD2	45:A3:21:GLU:N	2.48	0.46
45:A3:95:ARG:HE	45:A3:95:ARG:HB2	1.56	0.46
68:A6:37:CYS:O	68:A6:40:GLU:HG3	2.16	0.46
83:A4:43:LEU:HD23	83:A4:43:LEU:HA	1.75	0.46
84:A7:66:HIS:H	84:A7:92:ARG:NH1	2.13	0.46
1:AA:1303:A:H61	50:Bz:3:THR:HG22	1.80	0.46
3:BA:1608:OMC:H1'	3:BA:1608:OMC:HM23	1.69	0.46
4:BB:1514:U:C2	4:BB:1534:G:N1	2.80	0.46
22:Bw:246:ASP:OD1	22:Bw:247:THR:N	2.46	0.46
25:Bu:194:ASP:N	25:Bu:194:ASP:OD1	2.48	0.46
40:AP:131:VAL:O	40:AP:135:ILE:HG12	2.16	0.46
47:A1:120:MET:HE2	47:A1:120:MET:HB3	1.75	0.46
68:A6:91:LYS:O	68:A6:92:LEU:HB3	2.16	0.46
74:BG:178:G:H2'	74:BG:179:C:C6	2.51	0.46
1:AA:539:A:OP1	47:A1:56:LEU:HD23	2.15	0.46
1:AA:793:U:P	1:AA:793:U:O4'	2.74	0.46
1:AA:803:C:H2'	1:AA:804:C:C6	2.51	0.46
1:AA:2086:C:H2'	1:AA:2087:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BA:210:G:N2	3:BA:239:A:C6	2.84	0.46
3:BA:729:C:O2	24:Bl:54:GLN:NE2	2.43	0.46
4:BB:1105:A:H2'	4:BB:1106:G:H8	1.81	0.46
4:BB:1490:G:H2'	4:BB:1491:U:C6	2.51	0.46
4:BB:1521:G:H2'	4:BB:1522:C:C6	2.51	0.46
5:BC:71:A:N6	5:BC:86:U:H3	2.06	0.46
37:AL:104:GLN:HE22	48:AC:78:THR:HA	1.81	0.46
38:AM:40:ARG:O	38:AM:40:ARG:HG3	2.16	0.46
38:AM:52:ASP:OD2	38:AM:53:VAL:N	2.49	0.46
39:AO:127:LEU:HD12	39:AO:127:LEU:HA	1.81	0.46
43:AX:153:ASP:OD2	43:AX:154:GLY:N	2.47	0.46
43:AX:163:HIS:O	43:AX:167:VAL:HG12	2.16	0.46
60:Ba:5:LYS:HE2	60:Ba:5:LYS:HB3	1.79	0.46
1:AA:1697:G:H2'	1:AA:1698:U:C6	2.50	0.46
3:BA:562:G:H2'	3:BA:563:G:C8	2.51	0.46
4:BB:1516:G:P	72:Bh:36:ARG:HH12	2.39	0.46
27:A0:33:VAL:O	27:A0:100:THR:OG1	2.28	0.46
36:AJ:121:THR:OG1	36:AJ:122:GLY:N	2.43	0.46
37:AL:70:SER:O	37:AL:70:SER:OG	2.29	0.46
38:AM:39:ILE:O	38:AM:40:ARG:HB3	2.16	0.46
64:BK:30:ARG:HB3	64:BK:30:ARG:CZ	2.46	0.46
64:BK:66:GLU:HA	64:BK:66:GLU:OE2	2.15	0.46
67:AK:45:ILE:HG22	67:AK:47:PRO:HD2	1.97	0.46
1:AA:1607:A:N6	1:AA:1924:G:OP1	2.45	0.46
1:AA:1638:G:H1	1:AA:1657:C:H5	1.64	0.46
1:AA:1946:U:OP1	39:AO:73:ARG:NH1	2.49	0.46
1:AA:2136:C:H5''	50:Bz:9:GLY:HA2	1.98	0.46
1:AA:2163:A:H2'	1:AA:2164:C:O4'	2.16	0.46
3:BA:895:G:C2'	3:BA:896:G:H5'	2.46	0.46
3:BA:1685:C:H2'	3:BA:1686:G:C8	2.51	0.46
4:BB:1335:C:H2'	4:BB:1336:U:C6	2.51	0.46
68:A6:137:LYS:HA	68:A6:137:LYS:HE3	1.98	0.46
1:AA:982:G:H1	1:AA:1012:A:H61	1.64	0.45
3:BA:178:U:H3'	3:BA:179:A:H5''	1.98	0.45
3:BA:1088:G:H2'	3:BA:1089:C:C6	2.51	0.45
3:BA:1261:G:OP2	64:BK:98:ARG:NH1	2.49	0.45
25:Bu:132:VAL:HG21	25:Bu:178:ALA:HA	1.97	0.45
25:Bu:263:ARG:HH11	25:Bu:263:ARG:C	2.24	0.45
71:Bv:169:LYS:HE2	71:Bv:169:LYS:HB2	1.75	0.45
84:A7:50:HIS:ND1	84:A7:54:CYS:SG	2.87	0.45
1:AA:799:A:H2'	1:AA:799:A:N3	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BB:767:G:H2'	4:BB:768:U:C6	2.51	0.45
4:BB:811:A:H2'	4:BB:812:G:C8	2.51	0.45
5:BC:146:U:H4'	16:BX:69:SER:O	2.16	0.45
84:A7:46:ASN:ND2	84:A7:55:SER:O	2.42	0.45
1:AA:306:C:H4'	1:AA:322:G:H22	1.80	0.45
1:AA:331:A:H62	1:AA:871:U:H4'	1.81	0.45
1:AA:827:G:O2'	1:AA:828:A:N3	2.35	0.45
1:AA:1984:C:H41	1:AA:2005:G:H1	1.64	0.45
1:AA:2029:C:OP2	42:AU:44:ASN:ND2	2.50	0.45
1:AA:2096:A2M:H5''	1:AA:2096:A2M:H8	1.98	0.45
4:BB:8:U:H5''	18:Bp:19:ASP:OD2	2.16	0.45
5:BC:157:U:H3'	5:BC:158:U:C5	2.51	0.45
28:A2:84:GLU:H	28:A2:84:GLU:CD	2.20	0.45
43:AX:141:ILE:HG22	43:AX:142:LYS:HE2	1.98	0.45
47:A1:172:ILE:HD12	47:A1:172:ILE:HA	1.88	0.45
64:BK:78:LYS:HE3	64:BK:78:LYS:HB2	1.72	0.45
1:AA:221:C:H1'	29:A5:155:SER:HA	1.99	0.45
1:AA:483:G:H1	1:AA:500:A:H61	1.63	0.45
1:AA:770:U:H2'	1:AA:771:C:C6	2.51	0.45
3:BA:1191:A:H2'	3:BA:1192:C:H6	1.81	0.45
4:BB:1531:G:H2'	4:BB:1532:G:C8	2.51	0.45
14:BW:15:VAL:HG22	14:BW:55:ALA:HB1	1.99	0.45
32:AE:32:GLU:H	32:AE:32:GLU:CD	2.15	0.45
64:BK:175:ASN:OD1	64:BK:175:ASN:N	2.42	0.45
78:Az:175:GLU:O	78:Az:175:GLU:HG2	2.14	0.45
83:A4:87:LEU:HD12	83:A4:96:VAL:HG11	1.97	0.45
84:A7:257:GLU:HA	84:A7:287:GLU:HG2	1.98	0.45
1:AA:571:A:H3'	1:AA:572:A:H8	1.80	0.45
1:AA:889:G:H2'	1:AA:890:U:H5''	1.98	0.45
1:AA:962:A:H2	1:AA:963:A:C8	2.34	0.45
3:BA:456:A:H2'	3:BA:457:A:C8	2.52	0.45
3:BA:1037:A:H4'	4:BB:401:U:H4'	1.98	0.45
4:BB:670:C:H2'	4:BB:671:C:C6	2.51	0.45
25:Bu:50:ARG:NH1	25:Bu:153:ASP:OD2	2.49	0.45
45:A3:14:LYS:HA	45:A3:14:LYS:HD3	1.60	0.45
54:Bk:126:LYS:HA	62:BN:127:LYS:HG3	1.97	0.45
60:Ba:2:LYS:HB3	60:Ba:2:LYS:HE3	1.79	0.45
65:BI:38:LYS:HG3	65:BI:39:ARG:HG2	1.99	0.45
66:Be:28:LYS:HA	66:Be:28:LYS:HD2	1.82	0.45
66:Be:117:GLU:HG2	66:Be:124:GLY:H	1.81	0.45
71:Bv:75:ARG:NH2	73:BF:69:U:OP2	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:BV:49:GLN:OE1	77:BV:49:GLN:HA	2.15	0.45
1:AA:173:C:O2'	1:AA:174:U:OP1	2.29	0.45
1:AA:384:U:H2'	1:AA:385:C:O2	2.16	0.45
1:AA:767:C:H2'	1:AA:768:A:C8	2.51	0.45
3:BA:1652:U:C5	10:BR:46:GLN:HG3	2.51	0.45
4:BB:1139:A:H2'	4:BB:1140:A:C8	2.52	0.45
10:BR:116:HIS:O	10:BR:148:LEU:HA	2.16	0.45
38:AM:7:SER:C	38:AM:9:SER:H	2.25	0.45
41:AS:124:LYS:HD2	41:AS:127:SER:HA	1.97	0.45
48:AC:227:ARG:HH11	80:AR:48:GLY:HA3	1.80	0.45
54:Bk:38:MET:H	54:Bk:38:MET:HG2	1.58	0.45
62:BN:145:GLU:OE2	62:BN:149:LYS:NZ	2.49	0.45
67:AK:112:LYS:O	67:AK:116:LEU:HD12	2.17	0.45
75:BH:29:G:H2'	75:BH:30:C:C6	2.52	0.45
1:AA:427:A:N7	29:A5:49:ARG:HD2	2.32	0.45
1:AA:584:C:H2'	1:AA:585:G:C8	2.52	0.45
1:AA:771:C:H2'	1:AA:772:C:O4'	2.17	0.45
1:AA:1468:C:H2'	1:AA:1469:G:H8	1.82	0.45
1:AA:1639:A:H4'	1:AA:1640:C:OP1	2.16	0.45
3:BA:954:U:H2'	3:BA:955:G:O4'	2.16	0.45
3:BA:1314:A:H4'	3:BA:1315:C:OP2	2.17	0.45
18:Bp:52:LYS:O	18:Bp:52:LYS:HG2	2.17	0.45
34:AI:123:LEU:HD12	34:AI:123:LEU:HA	1.81	0.45
74:BG:149:U:H5	74:BG:151:A:N7	2.15	0.45
83:A4:87:LEU:HB3	83:A4:96:VAL:HG21	1.98	0.45
84:A7:50:HIS:CD2	84:A7:50:HIS:N	2.83	0.45
1:AA:631:U:H2'	1:AA:632:C:C5	2.52	0.45
1:AA:756:U:N3	1:AA:757:G:N7	2.65	0.45
1:AA:1644:U:H4'	1:AA:1644:U:OP1	2.17	0.45
1:AA:1853:A:H1'	1:AA:1854:U:OP2	2.17	0.45
3:BA:727:C:H2'	3:BA:728:C:C6	2.52	0.45
3:BA:762:A2M:N1	3:BA:917:U:H5	2.14	0.45
4:BB:1532:G:C2	4:BB:1533:C:C5	3.05	0.45
5:BC:6:G:H2'	5:BC:7:OMU:H6	1.98	0.45
16:BX:62:ARG:HG3	16:BX:62:ARG:NH1	2.32	0.45
40:AP:90:MET:HE3	40:AP:90:MET:HA	1.99	0.45
72:Bh:31:LYS:O	72:Bh:33:ARG:NE	2.41	0.45
74:BG:17:A:H2'	74:BG:18:U:C6	2.51	0.45
74:BG:19:C:H2'	74:BG:20:U:C6	2.52	0.45
1:AA:1652:OMU:HM23	1:AA:1652:OMU:H1'	1.62	0.45
1:AA:2167:G:H2'	1:AA:2168:U:H6	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BA:1815:A:H2'	3:BA:1816:A:C8	2.52	0.45
4:BB:683:A:H2'	4:BB:684:C:C6	2.51	0.45
4:BB:707:A:H2'	4:BB:708:C:C6	2.52	0.45
4:BB:1490:G:H2'	4:BB:1491:U:H6	1.82	0.45
64:BK:115:MET:HE3	64:BK:115:MET:HB3	1.81	0.45
68:A6:15:ARG:HE	68:A6:15:ARG:HB3	1.61	0.45
74:BG:149:U:H1'	74:BG:150:A:H5''	1.98	0.45
80:AR:85:ILE:HD11	82:AW:4:PHE:CD1	2.52	0.45
1:AA:489:G:H5'	1:AA:490:A:OP2	2.17	0.45
1:AA:768:A:H61	1:AA:782:C:H42	1.64	0.45
1:AA:2110:C:OP1	44:AZ:49:ARG:NH2	2.49	0.45
1:AA:2234:A:OP1	41:AS:61:GLN:NE2	2.50	0.45
3:BA:1024:A2M:HM'3	3:BA:1024:A2M:H1'	1.73	0.45
4:BB:1350:C:P	76:Bs:102:ARG:HH21	2.40	0.45
40:AP:205:ASP:OD2	40:AP:205:ASP:C	2.60	0.45
66:Be:247:ARG:HA	66:Be:247:ARG:HD3	1.82	0.45
68:A6:28:LYS:HG3	70:AY:44:TYR:CE2	2.52	0.45
84:A7:34:THR:HG22	84:A7:40:LEU:HG	1.98	0.45
1:AA:528:C:H5''	41:AS:48:LYS:HE3	1.99	0.44
1:AA:877:A:H2'	1:AA:878:U:C6	2.52	0.44
3:BA:189:C:H5	3:BA:309:G:H1	1.65	0.44
3:BA:1065:A:H2'	3:BA:1066:C:C6	2.53	0.44
3:BA:1134:A:H2'	3:BA:1135:G:C8	2.51	0.44
3:BA:1181:OMU:O5'	3:BA:1181:OMU:H6	2.17	0.44
4:BB:997:G:N2	4:BB:1014:U:H3	2.13	0.44
21:Bt:96:LYS:HD3	21:Bt:96:LYS:HA	1.70	0.44
38:AM:26:LYS:HA	38:AM:26:LYS:HD2	1.82	0.44
39:AO:157:LEU:HD23	39:AO:157:LEU:HA	1.87	0.44
40:AP:116:ASP:OD1	40:AP:116:ASP:C	2.61	0.44
51:Bo:67:GLY:O	51:Bo:69:TYR:N	2.49	0.44
51:Bo:87:ARG:HD3	66:Be:96:LEU:O	2.17	0.44
67:AK:100:GLN:NE2	84:A7:64:GLU:OE1	2.50	0.44
1:AA:770:U:H2'	1:AA:771:C:H6	1.82	0.44
1:AA:908:A:C6	1:AA:909:C:C4	3.05	0.44
1:AA:1007:U:O2'	1:AA:1008:U:H5''	2.17	0.44
3:BA:652:U:H1'	22:Bw:87:HIS:HD2	1.82	0.44
32:AE:118:LYS:O	41:AS:11:ARG:NH2	2.46	0.44
45:A3:30:ASP:OD1	45:A3:30:ASP:N	2.32	0.44
63:BL:102:ASN:HD22	63:BL:102:ASN:HA	1.60	0.44
64:BK:76:MET:HE2	64:BK:138:MET:SD	2.58	0.44
64:BK:145:VAL:N	64:BK:146:PRO:HD2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:BH:56:C:H2'	75:BH:57:A:C8	2.53	0.44
1:AA:398:A:H2'	1:AA:399:C:H5	1.83	0.44
1:AA:474:C:OP1	47:A1:7:LYS:HE2	2.17	0.44
1:AA:953:G:C2	1:AA:954:C:C4	3.05	0.44
1:AA:1630:U:O2	1:AA:1635:A:O2'	2.27	0.44
1:AA:1947:G:H2'	1:AA:1948:A:C8	2.53	0.44
3:BA:508:C:H2'	3:BA:509:A:C8	2.52	0.44
3:BA:619[B]:C:O2	3:BA:619[B]:C:H2'	2.17	0.44
4:BB:985:C:H3'	4:BB:986:G:H21	1.81	0.44
4:BB:1512:C:H2'	4:BB:1513:G:C8	2.53	0.44
40:AP:188:ILE:HG23	40:AP:206:VAL:HG12	1.99	0.44
47:A1:104:GLY:O	47:A1:186:ARG:NH2	2.42	0.44
59:Bb:84:LYS:HD2	59:Bb:84:LYS:HA	1.76	0.44
61:BO:206:LYS:HB2	61:BO:206:LYS:HE3	1.72	0.44
67:AK:14:THR:HG21	67:AK:94:GLY:HA2	1.99	0.44
83:A4:135:ILE:HD12	83:A4:135:ILE:O	2.17	0.44
83:A4:155:MET:HE2	83:A4:186:VAL:HG23	1.99	0.44
1:AA:132:C:H2'	1:AA:133:A:H8	1.83	0.44
1:AA:320:C:H1'	1:AA:321:A:C2	2.52	0.44
1:AA:669:A:P	70:AY:10:ARG:HH21	2.41	0.44
1:AA:1595:C:H4'	1:AA:1596:B8N:P	2.58	0.44
1:AA:2001:G:H3'	1:AA:2002:C:H5''	1.99	0.44
3:BA:509:A:H2'	3:BA:510:U:H6	1.82	0.44
3:BA:1088:G:H2'	3:BA:1089:C:H6	1.82	0.44
4:BB:1514:U:N3	4:BB:1534:G:N1	2.56	0.44
6:BD:52:U:O2'	6:BD:54:A:N7	2.51	0.44
8:BP:39:GLU:HG3	8:BP:40:ASN:N	2.32	0.44
27:A0:29:TRP:HE1	35:AH:11:GLY:HA2	1.83	0.44
64:BK:179:ASN:OD1	64:BK:179:ASN:N	2.42	0.44
69:Bf:215:GLN:HB2	69:Bf:218:GLU:HG3	1.99	0.44
80:AR:4:ILE:HG23	80:AR:18:ILE:HG12	1.99	0.44
1:AA:224:U:H2'	1:AA:225:C:C6	2.52	0.44
3:BA:7:A:O2'	3:BA:8:G:H8	1.98	0.44
3:BA:682:C:H2'	3:BA:683:C:H6	1.83	0.44
4:BB:362:G:H2'	4:BB:363:C:C6	2.52	0.44
30:AD:5:VAL:HB	30:AD:6:PRO:HD3	1.99	0.44
31:A8:10:ARG:HD3	31:A8:13:ILE:HD12	1.99	0.44
35:AH:56:LYS:HE2	35:AH:56:LYS:HB2	1.74	0.44
37:AL:5:ARG:O	37:AL:10:LYS:NZ	2.47	0.44
51:Bo:8:MET:HE3	51:Bo:12:GLY:HA2	1.98	0.44
71:Bv:145:ASP:O	71:Bv:149:GLN:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BA:759:U:H2'	3:BA:760:OMC:C6	2.53	0.44
3:BA:870:G:N2	3:BA:1096:U:H4'	2.32	0.44
3:BA:874:A:H5''	58:Bd:32:SER:HB3	2.00	0.44
4:BB:812:G:H1	4:BB:821:C:H41	1.66	0.44
6:BD:69:U:H2'	6:BD:70:C:C6	2.52	0.44
9:BQ:22:MET:HE2	9:BQ:22:MET:HB3	1.78	0.44
13:BU:128:LYS:HD3	13:BU:128:LYS:HA	1.70	0.44
29:A5:173:LYS:HA	29:A5:173:LYS:HD3	1.86	0.44
36:AJ:87:GLU:OE1	36:AJ:87:GLU:C	2.60	0.44
40:AP:118:ASN:N	40:AP:118:ASN:OD1	2.50	0.44
1:AA:352:U:H2'	1:AA:353:C:O2	2.18	0.44
1:AA:762:C:H3'	1:AA:763:G:H8	1.82	0.44
1:AA:2063:C:H5''	1:AA:2064:A:H5'	1.98	0.44
3:BA:400:G:OP2	52:Bn:58:ARG:NH2	2.38	0.44
3:BA:1192:C:H2'	3:BA:1193:C:C6	2.53	0.44
4:BB:361:U:H2'	4:BB:362:G:H8	1.83	0.44
4:BB:487:G:H2'	4:BB:488:A:C8	2.53	0.44
4:BB:1270:G:O4'	4:BB:1324:5MC:HM53	2.18	0.44
13:BU:79:PRO:HA	13:BU:84:THR:HA	2.00	0.44
34:AI:130:TYR:OH	38:AM:125:ARG:NH1	2.50	0.44
46:AT:42:PRO:HG2	46:AT:44:LYS:HZ2	1.83	0.44
71:Bv:53:GLN:HG3	71:Bv:60:LEU:HD23	1.99	0.44
79:AQ:108:ASP:C	79:AQ:108:ASP:OD2	2.61	0.44
83:A4:76:VAL:HA	83:A4:79:ILE:HG13	1.99	0.44
84:A7:264:ASP:O	84:A7:268:LYS:N	2.47	0.44
1:AA:586:U:O2	1:AA:599:G:N2	2.50	0.44
1:AA:1755:U:H2'	1:AA:1756:G:H5''	2.00	0.44
3:BA:1852:A:OP2	18:Bp:21:ARG:NH2	2.51	0.44
8:BP:105:SER:HB2	8:BP:110:ARG:HG3	2.00	0.44
21:Bt:9:LYS:HE2	21:Bt:9:LYS:HB3	1.86	0.44
22:Bw:65:LYS:HE3	22:Bw:65:LYS:HB3	1.74	0.44
28:A2:187:LYS:HE2	28:A2:187:LYS:HB2	1.74	0.44
41:AS:7:GLN:O	41:AS:7:GLN:HG3	2.17	0.44
44:AZ:78:ARG:HA	44:AZ:78:ARG:HD2	1.67	0.44
46:AT:28:PHE:CE2	46:AT:82:ILE:HG13	2.52	0.44
70:AY:37:ARG:O	70:AY:41:THR:HG23	2.17	0.44
71:Bv:65:PRO:HA	71:Bv:155:ASP:OD2	2.18	0.44
83:A4:43:LEU:N	83:A4:44:PRO:HD2	2.33	0.44
84:A7:122:ARG:NE	84:A7:122:ARG:HA	2.32	0.44
1:AA:1010:G:C4	1:AA:1011:A:C8	3.06	0.44
3:BA:501:G:H2'	3:BA:502:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BA:1683:U:H5	4:BB:18:A:N1	2.15	0.44
3:BA:1863:G:H2'	3:BA:1864:U:H6	1.81	0.44
4:BB:60:A:H5'	4:BB:61:C:OP1	2.17	0.44
4:BB:400:A2M:OP2	4:BB:400:A2M:H8	2.17	0.44
4:BB:837:C:N4	4:BB:970:C:H42	2.16	0.44
4:BB:1062:OMG:HM23	4:BB:1062:OMG:H1'	1.80	0.44
9:BQ:220:LYS:O	20:Br:113:LYS:HD2	2.17	0.44
20:Br:171:LYS:HB3	20:Br:171:LYS:HE2	1.81	0.44
29:A5:66:ALA:HA	29:A5:73:ALA:HA	2.00	0.44
29:A5:171:ILE:O	32:AE:8:TYR:N	2.51	0.44
30:AD:80:ILE:HA	30:AD:83:MET:HB2	2.00	0.44
40:AP:85:ASP:O	40:AP:116:ASP:HA	2.18	0.44
47:A1:36:ARG:HD3	47:A1:36:ARG:HA	1.75	0.44
52:Bn:39:TYR:CD1	52:Bn:40:PRO:HA	2.53	0.44
76:Bs:123:MET:HE3	76:Bs:123:MET:HB3	1.93	0.44
1:AA:623:A:H2'	1:AA:624:A:H8	1.83	0.43
1:AA:1123:C:N4	1:AA:1124:G:O6	2.50	0.43
1:AA:1651:U:H2'	1:AA:1652:OMU:H6	2.00	0.43
3:BA:484:U:H2'	3:BA:485:G:C8	2.52	0.43
4:BB:1132:G:H2'	4:BB:1132:G:N3	2.33	0.43
4:BB:1152:U:H2'	4:BB:1153:G:C8	2.53	0.43
8:BP:110:ARG:NH2	71:Bv:192:TRP:H	2.16	0.43
67:AK:36:ARG:HA	67:AK:41:PRO:HA	2.00	0.43
79:AQ:43:GLU:OE2	79:AQ:45:VAL:HG13	2.18	0.43
1:AA:133:A:H2'	1:AA:134:G:H8	1.82	0.43
1:AA:315:G:O2'	1:AA:316:G:H8	2.01	0.43
1:AA:796:C:H2'	1:AA:797:C:C6	2.53	0.43
1:AA:877:A:OP2	1:AA:877:A:H8	2.01	0.43
1:AA:953:G:C2	1:AA:954:C:N3	2.86	0.43
1:AA:2087:A:H2'	1:AA:2088:G:C8	2.53	0.43
3:BA:505:C:OP2	24:Bl:88:LYS:NZ	2.51	0.43
3:BA:913:C:H2'	3:BA:914:U:C6	2.53	0.43
4:BB:379:U:H4'	4:BB:380:A:O5'	2.18	0.43
4:BB:412:U:H2'	4:BB:413:A:C8	2.52	0.43
29:A5:161:LYS:HE3	29:A5:161:LYS:HB2	1.78	0.43
36:AJ:88:LYS:HE2	36:AJ:88:LYS:HB3	1.49	0.43
39:AO:25:ASP:C	39:AO:25:ASP:OD2	2.60	0.43
43:AX:22:GLU:OE2	43:AX:26:ARG:NE	2.39	0.43
43:AX:47:ILE:HB	43:AX:85:LEU:HD22	1.99	0.43
44:AZ:72:ALA:O	44:AZ:73:ASN:ND2	2.34	0.43
46:AT:119:ASN:HA	46:AT:122:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:A1:15:TRP:HE3	47:A1:17:LEU:HD11	1.82	0.43
48:AC:204:ARG:H	48:AC:204:ARG:HG3	1.51	0.43
61:BO:18:LYS:HE2	61:BO:18:LYS:HB2	1.91	0.43
74:BG:144:G:H21	74:BG:144:G:P	2.39	0.43
84:A7:50:HIS:CE1	84:A7:54:CYS:HG	2.36	0.43
84:A7:221:ARG:HB3	84:A7:223:TRP:NE1	2.33	0.43
1:AA:425:G:H5'	29:A5:33:PRO:HA	2.00	0.43
1:AA:2123:OMU:HM23	1:AA:2123:OMU:H1'	1.79	0.43
1:AA:2211:U:H2'	1:AA:2212:A:C8	2.53	0.43
3:BA:1614:PSU:H2'	3:BA:1615:G:C8	2.53	0.43
4:BB:79:C:O2'	74:BG:81:G:H4'	2.19	0.43
7:BE:108:G:H21	7:BE:125:G:H21	1.64	0.43
8:BP:53:LEU:HD23	8:BP:53:LEU:HA	1.88	0.43
20:Br:139:ARG:HD3	20:Br:245:GLY:O	2.18	0.43
38:AM:117:LYS:HE2	38:AM:117:LYS:HB2	1.74	0.43
41:AS:68:LYS:O	41:AS:85:VAL:HG22	2.18	0.43
44:AZ:93:MET:HB3	44:AZ:94:GLU:OE2	2.18	0.43
46:AT:111:ARG:O	46:AT:115:LYS:HG2	2.17	0.43
51:Bo:56:ARG:HG3	51:Bo:56:ARG:NH1	2.34	0.43
57:Bg:110:ASP:OD1	57:Bg:110:ASP:N	2.51	0.43
62:BN:206:ARG:HG3	62:BN:209:ARG:NH2	2.33	0.43
65:BI:3:VAL:HB	65:BI:5:LEU:HD13	2.00	0.43
68:A6:64:ASN:OD1	68:A6:64:ASN:C	2.61	0.43
69:Bf:346:ARG:HH12	69:Bf:349:MET:HG2	1.83	0.43
1:AA:501:C:H2'	1:AA:502:C:C6	2.52	0.43
1:AA:542:U:H2'	1:AA:543:C:C6	2.53	0.43
1:AA:607:U:O2'	1:AA:608:C:H6	2.00	0.43
1:AA:1013:G:H2'	1:AA:1014:U:H6	1.83	0.43
1:AA:1227:C:H2'	1:AA:1228:A:C8	2.52	0.43
3:BA:885:G:N2	3:BA:892:G:C6	2.85	0.43
4:BB:360:U:H2'	4:BB:361:U:H6	1.83	0.43
8:BP:152:LYS:HD3	8:BP:152:LYS:HA	1.90	0.43
34:AI:88:ARG:NH2	34:AI:127:SER:O	2.51	0.43
41:AS:67:ARG:HG3	41:AS:115:ILE:HG12	2.00	0.43
45:A3:129:ASP:OD1	45:A3:129:ASP:N	2.51	0.43
69:Bf:392:LYS:H	69:Bf:392:LYS:HG3	1.60	0.43
1:AA:500:A:H2'	1:AA:501:C:C6	2.54	0.43
1:AA:599:G:H2'	1:AA:600:G:N2	2.32	0.43
1:AA:947:U:O2'	1:AA:948:A:H5'	2.19	0.43
1:AA:1461:C:H6	27:A0:202:ARG:HH22	1.67	0.43
3:BA:1673:G:N2	55:Bj:5:ARG:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BA:1721:C:H2'	3:BA:1722:U:C6	2.54	0.43
4:BB:1103:C:OP1	4:BB:1194:C:O2'	2.35	0.43
6:BD:4:U:H2'	6:BD:5:A:H8	1.83	0.43
26:By:141:GLU:OE1	26:By:141:GLU:HA	2.18	0.43
28:A2:35:VAL:HG21	67:AK:49:THR:HG23	1.99	0.43
35:AH:136:LYS:HB3	35:AH:136:LYS:HE3	1.70	0.43
37:AL:3:LYS:HA	37:AL:3:LYS:HD2	1.74	0.43
46:AT:40:THR:HG22	46:AT:41:VAL:H	1.83	0.43
54:Bk:64:LYS:HB3	54:Bk:64:LYS:HE3	1.78	0.43
60:Ba:86:MET:HE3	60:Ba:118:ARG:HD3	2.00	0.43
61:BO:6:ARG:NH2	74:BG:181:C:N3	2.66	0.43
63:BL:97:GLU:OE2	63:BL:177:ILE:N	2.52	0.43
83:A4:80:GLN:O	83:A4:82:THR:N	2.48	0.43
84:A7:207:ASP:OD1	84:A7:208:GLY:N	2.51	0.43
1:AA:368:G:N3	1:AA:369:C:H1'	2.34	0.43
1:AA:829:U:H2'	1:AA:830:A:C8	2.54	0.43
1:AA:1835:A:H4'	1:AA:1836:G:H5'	2.01	0.43
2:AB:69:G:H2'	2:AB:70:G:O4'	2.19	0.43
3:BA:743:A2M:HM'3	3:BA:743:A2M:H1'	1.74	0.43
3:BA:840:G:N2	3:BA:874:A:H2	2.14	0.43
4:BB:1351:C:OP2	4:BB:1353:C:N4	2.49	0.43
4:BB:1523:A:N6	69:Bf:327:ASP:H	2.11	0.43
8:BP:6:TYR:HB2	73:BF:37:C:OP1	2.19	0.43
8:BP:141:LYS:HD3	8:BP:141:LYS:HA	1.85	0.43
22:Bw:100:VAL:HG13	22:Bw:131:PHE:CE1	2.53	0.43
25:Bu:99:TYR:HE2	25:Bu:170:LYS:HG3	1.83	0.43
38:AM:60:LEU:HD23	38:AM:60:LEU:HA	1.80	0.43
44:AZ:91:SER:O	44:AZ:91:SER:OG	2.32	0.43
46:AT:21:LYS:NZ	47:A1:92:THR:HG23	2.33	0.43
56:Bi:129:ARG:HE	56:Bi:129:ARG:HB3	1.69	0.43
78:Az:186:ARG:O	78:Az:186:ARG:NH1	2.38	0.43
1:AA:57:OMU:H1'	1:AA:57:OMU:HM23	1.54	0.43
3:BA:316:C:H2'	3:BA:317:U:C6	2.54	0.43
3:BA:556:U:H2'	3:BA:557:U:H6	1.84	0.43
3:BA:687:C:O2'	20:Br:348:ASN:OD1	2.27	0.43
3:BA:717:A:H2'	3:BA:718:A:C8	2.53	0.43
4:BB:991:C:H5''	4:BB:992:G:H21	1.83	0.43
6:BD:37:G:N2	6:BD:41:G:N3	2.67	0.43
12:BT:178:LEU:O	12:BT:179:LYS:HB3	2.17	0.43
26:By:91:ARG:HG3	26:By:180:GLN:HG3	2.00	0.43
26:By:171:ARG:HA	76:Bs:91:TRP:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:By:174:LEU:HB3	76:Bs:86:ALA:HB1	2.01	0.43
40:AP:151:ARG:HB3	40:AP:161:PRO:HB2	2.00	0.43
43:AX:145:ARG:HA	43:AX:145:ARG:HD2	1.82	0.43
46:AT:64:VAL:HB	46:AT:67:PHE:HE1	1.83	0.43
48:AC:125:LYS:NZ	48:AC:237:LEU:HD23	2.34	0.43
62:BN:134:ASN:OD1	62:BN:137:LYS:N	2.38	0.43
68:A6:28:LYS:HG3	70:AY:44:TYR:HE2	1.84	0.43
71:Bv:77:ASP:HB3	71:Bv:80:TYR:HD2	1.84	0.43
77:BV:93:LEU:HD12	77:BV:93:LEU:HA	1.83	0.43
1:AA:211:C:H2'	1:AA:212:A:O4'	2.19	0.43
1:AA:845:G:H1	47:A1:176:LYS:NZ	2.17	0.43
1:AA:2110:C:OP2	28:A2:46:ARG:NH1	2.52	0.43
3:BA:559:C:O2'	3:BA:560:G:OP1	2.30	0.43
3:BA:596:U:H5''	3:BA:597:U:O2	2.19	0.43
3:BA:804:C:H2'	3:BA:805:U:C6	2.53	0.43
5:BC:162:C:H2'	5:BC:163:A2M:H8	2.00	0.43
6:BD:2:G:C6	6:BD:118:C:N4	2.87	0.43
7:BE:62:U:H2'	7:BE:63:U:O2	2.19	0.43
33:AG:72:LEU:HD12	33:AG:72:LEU:HA	1.89	0.43
35:AH:75:VAL:HG22	35:AH:117:MET:HG3	2.01	0.43
39:AO:24:ARG:HA	39:AO:24:ARG:HD2	1.74	0.43
45:A3:59:LYS:HE2	45:A3:59:LYS:HB2	1.59	0.43
48:AC:86:ASP:OD1	48:AC:86:ASP:C	2.61	0.43
53:Bm:95:ARG:HE	53:Bm:95:ARG:HB3	1.64	0.43
62:BN:133:LEU:HD12	62:BN:133:LEU:HA	1.88	0.43
1:AA:188:A:H2'	1:AA:189:A:O4'	2.19	0.43
1:AA:319:G:O2'	1:AA:320:C:O2	2.31	0.43
1:AA:406:A:H4'	1:AA:407:U:O5'	2.18	0.43
1:AA:747:C:O2	1:AA:801:G:C6	2.72	0.43
1:AA:845:G:O6	47:A1:170:ILE:HA	2.19	0.43
1:AA:1236:C:H5''	33:AG:15:ALA:O	2.19	0.43
3:BA:728:C:H2'	3:BA:729:C:C6	2.54	0.43
3:BA:1835:U:P	55:Bj:9:ARG:HH22	2.42	0.43
4:BB:1302:G:OP1	76:Bs:100:TYR:OH	2.31	0.43
23:Bx:179:MET:HE2	23:Bx:179:MET:HB3	1.86	0.43
25:Bu:116:ALA:C	25:Bu:118:LYS:H	2.27	0.43
33:AG:35:ASP:C	33:AG:35:ASP:OD2	2.62	0.43
35:AH:39:ASP:OD2	35:AH:44:GLU:HB2	2.18	0.43
49:Bc:133:LYS:HE2	49:Bc:133:LYS:HB3	1.85	0.43
60:Ba:90:ARG:HD3	60:Ba:90:ARG:HA	1.83	0.43
80:AR:43:ASN:OD1	80:AR:53:THR:OG1	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:A4:103:LYS:HB3	83:A4:103:LYS:HE3	1.28	0.43
84:A7:192:LEU:HD13	84:A7:223:TRP:HE3	1.83	0.43
84:A7:261:ARG:HG2	84:A7:273:GLU:OE2	2.18	0.43
1:AA:314:C:H3'	1:AA:315:G:C8	2.54	0.43
1:AA:492:A:OP1	29:A5:49:ARG:NH2	2.52	0.43
1:AA:1639:A:OP2	1:AA:1650:G:O2'	2.32	0.43
1:AA:1655:U:O2'	1:AA:1656:U:H5'	2.18	0.43
3:BA:1253:C:H2'	3:BA:1254:U:C6	2.54	0.43
3:BA:1315:C:N4	11:BS:179:ALA:HB1	2.34	0.43
3:BA:1574:G:N2	3:BA:1577:A:OP2	2.36	0.43
12:BT:92:LYS:HG2	12:BT:96:MET:HE2	2.01	0.43
21:Bt:14:ASP:OD1	21:Bt:15:GLU:N	2.51	0.43
23:Bx:119:ARG:O	23:Bx:123:THR:OG1	2.34	0.43
29:A5:163:GLU:CD	29:A5:163:GLU:N	2.77	0.43
30:AD:52:LEU:HD23	30:AD:52:LEU:HA	1.86	0.43
33:AG:4:MET:CE	33:AG:121:ARG:HG3	2.49	0.43
39:AO:92:LEU:HB2	39:AO:117:LEU:HD13	2.00	0.43
46:AT:21:LYS:HE2	46:AT:21:LYS:HB2	1.85	0.43
55:Bj:18:GLY:HA2	55:Bj:38:LYS:HD3	2.00	0.43
64:BK:183:GLU:OE1	64:BK:183:GLU:HA	2.19	0.43
74:BG:16:G:H2'	74:BG:17:A:H8	1.82	0.43
74:BG:167:C:H2'	74:BG:168:A:O4'	2.18	0.43
77:BV:43:ILE:HA	77:BV:46:ASN:HD21	1.83	0.43
1:AA:957:G:H8	36:AJ:107:SER:HG	1.64	0.42
1:AA:1478:U:HO2'	1:AA:1479:U:P	2.42	0.42
1:AA:1998:A:O2'	1:AA:1999:G:N3	2.38	0.42
3:BA:1349:U:H2'	3:BA:1350:U:C6	2.53	0.42
4:BB:1498:U:O2'	24:Bl:13:ALA:HB2	2.18	0.42
6:BD:4:U:H2'	6:BD:5:A:C8	2.54	0.42
20:Br:298:ARG:HG3	20:Br:298:ARG:HH11	1.84	0.42
21:Bt:34:ARG:O	21:Bt:35:LEU:HB3	2.19	0.42
28:A2:140:MET:HA	28:A2:162:GLU:OE2	2.19	0.42
47:A1:153:ARG:NE	89:A1:301:HOH:O	2.42	0.42
47:A1:202:PHE:CD1	47:A1:202:PHE:N	2.87	0.42
47:A1:255:ILE:O	47:A1:259:THR:HG23	2.18	0.42
61:BO:43:LYS:HB2	61:BO:43:LYS:HE2	1.87	0.42
65:BI:114:LYS:HB2	65:BI:114:LYS:HE2	1.77	0.42
84:A7:9:LEU:HB2	84:A7:309:ILE:HB	2.01	0.42
1:AA:182:U:HO2'	1:AA:183:U:H6	1.67	0.42
1:AA:746:C:C2'	1:AA:747:C:H4'	2.49	0.42
1:AA:1145:G:H21	33:AG:52:MET:CE	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1948:A:H2'	1:AA:1949:G:O4'	2.19	0.42
4:BB:1480:A:H2'	4:BB:1481:G:O4'	2.19	0.42
13:BU:68:THR:HG22	13:BU:71:GLY:N	2.34	0.42
27:A0:207:ILE:HG23	27:A0:209:LEU:HG	2.00	0.42
56:Bi:80:VAL:HG13	56:Bi:112:LYS:HG2	2.01	0.42
68:A6:173:ARG:O	68:A6:177:ASN:ND2	2.44	0.42
84:A7:139:LYS:HE3	84:A7:139:LYS:HB3	1.77	0.42
1:AA:141:U:H2'	1:AA:142:C:C6	2.54	0.42
1:AA:220:G:H3'	1:AA:221:C:H4'	2.02	0.42
1:AA:359:G:O2'	1:AA:360:A:OP2	2.31	0.42
1:AA:628:C:C5	1:AA:629:A:C8	3.08	0.42
1:AA:2025:G:H2'	1:AA:2026:A:H8	1.83	0.42
1:AA:2032:U:C4	1:AA:2034:G:C8	3.07	0.42
3:BA:527:G:H1	56:Bi:3:LYS:HZ3	1.67	0.42
3:BA:681:U:HO2'	3:BA:682:C:C5'	2.33	0.42
3:BA:1188:A:H2	3:BA:1192:C:H1'	1.84	0.42
4:BB:1199:C:H42	13:BU:49:ARG:NH2	2.18	0.42
4:BB:1306:C:N3	64:BK:158:LYS:NZ	2.68	0.42
6:BD:3:G:H2'	6:BD:4:U:C6	2.55	0.42
28:A2:45:LYS:HG2	28:A2:48:ARG:NH2	2.33	0.42
43:AX:177:ARG:HH12	70:AY:63:GLY:HA2	1.83	0.42
48:AC:37:VAL:HG13	48:AC:40:GLY:HA2	2.01	0.42
63:BL:18:GLU:H	63:BL:18:GLU:CD	2.23	0.42
63:BL:48:CYS:SG	63:BL:50:GLN:HB3	2.58	0.42
71:Bv:171:MET:HE2	71:Bv:171:MET:HB3	1.80	0.42
80:AR:8:ASN:HB3	80:AR:9:GLU:OE2	2.19	0.42
83:A4:65:ILE:HA	83:A4:97:VAL:HG22	2.01	0.42
1:AA:96:A:OP1	45:A3:163:ARG:NH2	2.47	0.42
1:AA:601:U:H2'	1:AA:602:U:C4	2.54	0.42
1:AA:848:G:N2	1:AA:848:G:OP2	2.52	0.42
1:AA:1762:A:H2'	1:AA:1763:U:C6	2.54	0.42
3:BA:1442:A:O2'	3:BA:1443:A:O5'	2.37	0.42
4:BB:1272:U:H5'	4:BB:1272:U:H6	1.85	0.42
4:BB:1414:C:H2'	4:BB:1415:G:H8	1.84	0.42
4:BB:1503:U:H2'	4:BB:1504:G:C8	2.55	0.42
5:BC:43:A2M:HM'3	5:BC:43:A2M:H1'	1.84	0.42
10:BR:7:LYS:HE3	10:BR:7:LYS:HB3	1.84	0.42
26:By:2:LYS:HB3	26:By:2:LYS:HE2	1.56	0.42
32:AE:71:ASP:OD1	32:AE:129:PRO:HD3	2.19	0.42
32:AE:121:ARG:NH1	32:AE:122:ASN:O	2.53	0.42
48:AC:73:TYR:CD1	48:AC:89:MET:HE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:BV:103:LEU:HD23	77:BV:103:LEU:HA	1.86	0.42
1:AA:747:C:C4	1:AA:748:A:C6	3.07	0.42
1:AA:764:U:H2'	1:AA:765:A:C8	2.55	0.42
1:AA:1656:U:O2'	1:AA:1657:C:O4'	2.32	0.42
3:BA:1849:A:H2	3:BA:1850:A:H62	1.67	0.42
5:BC:67:U:H2'	5:BC:68:A:H8	1.83	0.42
6:BD:111:U:H2'	6:BD:112:U:O4'	2.19	0.42
7:BE:7:G:N2	7:BE:10:A:OP2	2.36	0.42
12:BT:187:ARG:NH1	12:BT:191:ASP:HB2	2.34	0.42
40:AP:154:TRP:CE3	40:AP:183:PRO:HB3	2.54	0.42
43:AX:110:SER:O	43:AX:110:SER:OG	2.33	0.42
64:BK:48:VAL:O	64:BK:139:ARG:HA	2.20	0.42
64:BK:52:VAL:HG12	64:BK:152:LEU:HD13	2.00	0.42
64:BK:61:SER:OG	64:BK:63:GLU:OE2	2.34	0.42
72:Bh:128:ASP:OD1	72:Bh:129:ALA:N	2.51	0.42
74:BG:26:G:H2'	74:BG:27:C:C6	2.54	0.42
79:AQ:22:THR:HB	79:AQ:83:LYS:HG2	2.01	0.42
82:AW:21:LYS:O	82:AW:22:ARG:HB2	2.19	0.42
84:A7:159:ARG:HD2	84:A7:159:ARG:HA	1.95	0.42
1:AA:99:G:OP2	45:A3:167:LYS:NZ	2.52	0.42
1:AA:325:A:H61	1:AA:332:G:H5'	1.85	0.42
1:AA:629:A:N3	46:AT:69:THR:OG1	2.47	0.42
1:AA:801:G:H2'	1:AA:802:C:H6	1.83	0.42
3:BA:717:A:H2'	3:BA:718:A:H8	1.85	0.42
23:Bx:100:ARG:NH1	23:Bx:101:ASN:OD1	2.52	0.42
27:A0:55:LYS:HB3	27:A0:60:PHE:HE2	1.84	0.42
40:AP:240:TRP:O	80:AR:21:LYS:HE2	2.20	0.42
42:AU:58:LYS:O	42:AU:62:LYS:NZ	2.48	0.42
47:A1:145:ARG:HA	47:A1:145:ARG:HD2	1.86	0.42
54:Bk:79:LEU:O	54:Bk:81:SER:N	2.52	0.42
68:A6:44:VAL:HG21	68:A6:104:LEU:HD21	2.01	0.42
68:A6:109:GLN:NE2	68:A6:125:ARG:HB2	2.35	0.42
79:AQ:15:GLN:N	79:AQ:89:ARG:HH21	2.17	0.42
1:AA:448:C:OP1	29:A5:14:THR:OG1	2.25	0.42
1:AA:660:U:OP1	70:AY:56:ARG:NH2	2.51	0.42
1:AA:969:C:H4'	1:AA:970:A:O5'	2.19	0.42
1:AA:1763:U:OP1	39:AO:146:LYS:NZ	2.49	0.42
3:BA:885:G:H8	3:BA:885:G:O5'	2.02	0.42
3:BA:895:G:H2'	3:BA:896:G:H5'	2.02	0.42
4:BB:1040:U:H2'	4:BB:1041:G:H8	1.82	0.42
28:A2:78:LEU:O	28:A2:82:THR:OG1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:A3:6:ALA:HB3	45:A3:115:THR:HG22	2.00	0.42
61:BO:10:ASN:O	61:BO:14:ARG:HG3	2.19	0.42
66:Be:89:LEU:HD12	66:Be:95:PRO:HD2	2.01	0.42
70:AY:47:LYS:HD3	70:AY:47:LYS:HA	1.67	0.42
84:A7:41:LEU:HD23	84:A7:41:LEU:HA	1.84	0.42
1:AA:488:U:H2'	1:AA:489:G:O4'	2.19	0.42
1:AA:753:G:H2'	1:AA:754:U:H6	1.81	0.42
1:AA:965:G:H2'	1:AA:966:A:H8	1.83	0.42
1:AA:1026:U:O2'	1:AA:1027:A:H4'	2.20	0.42
1:AA:1303:A:H61	50:Bz:3:THR:CG2	2.33	0.42
8:BP:110:ARG:HH22	71:Bv:192:TRP:H	1.67	0.42
9:BQ:202:ARG:HD2	9:BQ:202:ARG:HA	1.85	0.42
28:A2:45:LYS:HA	28:A2:45:LYS:HD2	1.67	0.42
54:Bk:6:LYS:HD2	54:Bk:8:ARG:HH21	1.85	0.42
64:BK:177:LEU:H	64:BK:177:LEU:HD22	1.84	0.42
75:BH:54:U:H2'	75:BH:55:C:H6	1.85	0.42
84:A7:209:SER:OG	84:A7:210:LEU:HD23	2.20	0.42
1:AA:45:C:H2'	1:AA:46:OMC:C6	2.55	0.42
1:AA:602:U:C2	1:AA:603:G:N1	2.88	0.42
3:BA:550:A:H8	3:BA:550:A:OP1	2.02	0.42
3:BA:1321:G:N2	11:BS:114:SER:HB3	2.35	0.42
4:BB:96:U:H2'	4:BB:97:A:O4'	2.20	0.42
4:BB:671:C:H2'	4:BB:672:U:H6	1.85	0.42
12:BT:178:LEU:C	12:BT:180:LYS:H	2.27	0.42
22:Bw:233:ARG:O	22:Bw:234:ARG:HB2	2.19	0.42
35:AH:80:GLU:C	35:AH:80:GLU:OE1	2.63	0.42
43:AX:66:ARG:O	43:AX:69:THR:OG1	2.26	0.42
57:Bg:28:VAL:HG11	57:Bg:103:ILE:HG12	2.01	0.42
66:Be:33:ASP:OD1	66:Be:33:ASP:N	2.51	0.42
81:AV:35:ASP:OD1	81:AV:35:ASP:N	2.42	0.42
1:AA:340:G:N3	32:AE:55:GLY:HA3	2.35	0.42
1:AA:347:U:H2'	1:AA:348:U:C6	2.54	0.42
1:AA:361:A:H3'	1:AA:362:A:H5''	2.02	0.42
1:AA:424:U:H2'	1:AA:425:G:C8	2.55	0.42
1:AA:538:A:H61	1:AA:560:G:H1'	1.85	0.42
1:AA:762:C:H6	1:AA:762:C:H2'	1.70	0.42
1:AA:966:A:O2'	1:AA:967:A:H5'	2.19	0.42
1:AA:1238:U:H2'	1:AA:1239:C:C6	2.55	0.42
4:BB:533:U:H2'	4:BB:535:A:OP2	2.19	0.42
29:A5:175:LEU:HA	29:A5:175:LEU:HD23	1.81	0.42
43:AX:32:GLY:HA3	43:AX:52:THR:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:BN:146:GLU:H	62:BN:149:LYS:HZ1	1.66	0.42
83:A4:79:ILE:C	83:A4:79:ILE:HD12	2.45	0.42
1:AA:275:G:H2'	1:AA:276:U:H6	1.85	0.41
1:AA:582:A:H2	1:AA:603:G:C2	2.37	0.41
3:BA:626:G:O2'	3:BA:628:G:H2'	2.20	0.41
3:BA:645:U:N3	3:BA:646:G:O6	2.53	0.41
3:BA:1278:U:OP2	56:Bi:44:ARG:NH2	2.53	0.41
4:BB:609:A2M:HM'3	4:BB:609:A2M:H1'	1.79	0.41
4:BB:1129:C:H2'	4:BB:1130:G:O4'	2.20	0.41
7:BE:49:G:H2'	7:BE:50:G:H8	1.85	0.41
20:Br:177:ASP:OD1	20:Br:177:ASP:N	2.52	0.41
24:Bl:103:SER:OG	24:Bl:104:ASN:N	2.53	0.41
25:Bu:203:ASP:HB3	25:Bu:208:ARG:HB2	2.02	0.41
47:A1:179:MET:HE3	47:A1:187:GLY:HA2	2.02	0.41
61:BO:188:LYS:HA	61:BO:188:LYS:HE3	2.02	0.41
64:BK:116:ARG:HG2	64:BK:117:GLN:HG3	2.01	0.41
70:AY:55:LEU:HD23	70:AY:55:LEU:H	1.85	0.41
79:AQ:43:GLU:CD	79:AQ:94:LEU:HD21	2.45	0.41
83:A4:47:HIS:ND1	83:A4:47:HIS:C	2.77	0.41
83:A4:171:LEU:HA	83:A4:171:LEU:HD13	1.75	0.41
1:AA:343:U:C4	32:AE:29:ALA:HB2	2.54	0.41
1:AA:1478:U:O2'	1:AA:1479:U:H6	2.03	0.41
1:AA:2034:G:H2'	1:AA:2035:G:H5'	2.02	0.41
1:AA:2036:G:H5''	39:AO:103:GLY:HA2	2.02	0.41
1:AA:2108:U:H2'	1:AA:2109:A:H8	1.85	0.41
2:AB:76:A:H62	4:BB:1248:G:H5'	1.85	0.41
3:BA:212:A:N6	3:BA:228:U:O2'	2.53	0.41
3:BA:527:G:H22	56:Bi:3:LYS:NZ	2.18	0.41
3:BA:702:C:O3'	56:Bi:63:ARG:NH2	2.51	0.41
3:BA:1195:A:H2'	3:BA:1196:G:C8	2.55	0.41
12:BT:186:GLU:HA	12:BT:189:ARG:CZ	2.50	0.41
14:BW:106:ASN:OD1	14:BW:110:GLU:N	2.43	0.41
18:Bp:49:ASP:OD1	18:Bp:51:LYS:N	2.53	0.41
26:By:105:ASN:HB3	26:By:106:GLN:H	1.65	0.41
32:AE:65:ILE:HG22	32:AE:66:ASN:OD1	2.20	0.41
34:AI:117:GLU:OE1	34:AI:117:GLU:N	2.40	0.41
39:AO:27:HIS:CE1	39:AO:29:TRP:HB3	2.55	0.41
39:AO:116:LEU:HD12	39:AO:116:LEU:HA	1.85	0.41
41:AS:16:LEU:HD12	41:AS:16:LEU:HA	1.91	0.41
46:AT:45:LEU:HD23	46:AT:45:LEU:HA	1.80	0.41
58:Bd:31:ASN:OD1	58:Bd:31:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:BO:3:LEU:HD23	61:BO:3:LEU:HA	1.73	0.41
74:BG:19:C:H2'	74:BG:20:U:H6	1.85	0.41
74:BG:145:C:H6	74:BG:145:C:P	2.43	0.41
1:AA:2096:A2M:H1'	1:AA:2096:A2M:HM'3	1.72	0.41
3:BA:179:A:H2'	3:BA:180:G:C8	2.56	0.41
3:BA:1686:G:H2'	3:BA:1687:U:C6	2.55	0.41
4:BB:601:OMC:H1'	4:BB:601:OMC:HM23	1.83	0.41
7:BE:202:A:H2'	7:BE:203:A:C8	2.56	0.41
24:Bl:30:LYS:NZ	73:BF:11:C:H5''	2.35	0.41
24:Bl:149:ILE:HG22	71:Bv:82:ILE:HG23	2.02	0.41
32:AE:56:LEU:HD21	47:A1:200:GLY:HA3	2.02	0.41
33:AG:84:ILE:HG22	33:AG:135:LEU:HD21	2.02	0.41
37:AL:90:HIS:NE2	48:AC:57:MET:HE1	2.36	0.41
40:AP:82:ARG:O	40:AP:83:GLU:HB3	2.20	0.41
40:AP:87:ARG:HH21	40:AP:117:GLY:HA2	1.83	0.41
47:A1:16:MET:CE	47:A1:105:ARG:HD2	2.50	0.41
69:Bf:80:GLU:OE1	69:Bf:321:TYR:OH	2.29	0.41
70:AY:26:LYS:HE2	70:AY:26:LYS:HB2	1.87	0.41
71:Bv:25:THR:O	71:Bv:25:THR:OG1	2.29	0.41
82:AW:42:LYS:O	82:AW:42:LYS:HG2	2.19	0.41
83:A4:90:ARG:HA	83:A4:90:ARG:HD3	1.84	0.41
83:A4:124:VAL:O	83:A4:128:GLU:HG2	2.20	0.41
1:AA:224:U:H2'	1:AA:225:C:H6	1.85	0.41
1:AA:585:G:N2	70:AY:48:THR:OG1	2.45	0.41
1:AA:1397:U:H2'	1:AA:1398:G:C8	2.55	0.41
1:AA:1773:A:O2'	1:AA:1774:G:H5'	2.20	0.41
3:BA:1427:U:H2'	3:BA:1428:C:H6	1.86	0.41
4:BB:1377:U:H2'	4:BB:1378:U:C6	2.56	0.41
4:BB:1428:U:H2'	4:BB:1429:PSU:C6	2.56	0.41
40:AP:238:ASP:OD2	40:AP:238:ASP:C	2.64	0.41
41:AS:88:ASP:OD1	70:AY:12:GLY:HA2	2.20	0.41
46:AT:86:LEU:O	46:AT:90:LYS:HG2	2.20	0.41
48:AC:80:ASP:OD2	48:AC:80:ASP:C	2.62	0.41
59:Bb:77:ASN:HB3	59:Bb:80:LYS:HE3	2.01	0.41
65:BI:75:THR:HA	65:BI:78:LEU:HG	2.02	0.41
68:A6:50:LYS:O	68:A6:54:THR:HG22	2.20	0.41
75:BH:5:G:H2'	75:BH:6:U:H6	1.84	0.41
83:A4:174:LEU:HD23	83:A4:174:LEU:HA	1.87	0.41
1:AA:764:U:H5	1:AA:787:G:H22	1.68	0.41
1:AA:1027:A:H2'	1:AA:1028:U:C6	2.55	0.41
1:AA:1478:U:O2'	1:AA:1479:U:P	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BA:485:G:H1'	74:BG:8:U:H5	1.85	0.41
3:BA:884:G:H2'	3:BA:885:G:C8	2.56	0.41
3:BA:1630:U:H2'	3:BA:1631:A:C8	2.55	0.41
8:BP:154:VAL:HG13	8:BP:155:ASP:OD2	2.21	0.41
12:BT:89:MET:HE3	12:BT:90:PRO:HD2	2.02	0.41
20:Br:23:LEU:HA	20:Br:24:PRO:HD3	1.93	0.41
23:Bx:76:ARG:HA	23:Bx:76:ARG:HD2	1.80	0.41
45:A3:32:ARG:HB2	45:A3:103:CYS:SG	2.61	0.41
47:A1:159:TYR:OH	47:A1:164:LYS:HB3	2.20	0.41
48:AC:167:HIS:HE1	48:AC:171:ARG:NH2	2.19	0.41
49:Bc:21:LYS:HG3	49:Bc:26:ARG:HG3	2.03	0.41
78:Az:211:ASN:OD1	78:Az:211:ASN:N	2.53	0.41
83:A4:95:ILE:HD12	83:A4:95:ILE:O	2.21	0.41
1:AA:909:C:H2'	1:AA:910:C:C2	2.55	0.41
1:AA:1635:A:H2	1:AA:1663:C:C2	2.39	0.41
12:BT:190:ARG:C	12:BT:190:ARG:HD2	2.46	0.41
20:Br:325:LEU:HD23	20:Br:325:LEU:HA	1.94	0.41
25:Bu:158:ARG:HE	25:Bu:158:ARG:HB2	1.74	0.41
40:AP:180:ILE:HB	40:AP:207:TYR:HB2	2.02	0.41
40:AP:189:VAL:O	40:AP:208:THR:HB	2.21	0.41
48:AC:103:ALA:HB2	80:AR:42:ALA:HB2	2.03	0.41
72:Bh:36:ARG:HE	72:Bh:37:ARG:N	2.18	0.41
74:BG:18:U:O2'	74:BG:19:C:OP1	2.35	0.41
74:BG:170:G:H4'	74:BG:171:A:H3'	2.03	0.41
83:A4:72:PHE:O	83:A4:76:VAL:HG13	2.20	0.41
1:AA:56:A2M:H2'	1:AA:57:OMU:C6	2.48	0.41
1:AA:827:G:C4	1:AA:828:A:C2	3.09	0.41
1:AA:909:C:O2'	1:AA:910:C:O5'	2.35	0.41
1:AA:2154:OMU:HM23	1:AA:2154:OMU:H1'	1.55	0.41
1:AA:2174:G:HO2'	1:AA:2200:A:N6	2.18	0.41
3:BA:253:G:H2'	3:BA:254:A2M:C8	2.51	0.41
3:BA:356:A:H2'	3:BA:357:G:C8	2.55	0.41
3:BA:762:A2M:H8	3:BA:762:A2M:O5'	2.21	0.41
3:BA:1451:C:H2'	3:BA:1452:G:O4'	2.20	0.41
3:BA:1738:C:H5'	52:Bn:41:ARG:HD2	2.02	0.41
4:BB:1020:G:OP2	4:BB:1021:A:O2'	2.29	0.41
11:BS:175:ARG:HD3	11:BS:175:ARG:HA	1.78	0.41
20:Br:346:LYS:HA	20:Br:349:ARG:HE	1.85	0.41
24:Bl:23:THR:O	24:Bl:24:LYS:HB3	2.21	0.41
27:A0:202:ARG:HD2	27:A0:202:ARG:HA	1.76	0.41
31:A8:8:ARG:O	31:A8:10:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:AE:109:PHE:HD1	32:AE:116:TYR:CE2	2.39	0.41
40:AP:89:GLU:HB3	40:AP:113:VAL:HG13	2.02	0.41
40:AP:193:VAL:HB	40:AP:194:PRO:HD3	2.03	0.41
64:BK:13:LYS:H	64:BK:13:LYS:HG2	1.67	0.41
79:AQ:37:LEU:O	79:AQ:41:ARG:N	2.48	0.41
1:AA:274:C:H2'	1:AA:275:G:C8	2.56	0.41
1:AA:317:A:H3'	1:AA:318:G:H21	1.86	0.41
1:AA:542:U:H5	1:AA:555:A:N1	2.19	0.41
1:AA:1233:U:OP1	1:AA:1474:U:O2'	2.34	0.41
1:AA:1512:G:H2'	1:AA:1513:G:C8	2.55	0.41
1:AA:1584:G:N2	1:AA:1927:A:N6	2.34	0.41
1:AA:1635:A:N6	1:AA:1660:G:H1'	2.36	0.41
1:AA:1658:U:H2'	1:AA:1659:C:C6	2.56	0.41
1:AA:2144:U:H2'	1:AA:2145:U:C6	2.55	0.41
3:BA:152:U:H5''	9:BQ:71:LYS:O	2.21	0.41
4:BB:1533:C:H2'	4:BB:1534:G:N9	2.35	0.41
36:AJ:84:ARG:HG2	36:AJ:84:ARG:HH11	1.86	0.41
68:A6:83:GLY:HA3	68:A6:106:ARG:HE	1.86	0.41
71:Bv:186:ALA:HB1	71:Bv:188:HIS:CE1	2.56	0.41
1:AA:175:G:H2'	1:AA:176:G:H8	1.83	0.41
1:AA:550:A:OP1	46:AT:105:LYS:NZ	2.49	0.41
1:AA:810:G:H21	1:AA:827:G:H22	1.69	0.41
1:AA:894:U:H2'	1:AA:895:G:N3	2.35	0.41
1:AA:1302:A:H2'	1:AA:1304:A:H5''	2.02	0.41
1:AA:1464:A:H61	82:AW:75:VAL:HA	1.85	0.41
1:AA:1503:A:H3'	1:AA:1504:C:H5'	2.02	0.41
1:AA:1658:U:H2'	1:AA:1659:C:H6	1.85	0.41
1:AA:1879:A:H1'	1:AA:1880:U:C5	2.56	0.41
1:AA:2028:C:OP2	38:AM:56:ARG:NH2	2.54	0.41
1:AA:2108:U:N3	1:AA:2109:A:N7	2.69	0.41
1:AA:2279:U:H3	27:A0:154:LYS:HB3	1.86	0.41
3:BA:405:A:H2'	3:BA:406:A:O4'	2.21	0.41
3:BA:502:U:H2'	3:BA:503:A:H8	1.84	0.41
3:BA:703:G:P	56:Bi:63:ARG:NH2	2.92	0.41
3:BA:753:A:H2'	3:BA:754:A:C8	2.56	0.41
3:BA:1434:G:H2'	3:BA:1435:C:C6	2.56	0.41
4:BB:659:OMG:H2'	4:BB:660:G:H5''	2.03	0.41
5:BC:135:A:H2'	5:BC:136:G:C8	2.55	0.41
18:Bp:12:LEU:HD13	18:Bp:12:LEU:HA	1.94	0.41
19:Bq:48:LYS:O	19:Bq:49:LEU:HB3	2.21	0.41
23:Bx:36:ALA:HB3	23:Bx:37:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AD:53:MET:HG3	30:AD:73:TRP:CD2	2.55	0.41
35:AH:79:LYS:HD2	35:AH:79:LYS:HA	1.96	0.41
37:AL:25:ASN:H	37:AL:31:ASN:HD21	1.69	0.41
38:AM:21:VAL:HA	38:AM:33:MET:HE2	2.03	0.41
38:AM:88:GLN:O	38:AM:96:THR:OG1	2.27	0.41
42:AU:49:ASP:O	42:AU:53:MET:N	2.53	0.41
43:AX:177:ARG:HH21	70:AY:65:ALA:HB2	1.85	0.41
48:AC:110:VAL:HG22	48:AC:157:VAL:HG12	2.02	0.41
52:Bn:67:LEU:HD23	52:Bn:67:LEU:HA	1.87	0.41
56:Bi:127:LEU:HD12	56:Bi:127:LEU:HA	1.83	0.41
61:BO:151:GLU:H	61:BO:151:GLU:CD	2.29	0.41
64:BK:84:CYS:O	64:BK:140:THR:OG1	2.29	0.41
67:AK:20:THR:OG1	67:AK:78:SER:HB2	2.21	0.41
68:A6:63:GLU:CD	68:A6:64:ASN:H	2.29	0.41
74:BG:138:C:H2'	74:BG:139:U:C6	2.56	0.41
83:A4:134:LEU:HD23	83:A4:134:LEU:HA	1.87	0.41
84:A7:175:ASP:OD1	84:A7:175:ASP:N	2.26	0.41
84:A7:238:ALA:HB2	84:A7:258:LYS:HG2	2.02	0.41
1:AA:2016:A:H2'	1:AA:2017:A:C8	2.56	0.41
1:AA:2261:MA6:H8	1:AA:2261:MA6:H5''	2.01	0.41
3:BA:773:A:N7	65:BI:111:ARG:NH2	2.69	0.41
3:BA:913:C:H2'	3:BA:914:U:H6	1.85	0.41
4:BB:444:G:OP1	66:Be:174:ARG:NH2	2.54	0.41
14:BW:126:GLU:H	14:BW:126:GLU:HG2	1.63	0.41
20:Br:285:THR:HG22	20:Br:286:ASP:N	2.31	0.41
24:Bl:66:VAL:HG23	24:Bl:67:ASN:N	2.34	0.41
26:By:116:GLU:OE2	26:By:120:ARG:NH2	2.53	0.41
35:AH:94:GLY:HA3	35:AH:127:PRO:HG2	2.03	0.41
38:AM:63:GLU:HG2	38:AM:64:GLU:N	2.36	0.41
64:BK:92:HIS:HA	64:BK:93:PRO:HD3	1.92	0.41
66:Be:104:LEU:HA	66:Be:107:ILE:HD12	2.03	0.41
75:BH:54:U:H2'	75:BH:55:C:C6	2.56	0.41
79:AQ:21:MET:HG2	79:AQ:109:VAL:HG22	2.03	0.41
1:AA:394:A:H2'	1:AA:395:A:C8	2.56	0.40
1:AA:692:C:N4	1:AA:693:A:H62	2.19	0.40
1:AA:1267:C:H2'	1:AA:1268:A:O4'	2.21	0.40
1:AA:1981:G:H2'	1:AA:1982:C:O4'	2.21	0.40
1:AA:2153:A2M:H1'	1:AA:2153:A2M:HM'3	1.77	0.40
3:BA:126:A:H5'	3:BA:127:U:OP2	2.20	0.40
3:BA:246:U:H2'	3:BA:247:U:C6	2.57	0.40
20:Br:127:LEU:HD23	20:Br:127:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AS:85:VAL:HA	41:AS:86:PRO:HD3	1.94	0.40
72:Bh:42:LEU:HD13	72:Bh:42:LEU:HA	1.92	0.40
1:AA:149:C:H2'	1:AA:150:A:C8	2.55	0.40
1:AA:467:U:H2'	1:AA:468:U:O4'	2.20	0.40
1:AA:907:G:O6	1:AA:953:G:N2	2.47	0.40
1:AA:1207:A:C2	27:A0:116:LEU:HD11	2.56	0.40
1:AA:1917:U:O2'	31:A8:7:TRP:O	2.27	0.40
3:BA:66:G:OP1	9:BQ:202:ARG:NH2	2.52	0.40
3:BA:619[B]:C:N4	3:BA:622:G:O6	2.54	0.40
3:BA:912:C:H2'	3:BA:913:C:H6	1.85	0.40
4:BB:1248:G:O2'	4:BB:1249:U:OP2	2.36	0.40
4:BB:1515:U:H5''	4:BB:1516:G:OP2	2.21	0.40
4:BB:1526:U:HO2'	4:BB:1527:G:N2	2.19	0.40
6:BD:110:G:H2'	6:BD:111:U:C6	2.56	0.40
9:BQ:162:ASP:HB3	9:BQ:165:ILE:HG22	2.03	0.40
19:Bq:48:LYS:HD2	19:Bq:48:LYS:HA	1.87	0.40
22:Bw:229:MET:HB2	22:Bw:241:ASP:OD2	2.21	0.40
46:AT:47:ARG:HG3	46:AT:62:ILE:HB	2.03	0.40
53:Bm:54:ASP:OD2	53:Bm:54:ASP:C	2.63	0.40
61:BO:204:ALA:O	61:BO:208:MET:HG3	2.21	0.40
65:BI:47:LEU:HD12	65:BI:47:LEU:HA	1.89	0.40
69:Bf:77:THR:OG1	69:Bf:333:GLY:O	2.40	0.40
83:A4:119:ARG:O	83:A4:122:THR:HG22	2.21	0.40
84:A7:169:ILE:HB	84:A7:181:TRP:HB2	2.03	0.40
1:AA:383:G:H2'	1:AA:384:U:O2	2.21	0.40
1:AA:961:U:C4	1:AA:962:A:N7	2.90	0.40
1:AA:1322:U:P	27:A0:155:ASN:HD22	2.43	0.40
3:BA:862:G:H2'	3:BA:863:U:C6	2.57	0.40
4:BB:705:C:H2'	4:BB:706:G:O4'	2.22	0.40
4:BB:1103:C:H2'	4:BB:1104:G:H8	1.86	0.40
7:BE:167:A:H2'	7:BE:168:C:O4'	2.21	0.40
18:Bp:59:SER:O	18:Bp:59:SER:OG	2.38	0.40
20:Br:347:LYS:HB2	20:Br:347:LYS:NZ	2.37	0.40
23:Bx:167:ALA:HB2	23:Bx:199:LEU:HD12	2.04	0.40
37:AL:104:GLN:NE2	48:AC:78:THR:HA	2.36	0.40
47:A1:174:ASN:OD1	47:A1:174:ASN:N	2.54	0.40
48:AC:119:GLY:O	48:AC:123:ILE:HG12	2.21	0.40
68:A6:106:ARG:HA	68:A6:106:ARG:HD2	1.93	0.40
69:Bf:291:GLY:HA3	69:Bf:328:TYR:CE1	2.57	0.40
71:Bv:182:LYS:HE2	71:Bv:182:LYS:HB2	1.78	0.40
77:BV:123:ASN:OD1	77:BV:123:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AQ:15:GLN:N	79:AQ:15:GLN:OE1	2.54	0.40
79:AQ:35:GLU:O	79:AQ:38:GLU:HG3	2.21	0.40
1:AA:132:C:OP1	1:AA:476:G:O2'	2.37	0.40
1:AA:755:G:H2'	1:AA:756:U:C6	2.57	0.40
1:AA:788:U:H2'	1:AA:789:G:N7	2.36	0.40
1:AA:1119:C:H2'	1:AA:1120:G:C8	2.56	0.40
1:AA:1848:G:H5'	79:AQ:84:ARG:HH22	1.85	0.40
1:AA:1917:U:H2'	1:AA:1918:C:H6	1.86	0.40
1:AA:1936:A:H2'	1:AA:1937:C:C6	2.56	0.40
3:BA:1192:C:O2'	3:BA:1193:C:H5'	2.22	0.40
4:BB:685:OMU:HM23	4:BB:685:OMU:H1'	1.90	0.40
4:BB:1211:U:H2'	4:BB:1212:G:H8	1.86	0.40
5:BC:163:A2M:H1'	5:BC:163:A2M:HM'3	1.68	0.40
6:BD:94:C:OP1	11:BS:45:ARG:NH2	2.55	0.40
13:BU:31:LEU:HD21	25:Bu:37:VAL:HG12	2.03	0.40
13:BU:131:SER:OG	13:BU:134:ASN:OD1	2.34	0.40
15:BY:14:HIS:HB3	15:BY:15:PRO:HD2	2.02	0.40
21:Bt:6:LYS:N	21:Bt:95:ASP:HB2	2.37	0.40
24:Bl:23:THR:C	24:Bl:25:LYS:H	2.29	0.40
31:A8:47:ASN:O	31:A8:51:ILE:HG12	2.22	0.40
35:AH:57:ALA:C	35:AH:59:ARG:H	2.29	0.40
39:AO:27:HIS:HE1	39:AO:29:TRP:HB3	1.85	0.40
59:Bb:92:LYS:HD2	59:Bb:92:LYS:HA	1.61	0.40
70:AY:20:LYS:NZ	70:AY:20:LYS:HB3	2.36	0.40
80:AR:7:TYR:CE1	80:AR:13:ASN:HB2	2.57	0.40
1:AA:58:G:H2'	1:AA:59:C:C6	2.56	0.40
1:AA:888:C:OP1	1:AA:888:C:H4'	2.22	0.40
1:AA:1213:G:O6	81:AV:17:ARG:HG2	2.22	0.40
1:AA:1562:A:H2'	1:AA:1565:A:N7	2.37	0.40
1:AA:1635:A:H62	1:AA:1660:G:H1'	1.87	0.40
1:AA:2044:A:H2'	1:AA:2045:PSU:C6	2.56	0.40
3:BA:440:U:H6	3:BA:440:U:H2'	1.68	0.40
3:BA:1427:U:H2'	3:BA:1428:C:C6	2.57	0.40
3:BA:1500:G:N7	49:Bc:104:LYS:HG3	2.37	0.40
4:BB:766:C:O2'	4:BB:767:G:H8	2.03	0.40
4:BB:1506:G:H8	4:BB:1506:G:O5'	2.05	0.40
5:BC:121:G:H2'	5:BC:122:A:H8	1.86	0.40
8:BP:126:LYS:HB3	8:BP:126:LYS:HE3	1.66	0.40
8:BP:145:LYS:HB3	8:BP:145:LYS:HE2	1.82	0.40
14:BW:91:ASP:OD1	14:BW:93:THR:OG1	2.32	0.40
14:BW:105:VAL:HG13	14:BW:106:ASN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Br:189:ARG:HB2	20:Br:201:VAL:HG13	2.04	0.40
25:Bu:116:ALA:O	25:Bu:118:LYS:HG3	2.20	0.40
39:AO:59:GLY:HA2	39:AO:100:LYS:HD2	2.04	0.40
43:AX:105:ARG:HG3	43:AX:174:CYS:HB3	2.03	0.40
53:Bm:100:GLU:C	53:Bm:100:GLU:OE2	2.65	0.40
62:BN:72:MET:N	62:BN:72:MET:SD	2.82	0.40
63:BL:37:LEU:HD23	63:BL:37:LEU:HA	1.93	0.40
68:A6:47:THR:O	68:A6:51:MET:HG3	2.21	0.40
72:Bh:127:ILE:HD13	72:Bh:127:ILE:HA	1.96	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	
8	BP	152/189 (80%)	146 (96%)	5 (3%)	1 (1%)	18	38
9	BQ	201/221 (91%)	192 (96%)	9 (4%)	0	100	100
10	BR	148/166 (89%)	145 (98%)	3 (2%)	0	100	100
11	BS	176/179 (98%)	160 (91%)	16 (9%)	0	100	100
12	BT	190/260 (73%)	186 (98%)	4 (2%)	0	100	100
13	BU	147/159 (92%)	135 (92%)	12 (8%)	0	100	100
14	BW	127/139 (91%)	125 (98%)	2 (2%)	0	100	100
15	BY	60/125 (48%)	57 (95%)	3 (5%)	0	100	100
16	BX	115/164 (70%)	113 (98%)	2 (2%)	0	100	100
17	BZ	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
18	Bp	71/82 (87%)	67 (94%)	4 (6%)	0	100	100
19	Bq	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
20	Br	364/374 (97%)	339 (93%)	25 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Bt	95/106 (90%)	87 (92%)	8 (8%)	0	100	100
22	Bw	228/257 (89%)	221 (97%)	7 (3%)	0	100	100
23	Bx	228/276 (83%)	217 (95%)	10 (4%)	1 (0%)	30	51
24	Bl	142/149 (95%)	135 (95%)	7 (5%)	0	100	100
25	Bu	236/308 (77%)	230 (98%)	6 (2%)	0	100	100
26	By	176/189 (93%)	168 (96%)	8 (4%)	0	100	100
27	A0	214/256 (84%)	203 (95%)	10 (5%)	1 (0%)	24	46
28	A2	179/190 (94%)	171 (96%)	8 (4%)	0	100	100
29	A5	182/220 (83%)	171 (94%)	11 (6%)	0	100	100
30	AD	85/172 (49%)	81 (95%)	4 (5%)	0	100	100
31	A8	51/57 (90%)	47 (92%)	3 (6%)	1 (2%)	6	12
32	AE	150/174 (86%)	131 (87%)	19 (13%)	0	100	100
33	AG	139/151 (92%)	129 (93%)	10 (7%)	0	100	100
34	AI	100/152 (66%)	98 (98%)	2 (2%)	0	100	100
35	AH	133/144 (92%)	122 (92%)	11 (8%)	0	100	100
36	AJ	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
37	AL	120/142 (84%)	116 (97%)	4 (3%)	0	100	100
38	AM	131/153 (86%)	116 (88%)	14 (11%)	1 (1%)	16	34
39	AO	147/167 (88%)	141 (96%)	6 (4%)	0	100	100
40	AP	218/266 (82%)	199 (91%)	19 (9%)	0	100	100
41	AS	138/143 (96%)	126 (91%)	12 (9%)	0	100	100
42	AU	69/113 (61%)	68 (99%)	1 (1%)	0	100	100
43	AX	206/214 (96%)	199 (97%)	7 (3%)	0	100	100
44	AZ	53/103 (52%)	50 (94%)	3 (6%)	0	100	100
45	A3	228/250 (91%)	217 (95%)	11 (5%)	0	100	100
46	AT	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
47	A1	258/273 (94%)	239 (93%)	19 (7%)	0	100	100
48	AC	206/277 (74%)	199 (97%)	7 (3%)	0	100	100
49	Bc	142/146 (97%)	133 (94%)	9 (6%)	0	100	100
50	Bz	31/34 (91%)	26 (84%)	5 (16%)	0	100	100
51	Bo	87/93 (94%)	82 (94%)	4 (5%)	1 (1%)	11	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	Bn	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
53	Bm	96/109 (88%)	84 (88%)	12 (12%)	0	100	100
54	Bk	121/127 (95%)	113 (93%)	8 (7%)	0	100	100
55	Bj	114/170 (67%)	112 (98%)	2 (2%)	0	100	100
56	Bi	129/132 (98%)	128 (99%)	1 (1%)	0	100	100
57	Bg	90/105 (86%)	89 (99%)	1 (1%)	0	100	100
58	Bd	67/71 (94%)	62 (92%)	5 (8%)	0	100	100
59	Bb	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
60	Ba	126/133 (95%)	121 (96%)	5 (4%)	0	100	100
61	BO	219/222 (99%)	213 (97%)	6 (3%)	0	100	100
62	BN	208/218 (95%)	194 (93%)	14 (7%)	0	100	100
63	BL	152/194 (78%)	145 (95%)	7 (5%)	0	100	100
64	BK	190/213 (89%)	181 (95%)	9 (5%)	0	100	100
65	BI	189/193 (98%)	180 (95%)	9 (5%)	0	100	100
66	Be	253/260 (97%)	247 (98%)	6 (2%)	0	100	100
67	AK	140/149 (94%)	132 (94%)	8 (6%)	0	100	100
68	A6	176/190 (93%)	169 (96%)	7 (4%)	0	100	100
69	Bf	398/429 (93%)	389 (98%)	9 (2%)	0	100	100
70	AY	57/66 (86%)	51 (90%)	6 (10%)	0	100	100
71	Bv	139/192 (72%)	133 (96%)	6 (4%)	0	100	100
72	Bh	139/188 (74%)	135 (97%)	4 (3%)	0	100	100
76	Bs	48/128 (38%)	46 (96%)	2 (4%)	0	100	100
77	BV	120/130 (92%)	116 (97%)	4 (3%)	0	100	100
78	Az	35/279 (12%)	32 (91%)	3 (9%)	0	100	100
79	AQ	98/117 (84%)	96 (98%)	2 (2%)	0	100	100
80	AR	86/194 (44%)	81 (94%)	5 (6%)	0	100	100
81	AV	101/111 (91%)	98 (97%)	3 (3%)	0	100	100
82	AW	83/86 (96%)	76 (92%)	7 (8%)	0	100	100
83	A4	196/202 (97%)	185 (94%)	11 (6%)	0	100	100
84	A7	295/318 (93%)	281 (95%)	14 (5%)	0	100	100
85	A	2/4 (50%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	10823/12853 (84%)	10283 (95%)	534 (5%)	6 (0%)	49	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	Bo	68	ALA
31	A8	9	SER
27	A0	108	THR
8	BP	32	ASP
23	Bx	52	ASP
38	AM	13	ILE

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	
8	BP	134/158 (85%)	126 (94%)	8 (6%)	17	37
9	BQ	176/193 (91%)	168 (96%)	8 (4%)	24	50
10	BR	128/144 (89%)	126 (98%)	2 (2%)	55	79
11	BS	159/160 (99%)	151 (95%)	8 (5%)	22	46
12	BT	153/198 (77%)	150 (98%)	3 (2%)	48	74
13	BU	125/134 (93%)	116 (93%)	9 (7%)	13	30
14	BW	101/108 (94%)	98 (97%)	3 (3%)	36	64
15	BY	55/102 (54%)	55 (100%)	0	100	100
16	BX	104/136 (76%)	100 (96%)	4 (4%)	29	56
17	BZ	105/125 (84%)	95 (90%)	10 (10%)	8	18
18	Bp	70/77 (91%)	65 (93%)	5 (7%)	13	31
19	Bq	46/47 (98%)	44 (96%)	2 (4%)	26	51
20	Br	303/310 (98%)	287 (95%)	16 (5%)	20	43
21	Bt	87/95 (92%)	82 (94%)	5 (6%)	18	40
22	Bw	193/213 (91%)	187 (97%)	6 (3%)	35	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	Bx	196/229 (86%)	186 (95%)	10 (5%)	21	45
24	Bl	122/126 (97%)	118 (97%)	4 (3%)	33	61
25	Bu	193/247 (78%)	188 (97%)	5 (3%)	40	68
26	By	165/172 (96%)	148 (90%)	17 (10%)	7	15
27	A0	189/218 (87%)	181 (96%)	8 (4%)	26	52
28	A2	157/160 (98%)	149 (95%)	8 (5%)	21	45
29	A5	145/180 (81%)	134 (92%)	11 (8%)	12	27
30	AD	76/131 (58%)	69 (91%)	7 (9%)	8	19
31	A8	47/50 (94%)	45 (96%)	2 (4%)	26	51
32	AE	135/156 (86%)	127 (94%)	8 (6%)	18	38
33	AG	124/131 (95%)	119 (96%)	5 (4%)	28	55
34	AI	90/128 (70%)	83 (92%)	7 (8%)	11	26
35	AH	102/112 (91%)	95 (93%)	7 (7%)	14	32
36	AJ	108/109 (99%)	101 (94%)	7 (6%)	15	35
37	AL	96/122 (79%)	88 (92%)	8 (8%)	10	23
38	AM	116/133 (87%)	109 (94%)	7 (6%)	17	37
39	AO	124/137 (90%)	117 (94%)	7 (6%)	19	40
40	AP	182/204 (89%)	166 (91%)	16 (9%)	9	21
41	AS	115/118 (98%)	110 (96%)	5 (4%)	26	51
42	AU	62/94 (66%)	59 (95%)	3 (5%)	23	47
43	AX	176/180 (98%)	164 (93%)	12 (7%)	14	32
44	AZ	48/84 (57%)	44 (92%)	4 (8%)	10	23
45	A3	184/207 (89%)	172 (94%)	12 (6%)	15	35
46	AT	103/116 (89%)	98 (95%)	5 (5%)	22	47
47	A1	219/231 (95%)	204 (93%)	15 (7%)	14	32
48	AC	183/243 (75%)	175 (96%)	8 (4%)	25	50
49	Bc	128/130 (98%)	119 (93%)	9 (7%)	14	31
50	Bz	30/31 (97%)	29 (97%)	1 (3%)	33	61
51	Bo	72/76 (95%)	71 (99%)	1 (1%)	59	81
52	Bn	68/71 (96%)	66 (97%)	2 (3%)	37	65
53	Bm	81/90 (90%)	79 (98%)	2 (2%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	Bk	106/114 (93%)	103 (97%)	3 (3%)	38	66
55	Bj	99/137 (72%)	96 (97%)	3 (3%)	36	64
56	Bi	116/117 (99%)	113 (97%)	3 (3%)	40	68
57	Bg	81/92 (88%)	80 (99%)	1 (1%)	63	83
58	Bd	57/59 (97%)	57 (100%)	0	100	100
59	Bb	115/116 (99%)	111 (96%)	4 (4%)	32	59
60	Ba	114/117 (97%)	110 (96%)	4 (4%)	32	59
61	BO	194/195 (100%)	189 (97%)	5 (3%)	40	68
62	BN	181/188 (96%)	171 (94%)	10 (6%)	19	41
63	BL	134/167 (80%)	119 (89%)	15 (11%)	6	12
64	BK	168/185 (91%)	160 (95%)	8 (5%)	23	47
65	BI	163/165 (99%)	158 (97%)	5 (3%)	35	63
66	Be	191/204 (94%)	187 (98%)	4 (2%)	47	73
67	AK	118/124 (95%)	112 (95%)	6 (5%)	21	45
68	A6	157/166 (95%)	146 (93%)	11 (7%)	14	31
69	Bf	341/360 (95%)	328 (96%)	13 (4%)	29	56
70	AY	48/53 (91%)	44 (92%)	4 (8%)	10	23
71	Bv	119/160 (74%)	109 (92%)	10 (8%)	10	23
72	Bh	128/162 (79%)	120 (94%)	8 (6%)	16	36
76	Bs	41/111 (37%)	39 (95%)	2 (5%)	22	47
77	BV	99/116 (85%)	93 (94%)	6 (6%)	17	37
78	Az	36/216 (17%)	30 (83%)	6 (17%)	2	4
79	AQ	90/104 (86%)	82 (91%)	8 (9%)	9	20
80	AR	71/151 (47%)	63 (89%)	8 (11%)	5	12
81	AV	90/97 (93%)	86 (96%)	4 (4%)	25	50
82	AW	74/75 (99%)	67 (90%)	7 (10%)	8	18
83	A4	172/187 (92%)	153 (89%)	19 (11%)	6	13
84	A7	255/268 (95%)	233 (91%)	22 (9%)	10	22
85	A	4/4 (100%)	4 (100%)	0	100	100
All	All	9337/10826 (86%)	8826 (94%)	511 (6%)	21	41

All (511) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	BP	20	ARG
8	BP	26	VAL
8	BP	31	VAL
8	BP	78	LEU
8	BP	80	SER
8	BP	126	LYS
8	BP	135	ASN
8	BP	142	VAL
9	BQ	78	VAL
9	BQ	106	VAL
9	BQ	117	VAL
9	BQ	138	VAL
9	BQ	145	LEU
9	BQ	152	VAL
9	BQ	172	VAL
9	BQ	204	SER
10	BR	7	LYS
10	BR	64	ASN
11	BS	25	THR
11	BS	65	VAL
11	BS	66	VAL
11	BS	70	LYS
11	BS	128	VAL
11	BS	136	VAL
11	BS	139	LEU
11	BS	166	VAL
12	BT	3	SER
12	BT	55	VAL
12	BT	115	ILE
13	BU	18	LYS
13	BU	28	SER
13	BU	64	VAL
13	BU	68	THR
13	BU	74	VAL
13	BU	84	THR
13	BU	99	SER
13	BU	130	VAL
13	BU	146	LEU
14	BW	15	VAL
14	BW	105	VAL
14	BW	132	SER
16	BX	53	GLN
16	BX	70	SER

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Mol	Chain	Res	Type
16	BX	127	VAL
16	BX	151	SER
17	BZ	47	VAL
17	BZ	57	ARG
17	BZ	59	LYS
17	BZ	90	THR
17	BZ	92	VAL
17	BZ	98	THR
17	BZ	99	SER
17	BZ	105	LYS
17	BZ	117	GLU
17	BZ	122	SER
18	Bp	31	VAL
18	Bp	45	LEU
18	Bp	46	VAL
18	Bp	61	HIS
18	Bp	63	SER
19	Bq	5	LYS
19	Bq	49	LEU
20	Br	47	SER
20	Br	62	SER
20	Br	68	THR
20	Br	84	SER
20	Br	86	SER
20	Br	124	VAL
20	Br	207	MET
20	Br	216	THR
20	Br	226	ASP
20	Br	227	LEU
20	Br	251	THR
20	Br	264	THR
20	Br	269	SER
20	Br	283	THR
20	Br	317	THR
20	Br	325	LEU
21	Bt	2	VAL
21	Bt	15	GLU
21	Bt	26	VAL
21	Bt	57	ILE
21	Bt	63	LYS
22	Bw	100	VAL
22	Bw	172	ASN

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Mol	Chain	Res	Type
22	Bw	211	ARG
22	Bw	231	GLN
22	Bw	232	LYS
22	Bw	248	LEU
23	Bx	49	ILE
23	Bx	99	SER
23	Bx	147	SER
23	Bx	207	THR
23	Bx	214	THR
23	Bx	216	VAL
23	Bx	221	GLN
23	Bx	231	VAL
23	Bx	239	SER
23	Bx	240	ASP
24	Bl	26	THR
24	Bl	27	THR
24	Bl	96	SER
24	Bl	103	SER
25	Bu	46	THR
25	Bu	56	THR
25	Bu	104	LEU
25	Bu	158	ARG
25	Bu	244	ASP
26	By	5	SER
26	By	16	THR
26	By	32	THR
26	By	46	VAL
26	By	82	VAL
26	By	90	VAL
26	By	99	ILE
26	By	129	LYS
26	By	130	VAL
26	By	133	THR
26	By	140	ASP
26	By	144	LEU
26	By	153	SER
26	By	163	CYS
26	By	179	VAL
26	By	181	THR
26	By	184	ASN
27	A0	51	THR
27	A0	54	THR

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Mol	Chain	Res	Type
27	A0	80	ASP
27	A0	108	THR
27	A0	128	GLU
27	A0	130	LYS
27	A0	228	GLN
27	A0	239	THR
28	A2	55	VAL
28	A2	79	VAL
28	A2	82	THR
28	A2	91	ASP
28	A2	92	GLN
28	A2	111	SER
28	A2	112	THR
28	A2	164	VAL
29	A5	4	VAL
29	A5	42	ARG
29	A5	55	LEU
29	A5	64	ASN
29	A5	82	VAL
29	A5	93	THR
29	A5	121	LEU
29	A5	150	ASP
29	A5	171	ILE
29	A5	175	LEU
29	A5	179	LEU
30	AD	23	VAL
30	AD	24	SER
30	AD	32	THR
30	AD	41	THR
30	AD	55	SER
30	AD	62	ILE
30	AD	76	ASN
31	A8	23	VAL
31	A8	56	LEU
32	AE	14	VAL
32	AE	28	THR
32	AE	78	SER
32	AE	86	ILE
32	AE	91	VAL
32	AE	95	LYS
32	AE	128	SER
32	AE	156	LEU

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Mol	Chain	Res	Type
33	AG	26	LEU
33	AG	38	CYS
33	AG	46	SER
33	AG	66	VAL
33	AG	87	ASP
34	AI	23	THR
34	AI	45	HIS
34	AI	74	VAL
34	AI	75	LYS
34	AI	99	SER
34	AI	107	ARG
34	AI	123	LEU
35	AH	29	SER
35	AH	45	THR
35	AH	68	MET
35	AH	74	VAL
35	AH	78	CYS
35	AH	100	SER
35	AH	142	ARG
36	AJ	2	THR
36	AJ	6	VAL
36	AJ	25	VAL
36	AJ	30	SER
36	AJ	54	ASP
36	AJ	78	ARG
36	AJ	111	MET
37	AL	32	LYS
37	AL	39	THR
37	AL	57	ILE
37	AL	67	ARG
37	AL	69	ILE
37	AL	91	VAL
37	AL	104	GLN
37	AL	114	THR
38	AM	3	LEU
38	AM	4	THR
38	AM	39	ILE
38	AM	100	THR
38	AM	102	SER
38	AM	104	VAL
38	AM	117	LYS
39	AO	49	ASN

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Mol	Chain	Res	Type
39	AO	56	THR
39	AO	57	SER
39	AO	77	VAL
39	AO	116	LEU
39	AO	123	SER
39	AO	129	LEU
40	AP	53	VAL
40	AP	68	SER
40	AP	86	LEU
40	AP	101	SER
40	AP	131	VAL
40	AP	132	SER
40	AP	138	SER
40	AP	146	ILE
40	AP	149	VAL
40	AP	167	LYS
40	AP	196	LYS
40	AP	210	SER
40	AP	211	CYS
40	AP	220	PHE
40	AP	231	THR
40	AP	254	SER
41	AS	32	THR
41	AS	45	SER
41	AS	57	VAL
41	AS	108	SER
41	AS	127	SER
42	AU	62	LYS
42	AU	75	LEU
42	AU	97	LEU
43	AX	4	LEU
43	AX	24	LEU
43	AX	38	HIS
43	AX	41	THR
43	AX	44	ARG
43	AX	83	LEU
43	AX	112	LEU
43	AX	148	SER
43	AX	152	ARG
43	AX	169	THR
43	AX	171	THR
43	AX	205	THR

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Mol	Chain	Res	Type
44	AZ	57	THR
44	AZ	61	VAL
44	AZ	73	ASN
44	AZ	75	THR
45	A3	19	THR
45	A3	57	SER
45	A3	64	MET
45	A3	72	SER
45	A3	75	SER
45	A3	83	VAL
45	A3	97	ARG
45	A3	147	LEU
45	A3	150	LEU
45	A3	156	VAL
45	A3	186	THR
45	A3	204	LYS
46	AT	40	THR
46	AT	41	VAL
46	AT	63	SER
46	AT	81	LEU
46	AT	86	LEU
47	A1	20	LEU
47	A1	49	LEU
47	A1	78	LYS
47	A1	92	THR
47	A1	101	ASP
47	A1	128	THR
47	A1	130	THR
47	A1	135	VAL
47	A1	138	THR
47	A1	155	ASP
47	A1	177	VAL
47	A1	181	THR
47	A1	224	VAL
47	A1	238	LYS
47	A1	247	ILE
48	AC	35	THR
48	AC	77	ARG
48	AC	127	SER
48	AC	133	SER
48	AC	135	LEU
48	AC	172	GLU

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Mol	Chain	Res	Type
48	AC	204	ARG
48	AC	208	SER
49	Bc	17	LYS
49	Bc	29	SER
49	Bc	63	THR
49	Bc	66	SER
49	Bc	69	THR
49	Bc	83	GLU
49	Bc	89	SER
49	Bc	90	VAL
49	Bc	135	HIS
50	Bz	33	SER
51	Bo	52	VAL
52	Bn	7	SER
52	Bn	59	THR
53	Bm	34	SER
53	Bm	95	ARG
54	Bk	40	VAL
54	Bk	86	THR
54	Bk	125	VAL
55	Bj	3	CYS
55	Bj	23	LEU
55	Bj	104	VAL
56	Bi	70	SER
56	Bi	77	VAL
56	Bi	121	ILE
57	Bg	72	THR
59	Bb	27	LYS
59	Bb	85	ASP
59	Bb	116	GLN
59	Bb	127	SER
60	Ba	52	VAL
60	Ba	89	SER
60	Ba	98	VAL
60	Ba	106	LYS
61	BO	8	SER
61	BO	40	ILE
61	BO	41	VAL
61	BO	144	ARG
61	BO	169	SER
62	BN	14	ARG
62	BN	97	THR

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Mol	Chain	Res	Type
62	BN	127	LYS
62	BN	129	VAL
62	BN	168	THR
62	BN	178	THR
62	BN	180	GLU
62	BN	183	THR
62	BN	188	LYS
62	BN	211	GLU
63	BL	21	VAL
63	BL	24	LEU
63	BL	55	SER
63	BL	72	ILE
63	BL	74	VAL
63	BL	76	CYS
63	BL	77	THR
63	BL	91	LEU
63	BL	102	ASN
63	BL	126	SER
63	BL	136	VAL
63	BL	153	SER
63	BL	158	ASN
63	BL	175	ASP
63	BL	178	ILE
64	BK	13	LYS
64	BK	33	THR
64	BK	43	VAL
64	BK	52	VAL
64	BK	53	VAL
64	BK	113	THR
64	BK	166	VAL
64	BK	197	VAL
65	BI	3	VAL
65	BI	76	VAL
65	BI	100	THR
65	BI	136	MET
65	BI	183	SER
66	Be	18	VAL
66	Be	80	GLU
66	Be	242	ARG
66	Be	245	ARG
67	AK	28	THR
67	AK	69	LEU

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Mol	Chain	Res	Type
67	AK	73	VAL
67	AK	75	VAL
67	AK	142	THR
67	AK	147	SER
68	A6	19	GLU
68	A6	30	CYS
68	A6	49	SER
68	A6	73	SER
68	A6	88	ASP
68	A6	100	VAL
68	A6	120	SER
68	A6	121	VAL
68	A6	126	VAL
68	A6	149	VAL
68	A6	172	LYS
69	Bf	2	SER
69	Bf	24	GLN
69	Bf	38	SER
69	Bf	60	VAL
69	Bf	135	GLN
69	Bf	178	VAL
69	Bf	217	SER
69	Bf	283	LEU
69	Bf	295	SER
69	Bf	335	VAL
69	Bf	339	ARG
69	Bf	370	SER
69	Bf	392	LYS
70	AY	14	VAL
70	AY	18	THR
70	AY	22	SER
70	AY	54	LYS
71	Bv	28	LYS
71	Bv	47	ARG
71	Bv	60	LEU
71	Bv	66	MET
71	Bv	78	SER
71	Bv	85	SER
71	Bv	86	THR
71	Bv	93	VAL
71	Bv	144	SER
71	Bv	154	ILE

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Mol	Chain	Res	Type
72	Bh	28	GLU
72	Bh	32	SER
72	Bh	42	LEU
72	Bh	56	VAL
72	Bh	59	THR
72	Bh	102	HIS
72	Bh	155	SER
72	Bh	168	THR
76	Bs	105	VAL
76	Bs	117	HIS
77	BV	39	PHE
77	BV	43	ILE
77	BV	81	THR
77	BV	82	THR
77	BV	93	LEU
77	BV	96	LYS
78	Az	166	THR
78	Az	175	GLU
78	Az	185	ILE
78	Az	187	THR
78	Az	213	THR
78	Az	222	VAL
79	AQ	19	VAL
79	AQ	45	VAL
79	AQ	51	VAL
79	AQ	53	LEU
79	AQ	61	THR
79	AQ	92	THR
79	AQ	100	SER
79	AQ	112	THR
80	AR	3	THR
80	AR	10	GLU
80	AR	14	VAL
80	AR	31	SER
80	AR	66	GLN
80	AR	70	ASP
80	AR	85	ILE
80	AR	87	THR
81	AV	30	ARG
81	AV	94	GLU
81	AV	102	SER
81	AV	104	VAL

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Mol	Chain	Res	Type
82	AW	5	ASP
82	AW	6	SER
82	AW	9	SER
82	AW	45	THR
82	AW	63	LEU
82	AW	68	THR
82	AW	76	THR
83	A4	6	HIS
83	A4	35	SER
83	A4	47	HIS
83	A4	48	ILE
83	A4	50	THR
83	A4	55	SER
83	A4	59	HIS
83	A4	62	THR
83	A4	76	VAL
83	A4	82	THR
83	A4	97	VAL
83	A4	103	LYS
83	A4	120	SER
83	A4	157	VAL
83	A4	171	LEU
83	A4	182	THR
83	A4	185	THR
83	A4	187	THR
83	A4	200	SER
84	A7	28	THR
84	A7	77	ASN
84	A7	101	CYS
84	A7	111	ASP
84	A7	130	ASP
84	A7	138	VAL
84	A7	146	LEU
84	A7	152	THR
84	A7	156	SER
84	A7	175	ASP
84	A7	189	VAL
84	A7	199	VAL
84	A7	200	THR
84	A7	202	VAL
84	A7	244	CYS
84	A7	250	TYR

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Mol	Chain	Res	Type
84	A7	256	THR
84	A7	265	LEU
84	A7	284	ILE
84	A7	299	THR
84	A7	311	VAL
84	A7	314	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
8	BP	21	GLN
9	BQ	25	ASN
9	BQ	129	ASN
9	BQ	175	HIS
10	BR	72	GLN
10	BR	97	ASN
11	BS	85	GLN
11	BS	147	HIS
13	BU	66	ASN
13	BU	107	GLN
16	BX	101	ASN
17	BZ	78	HIS
18	Bp	41	HIS
19	Bq	33	ASN
20	Br	33	HIS
21	Bt	59	HIS
22	Bw	125	GLN
22	Bw	209	HIS
22	Bw	231	GLN
23	Bx	168	ASN
23	Bx	186	ASN
24	Bl	52	HIS
24	Bl	55	ASN
24	Bl	65	ASN
25	Bu	197	ASN
26	By	6	HIS
26	By	41	GLN
27	A0	69	ASN
27	A0	94	GLN
27	A0	184	ASN
28	A2	16	ASN
28	A2	93	ASN

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Mol	Chain	Res	Type
29	A5	209	GLN
31	A8	21	HIS
31	A8	27	ASN
31	A8	28	GLN
32	AE	25	GLN
32	AE	126	HIS
33	AG	7	ASN
34	AI	121	HIS
36	AJ	113	HIS
37	AL	31	ASN
38	AM	135	GLN
39	AO	27	HIS
39	AO	101	ASN
40	AP	97	GLN
40	AP	104	GLN
40	AP	120	HIS
40	AP	156	ASN
41	AS	36	GLN
43	AX	77	ASN
44	AZ	39	GLN
46	AT	119	ASN
48	AC	168	GLN
49	Bc	34	ASN
50	Bz	15	HIS
52	Bn	10	GLN
52	Bn	25	ASN
52	Bn	71	HIS
55	Bj	72	GLN
56	Bi	9	ASN
56	Bi	21	HIS
57	Bg	22	ASN
58	Bd	9	ASN
58	Bd	70	GLN
59	Bb	116	GLN
60	Ba	124	ASN
61	BO	199	ASN
62	BN	16	HIS
62	BN	18	ASN
64	BK	59	GLN
65	BI	17	HIS
65	BI	49	HIS
65	BI	58	ASN

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Mol	Chain	Res	Type
65	BI	168	HIS
66	Be	86	GLN
66	Be	218	HIS
68	A6	115	HIS
68	A6	138	GLN
69	Bf	11	HIS
69	Bf	135	GLN
69	Bf	195	GLN
70	AY	24	GLN
70	AY	60	GLN
71	Bv	151	GLN
72	Bh	125	ASN
76	Bs	90	ASN
78	Az	211	ASN
82	AW	27	GLN
83	A4	94	ASN
83	A4	129	ASN
84	A7	23	GLN
84	A7	46	ASN
84	A7	97	GLN
84	A7	137	ASN
84	A7	242	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1811/2280 (79%)	485 (26%)	19 (1%)
2	AB	17/19 (89%)	8 (47%)	0
3	BA	1553/1920 (80%)	292 (18%)	8 (0%)
4	BB	1102/1536 (71%)	209 (18%)	3 (0%)
5	BC	157/209 (75%)	27 (17%)	0
6	BD	118/119 (99%)	16 (13%)	1 (0%)
7	BE	161/216 (74%)	23 (14%)	2 (1%)
73	BF	66/78 (84%)	18 (27%)	0
74	BG	182/183 (99%)	30 (16%)	1 (0%)
75	BH	114/136 (83%)	21 (18%)	0
All	All	5281/6696 (78%)	1129 (21%)	34 (0%)

All (1129) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	32	C
1	AA	34	G
1	AA	45	C
1	AA	46	OMC
1	AA	51	G
1	AA	53	C
1	AA	54	A
1	AA	62	G
1	AA	70	G
1	AA	73	U
1	AA	75	A
1	AA	79	A
1	AA	87	C
1	AA	91	G
1	AA	93	A
1	AA	94	U
1	AA	118	A
1	AA	128	A
1	AA	130	A
1	AA	135	A
1	AA	136	C
1	AA	139	A
1	AA	140	A
1	AA	141	U
1	AA	144	G
1	AA	148	C
1	AA	155	U
1	AA	158	G
1	AA	169	A
1	AA	172	A
1	AA	173	C
1	AA	174	U
1	AA	179	A
1	AA	182	U
1	AA	183	U
1	AA	185	G
1	AA	190	A
1	AA	191	C
1	AA	208	A
1	AA	209	A
1	AA	210	C
1	AA	211	C
1	AA	212	A

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Mol	Chain	Res	Type
1	AA	213	A
1	AA	221	C
1	AA	222	U
1	AA	223	C
1	AA	227	U
1	AA	270	G
1	AA	274	C
1	AA	280	G
1	AA	292	A
1	AA	293	A
1	AA	302	A
1	AA	303	A
1	AA	304	C
1	AA	305	G
1	AA	309	C
1	AA	315	G
1	AA	316	G
1	AA	317	A
1	AA	319	G
1	AA	320	C
1	AA	322	G
1	AA	324	A
1	AA	325	A
1	AA	326	C
1	AA	327	A
1	AA	329	U
1	AA	330	C
1	AA	331	A
1	AA	334	C
1	AA	340	G
1	AA	341	A
1	AA	344	C
1	AA	354	C
1	AA	355	G
1	AA	356	U
1	AA	360	A
1	AA	362	A
1	AA	363	G
1	AA	364	C
1	AA	367	A
1	AA	369	C
1	AA	376	G

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Mol	Chain	Res	Type
1	AA	390	G
1	AA	393	G
1	AA	395	A
1	AA	398	A
1	AA	399	C
1	AA	403	C
1	AA	407	U
1	AA	408	C
1	AA	410	G
1	AA	414	G
1	AA	419	G
1	AA	422	C
1	AA	425	G
1	AA	432	A
1	AA	447	A
1	AA	454	C
1	AA	463	A
1	AA	473	U
1	AA	483	G
1	AA	485	G
1	AA	489	G
1	AA	492	A
1	AA	493	A
1	AA	494	A
1	AA	495	U
1	AA	504	C
1	AA	511	G
1	AA	512	G
1	AA	517	C
1	AA	527	G
1	AA	532	U
1	AA	537	C
1	AA	538	A
1	AA	545	A
1	AA	546	A
1	AA	549	A
1	AA	550	A
1	AA	551	U
1	AA	552	A
1	AA	553	C
1	AA	558	A
1	AA	559	G

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Mol	Chain	Res	Type
1	AA	566	A
1	AA	573	A
1	AA	575	A
1	AA	578	G
1	AA	580	C
1	AA	583	C
1	AA	585	G
1	AA	586	U
1	AA	599	G
1	AA	601	U
1	AA	602	U
1	AA	603	G
1	AA	604	U
1	AA	605	U
1	AA	606	U
1	AA	607	U
1	AA	608	C
1	AA	612	G
1	AA	613	G
1	AA	614	G
1	AA	615	G
1	AA	616	G
1	AA	618	U
1	AA	619	A
1	AA	623	A
1	AA	624	A
1	AA	625	A
1	AA	631	U
1	AA	632	C
1	AA	633	A
1	AA	635	U
1	AA	636	A
1	AA	638	C
1	AA	640	A
1	AA	642	U
1	AA	643	A
1	AA	644	A
1	AA	658	A
1	AA	659	G
1	AA	660	U
1	AA	667	C
1	AA	673	C

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Mol	Chain	Res	Type
1	AA	681	A
1	AA	694	A
1	AA	695	A
1	AA	696	A
1	AA	712	G
1	AA	713	U
1	AA	721	A2M
1	AA	722	A
1	AA	725	G
1	AA	726	G
1	AA	740	U
1	AA	742	U
1	AA	743	G
1	AA	747	C
1	AA	748	A
1	AA	753	G
1	AA	754	U
1	AA	757	G
1	AA	758	G
1	AA	779	C
1	AA	781	U
1	AA	786	C
1	AA	789	G
1	AA	790	U
1	AA	793	U
1	AA	800	C
1	AA	801	G
1	AA	805	U
1	AA	806	C
1	AA	807	G
1	AA	809	G
1	AA	811	C
1	AA	826	A
1	AA	828	A
1	AA	829	U
1	AA	837	A
1	AA	839	A
1	AA	842	G
1	AA	844	A
1	AA	845	G
1	AA	846	C
1	AA	847	A

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Mol	Chain	Res	Type
1	AA	848	G
1	AA	851	C
1	AA	867	C
1	AA	868	A
1	AA	873	A
1	AA	874	U
1	AA	877	A
1	AA	879	G
1	AA	887	G
1	AA	888	C
1	AA	889	G
1	AA	890	U
1	AA	899	U
1	AA	900	U
1	AA	904	U
1	AA	907	G
1	AA	909	C
1	AA	911	A
1	AA	912	A
1	AA	917	A
1	AA	918	U
1	AA	920	C
1	AA	921	G
1	AA	922	A
1	AA	930	A
1	AA	931	G
1	AA	934	U
1	AA	935	G
1	AA	936	C
1	AA	938	G
1	AA	941	U
1	AA	948	A
1	AA	949	C
1	AA	954	C
1	AA	955	A
1	AA	956	U
1	AA	957	G
1	AA	959	G
1	AA	961	U
1	AA	963	A
1	AA	967	A
1	AA	968	G

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Mol	Chain	Res	Type
1	AA	969	C
1	AA	970	A
1	AA	971	U
1	AA	972	C
1	AA	974	G
1	AA	997	U
1	AA	998	A
1	AA	999	U
1	AA	1000	G
1	AA	1005	U
1	AA	1006	U
1	AA	1007	U
1	AA	1008	U
1	AA	1009	A
1	AA	1013	G
1	AA	1017	U
1	AA	1020	G
1	AA	1025	U
1	AA	1027	A
1	AA	1120	G
1	AA	1121	C
1	AA	1122	G
1	AA	1126	C
1	AA	1129	C
1	AA	1135	A
1	AA	1139	A
1	AA	1149	U
1	AA	1153	G
1	AA	1158	G
1	AA	1160	A
1	AA	1163	U
1	AA	1183	A
1	AA	1186	U
1	AA	1192	A
1	AA	1198	C
1	AA	1210	A
1	AA	1212	A
1	AA	1222	U
1	AA	1229	A
1	AA	1236	C
1	AA	1237	U
1	AA	1241	U

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Mol	Chain	Res	Type
1	AA	1243	A
1	AA	1265	A
1	AA	1269	A
1	AA	1275	A
1	AA	1282	A
1	AA	1291	G
1	AA	1298	C
1	AA	1301	C
1	AA	1303	A
1	AA	1305	C
1	AA	1316	A
1	AA	1318	G
1	AA	1401	U
1	AA	1462	U
1	AA	1463	C
1	AA	1464	A
1	AA	1479	U
1	AA	1482	U
1	AA	1483	C
1	AA	1484	A
1	AA	1485	C
1	AA	1496	G
1	AA	1501	U
1	AA	1502	U
1	AA	1504	C
1	AA	1505	A
1	AA	1506	G
1	AA	1519	G
1	AA	1536	A
1	AA	1541	U
1	AA	1543	A
1	AA	1555	G
1	AA	1556	A
1	AA	1560	G
1	AA	1563	C
1	AA	1564	C
1	AA	1590	U
1	AA	1596	B8N
1	AA	1599	A
1	AA	1601	A
1	AA	1604	G
1	AA	1605	G

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Mol	Chain	Res	Type
1	AA	1606	G
1	AA	1607	A
1	AA	1617	G
1	AA	1619	PSU
1	AA	1622	G
1	AA	1623	G
1	AA	1628	G
1	AA	1629	G
1	AA	1633	G
1	AA	1634	G
1	AA	1638	G
1	AA	1640	C
1	AA	1642	G
1	AA	1644	U
1	AA	1651	U
1	AA	1656	U
1	AA	1657	C
1	AA	1661	A
1	AA	1668	G
1	AA	1669	A
1	AA	1676	OMG
1	AA	1696	G
1	AA	1706	U
1	AA	1711	U
1	AA	1714	G
1	AA	1719	U
1	AA	1720	U
1	AA	1726	A
1	AA	1730	G
1	AA	1732	C
1	AA	1746	C
1	AA	1749	A
1	AA	1751	U
1	AA	1752	A
1	AA	1754	G
1	AA	1756	G
1	AA	1763	U
1	AA	1764	U
1	AA	1765	G
1	AA	1767	C
1	AA	1768	C
1	AA	1770	C

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Mol	Chain	Res	Type
1	AA	1774	G
1	AA	1775	G
1	AA	1776	A
1	AA	1780	C
1	AA	1822	U
1	AA	1824	C
1	AA	1825	U
1	AA	1827	C
1	AA	1830	U
1	AA	1837	G
1	AA	1841	C
1	AA	1850	G
1	AA	1853	A
1	AA	1854	U
1	AA	1855	U
1	AA	1857	C
1	AA	1862	U
1	AA	1863	U
1	AA	1865	U
1	AA	1870	C
1	AA	1875	U
1	AA	1876	G
1	AA	1879	A
1	AA	1880	U
1	AA	1881	U
1	AA	1882	U
1	AA	1885	G
1	AA	1892	G
1	AA	1894	A
1	AA	1895	OMG
1	AA	1899	OMU
1	AA	1902	G
1	AA	1903	A
1	AA	1906	C
1	AA	1912	A
1	AA	1926	C
1	AA	1927	A
1	AA	1928	C
1	AA	1936	A
1	AA	1938	A
1	AA	1941	G
1	AA	1946	U

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Mol	Chain	Res	Type
1	AA	1950	A
1	AA	1951	A
1	AA	1953	A
1	AA	1956	A
1	AA	1957	G
1	AA	1958	U
1	AA	1987	G
1	AA	1991	G
1	AA	1994	C
1	AA	1998	A
1	AA	1999	G
1	AA	2001	G
1	AA	2002	C
1	AA	2008	A
1	AA	2009	A
1	AA	2010	C
1	AA	2013	C
1	AA	2014	G
1	AA	2018	U
1	AA	2019	C
1	AA	2023	U
1	AA	2024	A
1	AA	2025	G
1	AA	2030	A
1	AA	2031	C
1	AA	2036	G
1	AA	2051	U
1	AA	2053	A
1	AA	2054	OMU
1	AA	2057	G
1	AA	2063	C
1	AA	2064	A
1	AA	2069	G
1	AA	2075	U
1	AA	2078	C
1	AA	2079	G
1	AA	2080	U
1	AA	2085	G
1	AA	2096	A2M
1	AA	2102	G
1	AA	2104	C
1	AA	2111	G

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Mol	Chain	Res	Type
1	AA	2126	A
1	AA	2129	C
1	AA	2161	A
1	AA	2175	A
1	AA	2178	G
1	AA	2200	A
1	AA	2228	A
1	AA	2235	A
1	AA	2236	G
1	AA	2239	G
1	AA	2241	A
1	AA	2245	A
1	AA	2248	U
1	AA	2249	A
1	AA	2259	G
1	AA	2261	MA6
1	AA	2271	G
1	AA	2272	G
1	AA	2273	A
1	AA	2274	U
1	AA	2275	C
1	AA	2278	U
2	AB	4	C
2	AB	66	U
2	AB	67	C
2	AB	70	G
2	AB	71	G
2	AB	74	C
2	AB	75	C
2	AB	76	A
3	BA	8	G
3	BA	28	A
3	BA	33	C
3	BA	42	A
3	BA	45	A
3	BA	51	C
3	BA	62	A
3	BA	68	A
3	BA	91	A
3	BA	95	G
3	BA	96	C
3	BA	102	A

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Mol	Chain	Res	Type
3	BA	112	C
3	BA	113	A
3	BA	114	A
3	BA	125	A
3	BA	135	U
3	BA	138	A
3	BA	139	U
3	BA	140	G
3	BA	146	G
3	BA	156	A
3	BA	179	A
3	BA	184	U
3	BA	190	A
3	BA	197	G
3	BA	204	U
3	BA	205	C
3	BA	212	A
3	BA	213	A
3	BA	218	A
3	BA	221	C
3	BA	224	U
3	BA	225	U
3	BA	226	G
3	BA	228	U
3	BA	231	A
3	BA	242	A
3	BA	249	A
3	BA	250	U
3	BA	252	U
3	BA	253	G
3	BA	268	G
3	BA	269	A
3	BA	270	A
3	BA	274	G
3	BA	275	U
3	BA	276	C
3	BA	285	A
3	BA	286	C
3	BA	298	A
3	BA	308	C
3	BA	336	G
3	BA	353	U

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Mol	Chain	Res	Type
3	BA	362	A
3	BA	365	C
3	BA	366	C
3	BA	373	U
3	BA	391	A
3	BA	397	A
3	BA	398	G
3	BA	399	A
3	BA	400	G
3	BA	403	G
3	BA	404	G
3	BA	406	A
3	BA	420	C
3	BA	421	A
3	BA	439	U
3	BA	440	U
3	BA	447	G
3	BA	470	A
3	BA	473	A
3	BA	474	C
3	BA	475	C
3	BA	489	A
3	BA	491	G
3	BA	493	C
3	BA	494	A
3	BA	495	A
3	BA	501	G
3	BA	506	U
3	BA	507	U
3	BA	508	C
3	BA	514	U
3	BA	527	G
3	BA	545	G
3	BA	550	A
3	BA	552	U
3	BA	553	U
3	BA	554	C
3	BA	557	U
3	BA	560	G
3	BA	575	G
3	BA	579	G
3	BA	580	U

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Mol	Chain	Res	Type
3	BA	587	U
3	BA	591	C
3	BA	597	U
3	BA	598	C
3	BA	611	A
3	BA	615	G
3	BA	616	G
3	BA	617	U
3	BA	621	U
3	BA	627	G
3	BA	635	A
3	BA	636	A
3	BA	637	A
3	BA	638	G
3	BA	639	G
3	BA	646	G
3	BA	654	U
3	BA	677	U
3	BA	681	U
3	BA	682	C
3	BA	686	C
3	BA	690	G
3	BA	697	C
3	BA	699	U
3	BA	705	C
3	BA	706	G
3	BA	716	G
3	BA	717	A
3	BA	718	A
3	BA	733	C
3	BA	742	1MA
3	BA	745	C
3	BA	746	A2M
3	BA	757	A
3	BA	774	A
3	BA	785	U
3	BA	791	U
3	BA	792	G
3	BA	793	A
3	BA	802	U
3	BA	803	U
3	BA	809	A

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Mol	Chain	Res	Type
3	BA	816	G
3	BA	819	A
3	BA	834	C
3	BA	836	C
3	BA	837	G
3	BA	838	U
3	BA	845	C
3	BA	846	G
3	BA	868	U
3	BA	876	C
3	BA	883	C
3	BA	886	C
3	BA	894	G
3	BA	896	G
3	BA	900	C
3	BA	901	G
3	BA	905	G
3	BA	919	G
3	BA	926	A
3	BA	937	A
3	BA	950	A
3	BA	963	G
3	BA	967	A
3	BA	969	C
3	BA	981	C
3	BA	994	U
3	BA	999	U
3	BA	1027	G
3	BA	1028	OMG
3	BA	1029	A
3	BA	1034	A
3	BA	1036	G
3	BA	1041	A
3	BA	1043	C
3	BA	1044	G
3	BA	1045	A
3	BA	1057	G
3	BA	1064	C
3	BA	1079	C
3	BA	1080	U
3	BA	1094	G
3	BA	1097	U

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Mol	Chain	Res	Type
3	BA	1105	A
3	BA	1107	A
3	BA	1119	G
3	BA	1127	A
3	BA	1172	A
3	BA	1174	C
3	BA	1182	G
3	BA	1189	C
3	BA	1190	A
3	BA	1193	C
3	BA	1202	G
3	BA	1212	C
3	BA	1235	U
3	BA	1236	U
3	BA	1238	A
3	BA	1242	A
3	BA	1251	G
3	BA	1265	G
3	BA	1278	U
3	BA	1284	A
3	BA	1288	A
3	BA	1293	U
3	BA	1312	A
3	BA	1316	U
3	BA	1317	U
3	BA	1319	U
3	BA	1320	G
3	BA	1322	G
3	BA	1327	U
3	BA	1328	U
3	BA	1330	U
3	BA	1331	C
3	BA	1334	U
3	BA	1337	G
3	BA	1339	G
3	BA	1340	A
3	BA	1341	A
3	BA	1347	U
3	BA	1442	A
3	BA	1447	A
3	BA	1448	OMU
3	BA	1452	G

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Mol	Chain	Res	Type
3	BA	1455	U
3	BA	1456	A
3	BA	1461	C
3	BA	1469	G
3	BA	1470	U
3	BA	1471	G
3	BA	1472	A
3	BA	1480	U
3	BA	1481	U
3	BA	1491	G
3	BA	1492	U
3	BA	1499	G
3	BA	1500	G
3	BA	1501	C
3	BA	1502	U
3	BA	1503	A
3	BA	1505	A
3	BA	1519	A
3	BA	1526	G
3	BA	1545	G
3	BA	1562	G
3	BA	1571	G
3	BA	1585	A
3	BA	1586	U
3	BA	1590	C
3	BA	1602	G
3	BA	1605	OMG
3	BA	1608	OMC
3	BA	1615	G
3	BA	1617	C
3	BA	1626	G
3	BA	1637	A
3	BA	1638	U
3	BA	1639	A
3	BA	1642	U
3	BA	1643	U
3	BA	1650	A
3	BA	1652	U
3	BA	1653	G
3	BA	1654	C
3	BA	1665	A2M
3	BA	1669	G

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Mol	Chain	Res	Type
3	BA	1672	C
3	BA	1673	G
3	BA	1696	C
3	BA	1710	U
3	BA	1722	U
3	BA	1728	C
3	BA	1737	A
3	BA	1738	C
3	BA	1744	U
3	BA	1746	U
3	BA	1749	G
3	BA	1750	G
3	BA	1751	A
3	BA	1754	G
3	BA	1816	A
3	BA	1818	A
3	BA	1827	A
3	BA	1832	A
3	BA	1835	U
3	BA	1839	A
3	BA	1844	A
3	BA	1846	U
3	BA	1851	A
3	BA	1854	G
3	BA	1858	U
3	BA	1861	A
3	BA	1865	G
3	BA	1867	G
4	BB	12	G
4	BB	18	A
4	BB	22	A
4	BB	25	A
4	BB	29	C
4	BB	30	A
4	BB	33	A
4	BB	61	C
4	BB	63	U
4	BB	64	A
4	BB	68	A
4	BB	69	A
4	BB	75	C
4	BB	90	G

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Mol	Chain	Res	Type
4	BB	136	A
4	BB	367	C
4	BB	380	A
4	BB	381	C
4	BB	386	G
4	BB	395	A
4	BB	398	G
4	BB	400	A2M
4	BB	404	U
4	BB	422	A
4	BB	434	G
4	BB	452	A
4	BB	469	U
4	BB	470	G
4	BB	471	A
4	BB	478	A
4	BB	483	A
4	BB	487	G
4	BB	513	G
4	BB	520	A
4	BB	521	C
4	BB	522	PSU
4	BB	525	G
4	BB	527	C
4	BB	531	C
4	BB	536	G
4	BB	537	G
4	BB	545	A2M
4	BB	548	C
4	BB	552	OMG
4	BB	571	G
4	BB	574	U
4	BB	577	A
4	BB	578	OMU
4	BB	579	G
4	BB	598	U
4	BB	600	U
4	BB	629	PSU
4	BB	637	A
4	BB	638	C
4	BB	639	G
4	BB	650	G

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Mol	Chain	Res	Type
4	BB	657	G
4	BB	660	G
4	BB	661	A
4	BB	665	A
4	BB	666	A
4	BB	667	G
4	BB	668	A
4	BB	675	U
4	BB	676	G
4	BB	683	A
4	BB	704	G
4	BB	766	C
4	BB	767	G
4	BB	768	U
4	BB	772	U
4	BB	778	U
4	BB	779	A
4	BB	786	G
4	BB	787	A
4	BB	789	G
4	BB	790	A
4	BB	798	G
4	BB	799	G
4	BB	800	U
4	BB	803	U
4	BB	804	U
4	BB	806	U
4	BB	807	G
4	BB	819	G
4	BB	825	G
4	BB	831	U
4	BB	837	C
4	BB	975	G
4	BB	977	A
4	BB	978	A
4	BB	980	U
4	BB	983	U
4	BB	985	C
4	BB	990	A
4	BB	991	C
4	BB	995	G
4	BB	996	U

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Mol	Chain	Res	Type
4	BB	1017	C
4	BB	1023	U
4	BB	1026	U
4	BB	1027	G
4	BB	1028	U
4	BB	1035	A
4	BB	1038	U
4	BB	1049	G
4	BB	1050	G
4	BB	1057	G
4	BB	1062	OMG
4	BB	1069	A
4	BB	1095	U
4	BB	1098	U
4	BB	1099	A
4	BB	1132	G
4	BB	1134	A
4	BB	1137	A
4	BB	1139	A
4	BB	1147	A
4	BB	1157	G
4	BB	1162	A
4	BB	1163	C
4	BB	1172	G
4	BB	1173	U
4	BB	1190	A
4	BB	1191	A
4	BB	1193	G
4	BB	1197	G
4	BB	1199	C
4	BB	1205	A
4	BB	1215	A
4	BB	1221	A
4	BB	1222	G
4	BB	1223	G
4	BB	1225	A
4	BB	1226	A
4	BB	1231	A
4	BB	1232	A
4	BB	1241	A
4	BB	1250	G
4	BB	1253	A

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Mol	Chain	Res	Type
4	BB	1254	G
4	BB	1255	A
4	BB	1257	U
4	BB	1264	OMC
4	BB	1268	G
4	BB	1271	A
4	BB	1272	U
4	BB	1287	G
4	BB	1292	A
4	BB	1298	C
4	BB	1299	A
4	BB	1303	C
4	BB	1314	U
4	BB	1321	C
4	BB	1325	G
4	BB	1327	U
4	BB	1329	U
4	BB	1341	A
4	BB	1343	C
4	BB	1352	G
4	BB	1354	A
4	BB	1365	A
4	BB	1377	U
4	BB	1384	A
4	BB	1389	C
4	BB	1390	A
4	BB	1396	C
4	BB	1401	G
4	BB	1408	U
4	BB	1425	A
4	BB	1426	G
4	BB	1432	U
4	BB	1437	C
4	BB	1444	U
4	BB	1446	G
4	BB	1452	G
4	BB	1453	A
4	BB	1457	C
4	BB	1458	G
4	BB	1459	A
4	BB	1460	G
4	BB	1461	U

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Mol	Chain	Res	Type
4	BB	1464	A
4	BB	1468	U
4	BB	1470	A
4	BB	1478	A
4	BB	1479	A
4	BB	1486	G
4	BB	1487	G
4	BB	1494	G
4	BB	1495	U
4	BB	1496	U
4	BB	1498	U
4	BB	1500	U
4	BB	1502	C
4	BB	1505	G
4	BB	1506	G
4	BB	1507	U
4	BB	1509	U
4	BB	1514	U
4	BB	1516	G
4	BB	1519	U
4	BB	1523	A
4	BB	1524	U
4	BB	1526	U
4	BB	1527	G
4	BB	1530	U
4	BB	1532	G
4	BB	1536	U
5	BC	2	A
5	BC	22	U
5	BC	33	U
5	BC	34	U
5	BC	48	A
5	BC	59	A
5	BC	62	A
5	BC	63	G
5	BC	75	OMG
5	BC	77	A
5	BC	79	A
5	BC	87	C
5	BC	88	A
5	BC	94	C
5	BC	103	A

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Mol	Chain	Res	Type
5	BC	105	C
5	BC	110	A
5	BC	120	G
5	BC	124	A
5	BC	138	C
5	BC	149	A
5	BC	157	U
5	BC	158	U
5	BC	159	U
5	BC	162	C
5	BC	165	U
5	BC	169	G
6	BD	12	U
6	BD	22	A
6	BD	25	G
6	BD	40	C
6	BD	49	A
6	BD	50	A
6	BD	52	U
6	BD	53	U
6	BD	54	A
6	BD	63	C
6	BD	64	A
6	BD	73	U
6	BD	97	U
6	BD	100	A
6	BD	110	G
6	BD	117	U
7	BE	11	U
7	BE	23	G
7	BE	32	C
7	BE	34	C
7	BE	35	A
7	BE	40	U
7	BE	44	C
7	BE	46	C
7	BE	57	U
7	BE	59	C
7	BE	70	A
7	BE	97	U
7	BE	107	C
7	BE	108	G

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Mol	Chain	Res	Type
7	BE	122	C
7	BE	123	U
7	BE	148	A
7	BE	149	A
7	BE	172	C
7	BE	186	U
7	BE	187	C
7	BE	191	G
7	BE	198	A
73	BF	10	G
73	BF	11	C
73	BF	12	C
73	BF	13	A
73	BF	14	C
73	BF	16	U
73	BF	23	U
73	BF	24	C
73	BF	25	C
73	BF	29	G
73	BF	36	G
73	BF	55	C
73	BF	57	G
73	BF	58	U
73	BF	60	C
73	BF	63	U
73	BF	72	C
73	BF	73	A
74	BG	8	U
74	BG	9	G
74	BG	11	G
74	BG	19	C
74	BG	25	G
74	BG	39	A
74	BG	40	G
74	BG	42	A
74	BG	53	C
74	BG	56	G
74	BG	60	A
74	BG	74	G
74	BG	77	U
74	BG	85	C
74	BG	86	U

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Mol	Chain	Res	Type
74	BG	102	G
74	BG	114	A
74	BG	120	U
74	BG	121	C
74	BG	123	C
74	BG	127	G
74	BG	132	U
74	BG	139	U
74	BG	145	C
74	BG	149	U
74	BG	150	A
74	BG	157	A
74	BG	159	A
74	BG	168	A
74	BG	173	C
75	BH	14	C
75	BH	23	G
75	BH	26	C
75	BH	28	U
75	BH	29	G
75	BH	49	C
75	BH	50	A
75	BH	51	C
75	BH	69	C
75	BH	71	C
75	BH	72	G
75	BH	73	A
75	BH	80	C
75	BH	86	G
75	BH	99	G
75	BH	106	G
75	BH	109	G
75	BH	113	G
75	BH	114	G
75	BH	125	U
75	BH	128	G

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	172	A
1	AA	273	A

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Mol	Chain	Res	Type
1	AA	301	C
1	AA	406	A
1	AA	462	U
1	AA	550	A
1	AA	604	U
1	AA	623	A
1	AA	789	G
1	AA	846	C
1	AA	867	C
1	AA	911	A
1	AA	921	G
1	AA	967	A
1	AA	969	C
1	AA	1639	A
1	AA	1836	G
1	AA	1853	A
1	AA	2160	A
3	BA	212	A
3	BA	268	G
3	BA	399	A
3	BA	559	C
3	BA	610	C
3	BA	1028	OMG
3	BA	1316	U
3	BA	1864	U
4	BB	379	U
4	BB	1272	U
4	BB	1508	C
6	BD	51	G
7	BE	58	U
7	BE	96	C
74	BG	18	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

129 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
3	OMG	BA	915	3	23,26,27	2.38	9 (39%)	32,38,41	2.48	12 (37%)
4	OMU	BB	685	4	19,22,23	2.99	8 (42%)	25,31,34	1.88	4 (16%)
4	PSU	BB	1280	4	18,21,22	4.57	8 (44%)	21,30,33	2.00	6 (28%)
1	OMG	AA	2227	1	23,26,27	2.34	8 (34%)	32,38,41	2.51	10 (31%)
4	OMC	BB	1264	4	19,22,23	2.94	8 (42%)	25,31,34	0.87	1 (4%)
1	PSU	AA	2045	1	18,21,22	4.57	7 (38%)	21,30,33	1.88	5 (23%)
3	PSU	BA	1086	3,86	18,21,22	4.57	7 (38%)	21,30,33	1.99	5 (23%)
3	OMC	BA	1006	3	19,22,23	2.90	8 (42%)	25,31,34	0.77	0
1	MA6	AA	2260	1	23,26,27	1.51	4 (17%)	33,38,41	3.00	9 (27%)
4	A2M	BB	1400	4,86	22,25,26	3.23	10 (45%)	30,36,39	3.11	12 (40%)
3	OMU	BA	1181	3	19,22,23	3.01	8 (42%)	25,31,34	1.90	5 (20%)
4	5MC	BB	542	4,86	19,22,23	3.64	8 (42%)	26,32,35	1.03	2 (7%)
4	PSU	BB	1160	4	18,21,22	4.55	7 (38%)	21,30,33	2.03	5 (23%)
5	PSU	BC	74	5	18,21,22	4.64	7 (38%)	21,30,33	1.94	5 (23%)
3	PSU	BA	258	3	18,21,22	4.63	7 (38%)	21,30,33	1.99	5 (23%)
4	PSU	BB	1409	4	18,21,22	4.60	7 (38%)	21,30,33	1.90	5 (23%)
3	OMU	BA	1448	3	19,22,23	3.02	8 (42%)	25,31,34	1.90	5 (20%)
1	PSU	AA	1619	1	18,21,22	4.66	8 (44%)	21,30,33	1.81	4 (19%)
1	MA6	AA	2261	1	23,26,27	1.57	5 (21%)	33,38,41	2.98	13 (39%)
4	OMC	BB	1413	4	19,22,23	2.87	8 (42%)	25,31,34	0.85	0
3	A2M	BA	1620	4,3,86	22,25,26	3.23	10 (45%)	30,36,39	3.05	12 (40%)
3	OMG	BA	1605	3	23,26,27	2.39	9 (39%)	32,38,41	2.58	12 (37%)
1	A2M	AA	2153	1	22,25,26	3.24	10 (45%)	30,36,39	3.11	12 (40%)
3	PSU	BA	1009	3	18,21,22	4.57	7 (38%)	21,30,33	2.04	5 (23%)
4	A2M	BB	400	4	22,25,26	3.26	9 (40%)	30,36,39	2.97	13 (43%)
1	OMU	AA	2054	1	19,22,23	3.02	8 (42%)	25,31,34	1.83	5 (20%)
1	OMU	AA	57	1	19,22,23	2.98	8 (42%)	25,31,34	1.85	5 (20%)
3	PSU	BA	1169	3	18,21,22	4.63	7 (38%)	21,30,33	2.00	5 (23%)
1	B8N	AA	1596	1	25,29,30	3.35	7 (28%)	28,42,45	2.00	7 (25%)
3	PSU	BA	452	3	18,21,22	4.63	7 (38%)	21,30,33	1.93	5 (23%)
4	PSU	BB	518	4	18,21,22	4.63	7 (38%)	21,30,33	2.00	5 (23%)
5	A2M	BC	41	5	22,25,26	3.23	10 (45%)	30,36,39	3.11	12 (40%)
4	A2M	BB	609	4	22,25,26	3.23	10 (45%)	30,36,39	2.94	12 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	AA	2146	1	18,21,22	4.46	7 (38%)	21,30,33	1.89	5 (23%)
3	A2M	BA	1665	4,3	22,25,26	3.23	9 (40%)	30,36,39	2.98	12 (40%)
1	OMU	AA	2154	1	19,22,23	3.04	8 (42%)	25,31,34	1.97	5 (20%)
4	A2M	BB	1388	4	22,25,26	3.24	10 (45%)	30,36,39	3.10	11 (36%)
3	A2M	BA	1024	3	22,25,26	3.20	9 (40%)	30,36,39	3.06	11 (36%)
1	PSU	AA	1276	1	18,21,22	4.43	7 (38%)	21,30,33	1.95	5 (23%)
3	PSU	BA	737	3	18,21,22	4.50	7 (38%)	21,30,33	2.01	6 (28%)
5	A2M	BC	163	5,3	22,25,26	3.20	9 (40%)	30,36,39	3.08	11 (36%)
4	OMG	BB	659	4	23,26,27	2.37	9 (39%)	32,38,41	2.54	10 (31%)
4	OMU	BB	578	88,4	19,22,23	3.01	8 (42%)	25,31,34	1.94	5 (20%)
3	A2M	BA	927	3	22,25,26	3.21	9 (40%)	30,36,39	3.10	13 (43%)
4	5MC	BB	1324	4	19,22,23	3.70	8 (42%)	26,32,35	1.23	1 (3%)
4	OMU	BB	1375	4	19,22,23	2.98	8 (42%)	25,31,34	1.90	5 (20%)
3	OMU	BA	1742	3	19,22,23	2.98	8 (42%)	25,31,34	1.84	5 (20%)
1	OMU	AA	714	1	19,22,23	2.88	8 (42%)	25,31,34	1.88	5 (20%)
1	PSU	AA	131	1	18,21,22	4.53	7 (38%)	21,30,33	2.11	5 (23%)
5	OMG	BC	75	5	23,26,27	2.42	9 (39%)	32,38,41	2.56	10 (31%)
4	A2M	BB	95	4	22,25,26	3.22	9 (40%)	30,36,39	2.98	12 (40%)
4	PSU	BB	524	4	18,21,22	4.56	7 (38%)	21,30,33	1.89	5 (23%)
1	OMG	AA	1700	1	23,26,27	2.38	9 (39%)	32,38,41	2.57	12 (37%)
3	A2M	BA	743	4,3	22,25,26	3.22	9 (40%)	30,36,39	3.00	13 (43%)
4	A2M	BB	646	4	22,25,26	3.22	9 (40%)	30,36,39	3.02	11 (36%)
4	PSU	BB	1229	4	18,21,22	4.61	7 (38%)	21,30,33	2.03	5 (23%)
4	OMG	BB	552	4	23,26,27	2.38	9 (39%)	32,38,41	2.50	11 (34%)
1	A2M	AA	2096	1	22,25,26	3.23	10 (45%)	30,36,39	3.17	11 (36%)
4	A2M	BB	545	4,86	22,25,26	3.23	10 (45%)	30,36,39	3.34	15 (50%)
5	OMU	BC	7	5,3	19,22,23	3.02	8 (42%)	25,31,34	1.85	4 (16%)
1	OMG	AA	1531	1	23,26,27	2.32	9 (39%)	32,38,41	2.44	12 (37%)
3	A2M	BA	996	3	22,25,26	3.22	9 (40%)	30,36,39	2.98	12 (40%)
1	OMC	AA	46	1	19,22,23	2.84	8 (42%)	25,31,34	0.86	0
3	OMU	BA	46	3	19,22,23	3.01	8 (42%)	25,31,34	1.90	5 (20%)
3	OMC	BA	1608	3	19,22,23	2.90	8 (42%)	25,31,34	0.80	0
1	A2M	AA	56	1,86	22,25,26	3.24	9 (40%)	30,36,39	3.01	11 (36%)
3	PSU	BA	1248	3,86	18,21,22	4.59	7 (38%)	21,30,33	1.86	5 (23%)
1	PSU	AA	1592	1	18,21,22	4.55	7 (38%)	21,30,33	1.89	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	BA	925	3	23,26,27	2.38	9 (39%)	32,38,41	2.44	11 (34%)
3	OMG	BA	1028	3	23,26,27	2.39	9 (39%)	32,38,41	2.36	10 (31%)
4	OMC	BB	601	4	19,22,23	2.94	8 (42%)	25,31,34	0.77	0
4	PSU	BB	1076	4	18,21,22	4.54	7 (38%)	21,30,33	2.07	5 (23%)
4	OMC	BB	377	4	19,22,23	3.00	8 (42%)	25,31,34	0.72	0
4	OMU	BB	73	4	19,22,23	3.04	8 (42%)	25,31,34	1.83	5 (20%)
4	PSU	BB	615	4	18,21,22	4.54	7 (38%)	21,30,33	1.92	5 (23%)
3	PSU	BA	1258	3	18,21,22	4.61	7 (38%)	21,30,33	1.98	5 (23%)
1	OMU	AA	1652	1	19,22,23	3.12	8 (42%)	25,31,34	1.75	4 (16%)
1	OMC	AA	2134	1	19,22,23	2.84	8 (42%)	25,31,34	0.76	0
1	PSU	AA	61	1	18,21,22	4.59	7 (38%)	21,30,33	1.97	5 (23%)
4	OMG	BB	1062	4	23,26,27	2.41	9 (39%)	32,38,41	2.55	10 (31%)
1	OMG	AA	1895	1,86	23,26,27	2.38	9 (39%)	32,38,41	2.58	10 (31%)
3	PSU	BA	1129	3	18,21,22	4.60	7 (38%)	21,30,33	1.98	5 (23%)
4	PSU	BB	530	4	18,21,22	1.43	3 (16%)	21,30,33	2.27	5 (23%)
4	OMG	BB	1245	4	23,26,27	2.38	9 (39%)	32,38,41	2.51	11 (34%)
1	OMC	AA	66	1	19,22,23	2.91	8 (42%)	25,31,34	0.77	0
4	A2M	BB	622	4,3	22,25,26	3.22	10 (45%)	30,36,39	3.05	11 (36%)
3	OMC	BA	760	3	19,22,23	2.93	8 (42%)	25,31,34	0.76	0
4	OMG	BB	1094	4	23,26,27	2.38	9 (39%)	32,38,41	2.46	11 (34%)
4	PSU	BB	528	4	18,21,22	1.50	4 (22%)	21,30,33	2.17	5 (23%)
4	PSU	BB	1429	4	18,21,22	4.50	8 (44%)	21,30,33	2.05	5 (23%)
4	PSU	BB	644	4	18,21,22	4.56	7 (38%)	21,30,33	1.99	5 (23%)
1	OMG	AA	1931	1	23,26,27	2.40	9 (39%)	32,38,41	2.57	11 (34%)
4	OMU	BB	1435	4	19,22,23	3.01	8 (42%)	25,31,34	1.80	4 (16%)
1	OMU	AA	2123	1	19,22,23	2.91	7 (36%)	25,31,34	1.91	4 (16%)
4	PSU	BB	522	4	18,21,22	4.64	7 (38%)	21,30,33	1.90	5 (23%)
4	OMG	BB	71	4	23,26,27	2.40	9 (39%)	32,38,41	2.51	11 (34%)
4	PSU	BB	680	4,86	18,21,22	4.53	8 (44%)	21,30,33	2.02	6 (28%)
1	OMG	AA	1517	1	23,26,27	2.41	8 (34%)	32,38,41	2.68	10 (31%)
4	OMU	BB	1093	4	19,22,23	3.04	8 (42%)	25,31,34	1.84	4 (16%)
1	7MG	AA	2070	1	23,26,27	3.82	11 (47%)	27,39,42	2.21	9 (33%)
1	A2M	AA	721	1,88,86	22,25,26	3.29	10 (45%)	30,36,39	3.12	12 (40%)
3	OMU	BA	916	3	19,22,23	3.01	8 (42%)	25,31,34	1.85	5 (20%)
4	OMC	BB	1175	4	19,22,23	2.93	8 (42%)	25,31,34	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	AA	36	1	19,22,23	2.85	7 (36%)	25,31,34	1.99	5 (20%)
4	PSU	BB	611	4	18,21,22	4.54	7 (38%)	21,30,33	1.86	4 (19%)
1	OMU	AA	1899	1	19,22,23	3.04	8 (42%)	25,31,34	1.86	5 (20%)
4	PSU	BB	455	4	18,21,22	4.49	7 (38%)	21,30,33	2.10	5 (23%)
3	PSU	BA	1614	4,3	18,21,22	4.55	7 (38%)	21,30,33	2.02	5 (23%)
4	PSU	BB	1319	4	18,21,22	4.55	7 (38%)	21,30,33	2.02	6 (28%)
4	PSU	BB	1398	4	18,21,22	4.58	8 (44%)	21,30,33	2.04	6 (28%)
4	PSU	BB	1334	4	18,21,22	4.55	7 (38%)	21,30,33	1.99	5 (23%)
3	A2M	BA	254	3	22,25,26	3.23	9 (40%)	30,36,39	3.06	11 (36%)
4	PSU	BB	629	4	18,21,22	4.56	7 (38%)	21,30,33	1.81	4 (19%)
4	OMG	BB	673	4	23,26,27	2.38	9 (39%)	32,38,41	2.54	10 (31%)
4	OMG	BB	1247	4	23,26,27	2.40	9 (39%)	32,38,41	2.58	10 (31%)
4	A2M	BB	588	3,4,87	22,25,26	3.22	10 (45%)	30,36,39	3.16	14 (46%)
3	OMC	BA	1329	3	19,22,23	3.05	8 (42%)	25,31,34	0.76	0
4	OMG	BB	1269	4	23,26,27	2.36	9 (39%)	32,38,41	2.49	10 (31%)
3	OMG	BA	1267	3	23,26,27	2.37	9 (39%)	32,38,41	2.44	13 (40%)
3	A2M	BA	746	3	22,25,26	3.21	10 (45%)	30,36,39	3.10	11 (36%)
3	1MA	BA	742	3,86	21,25,26	2.82	5 (23%)	30,37,40	1.85	6 (20%)
1	OMG	AA	1676	1,88	23,26,27	2.42	9 (39%)	32,38,41	2.67	10 (31%)
5	A2M	BC	43	5	22,25,26	3.22	9 (40%)	30,36,39	3.06	11 (36%)
3	A2M	BA	762	3	22,25,26	3.24	10 (45%)	30,36,39	3.13	12 (40%)
3	OMG	BA	1621	4,3	23,26,27	2.37	9 (39%)	32,38,41	2.56	11 (34%)
3	PSU	BA	1609	3	18,21,22	4.62	7 (38%)	21,30,33	1.99	5 (23%)
4	PSU	BB	1210	4	18,21,22	4.57	7 (38%)	21,30,33	1.94	5 (23%)
3	OMG	BA	1709	3	23,26,27	2.39	9 (39%)	32,38,41	2.55	11 (34%)
4	A2M	BB	1201	4	22,25,26	3.23	9 (40%)	30,36,39	3.10	13 (43%)

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
3	OMG	BA	915	3	-	0/9/27/28	0/3/3/3
4	OMU	BB	685	4	-	0/9/27/28	0/2/2/2
4	PSU	BB	1280	4	-	0/7/25/26	0/2/2/2
1	OMG	AA	2227	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMC	BB	1264	4	-	1/9/27/28	0/2/2/2
1	PSU	AA	2045	1	-	0/7/25/26	0/2/2/2
3	PSU	BA	1086	3,86	-	0/7/25/26	0/2/2/2
3	OMC	BA	1006	3	-	0/9/27/28	0/2/2/2
1	MA6	AA	2260	1	-	2/11/29/30	0/3/3/3
4	A2M	BB	1400	4,86	-	0/9/27/28	0/3/3/3
3	OMU	BA	1181	3	-	0/9/27/28	0/2/2/2
4	5MC	BB	542	4,86	-	0/7/25/26	0/2/2/2
4	PSU	BB	1160	4	-	0/7/25/26	0/2/2/2
5	PSU	BC	74	5	-	2/7/25/26	0/2/2/2
3	PSU	BA	258	3	-	0/7/25/26	0/2/2/2
4	PSU	BB	1409	4	-	0/7/25/26	0/2/2/2
3	OMU	BA	1448	3	-	2/9/27/28	0/2/2/2
1	PSU	AA	1619	1	-	2/7/25/26	0/2/2/2
1	MA6	AA	2261	1	-	0/11/29/30	0/3/3/3
4	OMC	BB	1413	4	-	0/9/27/28	0/2/2/2
3	A2M	BA	1620	4,3,86	-	0/9/27/28	0/3/3/3
3	OMG	BA	1605	3	-	1/9/27/28	0/3/3/3
1	A2M	AA	2153	1	-	1/9/27/28	0/3/3/3
3	PSU	BA	1009	3	-	0/7/25/26	0/2/2/2
4	A2M	BB	400	4	-	2/9/27/28	0/3/3/3
1	OMU	AA	2054	1	-	2/9/27/28	0/2/2/2
1	OMU	AA	57	1	-	1/9/27/28	0/2/2/2
3	PSU	BA	1169	3	-	0/7/25/26	0/2/2/2
1	B8N	AA	1596	1	-	3/16/34/35	0/2/2/2
3	PSU	BA	452	3	-	0/7/25/26	0/2/2/2
4	PSU	BB	518	4	-	0/7/25/26	0/2/2/2
5	A2M	BC	41	5	-	0/9/27/28	0/3/3/3
4	A2M	BB	609	4	-	1/9/27/28	0/3/3/3
1	PSU	AA	2146	1	-	1/7/25/26	0/2/2/2
3	A2M	BA	1665	4,3	-	3/9/27/28	0/3/3/3
1	OMU	AA	2154	1	-	3/9/27/28	0/2/2/2
4	A2M	BB	1388	4	-	0/9/27/28	0/3/3/3
3	A2M	BA	1024	3	-	1/9/27/28	0/3/3/3
1	PSU	AA	1276	1	-	0/7/25/26	0/2/2/2
3	PSU	BA	737	3	-	4/7/25/26	0/2/2/2
5	A2M	BC	163	5,3	-	1/9/27/28	0/3/3/3
4	OMG	BB	659	4	-	2/9/27/28	0/3/3/3
4	OMU	BB	578	88,4	-	5/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	BA	927	3	-	1/9/27/28	0/3/3/3
4	5MC	BB	1324	4	-	4/7/25/26	0/2/2/2
4	OMU	BB	1375	4	-	0/9/27/28	0/2/2/2
3	OMU	BA	1742	3	-	0/9/27/28	0/2/2/2
1	OMU	AA	714	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	131	1	-	0/7/25/26	0/2/2/2
5	OMG	BC	75	5	-	2/9/27/28	0/3/3/3
4	A2M	BB	95	4	-	1/9/27/28	0/3/3/3
4	PSU	BB	524	4	-	1/7/25/26	0/2/2/2
1	OMG	AA	1700	1	-	0/9/27/28	0/3/3/3
3	A2M	BA	743	4,3	-	1/9/27/28	0/3/3/3
4	A2M	BB	646	4	-	0/9/27/28	0/3/3/3
4	PSU	BB	1229	4	-	0/7/25/26	0/2/2/2
4	OMG	BB	552	4	-	2/9/27/28	0/3/3/3
1	A2M	AA	2096	1	-	1/9/27/28	0/3/3/3
4	A2M	BB	545	4,86	-	2/9/27/28	0/3/3/3
5	OMU	BC	7	5,3	-	0/9/27/28	0/2/2/2
1	OMG	AA	1531	1	-	1/9/27/28	0/3/3/3
3	A2M	BA	996	3	-	0/9/27/28	0/3/3/3
1	OMC	AA	46	1	-	2/9/27/28	0/2/2/2
3	OMU	BA	46	3	-	0/9/27/28	0/2/2/2
3	OMC	BA	1608	3	-	2/9/27/28	0/2/2/2
1	A2M	AA	56	1,86	-	0/9/27/28	0/3/3/3
3	PSU	BA	1248	3,86	-	2/7/25/26	0/2/2/2
1	PSU	AA	1592	1	-	0/7/25/26	0/2/2/2
3	OMG	BA	925	3	-	0/9/27/28	0/3/3/3
3	OMG	BA	1028	3	-	0/9/27/28	0/3/3/3
4	OMC	BB	601	4	-	0/9/27/28	0/2/2/2
4	PSU	BB	1076	4	-	0/7/25/26	0/2/2/2
4	OMC	BB	377	4	-	0/9/27/28	0/2/2/2
4	OMU	BB	73	4	-	0/9/27/28	0/2/2/2
4	PSU	BB	615	4	-	0/7/25/26	0/2/2/2
3	PSU	BA	1258	3	-	2/7/25/26	0/2/2/2
1	OMU	AA	1652	1	-	1/9/27/28	0/2/2/2
1	OMC	AA	2134	1	-	1/9/27/28	0/2/2/2
1	PSU	AA	61	1	-	2/7/25/26	0/2/2/2
4	OMG	BB	1062	4	-	3/9/27/28	0/3/3/3
1	OMG	AA	1895	1,86	-	0/9/27/28	0/3/3/3
3	PSU	BA	1129	3	-	0/7/25/26	0/2/2/2
4	PSU	BB	530	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	BB	1245	4	-	0/9/27/28	0/3/3/3
1	OMC	AA	66	1	-	0/9/27/28	0/2/2/2
4	A2M	BB	622	4,3	-	0/9/27/28	0/3/3/3
3	OMC	BA	760	3	-	0/9/27/28	0/2/2/2
4	OMG	BB	1094	4	-	0/9/27/28	0/3/3/3
4	PSU	BB	528	4	-	2/7/25/26	0/2/2/2
4	PSU	BB	1429	4	-	0/7/25/26	0/2/2/2
4	PSU	BB	644	4	-	0/7/25/26	0/2/2/2
1	OMG	AA	1931	1	-	0/9/27/28	0/3/3/3
4	OMU	BB	1435	4	-	0/9/27/28	0/2/2/2
1	OMU	AA	2123	1	-	0/9/27/28	0/2/2/2
4	PSU	BB	522	4	-	2/7/25/26	0/2/2/2
4	OMG	BB	71	4	-	0/9/27/28	0/3/3/3
4	PSU	BB	680	4,86	-	0/7/25/26	0/2/2/2
1	OMG	AA	1517	1	-	0/9/27/28	0/3/3/3
4	OMU	BB	1093	4	-	0/9/27/28	0/2/2/2
1	7MG	AA	2070	1	-	2/7/37/38	0/3/3/3
1	A2M	AA	721	1,88,86	-	3/9/27/28	0/3/3/3
3	OMU	BA	916	3	-	0/9/27/28	0/2/2/2
4	OMC	BB	1175	4	-	0/9/27/28	0/2/2/2
1	OMU	AA	36	1	-	6/9/27/28	0/2/2/2
4	PSU	BB	611	4	-	0/7/25/26	0/2/2/2
1	OMU	AA	1899	1	-	3/9/27/28	0/2/2/2
4	PSU	BB	455	4	-	0/7/25/26	0/2/2/2
3	PSU	BA	1614	4,3	-	2/7/25/26	0/2/2/2
4	PSU	BB	1319	4	-	0/7/25/26	0/2/2/2
4	PSU	BB	1398	4	-	0/7/25/26	0/2/2/2
4	PSU	BB	1334	4	-	0/7/25/26	0/2/2/2
3	A2M	BA	254	3	-	1/9/27/28	0/3/3/3
4	PSU	BB	629	4	-	2/7/25/26	0/2/2/2
4	OMG	BB	673	4	-	1/9/27/28	0/3/3/3
4	OMG	BB	1247	4	-	0/9/27/28	0/3/3/3
4	A2M	BB	588	3,4,87	-	5/9/27/28	0/3/3/3
3	OMC	BA	1329	3	-	1/9/27/28	0/2/2/2
4	OMG	BB	1269	4	-	0/9/27/28	0/3/3/3
3	OMG	BA	1267	3	-	0/9/27/28	0/3/3/3
3	A2M	BA	746	3	-	0/9/27/28	0/3/3/3
3	1MA	BA	742	3,86	-	4/7/25/26	0/3/3/3
1	OMG	AA	1676	1,88	-	2/9/27/28	0/3/3/3
5	A2M	BC	43	5	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	BA	762	3	-	0/9/27/28	0/3/3/3
3	OMG	BA	1621	4,3	-	0/9/27/28	0/3/3/3
3	PSU	BA	1609	3	-	0/7/25/26	0/2/2/2
4	PSU	BB	1210	4	-	0/7/25/26	0/2/2/2
3	OMG	BA	1709	3	-	0/9/27/28	0/3/3/3
4	A2M	BB	1201	4	-	2/9/27/28	0/3/3/3

All (1041) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1619	PSU	C6-C5	12.33	1.48	1.35
3	BA	452	PSU	C6-C5	12.26	1.48	1.35
4	BB	522	PSU	C6-C5	12.25	1.48	1.35
3	BA	1609	PSU	C6-C5	12.24	1.48	1.35
4	BB	1409	PSU	C6-C5	12.17	1.48	1.35
3	BA	258	PSU	C6-C5	12.17	1.48	1.35
3	BA	1086	PSU	C6-C5	12.16	1.48	1.35
3	BA	1248	PSU	C6-C5	12.16	1.48	1.35
5	BC	74	PSU	C6-C5	12.13	1.48	1.35
4	BB	644	PSU	C6-C5	12.13	1.48	1.35
3	BA	1258	PSU	C6-C5	12.11	1.48	1.35
4	BB	1229	PSU	C6-C5	12.10	1.48	1.35
3	BA	1129	PSU	C6-C5	12.10	1.48	1.35
4	BB	518	PSU	C6-C5	12.09	1.48	1.35
4	BB	1398	PSU	C6-C5	12.08	1.48	1.35
4	BB	629	PSU	C6-C5	12.07	1.48	1.35
3	BA	1169	PSU	C6-C5	12.06	1.48	1.35
4	BB	1210	PSU	C6-C5	12.04	1.48	1.35
4	BB	611	PSU	C6-C5	12.04	1.48	1.35
1	AA	61	PSU	C6-C5	12.02	1.48	1.35
4	BB	1280	PSU	C6-C5	12.00	1.48	1.35
4	BB	615	PSU	C6-C5	11.98	1.48	1.35
3	BA	737	PSU	C6-C5	11.97	1.48	1.35
4	BB	1334	PSU	C6-C5	11.95	1.48	1.35
4	BB	524	PSU	C6-C5	11.94	1.48	1.35
4	BB	1160	PSU	C6-C5	11.93	1.48	1.35
3	BA	1009	PSU	C6-C5	11.92	1.48	1.35
4	BB	1076	PSU	C6-C5	11.91	1.48	1.35
1	AA	1592	PSU	C6-C5	11.90	1.48	1.35
3	BA	1614	PSU	C6-C5	11.90	1.48	1.35
1	AA	2045	PSU	C6-C5	11.89	1.48	1.35
4	BB	1429	PSU	C6-C5	11.89	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	1319	PSU	C6-C5	11.89	1.48	1.35
4	BB	680	PSU	C6-C5	11.88	1.48	1.35
1	AA	131	PSU	C6-C5	11.84	1.48	1.35
4	BB	455	PSU	C6-C5	11.79	1.48	1.35
1	AA	2146	PSU	C6-C5	11.69	1.48	1.35
1	AA	1276	PSU	C6-C5	11.55	1.48	1.35
3	BA	1248	PSU	C2-N1	10.09	1.49	1.36
3	BA	1169	PSU	C2-N1	10.05	1.49	1.36
4	BB	518	PSU	C2-N1	10.05	1.49	1.36
3	BA	1009	PSU	C2-N1	10.02	1.49	1.36
5	BC	74	PSU	C2-N1	10.01	1.49	1.36
4	BB	522	PSU	C2-N1	10.00	1.49	1.36
4	BB	1229	PSU	C2-N1	9.99	1.49	1.36
3	BA	1258	PSU	C2-N1	9.98	1.49	1.36
3	BA	258	PSU	C2-N1	9.96	1.49	1.36
4	BB	1398	PSU	C2-N1	9.91	1.49	1.36
3	BA	452	PSU	C2-N1	9.91	1.49	1.36
1	AA	61	PSU	C2-N1	9.90	1.49	1.36
1	AA	2045	PSU	C2-N1	9.89	1.49	1.36
3	BA	1129	PSU	C2-N1	9.89	1.49	1.36
3	BA	1609	PSU	C2-N1	9.89	1.49	1.36
4	BB	1334	PSU	C2-N1	9.89	1.49	1.36
1	AA	1619	PSU	C2-N1	9.86	1.49	1.36
4	BB	1280	PSU	C2-N1	9.86	1.49	1.36
4	BB	1319	PSU	C2-N1	9.85	1.49	1.36
4	BB	1160	PSU	C2-N1	9.85	1.49	1.36
1	AA	1592	PSU	C2-N1	9.84	1.49	1.36
3	BA	737	PSU	C2-N1	9.81	1.49	1.36
1	AA	131	PSU	C2-N1	9.81	1.49	1.36
4	BB	1409	PSU	C2-N1	9.78	1.49	1.36
4	BB	629	PSU	C2-N1	9.76	1.49	1.36
3	BA	1614	PSU	C2-N1	9.76	1.49	1.36
4	BB	1210	PSU	C2-N1	9.75	1.49	1.36
4	BB	524	PSU	C2-N1	9.74	1.49	1.36
4	BB	611	PSU	C2-N1	9.73	1.49	1.36
4	BB	1076	PSU	C2-N1	9.73	1.49	1.36
4	BB	615	PSU	C2-N1	9.73	1.49	1.36
3	BA	1086	PSU	C2-N1	9.73	1.49	1.36
4	BB	680	PSU	C2-N1	9.72	1.49	1.36
4	BB	455	PSU	C2-N1	9.67	1.49	1.36
4	BB	644	PSU	C2-N1	9.61	1.49	1.36
4	BB	1429	PSU	C2-N1	9.55	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	2146	PSU	C2-N1	9.55	1.49	1.36
1	AA	1276	PSU	C2-N1	9.55	1.49	1.36
1	AA	2070	7MG	C8-N9	9.37	1.51	1.45
4	BB	1324	5MC	C6-C5	9.21	1.49	1.34
4	BB	400	A2M	C3'-C4'	-9.12	1.29	1.53
1	AA	56	A2M	C3'-C4'	-9.01	1.30	1.53
1	AA	721	A2M	C3'-C4'	-9.00	1.30	1.53
1	AA	2153	A2M	C3'-C4'	-8.94	1.30	1.53
3	BA	1665	A2M	C3'-C4'	-8.93	1.30	1.53
4	BB	542	5MC	C6-C5	8.93	1.49	1.34
3	BA	1620	A2M	C3'-C4'	-8.87	1.30	1.53
4	BB	1400	A2M	C3'-C4'	-8.86	1.30	1.53
1	AA	2096	A2M	C3'-C4'	-8.86	1.30	1.53
3	BA	927	A2M	C3'-C4'	-8.84	1.30	1.53
4	BB	1201	A2M	C3'-C4'	-8.84	1.30	1.53
5	BC	163	A2M	C3'-C4'	-8.82	1.30	1.53
4	BB	95	A2M	C3'-C4'	-8.80	1.30	1.53
3	BA	254	A2M	C3'-C4'	-8.80	1.30	1.53
4	BB	646	A2M	C3'-C4'	-8.80	1.30	1.53
3	BA	762	A2M	C3'-C4'	-8.80	1.30	1.53
5	BC	41	A2M	C3'-C4'	-8.79	1.30	1.53
3	BA	996	A2M	C3'-C4'	-8.78	1.30	1.53
4	BB	1388	A2M	C3'-C4'	-8.78	1.30	1.53
3	BA	743	A2M	C3'-C4'	-8.77	1.30	1.53
5	BC	43	A2M	C3'-C4'	-8.77	1.30	1.53
3	BA	1024	A2M	C3'-C4'	-8.76	1.30	1.53
4	BB	609	A2M	C3'-C4'	-8.73	1.30	1.53
4	BB	622	A2M	C3'-C4'	-8.73	1.30	1.53
4	BB	588	A2M	C3'-C4'	-8.64	1.31	1.53
3	BA	742	1MA	C2-N3	8.58	1.46	1.30
3	BA	746	A2M	C3'-C4'	-8.52	1.31	1.53
4	BB	545	A2M	C3'-C4'	-8.44	1.31	1.53
1	AA	1596	B8N	C6-N1	8.33	1.56	1.36
1	AA	2070	7MG	C5-N7	8.20	1.46	1.35
1	AA	1619	PSU	C2-N3	7.86	1.50	1.37
1	AA	1596	B8N	C4-N3	-7.86	1.26	1.40
4	BB	522	PSU	C2-N3	7.79	1.50	1.37
4	BB	609	A2M	O4'-C4'	7.78	1.62	1.45
3	BA	258	PSU	C2-N3	7.77	1.50	1.37
5	BC	74	PSU	C2-N3	7.76	1.50	1.37
4	BB	588	A2M	O4'-C4'	7.76	1.62	1.45
5	BC	43	A2M	O4'-C4'	7.75	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BA	1169	PSU	C2-N3	7.75	1.50	1.37
3	BA	254	A2M	O4'-C4'	7.74	1.62	1.45
4	BB	646	A2M	O4'-C4'	7.73	1.62	1.45
3	BA	762	A2M	O4'-C4'	7.72	1.62	1.45
3	BA	1614	PSU	C2-N3	7.71	1.50	1.37
1	AA	61	PSU	C2-N3	7.71	1.50	1.37
3	BA	452	PSU	C2-N3	7.71	1.50	1.37
4	BB	622	A2M	O4'-C4'	7.71	1.62	1.45
4	BB	545	A2M	O4'-C4'	7.70	1.62	1.45
4	BB	524	PSU	C2-N3	7.69	1.50	1.37
4	BB	1229	PSU	C2-N3	7.69	1.50	1.37
4	BB	1409	PSU	C2-N3	7.68	1.50	1.37
4	BB	1388	A2M	O4'-C4'	7.68	1.62	1.45
3	BA	1665	A2M	O4'-C4'	7.68	1.62	1.45
4	BB	518	PSU	C2-N3	7.68	1.50	1.37
1	AA	2045	PSU	C2-N3	7.67	1.50	1.37
3	BA	996	A2M	O4'-C4'	7.66	1.62	1.45
3	BA	746	A2M	O4'-C4'	7.66	1.62	1.45
1	AA	2153	A2M	O4'-C4'	7.66	1.62	1.45
3	BA	1609	PSU	C2-N3	7.66	1.50	1.37
3	BA	1258	PSU	C2-N3	7.66	1.50	1.37
4	BB	1400	A2M	O4'-C4'	7.65	1.62	1.45
4	BB	1210	PSU	C2-N3	7.65	1.50	1.37
3	BA	1129	PSU	C2-N3	7.65	1.50	1.37
1	AA	131	PSU	C2-N3	7.64	1.50	1.37
4	BB	95	A2M	O4'-C4'	7.64	1.62	1.45
4	BB	400	A2M	O4'-C4'	7.63	1.62	1.45
1	AA	1592	PSU	C2-N3	7.62	1.50	1.37
3	BA	743	A2M	O4'-C4'	7.62	1.61	1.45
4	BB	1076	PSU	C2-N3	7.62	1.50	1.37
1	AA	56	A2M	O4'-C4'	7.61	1.61	1.45
5	BC	41	A2M	O4'-C4'	7.60	1.61	1.45
4	BB	1319	PSU	C2-N3	7.60	1.50	1.37
1	AA	2096	A2M	O4'-C4'	7.59	1.61	1.45
4	BB	1160	PSU	C2-N3	7.59	1.50	1.37
3	BA	1024	A2M	O4'-C4'	7.58	1.61	1.45
3	BA	1086	PSU	C2-N3	7.58	1.50	1.37
4	BB	629	PSU	C2-N3	7.57	1.49	1.37
4	BB	1280	PSU	C2-N3	7.56	1.49	1.37
4	BB	644	PSU	C2-N3	7.55	1.49	1.37
5	BC	163	A2M	O4'-C4'	7.54	1.61	1.45
3	BA	1620	A2M	O4'-C4'	7.54	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	1201	A2M	O4'-C4'	7.50	1.61	1.45
3	BA	1009	PSU	C2-N3	7.50	1.49	1.37
4	BB	1334	PSU	C2-N3	7.49	1.49	1.37
4	BB	680	PSU	C2-N3	7.48	1.49	1.37
4	BB	615	PSU	C2-N3	7.47	1.49	1.37
4	BB	1398	PSU	C2-N3	7.47	1.49	1.37
4	BB	1429	PSU	C2-N3	7.44	1.49	1.37
4	BB	611	PSU	C2-N3	7.42	1.49	1.37
3	BA	927	A2M	O4'-C4'	7.40	1.61	1.45
1	AA	2154	OMU	C2-N1	7.39	1.50	1.38
1	AA	2146	PSU	C2-N3	7.36	1.49	1.37
4	BB	455	PSU	C2-N3	7.34	1.49	1.37
1	AA	1652	OMU	C2-N1	7.29	1.49	1.38
1	AA	1596	B8N	C4-C5	7.27	1.64	1.47
1	AA	1276	PSU	C2-N3	7.23	1.49	1.37
4	BB	578	OMU	C2-N1	7.22	1.49	1.38
1	AA	721	A2M	O4'-C4'	7.21	1.61	1.45
4	BB	1093	OMU	C2-N1	7.21	1.49	1.38
3	BA	737	PSU	C2-N3	7.19	1.49	1.37
3	BA	1248	PSU	C2-N3	7.13	1.49	1.37
1	AA	1652	OMU	C2-N3	7.11	1.50	1.38
4	BB	685	OMU	C2-N1	7.10	1.49	1.38
4	BB	73	OMU	C2-N1	7.09	1.49	1.38
3	BA	742	1MA	C4-N3	7.05	1.50	1.35
3	BA	46	OMU	C2-N1	7.04	1.49	1.38
5	BC	7	OMU	C2-N1	7.02	1.49	1.38
1	AA	1899	OMU	C2-N1	7.02	1.49	1.38
4	BB	1435	OMU	C2-N1	7.01	1.49	1.38
3	BA	1448	OMU	C2-N1	7.01	1.49	1.38
1	AA	1899	OMU	C2-N3	6.96	1.50	1.38
3	BA	1181	OMU	C2-N1	6.96	1.49	1.38
3	BA	1742	OMU	C2-N1	6.92	1.49	1.38
4	BB	1375	OMU	C2-N1	6.92	1.49	1.38
1	AA	2054	OMU	C2-N1	6.91	1.49	1.38
3	BA	916	OMU	C2-N1	6.90	1.49	1.38
1	AA	2054	OMU	C2-N3	6.86	1.49	1.38
4	BB	73	OMU	C2-N3	6.86	1.49	1.38
1	AA	2070	7MG	C4-N9	6.86	1.46	1.37
1	AA	57	OMU	C2-N3	6.85	1.49	1.38
1	AA	2154	OMU	C2-N3	6.81	1.49	1.38
3	BA	916	OMU	C2-N3	6.81	1.49	1.38
5	BC	7	OMU	C2-N3	6.80	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	2123	OMU	C2-N1	6.79	1.49	1.38
3	BA	1448	OMU	C2-N3	6.77	1.49	1.38
4	BB	1093	OMU	C2-N3	6.77	1.49	1.38
3	BA	1181	OMU	C2-N3	6.76	1.49	1.38
1	AA	57	OMU	C2-N1	6.75	1.49	1.38
4	BB	1435	OMU	C2-N3	6.72	1.49	1.38
3	BA	46	OMU	C2-N3	6.67	1.49	1.38
4	BB	1375	OMU	C2-N3	6.67	1.49	1.38
3	BA	1742	OMU	C2-N3	6.62	1.49	1.38
1	AA	714	OMU	C2-N1	6.60	1.48	1.38
4	BB	685	OMU	C2-N3	6.58	1.49	1.38
4	BB	578	OMU	C2-N3	6.56	1.49	1.38
3	BA	1329	OMC	C2-N3	6.55	1.49	1.36
1	AA	1676	OMG	C4-N3	6.50	1.49	1.34
4	BB	377	OMC	C2-N3	6.50	1.49	1.36
1	AA	36	OMU	C2-N1	6.49	1.48	1.38
5	BC	75	OMG	C4-N3	6.47	1.49	1.34
1	AA	1517	OMG	C4-N3	6.45	1.49	1.34
4	BB	1062	OMG	C4-N3	6.44	1.49	1.34
3	BA	1028	OMG	C4-N3	6.42	1.48	1.34
4	BB	71	OMG	C4-N3	6.39	1.48	1.34
1	AA	2123	OMU	C2-N3	6.38	1.49	1.38
4	BB	1247	OMG	C4-N3	6.38	1.48	1.34
3	BA	1605	OMG	C4-N3	6.36	1.48	1.34
3	BA	1709	OMG	C4-N3	6.36	1.48	1.34
3	BA	925	OMG	C4-N3	6.35	1.48	1.34
4	BB	601	OMC	C2-N3	6.34	1.48	1.36
3	BA	915	OMG	C4-N3	6.33	1.48	1.34
1	AA	714	OMU	C2-N3	6.33	1.49	1.38
1	AA	66	OMC	C2-N3	6.33	1.48	1.36
4	BB	673	OMG	C4-N3	6.33	1.48	1.34
1	AA	1895	OMG	C4-N3	6.33	1.48	1.34
1	AA	1931	OMG	C4-N3	6.32	1.48	1.34
4	BB	1245	OMG	C4-N3	6.31	1.48	1.34
4	BB	659	OMG	C4-N3	6.31	1.48	1.34
1	AA	36	OMU	C2-N3	6.30	1.48	1.38
4	BB	1094	OMG	C4-N3	6.30	1.48	1.34
4	BB	552	OMG	C4-N3	6.29	1.48	1.34
3	BA	1621	OMG	C4-N3	6.27	1.48	1.34
4	BB	1269	OMG	C4-N3	6.26	1.48	1.34
4	BB	1324	5MC	C4-N3	6.25	1.44	1.34
3	BA	1267	OMG	C4-N3	6.25	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	1175	OMC	C2-N3	6.25	1.48	1.36
1	AA	2227	OMG	C4-N3	6.21	1.48	1.34
3	BA	1608	OMC	C2-N3	6.21	1.48	1.36
3	BA	760	OMC	C2-N3	6.20	1.48	1.36
1	AA	2070	7MG	C2-N3	6.19	1.48	1.33
4	BB	1264	OMC	C2-N3	6.19	1.48	1.36
4	BB	542	5MC	C4-N3	6.19	1.44	1.34
3	BA	1006	OMC	C2-N3	6.14	1.48	1.36
1	AA	1700	OMG	C4-N3	6.10	1.48	1.34
4	BB	1413	OMC	C2-N3	6.10	1.48	1.36
1	AA	46	OMC	C2-N3	6.10	1.48	1.36
1	AA	2134	OMC	C2-N3	6.06	1.48	1.36
1	AA	1531	OMG	C4-N3	6.06	1.48	1.34
3	BA	1329	OMC	C6-C5	6.02	1.49	1.35
4	BB	542	5MC	C5-C4	5.97	1.48	1.44
4	BB	542	5MC	C2-N3	5.95	1.48	1.36
4	BB	377	OMC	C6-C5	5.94	1.48	1.35
4	BB	1264	OMC	C6-C5	5.94	1.48	1.35
4	BB	1324	5MC	C5-C4	5.89	1.48	1.44
1	AA	66	OMC	C6-C5	5.87	1.48	1.35
3	BA	760	OMC	C6-C5	5.86	1.48	1.35
4	BB	1175	OMC	C6-C5	5.85	1.48	1.35
4	BB	1324	5MC	C2-N3	5.83	1.47	1.36
4	BB	1413	OMC	C6-C5	5.81	1.48	1.35
3	BA	1006	OMC	C6-C5	5.81	1.48	1.35
1	AA	2134	OMC	C6-C5	5.77	1.48	1.35
1	AA	1652	OMU	C6-C5	5.76	1.48	1.35
4	BB	601	OMC	C6-C5	5.76	1.48	1.35
3	BA	1608	OMC	C6-C5	5.74	1.48	1.35
1	AA	46	OMC	C6-C5	5.72	1.48	1.35
1	AA	1596	B8N	C2-N1	5.70	1.55	1.39
1	AA	2054	OMU	C6-C5	5.64	1.48	1.35
3	BA	916	OMU	C6-C5	5.61	1.48	1.35
3	BA	1181	OMU	C6-C5	5.59	1.48	1.35
4	BB	73	OMU	C6-C5	5.58	1.48	1.35
3	BA	46	OMU	C6-C5	5.58	1.48	1.35
4	BB	1093	OMU	C6-C5	5.57	1.48	1.35
4	BB	578	OMU	C6-C5	5.55	1.47	1.35
3	BA	1448	OMU	C6-C5	5.54	1.47	1.35
5	BC	7	OMU	C6-C5	5.54	1.47	1.35
1	AA	1899	OMU	C6-C5	5.53	1.47	1.35
4	BB	1375	OMU	C6-C5	5.52	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	2154	OMU	C6-C5	5.51	1.47	1.35
1	AA	57	OMU	C6-C5	5.51	1.47	1.35
4	BB	685	OMU	C6-C5	5.50	1.47	1.35
1	AA	2070	7MG	C4-N3	5.50	1.46	1.34
4	BB	1435	OMU	C6-C5	5.49	1.47	1.35
3	BA	1742	OMU	C6-C5	5.48	1.47	1.35
1	AA	714	OMU	C6-C5	5.47	1.47	1.35
1	AA	2123	OMU	C6-C5	5.45	1.47	1.35
1	AA	36	OMU	C6-C5	5.41	1.47	1.35
5	BC	74	PSU	C6-N1	5.40	1.45	1.36
3	BA	1329	OMC	C4-N3	5.36	1.45	1.34
1	AA	1619	PSU	C6-N1	5.36	1.45	1.36
3	BA	258	PSU	C6-N1	5.35	1.45	1.36
3	BA	1169	PSU	C6-N1	5.35	1.45	1.36
3	BA	1248	PSU	C6-N1	5.33	1.45	1.36
4	BB	518	PSU	C6-N1	5.32	1.45	1.36
4	BB	545	A2M	O4'-C1'	-5.29	1.29	1.42
3	BA	1129	PSU	C6-N1	5.28	1.44	1.36
1	AA	1676	OMG	C2-N3	5.28	1.46	1.33
4	BB	522	PSU	C6-N1	5.28	1.44	1.36
3	BA	452	PSU	C6-N1	5.28	1.44	1.36
1	AA	2045	PSU	C6-N1	5.27	1.44	1.36
5	BC	75	OMG	C2-N3	5.25	1.45	1.33
3	BA	1609	PSU	C6-N1	5.24	1.44	1.36
4	BB	1409	PSU	C6-N1	5.22	1.44	1.36
4	BB	629	PSU	C6-N1	5.22	1.44	1.36
1	AA	1517	OMG	C2-N3	5.22	1.45	1.33
4	BB	1229	PSU	C6-N1	5.21	1.44	1.36
4	BB	1160	PSU	C6-N1	5.20	1.44	1.36
4	BB	524	PSU	C6-N1	5.20	1.44	1.36
1	AA	1592	PSU	C6-N1	5.19	1.44	1.36
4	BB	1210	PSU	C6-N1	5.18	1.44	1.36
3	BA	1258	PSU	C6-N1	5.17	1.44	1.36
4	BB	377	OMC	C4-N3	5.17	1.44	1.34
3	BA	1009	PSU	C6-N1	5.17	1.44	1.36
1	AA	721	A2M	O4'-C1'	-5.17	1.30	1.42
1	AA	61	PSU	C6-N1	5.16	1.44	1.36
4	BB	611	PSU	C6-N1	5.16	1.44	1.36
1	AA	131	PSU	C6-N1	5.15	1.44	1.36
3	BA	1605	OMG	C2-N3	5.15	1.45	1.33
3	BA	1028	OMG	C2-N3	5.13	1.45	1.33
4	BB	615	PSU	C6-N1	5.13	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	644	PSU	C6-N1	5.13	1.44	1.36
4	BB	1319	PSU	C6-N1	5.12	1.44	1.36
4	BB	1062	OMG	C2-N3	5.12	1.45	1.33
4	BB	1398	PSU	C6-N1	5.11	1.44	1.36
4	BB	1280	PSU	C6-N1	5.11	1.44	1.36
4	BB	1247	OMG	C2-N3	5.08	1.45	1.33
4	BB	601	OMC	C4-N3	5.07	1.44	1.34
1	AA	1276	PSU	C6-N1	5.07	1.44	1.36
4	BB	71	OMG	C2-N3	5.06	1.45	1.33
1	AA	1931	OMG	C2-N3	5.05	1.45	1.33
1	AA	1895	OMG	C2-N3	5.05	1.45	1.33
4	BB	1076	PSU	C6-N1	5.05	1.44	1.36
4	BB	1429	PSU	C6-N1	5.04	1.44	1.36
1	AA	2146	PSU	C6-N1	5.04	1.44	1.36
3	BA	746	A2M	O4'-C1'	-5.04	1.30	1.42
3	BA	1614	PSU	C6-N1	5.03	1.44	1.36
3	BA	1086	PSU	C6-N1	5.02	1.44	1.36
4	BB	455	PSU	C6-N1	5.02	1.44	1.36
3	BA	1709	OMG	C2-N3	5.02	1.45	1.33
4	BB	1334	PSU	C6-N1	5.01	1.44	1.36
4	BB	1175	OMC	C4-N3	5.01	1.44	1.34
4	BB	680	PSU	C6-N1	5.01	1.44	1.36
3	BA	760	OMC	C4-N3	5.00	1.44	1.34
4	BB	673	OMG	C2-N3	4.99	1.45	1.33
4	BB	659	OMG	C2-N3	4.98	1.45	1.33
3	BA	737	PSU	C6-N1	4.96	1.44	1.36
4	BB	1245	OMG	C2-N3	4.96	1.45	1.33
3	BA	1621	OMG	C2-N3	4.96	1.45	1.33
1	AA	66	OMC	C4-N3	4.96	1.44	1.34
3	BA	1608	OMC	C4-N3	4.94	1.44	1.34
3	BA	927	A2M	O4'-C1'	-4.94	1.30	1.42
4	BB	552	OMG	C2-N3	4.93	1.45	1.33
3	BA	915	OMG	C2-N3	4.93	1.45	1.33
4	BB	1094	OMG	C2-N3	4.90	1.45	1.33
4	BB	1264	OMC	C4-N3	4.89	1.44	1.34
3	BA	1006	OMC	C4-N3	4.89	1.44	1.34
4	BB	1269	OMG	C2-N3	4.89	1.45	1.33
1	AA	1596	B8N	C6-C5	4.87	1.42	1.35
1	AA	1700	OMG	C2-N3	4.87	1.45	1.33
5	BC	41	A2M	O4'-C1'	-4.86	1.30	1.42
3	BA	925	OMG	C2-N3	4.86	1.45	1.33
1	AA	2096	A2M	O4'-C1'	-4.85	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BA	1620	A2M	O4'-C1'	-4.83	1.30	1.42
4	BB	588	A2M	O4'-C1'	-4.83	1.30	1.42
5	BC	163	A2M	O4'-C1'	-4.81	1.30	1.42
4	BB	1413	OMC	C4-N3	4.81	1.44	1.34
1	AA	2227	OMG	C2-N3	4.80	1.44	1.33
3	BA	743	A2M	O4'-C1'	-4.80	1.30	1.42
3	BA	762	A2M	O4'-C1'	-4.79	1.30	1.42
3	BA	996	A2M	O4'-C1'	-4.79	1.30	1.42
3	BA	1267	OMG	C2-N3	4.79	1.44	1.33
3	BA	254	A2M	O4'-C1'	-4.78	1.30	1.42
4	BB	609	A2M	O4'-C1'	-4.77	1.31	1.42
1	AA	2153	A2M	O4'-C1'	-4.77	1.31	1.42
4	BB	95	A2M	O4'-C1'	-4.76	1.31	1.42
4	BB	1201	A2M	O4'-C1'	-4.76	1.31	1.42
1	AA	2134	OMC	C4-N3	4.76	1.44	1.34
1	AA	46	OMC	C4-N3	4.75	1.43	1.34
4	BB	1388	A2M	O4'-C1'	-4.75	1.31	1.42
4	BB	1400	A2M	O4'-C1'	-4.74	1.31	1.42
3	BA	1665	A2M	O4'-C1'	-4.73	1.31	1.42
4	BB	622	A2M	O4'-C1'	-4.73	1.31	1.42
5	BC	43	A2M	O4'-C1'	-4.71	1.31	1.42
1	AA	1931	OMG	C2-N2	4.71	1.45	1.34
4	BB	646	A2M	O4'-C1'	-4.69	1.31	1.42
1	AA	56	A2M	O4'-C1'	-4.69	1.31	1.42
4	BB	377	OMC	C4-N4	4.68	1.45	1.33
1	AA	1676	OMG	C2-N2	4.67	1.45	1.34
4	BB	1245	OMG	C2-N2	4.67	1.45	1.34
3	BA	1329	OMC	C4-N4	4.67	1.45	1.33
4	BB	1247	OMG	C2-N2	4.65	1.45	1.34
3	BA	1024	A2M	O4'-C1'	-4.65	1.31	1.42
5	BC	75	OMG	C2-N2	4.64	1.45	1.34
4	BB	400	A2M	O4'-C1'	-4.63	1.31	1.42
1	AA	1895	OMG	C2-N2	4.63	1.45	1.34
3	BA	1329	OMC	C2-N1	4.61	1.49	1.40
3	BA	915	OMG	C2-N2	4.60	1.44	1.34
4	BB	1062	OMG	C2-N2	4.60	1.44	1.34
4	BB	71	OMG	C2-N2	4.60	1.44	1.34
4	BB	680	PSU	C1'-C5	-4.60	1.39	1.50
4	BB	1175	OMC	C4-N4	4.60	1.45	1.33
4	BB	1264	OMC	C2-N1	4.59	1.49	1.40
3	BA	1709	OMG	C2-N2	4.58	1.44	1.34
4	BB	1324	5MC	C6-N1	4.57	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	1398	PSU	C1'-C5	-4.57	1.39	1.50
1	AA	1700	OMG	C2-N2	4.57	1.44	1.34
1	AA	66	OMC	C4-N4	4.57	1.45	1.33
3	BA	925	OMG	C2-N2	4.57	1.44	1.34
3	BA	1605	OMG	C2-N2	4.57	1.44	1.34
4	BB	1264	OMC	C4-N4	4.56	1.44	1.33
1	AA	1531	OMG	C2-N3	4.56	1.44	1.33
4	BB	659	OMG	C2-N2	4.55	1.44	1.34
3	BA	1086	PSU	C1'-C5	-4.55	1.40	1.50
1	AA	1596	B8N	C1'-C5	-4.54	1.40	1.50
3	BA	760	OMC	C4-N4	4.54	1.44	1.33
4	BB	1094	OMG	C2-N2	4.54	1.44	1.34
4	BB	601	OMC	C4-N4	4.53	1.44	1.33
4	BB	673	OMG	C2-N2	4.53	1.44	1.34
4	BB	552	OMG	C2-N2	4.53	1.44	1.34
3	BA	1621	OMG	C2-N2	4.52	1.44	1.34
1	AA	2134	OMC	C4-N4	4.52	1.44	1.33
4	BB	1229	PSU	C1'-C5	-4.52	1.40	1.50
4	BB	455	PSU	C1'-C5	-4.52	1.40	1.50
4	BB	615	PSU	C1'-C5	-4.52	1.40	1.50
3	BA	1028	OMG	C2-N2	4.51	1.44	1.34
5	BC	74	PSU	C1'-C5	-4.51	1.40	1.50
3	BA	1006	OMC	C4-N4	4.51	1.44	1.33
4	BB	518	PSU	C1'-C5	-4.51	1.40	1.50
3	BA	1009	PSU	C1'-C5	-4.50	1.40	1.50
3	BA	1169	PSU	C1'-C5	-4.50	1.40	1.50
1	AA	1517	OMG	C2-N2	4.50	1.44	1.34
4	BB	1076	PSU	C1'-C5	-4.50	1.40	1.50
1	AA	46	OMC	C4-N4	4.50	1.44	1.33
3	BA	1267	OMG	C2-N2	4.49	1.44	1.34
1	AA	1276	PSU	C1'-C5	-4.48	1.40	1.50
3	BA	452	PSU	C1'-C5	-4.47	1.40	1.50
3	BA	1258	PSU	C1'-C5	-4.47	1.40	1.50
4	BB	377	OMC	C2-N1	4.46	1.49	1.40
3	BA	1129	PSU	C1'-C5	-4.46	1.40	1.50
1	AA	2146	PSU	C1'-C5	-4.46	1.40	1.50
1	AA	2227	OMG	C2-N2	4.45	1.44	1.34
4	BB	1269	OMG	C2-N2	4.45	1.44	1.34
1	AA	1592	PSU	C1'-C5	-4.45	1.40	1.50
1	AA	61	PSU	C1'-C5	-4.44	1.40	1.50
3	BA	1608	OMC	C4-N4	4.44	1.44	1.33
4	BB	601	OMC	C2-N1	4.43	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BA	1614	PSU	C1'-C5	-4.43	1.40	1.50
4	BB	1413	OMC	C4-N4	4.43	1.44	1.33
4	BB	1160	PSU	C1'-C5	-4.43	1.40	1.50
3	BA	760	OMC	C2-N1	4.43	1.49	1.40
1	AA	131	PSU	C1'-C5	-4.42	1.40	1.50
4	BB	1319	PSU	C1'-C5	-4.42	1.40	1.50
4	BB	1429	PSU	C1'-C5	-4.42	1.40	1.50
4	BB	644	PSU	C1'-C5	-4.41	1.40	1.50
3	BA	1006	OMC	C2-N1	4.41	1.49	1.40
4	BB	1175	OMC	C2-N1	4.40	1.49	1.40
4	BB	1210	PSU	C1'-C5	-4.40	1.40	1.50
1	AA	2045	PSU	C1'-C5	-4.40	1.40	1.50
3	BA	1608	OMC	C2-N1	4.39	1.49	1.40
3	BA	258	PSU	C1'-C5	-4.37	1.40	1.50
4	BB	1280	PSU	C1'-C5	-4.37	1.40	1.50
4	BB	1334	PSU	C1'-C5	-4.37	1.40	1.50
1	AA	1652	OMU	C4-N3	4.37	1.46	1.38
1	AA	1531	OMG	C2-N2	4.35	1.44	1.34
4	BB	542	5MC	C6-N1	4.35	1.45	1.38
4	BB	1413	OMC	C2-N1	4.35	1.49	1.40
4	BB	524	PSU	C1'-C5	-4.35	1.40	1.50
3	BA	254	A2M	C6-N6	4.33	1.45	1.34
3	BA	1665	A2M	C6-N6	4.33	1.45	1.34
4	BB	1409	PSU	C1'-C5	-4.31	1.40	1.50
4	BB	622	A2M	C6-N6	4.29	1.45	1.34
4	BB	95	A2M	C6-N6	4.28	1.45	1.34
4	BB	1201	A2M	C6-N6	4.27	1.45	1.34
1	AA	2153	A2M	C6-N6	4.27	1.45	1.34
1	AA	2096	A2M	C6-N6	4.27	1.45	1.34
4	BB	1388	A2M	C6-N6	4.27	1.45	1.34
1	AA	56	A2M	C6-N6	4.26	1.45	1.34
4	BB	609	A2M	C6-N6	4.26	1.45	1.34
5	BC	163	A2M	C6-N6	4.26	1.45	1.34
4	BB	400	A2M	C6-N6	4.25	1.45	1.34
4	BB	611	PSU	C1'-C5	-4.25	1.40	1.50
3	BA	1609	PSU	C1'-C5	-4.24	1.40	1.50
4	BB	1324	5MC	C4-N4	4.24	1.44	1.34
3	BA	927	A2M	C6-N6	4.23	1.45	1.34
4	BB	646	A2M	C6-N6	4.23	1.45	1.34
4	BB	522	PSU	C1'-C5	-4.23	1.40	1.50
5	BC	43	A2M	C6-N6	4.23	1.45	1.34
3	BA	743	A2M	C6-N6	4.23	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BA	1620	A2M	C6-N6	4.23	1.45	1.34
3	BA	996	A2M	C6-N6	4.23	1.45	1.34
1	AA	1899	OMU	C4-N3	4.22	1.45	1.38
3	BA	1024	A2M	C6-N6	4.21	1.45	1.34
3	BA	746	A2M	C6-N6	4.19	1.44	1.34
3	BA	762	A2M	C6-N6	4.19	1.44	1.34
4	BB	1400	A2M	C6-N6	4.18	1.44	1.34
4	BB	588	A2M	C6-N6	4.17	1.44	1.34
3	BA	1248	PSU	C1'-C5	-4.16	1.40	1.50
4	BB	542	5MC	C4-N4	4.16	1.44	1.34
4	BB	629	PSU	C1'-C5	-4.16	1.40	1.50
5	BC	7	OMU	C4-N3	4.15	1.45	1.38
1	AA	2054	OMU	C4-N3	4.14	1.45	1.38
4	BB	545	A2M	C6-N6	4.14	1.44	1.34
1	AA	721	A2M	C6-N6	4.14	1.44	1.34
4	BB	1093	OMU	C4-N3	4.13	1.45	1.38
3	BA	737	PSU	C1'-C5	-4.12	1.41	1.50
3	BA	1181	OMU	C4-N3	4.12	1.45	1.38
1	AA	57	OMU	C4-N3	4.11	1.45	1.38
1	AA	1619	PSU	C1'-C5	-4.10	1.41	1.50
1	AA	66	OMC	C2-N1	4.08	1.48	1.40
3	BA	1448	OMU	C4-N3	4.07	1.45	1.38
4	BB	1324	5MC	C2-N1	4.06	1.48	1.40
5	BC	41	A2M	C6-N6	4.06	1.44	1.34
1	AA	46	OMC	C2-N1	4.05	1.48	1.40
3	BA	1742	OMU	C4-N3	4.05	1.45	1.38
4	BB	542	5MC	C2-N1	4.04	1.48	1.40
4	BB	1435	OMU	C4-N3	4.03	1.45	1.38
1	AA	2134	OMC	C2-N1	4.02	1.48	1.40
4	BB	73	OMU	C4-N3	3.99	1.45	1.38
3	BA	742	1MA	C2-N1	3.97	1.44	1.35
3	BA	46	OMU	C4-N3	3.96	1.45	1.38
3	BA	916	OMU	C4-N3	3.96	1.45	1.38
4	BB	1375	OMU	C4-N3	3.95	1.45	1.38
4	BB	522	PSU	C4-N3	3.91	1.46	1.38
1	AA	1619	PSU	C4-N3	3.88	1.46	1.38
4	BB	578	OMU	C4-N3	3.85	1.45	1.38
1	AA	2045	PSU	C4-N3	3.84	1.46	1.38
1	AA	2154	OMU	C4-N3	3.82	1.45	1.38
3	BA	258	PSU	C4-N3	3.80	1.46	1.38
1	AA	2261	MA6	C6-N6	3.79	1.47	1.36
4	BB	1409	PSU	C4-N3	3.79	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	685	OMU	C4-N3	3.78	1.45	1.38
4	BB	518	PSU	C4-N3	3.78	1.45	1.38
4	BB	629	PSU	C4-N3	3.76	1.45	1.38
3	BA	1129	PSU	C4-N3	3.76	1.45	1.38
3	BA	452	PSU	C4-N3	3.74	1.45	1.38
4	BB	524	PSU	C4-N3	3.73	1.45	1.38
3	BA	1169	PSU	C4-N3	3.73	1.45	1.38
5	BC	74	PSU	C4-N3	3.71	1.45	1.38
1	AA	61	PSU	C4-N3	3.71	1.45	1.38
4	BB	1210	PSU	C4-N3	3.69	1.45	1.38
3	BA	1609	PSU	C4-N3	3.67	1.45	1.38
1	AA	1592	PSU	C4-N3	3.67	1.45	1.38
1	AA	2260	MA6	C6-N6	3.67	1.46	1.36
4	BB	1280	PSU	C4-N3	3.66	1.45	1.38
1	AA	2123	OMU	C4-N3	3.65	1.44	1.38
1	AA	714	OMU	C4-N3	3.65	1.44	1.38
4	BB	644	PSU	C4-N3	3.65	1.45	1.38
3	BA	1258	PSU	C4-N3	3.62	1.45	1.38
3	BA	742	1MA	C5-C6	3.62	1.53	1.43
4	BB	1319	PSU	C4-N3	3.62	1.45	1.38
4	BB	1076	PSU	C4-N3	3.60	1.45	1.38
4	BB	1229	PSU	C4-N3	3.60	1.45	1.38
1	AA	721	A2M	C5-C4	-3.60	1.32	1.39
3	BA	1614	PSU	C4-N3	3.59	1.45	1.38
4	BB	615	PSU	C4-N3	3.58	1.45	1.38
4	BB	1160	PSU	C4-N3	3.57	1.45	1.38
1	AA	131	PSU	C4-N3	3.54	1.45	1.38
4	BB	611	PSU	C4-N3	3.54	1.45	1.38
4	BB	1429	PSU	C4-N3	3.54	1.45	1.38
4	BB	1334	PSU	C4-N3	3.54	1.45	1.38
3	BA	1086	PSU	C4-N3	3.53	1.45	1.38
1	AA	2146	PSU	C4-N3	3.52	1.45	1.38
4	BB	680	PSU	C4-N3	3.51	1.45	1.38
3	BA	1009	PSU	C4-N3	3.50	1.45	1.38
1	AA	2070	7MG	C2-N1	3.48	1.46	1.37
1	AA	2261	MA6	C5-C4	-3.47	1.32	1.39
4	BB	1398	PSU	C4-N3	3.45	1.45	1.38
1	AA	2070	7MG	C5-C6	3.43	1.52	1.43
1	AA	2070	7MG	C6-N1	3.42	1.45	1.38
3	BA	1248	PSU	C4-N3	3.40	1.45	1.38
4	BB	545	A2M	C5-C4	-3.39	1.33	1.39
1	AA	36	OMU	C4-N3	3.38	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BA	737	PSU	C4-N3	3.38	1.45	1.38
1	AA	1276	PSU	C4-N3	3.36	1.45	1.38
4	BB	455	PSU	C4-N3	3.35	1.45	1.38
1	AA	2070	7MG	C2-N2	3.35	1.42	1.34
1	AA	1517	OMG	C5-N7	-3.34	1.32	1.39
1	AA	36	OMU	O4-C4	-3.33	1.18	1.24
1	AA	2123	OMU	O4-C4	-3.32	1.18	1.24
3	BA	1329	OMC	C6-N1	3.31	1.46	1.38
3	BA	762	A2M	C5-C4	-3.29	1.33	1.39
5	BC	41	A2M	C5-C4	-3.28	1.33	1.39
1	AA	714	OMU	O4-C4	-3.27	1.18	1.24
3	BA	746	A2M	C5-C4	-3.26	1.33	1.39
4	BB	377	OMC	C6-N1	3.26	1.45	1.38
3	BA	46	OMU	O4-C4	-3.25	1.18	1.24
1	AA	2096	A2M	C5-C4	-3.25	1.33	1.39
4	BB	1400	A2M	C5-C4	-3.25	1.33	1.39
4	BB	1435	OMU	O4-C4	-3.23	1.18	1.24
1	AA	56	A2M	C5-C4	-3.22	1.33	1.39
1	AA	2153	A2M	C5-C4	-3.22	1.33	1.39
4	BB	1388	A2M	C5-C4	-3.21	1.33	1.39
3	BA	1608	OMC	C6-N1	3.21	1.45	1.38
3	BA	760	OMC	C6-N1	3.20	1.45	1.38
3	BA	1024	A2M	C5-C4	-3.20	1.33	1.39
4	BB	73	OMU	O4-C4	-3.20	1.18	1.24
4	BB	685	OMU	O4-C4	-3.19	1.18	1.24
4	BB	588	A2M	C5-C4	-3.19	1.33	1.39
3	BA	1620	A2M	C5-C4	-3.19	1.33	1.39
3	BA	743	A2M	C5-C4	-3.18	1.33	1.39
3	BA	1448	OMU	O4-C4	-3.18	1.18	1.24
4	BB	609	A2M	C5-C4	-3.17	1.33	1.39
4	BB	646	A2M	C5-C4	-3.17	1.33	1.39
3	BA	254	A2M	C5-C4	-3.17	1.33	1.39
1	AA	2070	7MG	O6-C6	-3.17	1.17	1.23
4	BB	400	A2M	C5-C4	-3.15	1.33	1.39
3	BA	1006	OMC	C6-N1	3.14	1.45	1.38
4	BB	528	PSU	C4-N3	-3.14	1.33	1.38
5	BC	163	A2M	C5-C4	-3.13	1.33	1.39
5	BC	43	A2M	C5-C4	-3.13	1.33	1.39
3	BA	916	OMU	O4-C4	-3.13	1.18	1.24
3	BA	927	A2M	C5-C4	-3.13	1.33	1.39
4	BB	1201	A2M	C5-C4	-3.11	1.33	1.39
3	BA	996	A2M	C5-C4	-3.11	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BA	1742	OMU	O4-C4	-3.11	1.18	1.24
1	AA	2134	OMC	O2-C2	-3.11	1.17	1.23
4	BB	1264	OMC	C6-N1	3.10	1.45	1.38
4	BB	1175	OMC	C6-N1	3.10	1.45	1.38
4	BB	601	OMC	C6-N1	3.10	1.45	1.38
4	BB	1413	OMC	C6-N1	3.09	1.45	1.38
4	BB	578	OMU	O4-C4	-3.08	1.18	1.24
4	BB	95	A2M	C5-C4	-3.08	1.33	1.39
3	BA	1248	PSU	O4-C4	-3.07	1.17	1.23
4	BB	622	A2M	C5-C4	-3.06	1.33	1.39
4	BB	1375	OMU	O4-C4	-3.06	1.18	1.24
5	BC	7	OMU	O4-C4	-3.05	1.18	1.24
1	AA	2154	OMU	O4-C4	-3.05	1.18	1.24
4	BB	1324	5MC	O2-C2	-3.05	1.18	1.23
1	AA	2260	MA6	C5-N7	-3.05	1.33	1.39
3	BA	1181	OMU	O4-C4	-3.05	1.18	1.24
1	AA	57	OMU	O4-C4	-3.04	1.18	1.24
1	AA	46	OMC	O2-C2	-3.04	1.18	1.23
1	AA	1700	OMG	C5-N7	-3.03	1.33	1.39
4	BB	601	OMC	O2-C2	-3.03	1.18	1.23
1	AA	1531	OMG	C5-N7	-3.03	1.33	1.39
3	BA	737	PSU	O4-C4	-3.03	1.17	1.23
3	BA	1665	A2M	C5-C4	-3.03	1.33	1.39
1	AA	1899	OMU	O4-C4	-3.03	1.18	1.24
1	AA	721	A2M	C8-N9	-3.01	1.32	1.37
4	BB	545	A2M	O3'-C3'	3.00	1.50	1.43
1	AA	36	OMU	O2-C2	-3.00	1.17	1.23
1	AA	2054	OMU	O4-C4	-3.00	1.18	1.24
4	BB	1269	OMG	C5-N7	-2.99	1.33	1.39
1	AA	1276	PSU	O4-C4	-2.99	1.17	1.23
4	BB	1093	OMU	O4-C4	-2.99	1.18	1.24
1	AA	1895	OMG	C5-N7	-2.99	1.33	1.39
1	AA	1531	OMG	O6-C6	-2.98	1.17	1.23
1	AA	1531	OMG	C4-N9	-2.98	1.30	1.38
1	AA	66	OMC	C6-N1	2.97	1.45	1.38
4	BB	530	PSU	C6-C5	2.97	1.38	1.35
3	BA	1608	OMC	O2-C2	-2.96	1.18	1.23
4	BB	530	PSU	C4-N3	-2.96	1.33	1.38
1	AA	2227	OMG	C5-N7	-2.96	1.33	1.39
3	BA	1006	OMC	O2-C2	-2.96	1.18	1.23
4	BB	552	OMG	C5-N7	-2.96	1.33	1.39
1	AA	1517	OMG	O6-C6	-2.96	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1652	OMU	C6-N1	2.96	1.45	1.38
1	AA	66	OMC	O2-C2	-2.96	1.18	1.23
4	BB	1264	OMC	O2-C2	-2.96	1.18	1.23
4	BB	1413	OMC	O2-C2	-2.95	1.18	1.23
1	AA	2261	MA6	C5-N7	-2.95	1.33	1.39
1	AA	1931	OMG	C5-N7	-2.94	1.33	1.39
4	BB	1398	PSU	O4-C4	-2.94	1.18	1.23
4	BB	455	PSU	O4-C4	-2.94	1.18	1.23
1	AA	56	A2M	O2'-C2'	-2.93	1.35	1.42
3	BA	760	OMC	O2-C2	-2.92	1.18	1.23
4	BB	400	A2M	C8-N9	-2.91	1.32	1.37
4	BB	1269	OMG	O6-C6	-2.91	1.18	1.23
4	BB	659	OMG	C5-N7	-2.90	1.33	1.39
4	BB	1388	A2M	C8-N9	-2.90	1.32	1.37
1	AA	721	A2M	O3'-C3'	2.90	1.50	1.43
4	BB	588	A2M	O3'-C3'	2.90	1.50	1.43
1	AA	2227	OMG	O6-C6	-2.90	1.18	1.23
3	BA	1621	OMG	C5-N7	-2.89	1.33	1.39
1	AA	1652	OMU	O4-C4	-2.89	1.18	1.24
4	BB	1388	A2M	O3'-C3'	2.89	1.50	1.43
1	AA	2146	PSU	O4-C4	-2.89	1.18	1.23
1	AA	721	A2M	O2'-C2'	-2.89	1.35	1.42
4	BB	673	OMG	O6-C6	-2.88	1.18	1.23
4	BB	588	A2M	C8-N9	-2.88	1.32	1.37
5	BC	41	A2M	C8-N9	-2.88	1.32	1.37
4	BB	680	PSU	O4-C4	-2.88	1.18	1.23
4	BB	1201	A2M	C8-N9	-2.88	1.32	1.37
1	AA	46	OMC	C6-N1	2.88	1.44	1.38
4	BB	528	PSU	C6-C5	2.87	1.38	1.35
4	BB	71	OMG	C5-N7	-2.87	1.33	1.39
1	AA	2123	OMU	O2-C2	-2.87	1.18	1.23
3	BA	1028	OMG	C5-N7	-2.87	1.33	1.39
3	BA	996	A2M	C8-N9	-2.87	1.32	1.37
3	BA	1181	OMU	C6-N1	2.86	1.44	1.38
1	AA	2260	MA6	C5-C4	-2.86	1.34	1.39
4	BB	609	A2M	C8-N9	-2.86	1.32	1.37
4	BB	1429	PSU	O4-C4	-2.86	1.18	1.23
4	BB	1247	OMG	C5-N7	-2.86	1.33	1.39
4	BB	1201	A2M	O3'-C3'	2.85	1.50	1.43
4	BB	400	A2M	O2'-C2'	-2.85	1.35	1.42
4	BB	673	OMG	C5-N7	-2.85	1.33	1.39
4	BB	71	OMG	O6-C6	-2.84	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	2134	OMC	C6-N1	2.84	1.44	1.38
4	BB	1175	OMC	O2-C2	-2.84	1.18	1.23
3	BA	1024	A2M	C8-N9	-2.84	1.32	1.37
3	BA	762	A2M	O2'-C2'	-2.84	1.35	1.42
4	BB	1334	PSU	O4-C4	-2.84	1.18	1.23
3	BA	915	OMG	C5-N7	-2.84	1.33	1.39
4	BB	1062	OMG	C5-N7	-2.83	1.33	1.39
4	BB	644	PSU	O4-C4	-2.83	1.18	1.23
3	BA	1605	OMG	C5-N7	-2.83	1.33	1.39
1	AA	1700	OMG	O6-C6	-2.83	1.18	1.23
4	BB	1280	PSU	O4-C4	-2.83	1.18	1.23
4	BB	1093	OMU	C6-N1	2.83	1.44	1.38
3	BA	1620	A2M	O2'-C2'	-2.82	1.35	1.42
1	AA	1676	OMG	C5-N7	-2.82	1.33	1.39
3	BA	746	A2M	C8-N9	-2.82	1.32	1.37
3	BA	1009	PSU	O4-C4	-2.82	1.18	1.23
4	BB	1062	OMG	O6-C6	-2.82	1.18	1.23
4	BB	552	OMG	O6-C6	-2.82	1.18	1.23
4	BB	622	A2M	O3'-C3'	2.82	1.49	1.43
3	BA	1609	PSU	O4-C4	-2.81	1.18	1.23
3	BA	1709	OMG	O6-C6	-2.81	1.18	1.23
4	BB	1210	PSU	O4-C4	-2.81	1.18	1.23
1	AA	56	A2M	C8-N9	-2.81	1.32	1.37
4	BB	542	5MC	O2-C2	-2.81	1.18	1.23
1	AA	1700	OMG	C4-N9	-2.81	1.30	1.38
4	BB	1435	OMU	C6-N1	2.81	1.44	1.38
5	BC	75	OMG	C5-N7	-2.80	1.33	1.39
3	BA	927	A2M	C8-N9	-2.80	1.32	1.37
3	BA	1086	PSU	O4-C4	-2.80	1.18	1.23
1	AA	1899	OMU	C6-N1	2.80	1.44	1.38
4	BB	646	A2M	O2'-C2'	-2.80	1.35	1.42
3	BA	743	A2M	O3'-C3'	2.80	1.49	1.43
1	AA	2096	A2M	O3'-C3'	2.80	1.49	1.43
3	BA	916	OMU	C6-N1	2.80	1.44	1.38
3	BA	254	A2M	O2'-C2'	-2.80	1.35	1.42
5	BC	75	OMG	C2-N1	2.80	1.44	1.37
3	BA	915	OMG	O6-C6	-2.79	1.18	1.23
3	BA	1621	OMG	O6-C6	-2.79	1.18	1.23
3	BA	746	A2M	O3'-C3'	2.79	1.49	1.43
4	BB	1076	PSU	O4-C4	-2.78	1.18	1.23
1	AA	721	A2M	C5-N7	-2.78	1.34	1.39
4	BB	1400	A2M	O2'-C2'	-2.78	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	73	OMU	C6-N1	2.78	1.44	1.38
5	BC	41	A2M	O2'-C2'	-2.78	1.35	1.42
4	BB	1201	A2M	O2'-C2'	-2.78	1.35	1.42
3	BA	1448	OMU	C6-N1	2.78	1.44	1.38
3	BA	762	A2M	C8-N9	-2.78	1.32	1.37
4	BB	95	A2M	C8-N9	-2.77	1.32	1.37
3	BA	927	A2M	O2'-C2'	-2.77	1.35	1.42
4	BB	646	A2M	C8-N9	-2.77	1.32	1.37
5	BC	7	OMU	C6-N1	2.77	1.44	1.38
3	BA	743	A2M	C8-N9	-2.77	1.32	1.37
4	BB	545	A2M	C8-N9	-2.77	1.32	1.37
3	BA	1267	OMG	O6-C6	-2.77	1.18	1.23
4	BB	629	PSU	O4-C4	-2.76	1.18	1.23
4	BB	646	A2M	O3'-C3'	2.76	1.49	1.43
4	BB	622	A2M	O2'-C2'	-2.76	1.35	1.42
4	BB	1245	OMG	C5-N7	-2.76	1.33	1.39
3	BA	1742	OMU	C6-N1	2.76	1.44	1.38
4	BB	1247	OMG	O6-C6	-2.76	1.18	1.23
1	AA	2054	OMU	C6-N1	2.76	1.44	1.38
3	BA	46	OMU	C6-N1	2.76	1.44	1.38
3	BA	927	A2M	O3'-C3'	2.76	1.49	1.43
4	BB	400	A2M	C5-N7	-2.76	1.34	1.39
4	BB	622	A2M	C8-N9	-2.76	1.32	1.37
3	BA	996	A2M	O2'-C2'	-2.76	1.35	1.42
5	BC	43	A2M	O2'-C2'	-2.75	1.35	1.42
4	BB	685	OMU	O2-C2	-2.75	1.18	1.23
3	BA	1258	PSU	O4-C4	-2.75	1.18	1.23
4	BB	1400	A2M	O3'-C3'	2.75	1.49	1.43
3	BA	1709	OMG	C5-N7	-2.75	1.33	1.39
1	AA	2153	A2M	O2'-C2'	-2.75	1.35	1.42
4	BB	1229	PSU	O4-C4	-2.74	1.18	1.23
3	BA	1267	OMG	C5-N7	-2.74	1.33	1.39
4	BB	1409	PSU	O4-C4	-2.74	1.18	1.23
1	AA	2260	MA6	C4-N9	-2.74	1.32	1.37
4	BB	611	PSU	O4-C4	-2.74	1.18	1.23
3	BA	1028	OMG	O6-C6	-2.73	1.18	1.23
4	BB	685	OMU	C6-N1	2.73	1.44	1.38
3	BA	1665	A2M	O3'-C3'	2.73	1.49	1.43
4	BB	377	OMC	O2-C2	-2.73	1.18	1.23
4	BB	578	OMU	O2-C2	-2.73	1.18	1.23
3	BA	925	OMG	C5-N7	-2.73	1.33	1.39
3	BA	1665	A2M	C8-N9	-2.73	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	545	A2M	O2'-C2'	-2.72	1.35	1.42
4	BB	1245	OMG	C2-N1	2.72	1.44	1.37
4	BB	1375	OMU	C6-N1	2.72	1.44	1.38
3	BA	925	OMG	O6-C6	-2.72	1.18	1.23
1	AA	2154	OMU	C6-N1	2.72	1.44	1.38
3	BA	1620	A2M	O3'-C3'	2.72	1.49	1.43
3	BA	1620	A2M	C8-N9	-2.72	1.32	1.37
4	BB	1094	OMG	O6-C6	-2.72	1.18	1.23
3	BA	1267	OMG	C4-N9	-2.72	1.31	1.38
4	BB	578	OMU	C6-N1	2.72	1.44	1.38
4	BB	659	OMG	O6-C6	-2.72	1.18	1.23
1	AA	714	OMU	O2-C2	-2.72	1.18	1.23
3	BA	1614	PSU	O4-C4	-2.72	1.18	1.23
5	BC	43	A2M	O3'-C3'	2.71	1.49	1.43
4	BB	1094	OMG	C2-N1	2.71	1.44	1.37
1	AA	2096	A2M	O2'-C2'	-2.71	1.36	1.42
4	BB	588	A2M	C5-N7	-2.71	1.34	1.39
5	BC	43	A2M	C8-N9	-2.71	1.32	1.37
3	BA	743	A2M	O2'-C2'	-2.71	1.36	1.42
3	BA	1329	OMC	O2-C2	-2.71	1.18	1.23
4	BB	1388	A2M	O2'-C2'	-2.71	1.36	1.42
3	BA	1709	OMG	C2-N1	2.71	1.44	1.37
4	BB	1094	OMG	C5-N7	-2.71	1.33	1.39
1	AA	1931	OMG	C2-N1	2.70	1.44	1.37
4	BB	1201	A2M	C5-N7	-2.70	1.34	1.39
4	BB	524	PSU	O4-C4	-2.70	1.18	1.23
4	BB	615	PSU	O4-C4	-2.70	1.18	1.23
1	AA	131	PSU	O4-C4	-2.70	1.18	1.23
3	BA	452	PSU	O4-C4	-2.70	1.18	1.23
4	BB	95	A2M	O3'-C3'	2.70	1.49	1.43
3	BA	1742	OMU	O2-C2	-2.70	1.18	1.23
4	BB	1319	PSU	O4-C4	-2.70	1.18	1.23
3	BA	925	OMG	C2-N1	2.70	1.44	1.37
3	BA	996	A2M	O3'-C3'	2.69	1.49	1.43
4	BB	71	OMG	C2-N1	2.69	1.44	1.37
4	BB	609	A2M	O3'-C3'	2.69	1.49	1.43
1	AA	1895	OMG	O6-C6	-2.69	1.18	1.23
3	BA	746	A2M	O2'-C2'	-2.69	1.36	1.42
3	BA	1267	OMG	C2-N1	2.69	1.44	1.37
3	BA	1024	A2M	C5-N7	-2.69	1.34	1.39
1	AA	1931	OMG	O6-C6	-2.69	1.18	1.23
3	BA	254	A2M	O3'-C3'	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BA	746	A2M	C5-N7	-2.68	1.34	1.39
3	BA	996	A2M	C5-N7	-2.68	1.34	1.39
5	BC	163	A2M	O2'-C2'	-2.68	1.36	1.42
3	BA	1665	A2M	O2'-C2'	-2.68	1.36	1.42
4	BB	1062	OMG	C2-N1	2.68	1.44	1.37
4	BB	1400	A2M	C8-N9	-2.68	1.33	1.37
5	BC	41	A2M	O3'-C3'	2.68	1.49	1.43
4	BB	609	A2M	C5-N7	-2.68	1.34	1.39
4	BB	95	A2M	O2'-C2'	-2.67	1.36	1.42
1	AA	1676	OMG	O6-C6	-2.67	1.18	1.23
4	BB	1160	PSU	O4-C4	-2.67	1.18	1.23
1	AA	2153	A2M	C8-N9	-2.67	1.33	1.37
3	BA	762	A2M	O3'-C3'	2.67	1.49	1.43
1	AA	1592	PSU	O4-C4	-2.67	1.18	1.23
3	BA	1024	A2M	O2'-C2'	-2.67	1.36	1.42
5	BC	41	A2M	C5-N7	-2.66	1.34	1.39
5	BC	74	PSU	O4-C4	-2.66	1.18	1.23
3	BA	925	OMG	C4-N9	-2.66	1.31	1.38
3	BA	1169	PSU	O4-C4	-2.66	1.18	1.23
3	BA	1448	OMU	O2-C2	-2.66	1.18	1.23
3	BA	1605	OMG	C2-N1	2.66	1.44	1.37
4	BB	552	OMG	C2-N1	2.66	1.44	1.37
3	BA	743	A2M	C5-N7	-2.66	1.34	1.39
3	BA	1620	A2M	C5-N7	-2.65	1.34	1.39
5	BC	163	A2M	O3'-C3'	2.65	1.49	1.43
4	BB	518	PSU	O4-C4	-2.65	1.18	1.23
3	BA	254	A2M	C8-N9	-2.65	1.33	1.37
4	BB	73	OMU	O2-C2	-2.65	1.18	1.23
3	BA	1621	OMG	C2-N1	2.65	1.44	1.37
1	AA	2096	A2M	C8-N9	-2.65	1.33	1.37
4	BB	609	A2M	O2'-C2'	-2.65	1.36	1.42
4	BB	1245	OMG	O6-C6	-2.65	1.18	1.23
1	AA	56	A2M	C5-N7	-2.64	1.34	1.39
1	AA	61	PSU	O4-C4	-2.64	1.18	1.23
3	BA	915	OMG	C2-N1	2.64	1.44	1.37
4	BB	95	A2M	C5-N7	-2.64	1.34	1.39
4	BB	1247	OMG	C2-N1	2.64	1.44	1.37
4	BB	1094	OMG	C4-N9	-2.64	1.31	1.38
3	BA	1024	A2M	O3'-C3'	2.64	1.49	1.43
3	BA	916	OMU	O2-C2	-2.63	1.18	1.23
3	BA	258	PSU	O4-C4	-2.63	1.18	1.23
1	AA	2154	OMU	O2-C2	-2.63	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BA	1665	A2M	C5-N7	-2.63	1.34	1.39
3	BA	1129	PSU	O4-C4	-2.62	1.18	1.23
4	BB	552	OMG	C4-N9	-2.62	1.31	1.38
5	BC	163	A2M	C8-N9	-2.62	1.33	1.37
3	BA	762	A2M	C5-N7	-2.62	1.34	1.39
1	AA	2045	PSU	O4-C4	-2.62	1.18	1.23
4	BB	673	OMG	C2-N1	2.61	1.44	1.37
3	BA	927	A2M	C5-N7	-2.61	1.34	1.39
4	BB	1375	OMU	O2-C2	-2.61	1.18	1.23
1	AA	56	A2M	O3'-C3'	2.61	1.49	1.43
1	AA	2153	A2M	O3'-C3'	2.61	1.49	1.43
1	AA	1895	OMG	C2-N1	2.61	1.44	1.37
5	BC	75	OMG	O6-C6	-2.60	1.18	1.23
3	BA	46	OMU	O2-C2	-2.60	1.18	1.23
4	BB	659	OMG	C2-N1	2.60	1.43	1.37
4	BB	1269	OMG	C4-N9	-2.60	1.31	1.38
3	BA	742	1MA	C5-N7	-2.60	1.33	1.39
1	AA	57	OMU	O2-C2	-2.60	1.18	1.23
1	AA	1676	OMG	C2-N1	2.59	1.43	1.37
4	BB	1435	OMU	O2-C2	-2.59	1.18	1.23
1	AA	57	OMU	C6-N1	2.58	1.44	1.38
3	BA	1028	OMG	C2-N1	2.57	1.43	1.37
5	BC	43	A2M	C5-N7	-2.57	1.34	1.39
3	BA	1605	OMG	O6-C6	-2.57	1.18	1.23
4	BB	1093	OMU	O2-C2	-2.57	1.18	1.23
4	BB	1388	A2M	C5-N7	-2.56	1.34	1.39
4	BB	622	A2M	C5-N7	-2.56	1.34	1.39
1	AA	2123	OMU	C6-N1	2.56	1.44	1.38
1	AA	2153	A2M	C5-N7	-2.56	1.34	1.39
1	AA	1619	PSU	O4-C4	-2.56	1.18	1.23
4	BB	1400	A2M	C5-N7	-2.55	1.34	1.39
5	BC	7	OMU	O2-C2	-2.55	1.18	1.23
3	BA	254	A2M	C5-N7	-2.54	1.34	1.39
1	AA	714	OMU	C6-N1	2.54	1.44	1.38
1	AA	2227	OMG	C4-N9	-2.54	1.31	1.38
1	AA	2054	OMU	O2-C2	-2.53	1.18	1.23
4	BB	1245	OMG	C4-N9	-2.51	1.31	1.38
3	BA	915	OMG	C4-N9	-2.50	1.31	1.38
3	BA	1028	OMG	C5-C6	2.50	1.53	1.44
3	BA	1621	OMG	C4-N9	-2.50	1.31	1.38
1	AA	1931	OMG	C4-N9	-2.50	1.31	1.38
1	AA	1899	OMU	O2-C2	-2.50	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	1269	OMG	C2-N1	2.50	1.43	1.37
4	BB	522	PSU	O4-C4	-2.49	1.18	1.23
3	BA	1329	OMC	C5-C4	2.49	1.48	1.42
3	BA	1605	OMG	C5-C6	2.49	1.53	1.44
4	BB	545	A2M	C5-N7	-2.49	1.34	1.39
1	AA	1700	OMG	C2-N1	2.49	1.43	1.37
4	BB	646	A2M	C5-N7	-2.48	1.34	1.39
3	BA	1709	OMG	C4-N9	-2.48	1.31	1.38
3	BA	915	OMG	C5-C6	2.48	1.53	1.44
1	AA	2261	MA6	C4-N9	-2.47	1.32	1.37
3	BA	1181	OMU	O2-C2	-2.47	1.18	1.23
1	AA	2096	A2M	C5-N7	-2.47	1.34	1.39
4	BB	673	OMG	C5-C6	2.46	1.53	1.44
5	BC	163	A2M	C5-N7	-2.46	1.34	1.39
1	AA	1652	OMU	C5-C4	2.45	1.49	1.43
1	AA	1517	OMG	C2-N1	2.45	1.43	1.37
1	AA	721	A2M	C4-N9	-2.45	1.32	1.37
4	BB	1247	OMG	C4-N9	-2.45	1.31	1.38
4	BB	1094	OMG	C5-C6	2.45	1.53	1.44
1	AA	2227	OMG	C2-N1	2.45	1.43	1.37
4	BB	400	A2M	O3'-C3'	2.44	1.49	1.43
5	BC	75	OMG	C5-C6	2.44	1.53	1.44
4	BB	659	OMG	C4-N9	-2.44	1.31	1.38
3	BA	1267	OMG	C5-C6	2.44	1.53	1.44
1	AA	1676	OMG	C5-C6	2.44	1.53	1.44
4	BB	673	OMG	C4-N9	-2.43	1.31	1.38
4	BB	71	OMG	C5-C6	2.43	1.53	1.44
4	BB	1062	OMG	C5-C6	2.43	1.53	1.44
3	BA	925	OMG	C5-C6	2.43	1.53	1.44
3	BA	1028	OMG	C4-N9	-2.43	1.31	1.38
3	BA	1709	OMG	C5-C6	2.42	1.53	1.44
4	BB	659	OMG	C5-C6	2.42	1.53	1.44
3	BA	1621	OMG	C5-C6	2.42	1.53	1.44
4	BB	1245	OMG	C5-C6	2.41	1.53	1.44
4	BB	71	OMG	C4-N9	-2.41	1.31	1.38
1	AA	36	OMU	C6-N1	2.41	1.43	1.38
5	BC	75	OMG	C6-N1	2.41	1.43	1.38
4	BB	588	A2M	O2'-C2'	-2.40	1.36	1.42
4	BB	1247	OMG	C5-C6	2.40	1.53	1.44
1	AA	1531	OMG	C2-N1	2.40	1.43	1.37
1	AA	1895	OMG	C4-N9	-2.39	1.32	1.38
4	BB	377	OMC	C5-C4	2.37	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	1245	OMG	C6-N1	2.37	1.43	1.38
4	BB	552	OMG	C5-C6	2.36	1.53	1.44
4	BB	1062	OMG	C4-N9	-2.35	1.32	1.38
4	BB	1264	OMC	C5-C4	2.34	1.48	1.42
4	BB	1093	OMU	C5-C4	2.34	1.48	1.43
4	BB	528	PSU	C2-N3	-2.33	1.33	1.37
3	BA	1605	OMG	C6-N1	2.33	1.43	1.38
1	AA	1931	OMG	C6-N1	2.32	1.43	1.38
3	BA	1267	OMG	C6-N1	2.31	1.43	1.38
1	AA	1931	OMG	C5-C6	2.31	1.53	1.44
4	BB	1175	OMC	C5-C4	2.31	1.48	1.42
5	BC	75	OMG	C4-N9	-2.30	1.32	1.38
3	BA	1181	OMU	C5-C4	2.30	1.48	1.43
3	BA	1006	OMC	C5-C4	2.30	1.48	1.42
3	BA	1709	OMG	C6-N1	2.30	1.43	1.38
1	AA	2227	OMG	C5-C6	2.30	1.53	1.44
4	BB	1269	OMG	C5-C6	2.29	1.53	1.44
3	BA	1605	OMG	C4-N9	-2.29	1.32	1.38
4	BB	1375	OMU	C5-C4	2.29	1.48	1.43
3	BA	925	OMG	C6-N1	2.29	1.43	1.38
1	AA	1895	OMG	C5-C6	2.28	1.52	1.44
3	BA	1448	OMU	C5-C4	2.28	1.48	1.43
1	AA	66	OMC	C5-C4	2.28	1.48	1.42
4	BB	1062	OMG	C6-N1	2.27	1.43	1.38
4	BB	685	OMU	C5-C4	2.27	1.48	1.43
4	BB	1094	OMG	C6-N1	2.27	1.43	1.38
1	AA	1700	OMG	C5-C6	2.27	1.52	1.44
3	BA	760	OMC	C5-C4	2.26	1.48	1.42
1	AA	2054	OMU	C5-C4	2.26	1.48	1.43
3	BA	1742	OMU	C5-C4	2.25	1.48	1.43
4	BB	578	OMU	C5-C4	2.25	1.48	1.43
4	BB	601	OMC	C5-C4	2.25	1.48	1.42
1	AA	1899	OMU	C5-C4	2.25	1.48	1.43
3	BA	762	A2M	C4-N9	-2.25	1.33	1.37
5	BC	7	OMU	C5-C4	2.25	1.48	1.43
1	AA	1652	OMU	O2-C2	-2.25	1.19	1.23
4	BB	1247	OMG	C6-N1	2.24	1.43	1.38
1	AA	1676	OMG	C4-N9	-2.23	1.32	1.38
3	BA	916	OMU	C5-C4	2.22	1.48	1.43
3	BA	746	A2M	C4-N9	-2.22	1.33	1.37
1	AA	1676	OMG	C6-N1	2.22	1.43	1.38
1	AA	1895	OMG	C6-N1	2.21	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	73	OMU	C5-C4	2.21	1.48	1.43
1	AA	2153	A2M	C4-N9	-2.21	1.33	1.37
3	BA	46	OMU	C5-C4	2.21	1.48	1.43
4	BB	1413	OMC	C5-C4	2.20	1.48	1.42
5	BC	41	A2M	C4-N9	-2.19	1.33	1.37
1	AA	1517	OMG	C5-C6	2.18	1.52	1.44
3	BA	915	OMG	C6-N1	2.18	1.42	1.38
4	BB	552	OMG	C6-N1	2.18	1.42	1.38
4	BB	71	OMG	C6-N1	2.17	1.42	1.38
1	AA	2134	OMC	C5-C4	2.17	1.48	1.42
4	BB	1388	A2M	C4-N9	-2.17	1.33	1.37
4	BB	1435	OMU	C5-C4	2.16	1.48	1.43
3	BA	1608	OMC	C5-C4	2.15	1.47	1.42
1	AA	1700	OMG	C6-N1	2.15	1.42	1.38
4	BB	530	PSU	C2-N3	-2.14	1.34	1.37
1	AA	2261	MA6	C8-N9	-2.14	1.33	1.37
1	AA	1531	OMG	C5-C6	2.14	1.52	1.44
3	BA	1028	OMG	C6-N1	2.14	1.42	1.38
1	AA	57	OMU	C5-C4	2.13	1.48	1.43
4	BB	1400	A2M	C4-N9	-2.12	1.33	1.37
1	AA	1517	OMG	C4-N9	-2.12	1.32	1.38
3	BA	1621	OMG	C6-N1	2.11	1.42	1.38
1	AA	2154	OMU	C5-C4	2.11	1.48	1.43
4	BB	673	OMG	C6-N1	2.11	1.42	1.38
4	BB	528	PSU	C2'-C1'	-2.10	1.50	1.53
3	BA	1620	A2M	C4-N9	-2.08	1.33	1.37
1	AA	1596	B8N	O2-C2	-2.07	1.18	1.22
1	AA	714	OMU	C5-C4	2.06	1.48	1.43
4	BB	680	PSU	O2-C2	-2.05	1.19	1.23
4	BB	659	OMG	C6-N1	2.05	1.42	1.38
4	BB	1269	OMG	C6-N1	2.05	1.42	1.38
4	BB	1280	PSU	O4'-C1'	-2.04	1.41	1.43
4	BB	545	A2M	C4-N9	-2.03	1.33	1.37
1	AA	1619	PSU	O4'-C1'	-2.03	1.41	1.43
4	BB	622	A2M	C4-N9	-2.03	1.33	1.37
1	AA	2096	A2M	C4-N9	-2.03	1.33	1.37
4	BB	588	A2M	C4-N9	-2.02	1.33	1.37
1	AA	46	OMC	C5-C4	2.02	1.47	1.42
1	AA	1531	OMG	C6-N1	2.02	1.42	1.38
4	BB	609	A2M	C4-N9	-2.02	1.33	1.37
4	BB	1398	PSU	O4'-C1'	-2.01	1.41	1.43
1	AA	2070	7MG	C8-N7	2.01	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	1429	PSU	O2-C2	-2.00	1.19	1.23

All (914) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2260	MA6	N1-C6-N6	-11.02	103.43	116.86
1	AA	2261	MA6	N1-C6-N6	-10.24	104.37	116.86
1	AA	1517	OMG	C1'-N9-C8	-8.00	104.00	126.73
1	AA	1676	OMG	C1'-N9-C8	-7.95	104.16	126.73
1	AA	1895	OMG	C1'-N9-C8	-7.81	104.55	126.73
3	BA	1621	OMG	C1'-N9-C8	-7.77	104.65	126.73
5	BC	75	OMG	C1'-N9-C8	-7.73	104.78	126.73
4	BB	1247	OMG	C1'-N9-C8	-7.70	104.86	126.73
4	BB	1062	OMG	C1'-N9-C8	-7.57	105.23	126.73
3	BA	1605	OMG	C1'-N9-C8	-7.54	105.31	126.73
1	AA	1931	OMG	C1'-N9-C8	-7.46	105.54	126.73
4	BB	1269	OMG	C1'-N9-C8	-7.44	105.58	126.73
4	BB	552	OMG	C1'-N9-C8	-7.43	105.62	126.73
4	BB	659	OMG	C1'-N9-C8	-7.43	105.63	126.73
1	AA	1700	OMG	C1'-N9-C8	-7.40	105.71	126.73
1	AA	2260	MA6	C5-C6-N6	7.40	137.04	125.33
1	AA	2227	OMG	C1'-N9-C8	-7.40	105.72	126.73
4	BB	673	OMG	C1'-N9-C8	-7.37	105.81	126.73
3	BA	1709	OMG	C1'-N9-C8	-7.34	105.87	126.73
4	BB	1245	OMG	C1'-N9-C8	-7.21	106.23	126.73
1	AA	1531	OMG	C1'-N9-C8	-7.12	106.50	126.73
4	BB	71	OMG	C1'-N9-C8	-7.10	106.55	126.73
1	AA	1517	OMG	C1'-N9-C4	7.09	147.43	126.49
3	BA	915	OMG	C1'-N9-C8	-6.99	106.87	126.73
3	BA	925	OMG	C1'-N9-C8	-6.99	106.88	126.73
4	BB	1094	OMG	C1'-N9-C8	-6.94	107.01	126.73
4	BB	530	PSU	N1-C2-N3	6.91	122.46	115.17
1	AA	1676	OMG	C1'-N9-C4	6.85	146.72	126.49
1	AA	2096	A2M	N6-C6-N1	-6.83	103.16	118.38
3	BA	746	A2M	N6-C6-N1	-6.81	103.20	118.38
4	BB	528	PSU	N1-C2-N3	6.78	122.32	115.17
1	AA	1895	OMG	C1'-N9-C4	6.72	146.34	126.49
5	BC	41	A2M	N6-C6-N1	-6.71	103.42	118.38
4	BB	622	A2M	N6-C6-N1	-6.70	103.45	118.38
3	BA	927	A2M	N6-C6-N1	-6.69	103.47	118.38
1	AA	2261	MA6	C5-C6-N6	6.68	135.90	125.33
5	BC	75	OMG	C1'-N9-C4	6.67	146.18	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BA	254	A2M	N6-C6-N1	-6.66	103.54	118.38
4	BB	1388	A2M	N6-C6-N1	-6.65	103.56	118.38
3	BA	743	A2M	N6-C6-N1	-6.65	103.57	118.38
3	BA	1620	A2M	N6-C6-N1	-6.64	103.59	118.38
4	BB	545	A2M	N6-C6-N1	-6.62	103.64	118.38
3	BA	1024	A2M	N6-C6-N1	-6.61	103.64	118.38
5	BC	43	A2M	N6-C6-N1	-6.61	103.66	118.38
4	BB	1400	A2M	N6-C6-N1	-6.60	103.67	118.38
3	BA	762	A2M	N6-C6-N1	-6.59	103.70	118.38
3	BA	1267	OMG	C1'-N9-C8	-6.59	108.02	126.73
3	BA	996	A2M	N6-C6-N1	-6.59	103.71	118.38
4	BB	1201	A2M	N6-C6-N1	-6.57	103.74	118.38
5	BC	163	A2M	N6-C6-N1	-6.57	103.75	118.38
3	BA	1621	OMG	C1'-N9-C4	6.57	145.89	126.49
4	BB	646	A2M	N6-C6-N1	-6.56	103.77	118.38
4	BB	1247	OMG	C1'-N9-C4	6.54	145.80	126.49
3	BA	1665	A2M	N6-C6-N1	-6.52	103.85	118.38
4	BB	588	A2M	N6-C6-N1	-6.52	103.86	118.38
1	AA	56	A2M	N6-C6-N1	-6.52	103.86	118.38
4	BB	95	A2M	N6-C6-N1	-6.51	103.87	118.38
1	AA	721	A2M	N6-C6-N1	-6.49	103.93	118.38
3	BA	1605	OMG	C1'-N9-C4	6.46	145.57	126.49
1	AA	721	A2M	C4-N9-C1'	-6.44	111.56	126.63
4	BB	1062	OMG	C1'-N9-C4	6.42	145.45	126.49
1	AA	2153	A2M	N6-C6-N1	-6.41	104.10	118.38
4	BB	400	A2M	N6-C6-N1	-6.38	104.18	118.38
4	BB	1269	OMG	C1'-N9-C4	6.34	145.22	126.49
4	BB	673	OMG	C1'-N9-C4	6.32	145.17	126.49
4	BB	659	OMG	C1'-N9-C4	6.32	145.16	126.49
3	BA	1028	OMG	C1'-N9-C8	-6.31	108.80	126.73
4	BB	552	OMG	C1'-N9-C4	6.31	145.12	126.49
4	BB	609	A2M	N6-C6-N1	-6.30	104.36	118.38
1	AA	1931	OMG	C1'-N9-C4	6.28	145.03	126.49
1	AA	2227	OMG	C1'-N9-C4	6.27	145.00	126.49
1	AA	36	OMU	C4-N3-C2	-6.17	118.95	126.61
3	BA	1709	OMG	C1'-N9-C4	6.17	144.72	126.49
4	BB	1388	A2M	C4-N9-C1'	-6.09	112.39	126.63
1	AA	2153	A2M	C4-N9-C1'	-6.07	112.43	126.63
1	AA	2096	A2M	C4-N9-C1'	-6.07	112.43	126.63
3	BA	762	A2M	C4-N9-C1'	-6.07	112.45	126.63
1	AA	1700	OMG	C1'-N9-C4	6.06	144.40	126.49
4	BB	1245	OMG	C1'-N9-C4	6.06	144.39	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	BC	41	A2M	C4-N9-C1'	-6.05	112.49	126.63
4	BB	71	OMG	C1'-N9-C4	6.04	144.32	126.49
4	BB	545	A2M	N9-C8-N7	-6.01	105.41	113.94
4	BB	1375	OMU	C4-N3-C2	-5.99	119.17	126.61
4	BB	578	OMU	C4-N3-C2	-5.99	119.17	126.61
1	AA	714	OMU	C4-N3-C2	-5.94	119.24	126.61
3	BA	762	A2M	N3-C2-N1	-5.93	119.61	128.58
3	BA	254	A2M	C4-N9-C1'	-5.92	112.79	126.63
1	AA	2096	A2M	N9-C8-N7	-5.89	105.58	113.94
3	BA	746	A2M	N3-C2-N1	-5.88	119.68	128.58
1	AA	2123	OMU	C4-N3-C2	-5.86	119.34	126.61
3	BA	1024	A2M	N3-C2-N1	-5.86	119.72	128.58
3	BA	1448	OMU	C4-N3-C2	-5.86	119.34	126.61
3	BA	925	OMG	C1'-N9-C4	5.85	143.78	126.49
3	BA	915	OMG	C1'-N9-C4	5.85	143.78	126.49
4	BB	545	A2M	C4-N9-C1'	-5.85	112.95	126.63
1	AA	2260	MA6	N1-C2-N3	-5.85	119.73	128.58
1	AA	1531	OMG	C1'-N9-C4	5.84	143.75	126.49
3	BA	46	OMU	C4-N3-C2	-5.84	119.36	126.61
4	BB	685	OMU	C4-N3-C2	-5.83	119.37	126.61
4	BB	1400	A2M	C4-N9-C1'	-5.83	113.01	126.63
4	BB	545	A2M	N3-C2-N1	-5.82	119.77	128.58
4	BB	1093	OMU	C4-N3-C2	-5.82	119.39	126.61
4	BB	1400	A2M	N9-C8-N7	-5.81	105.69	113.94
3	BA	1181	OMU	C4-N3-C2	-5.81	119.40	126.61
5	BC	163	A2M	N3-C2-N1	-5.80	119.80	128.58
4	BB	1388	A2M	N3-C2-N1	-5.80	119.81	128.58
1	AA	56	A2M	N3-C2-N1	-5.79	119.81	128.58
3	BA	746	A2M	C4-N9-C1'	-5.79	113.09	126.63
1	AA	2153	A2M	N9-C8-N7	-5.77	105.74	113.94
1	AA	721	A2M	N9-C8-N7	-5.77	105.75	113.94
4	BB	1201	A2M	N9-C8-N7	-5.77	105.75	113.94
4	BB	1388	A2M	N9-C8-N7	-5.75	105.78	113.94
5	BC	41	A2M	N9-C8-N7	-5.75	105.78	113.94
4	BB	1400	A2M	N3-C2-N1	-5.73	119.91	128.58
5	BC	163	A2M	N9-C8-N7	-5.73	105.81	113.94
3	BA	762	A2M	N9-C8-N7	-5.73	105.81	113.94
5	BC	43	A2M	N9-C8-N7	-5.72	105.82	113.94
4	BB	1094	OMG	C1'-N9-C4	5.71	143.34	126.49
5	BC	7	OMU	C4-N3-C2	-5.70	119.53	126.61
1	AA	2054	OMU	C4-N3-C2	-5.70	119.53	126.61
1	AA	2153	A2M	N3-C2-N1	-5.70	119.95	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	646	A2M	N3-C2-N1	-5.70	119.95	128.58
3	BA	1742	OMU	C4-N3-C2	-5.69	119.55	126.61
3	BA	916	OMU	C4-N3-C2	-5.68	119.56	126.61
5	BC	163	A2M	C4-N9-C1'	-5.68	113.34	126.63
5	BC	41	A2M	N3-C2-N1	-5.68	119.98	128.58
3	BA	927	A2M	N3-C2-N1	-5.66	120.02	128.58
3	BA	254	A2M	N3-C2-N1	-5.65	120.02	128.58
4	BB	622	A2M	N3-C2-N1	-5.64	120.04	128.58
3	BA	746	A2M	N9-C8-N7	-5.64	105.93	113.94
3	BA	1620	A2M	N3-C2-N1	-5.64	120.05	128.58
1	AA	2096	A2M	N3-C2-N1	-5.63	120.06	128.58
3	BA	1028	OMG	C1'-N9-C4	5.63	143.12	126.49
4	BB	646	A2M	N9-C8-N7	-5.63	105.95	113.94
1	AA	57	OMU	C4-N3-C2	-5.63	119.62	126.61
1	AA	721	A2M	N3-C2-N1	-5.63	120.07	128.58
1	AA	1899	OMU	C4-N3-C2	-5.62	119.64	126.61
3	BA	1024	A2M	N9-C8-N7	-5.62	105.97	113.94
5	BC	43	A2M	N3-C2-N1	-5.60	120.10	128.58
4	BB	73	OMU	C4-N3-C2	-5.59	119.68	126.61
4	BB	1201	A2M	C4-N9-C1'	-5.58	113.58	126.63
4	BB	622	A2M	N9-C8-N7	-5.57	106.03	113.94
3	BA	1665	A2M	N3-C2-N1	-5.56	120.16	128.58
4	BB	609	A2M	N3-C2-N1	-5.56	120.17	128.58
4	BB	1435	OMU	C4-N3-C2	-5.56	119.71	126.61
4	BB	622	A2M	C4-N9-C1'	-5.54	113.66	126.63
4	BB	1201	A2M	N3-C2-N1	-5.54	120.19	128.58
4	BB	588	A2M	N3-C2-N1	-5.53	120.20	128.58
1	AA	2261	MA6	N1-C2-N3	-5.53	120.20	128.58
4	BB	588	A2M	N9-C8-N7	-5.53	106.09	113.94
3	BA	927	A2M	N9-C8-N7	-5.52	106.10	113.94
1	AA	56	A2M	N9-C8-N7	-5.51	106.12	113.94
3	BA	996	A2M	N3-C2-N1	-5.51	120.24	128.58
3	BA	743	A2M	N3-C2-N1	-5.50	120.25	128.58
3	BA	254	A2M	N9-C8-N7	-5.50	106.13	113.94
3	BA	1620	A2M	C4-N9-C1'	-5.50	113.77	126.63
5	BC	43	A2M	C4-N9-C1'	-5.49	113.78	126.63
1	AA	2154	OMU	C4-N3-C2	-5.49	119.80	126.61
4	BB	646	A2M	C4-N9-C1'	-5.48	113.81	126.63
3	BA	1620	A2M	N9-C8-N7	-5.46	106.19	113.94
4	BB	545	A2M	C4-N9-C8	5.46	111.47	105.74
4	BB	95	A2M	N3-C2-N1	-5.46	120.32	128.58
3	BA	746	A2M	C5-C6-N6	5.44	136.75	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BA	1024	A2M	C4-N9-C1'	-5.43	113.94	126.63
4	BB	400	A2M	N3-C2-N1	-5.42	120.37	128.58
3	BA	1665	A2M	N9-C8-N7	-5.42	106.24	113.94
1	AA	1652	OMU	C4-N3-C2	-5.41	119.89	126.61
3	BA	1267	OMG	C1'-N9-C4	5.40	142.44	126.49
4	BB	95	A2M	N9-C8-N7	-5.40	106.28	113.94
3	BA	743	A2M	N9-C8-N7	-5.37	106.31	113.94
3	BA	996	A2M	N9-C8-N7	-5.36	106.33	113.94
1	AA	2153	A2M	C4-N9-C8	5.35	111.36	105.74
3	BA	1620	A2M	C5-C6-N6	5.34	136.51	123.29
1	AA	2096	A2M	C5-C6-N6	5.34	136.50	123.29
3	BA	762	A2M	C5-C6-N6	5.32	136.47	123.29
1	AA	1596	B8N	C5-C4-N3	5.32	125.81	116.15
4	BB	1388	A2M	C5-C6-N6	5.29	136.39	123.29
4	BB	622	A2M	C5-C6-N6	5.28	136.37	123.29
3	BA	996	A2M	C5-C6-N6	5.28	136.36	123.29
4	BB	400	A2M	N9-C8-N7	-5.28	106.45	113.94
3	BA	254	A2M	C5-C6-N6	5.27	136.34	123.29
5	BC	41	A2M	C5-C6-N6	5.27	136.33	123.29
5	BC	43	A2M	C5-C6-N6	5.26	136.32	123.29
3	BA	743	A2M	C5-C6-N6	5.26	136.31	123.29
4	BB	1388	A2M	C4-N9-C8	5.26	111.26	105.74
4	BB	609	A2M	N9-C8-N7	-5.25	106.48	113.94
4	BB	588	A2M	C4-N9-C1'	-5.25	114.35	126.63
4	BB	609	A2M	C4-N9-C1'	-5.25	114.36	126.63
4	BB	1400	A2M	C5-C6-N6	5.24	136.27	123.29
4	BB	1400	A2M	C4-N9-C8	5.24	111.24	105.74
3	BA	762	A2M	C4-N9-C8	5.23	111.23	105.74
3	BA	927	A2M	C5-C4-N3	-5.23	119.51	126.72
4	BB	1201	A2M	C5-C6-N6	5.23	136.24	123.29
5	BC	41	A2M	C4-N9-C8	5.22	111.22	105.74
5	BC	163	A2M	C5-C6-N6	5.21	136.18	123.29
3	BA	1024	A2M	C5-C6-N6	5.21	136.18	123.29
1	AA	721	A2M	C5-C6-N6	5.20	136.16	123.29
3	BA	742	1MA	N1-C2-N3	-5.20	119.82	126.00
3	BA	927	A2M	C5-C6-N6	5.20	136.15	123.29
4	BB	95	A2M	C5-C6-N6	5.18	136.11	123.29
4	BB	545	A2M	C5-C6-N6	5.17	136.09	123.29
4	BB	588	A2M	C5-C6-N6	5.16	136.07	123.29
1	AA	1517	OMG	C5-C4-N3	-5.16	120.18	128.39
3	BA	1665	A2M	C5-C6-N6	5.15	136.04	123.29
1	AA	721	A2M	C4-N9-C8	5.15	111.14	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	646	A2M	C5-C6-N6	5.15	136.03	123.29
1	AA	2096	A2M	C4-N9-C8	5.11	111.11	105.74
1	AA	2153	A2M	C5-C6-N6	5.10	135.91	123.29
4	BB	1201	A2M	C4-N9-C8	5.10	111.09	105.74
3	BA	1665	A2M	C5-C4-N3	-5.10	119.70	126.72
4	BB	455	PSU	C4-N3-C2	-5.10	119.35	126.37
1	AA	56	A2M	C5-C6-N6	5.09	135.90	123.29
3	BA	743	A2M	C5-C4-N3	-5.08	119.72	126.72
1	AA	2070	7MG	C5-C6-N1	5.08	119.88	110.94
1	AA	56	A2M	C5-C4-N3	-5.08	119.72	126.72
4	BB	400	A2M	C4-N9-C1'	-5.07	114.77	126.63
3	BA	1009	PSU	C4-N3-C2	-5.07	119.39	126.37
5	BC	163	A2M	C4-N9-C8	5.07	111.06	105.74
3	BA	746	A2M	C4-N9-C8	5.06	111.05	105.74
3	BA	737	PSU	C4-N3-C2	-5.06	119.40	126.37
4	BB	95	A2M	C4-N9-C1'	-5.06	114.80	126.63
4	BB	646	A2M	C4-N9-C8	5.06	111.05	105.74
4	BB	400	A2M	C5-C6-N6	5.05	135.80	123.29
4	BB	588	A2M	C5-C4-N3	-5.05	119.76	126.72
4	BB	1429	PSU	C4-N3-C2	-5.05	119.41	126.37
5	BC	43	A2M	C4-N9-C8	5.02	111.00	105.74
3	BA	996	A2M	C5-C4-N3	-5.02	119.81	126.72
1	AA	1676	OMG	C5-C4-N3	-5.01	120.42	128.39
4	BB	95	A2M	C5-C4-N3	-5.00	119.84	126.72
3	BA	1248	PSU	C4-N3-C2	-4.99	119.49	126.37
4	BB	1076	PSU	C4-N3-C2	-4.99	119.50	126.37
1	AA	56	A2M	C4-N9-C1'	-4.97	115.00	126.63
4	BB	609	A2M	C5-C6-N6	4.97	135.59	123.29
4	BB	455	PSU	N1-C2-N3	4.97	120.41	115.17
3	BA	1169	PSU	C4-N3-C2	-4.96	119.54	126.37
1	AA	131	PSU	C4-N3-C2	-4.96	119.54	126.37
4	BB	622	A2M	C4-N9-C8	4.96	110.94	105.74
3	BA	1024	A2M	C4-N9-C8	4.95	110.93	105.74
4	BB	1398	PSU	C4-N3-C2	-4.94	119.56	126.37
3	BA	1024	A2M	C5-C4-N3	-4.93	119.92	126.72
1	AA	1276	PSU	C4-N3-C2	-4.93	119.58	126.37
4	BB	1229	PSU	C4-N3-C2	-4.93	119.58	126.37
3	BA	927	A2M	C4-N9-C1'	-4.93	115.11	126.63
3	BA	996	A2M	C4-N9-C1'	-4.91	115.14	126.63
4	BB	400	A2M	C5-C4-N3	-4.91	119.95	126.72
4	BB	1280	PSU	C4-N3-C2	-4.90	119.62	126.37
3	BA	1665	A2M	C4-N9-C1'	-4.90	115.18	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	1334	PSU	C4-N3-C2	-4.89	119.64	126.37
1	AA	131	PSU	N1-C2-N3	4.89	120.32	115.17
4	BB	588	A2M	C4-N9-C8	4.88	110.86	105.74
4	BB	1429	PSU	N1-C2-N3	4.88	120.31	115.17
4	BB	1160	PSU	C4-N3-C2	-4.87	119.66	126.37
4	BB	644	PSU	C4-N3-C2	-4.87	119.67	126.37
4	BB	680	PSU	C4-N3-C2	-4.86	119.67	126.37
5	BC	43	A2M	C5-C4-N3	-4.86	120.03	126.72
3	BA	1609	PSU	C4-N3-C2	-4.86	119.68	126.37
3	BA	742	1MA	C5-C4-N3	-4.84	120.14	127.27
1	AA	56	A2M	C4-N9-C8	4.83	110.81	105.74
3	BA	927	A2M	C4-N9-C8	4.83	110.81	105.74
3	BA	258	PSU	C4-N3-C2	-4.83	119.72	126.37
4	BB	609	A2M	C5-C4-N3	-4.81	120.10	126.72
3	BA	1129	PSU	C4-N3-C2	-4.81	119.75	126.37
4	BB	622	A2M	C5-C4-N3	-4.81	120.10	126.72
4	BB	518	PSU	C4-N3-C2	-4.80	119.76	126.37
3	BA	1614	PSU	C4-N3-C2	-4.80	119.77	126.37
3	BA	737	PSU	N1-C2-N3	4.79	120.22	115.17
1	AA	61	PSU	C4-N3-C2	-4.78	119.79	126.37
4	BB	1076	PSU	N1-C2-N3	4.78	120.21	115.17
3	BA	1258	PSU	C4-N3-C2	-4.78	119.79	126.37
3	BA	743	A2M	C4-N9-C1'	-4.77	115.47	126.63
3	BA	1614	PSU	N1-C2-N3	4.77	120.20	115.17
4	BB	1201	A2M	C5-C4-N3	-4.76	120.16	126.72
5	BC	74	PSU	C4-N3-C2	-4.76	119.81	126.37
4	BB	1319	PSU	C4-N3-C2	-4.76	119.81	126.37
4	BB	400	A2M	C4-N9-C8	4.75	110.73	105.74
3	BA	1028	OMG	C5-C4-N3	-4.74	120.84	128.39
3	BA	452	PSU	C4-N3-C2	-4.74	119.84	126.37
3	BA	1086	PSU	C4-N3-C2	-4.74	119.85	126.37
4	BB	1210	PSU	C4-N3-C2	-4.74	119.85	126.37
4	BB	646	A2M	C5-C4-N3	-4.73	120.20	126.72
1	AA	1592	PSU	C4-N3-C2	-4.73	119.85	126.37
1	AA	2146	PSU	C4-N3-C2	-4.73	119.85	126.37
4	BB	1409	PSU	C4-N3-C2	-4.73	119.85	126.37
1	AA	2096	A2M	C5-C4-N3	-4.73	120.20	126.72
1	AA	2261	MA6	C5-C4-N3	-4.73	120.21	126.72
4	BB	95	A2M	C4-N9-C8	4.73	110.70	105.74
3	BA	254	A2M	C4-N9-C8	4.72	110.69	105.74
4	BB	1398	PSU	N1-C2-N3	4.71	120.14	115.17
3	BA	1665	A2M	C4-N9-C8	4.71	110.69	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	1160	PSU	N1-C2-N3	4.71	120.13	115.17
3	BA	743	A2M	C4-N9-C8	4.70	110.68	105.74
3	BA	1620	A2M	C4-N9-C8	4.69	110.66	105.74
5	BC	163	A2M	C5-C4-N3	-4.68	120.27	126.72
3	BA	1620	A2M	C5-C4-N3	-4.68	120.27	126.72
3	BA	1009	PSU	N1-C2-N3	4.68	120.11	115.17
3	BA	254	A2M	C5-C4-N3	-4.68	120.28	126.72
3	BA	1086	PSU	N1-C2-N3	4.67	120.09	115.17
1	AA	1596	B8N	C4-N3-C2	-4.67	119.87	125.62
3	BA	1258	PSU	N1-C2-N3	4.67	120.09	115.17
4	BB	1334	PSU	N1-C2-N3	4.65	120.07	115.17
4	BB	680	PSU	N1-C2-N3	4.64	120.07	115.17
4	BB	615	PSU	C4-N3-C2	-4.64	119.98	126.37
3	BA	1609	PSU	N1-C2-N3	4.64	120.06	115.17
4	BB	644	PSU	N1-C2-N3	4.64	120.06	115.17
3	BA	1605	OMG	C5-C4-N3	-4.64	121.01	128.39
4	BB	609	A2M	C4-N9-C8	4.64	110.61	105.74
4	BB	1319	PSU	N1-C2-N3	4.63	120.06	115.17
3	BA	1129	PSU	N1-C2-N3	4.63	120.05	115.17
4	BB	545	A2M	C5-C4-N3	-4.61	120.36	126.72
4	BB	522	PSU	C4-N3-C2	-4.61	120.02	126.37
4	BB	1229	PSU	N1-C2-N3	4.61	120.03	115.17
3	BA	996	A2M	C4-N9-C8	4.60	110.57	105.74
5	BC	75	OMG	C5-C4-N3	-4.60	121.07	128.39
1	AA	721	A2M	C1'-N9-C8	4.59	137.29	127.09
1	AA	61	PSU	N1-C2-N3	4.59	120.01	115.17
4	BB	524	PSU	C4-N3-C2	-4.58	120.06	126.37
1	AA	1676	OMG	C2-N3-C4	4.58	120.19	112.30
4	BB	1247	OMG	C5-C4-N3	-4.58	121.11	128.39
1	AA	2045	PSU	C4-N3-C2	-4.57	120.07	126.37
4	BB	629	PSU	C4-N3-C2	-4.57	120.07	126.37
3	BA	258	PSU	N1-C2-N3	4.55	119.97	115.17
4	BB	611	PSU	C4-N3-C2	-4.55	120.10	126.37
1	AA	2070	7MG	C2-N3-C4	4.55	120.14	112.30
1	AA	1517	OMG	C2-N3-C4	4.55	120.13	112.30
4	BB	673	OMG	C5-C4-N3	-4.54	121.16	128.39
3	BA	1709	OMG	C5-C4-N3	-4.53	121.17	128.39
4	BB	518	PSU	N1-C2-N3	4.53	119.94	115.17
4	BB	71	OMG	C5-C4-N3	-4.52	121.20	128.39
1	AA	1895	OMG	C5-C4-N3	-4.52	121.20	128.39
4	BB	1210	PSU	N1-C2-N3	4.51	119.93	115.17
4	BB	1400	A2M	C5-C4-N3	-4.51	120.50	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BA	1028	OMG	C2-N3-C4	4.51	120.07	112.30
4	BB	659	OMG	C5-C4-N3	-4.51	121.22	128.39
3	BA	1709	OMG	C2-N3-C4	4.50	120.06	112.30
3	BA	1169	PSU	N1-C2-N3	4.50	119.92	115.17
1	AA	1931	OMG	C5-C4-N3	-4.49	121.24	128.39
4	BB	530	PSU	C4-N3-C2	-4.49	120.19	126.37
4	BB	1062	OMG	C5-C4-N3	-4.49	121.25	128.39
4	BB	1280	PSU	N1-C2-N3	4.49	119.90	115.17
3	BA	746	A2M	C5-C4-N3	-4.47	120.56	126.72
4	BB	673	OMG	C2-N3-C4	4.47	119.99	112.30
4	BB	615	PSU	N1-C2-N3	4.46	119.87	115.17
1	AA	1931	OMG	C2-N3-C4	4.45	119.97	112.30
4	BB	1247	OMG	C2-N3-C4	4.45	119.96	112.30
4	BB	522	PSU	N1-C2-N3	4.45	119.86	115.17
1	AA	1619	PSU	C4-N3-C2	-4.44	120.25	126.37
4	BB	545	A2M	C2'-C1'-N9	-4.44	106.45	113.75
1	AA	36	OMU	N3-C2-N1	4.44	120.67	114.89
5	BC	74	PSU	N1-C2-N3	4.43	119.84	115.17
3	BA	452	PSU	N1-C2-N3	4.43	119.84	115.17
4	BB	1245	OMG	C2-N3-C4	4.43	119.92	112.30
4	BB	71	OMG	C2-N3-C4	4.42	119.91	112.30
3	BA	927	A2M	N3-C4-N9	4.42	134.68	127.17
5	BC	41	A2M	C5-C4-N3	-4.41	120.64	126.72
1	AA	1276	PSU	N1-C2-N3	4.41	119.82	115.17
4	BB	528	PSU	C4-N3-C2	-4.41	120.29	126.37
1	AA	2227	OMG	C5-C4-N3	-4.41	121.38	128.39
4	BB	611	PSU	N1-C2-N3	4.41	119.81	115.17
4	BB	1388	A2M	C5-C4-N3	-4.39	120.68	126.72
1	AA	1700	OMG	C2-N3-C4	4.39	119.86	112.30
4	BB	1062	OMG	C2-N3-C4	4.38	119.85	112.30
1	AA	2123	OMU	N3-C2-N1	4.38	120.59	114.89
3	BA	1621	OMG	C5-C4-N3	-4.37	121.43	128.39
1	AA	2153	A2M	C5-C4-N3	-4.37	120.70	126.72
4	BB	1409	PSU	N1-C2-N3	4.37	119.78	115.17
4	BB	552	OMG	C2-N3-C4	4.36	119.81	112.30
3	BA	915	OMG	C2-N3-C4	4.36	119.80	112.30
5	BC	75	OMG	C2-N3-C4	4.35	119.78	112.30
1	AA	1895	OMG	C2-N3-C4	4.34	119.77	112.30
3	BA	925	OMG	C2-N3-C4	4.33	119.77	112.30
3	BA	743	A2M	N3-C4-N9	4.33	134.53	127.17
4	BB	1245	OMG	C5-C4-N3	-4.33	121.50	128.39
3	BA	762	A2M	C5-C4-N3	-4.33	120.76	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BA	1605	OMG	C2-N3-C4	4.33	119.75	112.30
1	AA	56	A2M	N3-C4-N9	4.33	134.52	127.17
1	AA	2261	MA6	N9-C8-N7	-4.32	107.80	113.94
4	BB	659	OMG	C2-N3-C4	4.32	119.74	112.30
4	BB	552	OMG	C5-C4-N3	-4.32	121.52	128.39
1	AA	721	A2M	C5-C4-N3	-4.31	120.78	126.72
4	BB	524	PSU	N1-C2-N3	4.31	119.71	115.17
3	BA	915	OMG	C5-C4-N3	-4.31	121.53	128.39
3	BA	1621	OMG	C2-N3-C4	4.30	119.71	112.30
4	BB	1269	OMG	C5-C4-N3	-4.29	121.56	128.39
1	AA	2146	PSU	N1-C2-N3	4.29	119.69	115.17
1	AA	1700	OMG	C5-C4-N3	-4.28	121.57	128.39
4	BB	578	OMU	N3-C2-N1	4.28	120.47	114.89
4	BB	400	A2M	N3-C4-N9	4.28	134.44	127.17
1	AA	2070	7MG	C5-C4-N3	-4.27	120.11	128.13
1	AA	2045	PSU	N1-C2-N3	4.27	119.67	115.17
3	BA	1665	A2M	N3-C4-N9	4.27	134.43	127.17
4	BB	1094	OMG	C2-N3-C4	4.27	119.65	112.30
4	BB	685	OMU	N3-C2-N1	4.26	120.44	114.89
3	BA	254	A2M	C1'-N9-C8	4.24	136.50	127.09
4	BB	588	A2M	N3-C4-N9	4.23	134.36	127.17
1	AA	2227	OMG	C2-N3-C4	4.23	119.58	112.30
1	AA	2096	A2M	C1'-N9-C8	4.22	136.45	127.09
1	AA	1592	PSU	N1-C2-N3	4.21	119.60	115.17
3	BA	1267	OMG	C2-N3-C4	4.20	119.53	112.30
1	AA	1531	OMG	C2-N3-C4	4.20	119.53	112.30
3	BA	1248	PSU	N1-C2-N3	4.20	119.59	115.17
1	AA	1619	PSU	N1-C2-N3	4.19	119.59	115.17
4	BB	1269	OMG	C2-N3-C4	4.18	119.50	112.30
4	BB	95	A2M	N3-C4-N9	4.17	134.26	127.17
4	BB	1388	A2M	C1'-N9-C8	4.17	136.34	127.09
4	BB	629	PSU	N1-C2-N3	4.17	119.56	115.17
3	BA	1024	A2M	N3-C4-N9	4.16	134.24	127.17
3	BA	762	A2M	C1'-N9-C8	4.16	136.32	127.09
5	BC	41	A2M	C1'-N9-C8	4.14	136.28	127.09
4	BB	1375	OMU	N3-C2-N1	4.11	120.24	114.89
1	AA	2153	A2M	C1'-N9-C8	4.11	136.21	127.09
3	BA	996	A2M	N3-C4-N9	4.11	134.15	127.17
1	AA	2154	OMU	N3-C2-N1	4.10	120.23	114.89
3	BA	46	OMU	N3-C2-N1	4.10	120.23	114.89
4	BB	1094	OMG	C5-C4-N3	-4.09	121.88	128.39
1	AA	714	OMU	N3-C2-N1	4.08	120.20	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	1324	5MC	C5-C6-N1	-4.07	118.89	123.31
5	BC	43	A2M	N3-C4-N9	4.06	134.08	127.17
3	BA	925	OMG	C5-C4-N3	-4.06	121.93	128.39
3	BA	1267	OMG	C5-C4-N3	-4.05	121.95	128.39
1	AA	2260	MA6	C5-C4-N3	-4.03	121.16	126.72
4	BB	646	A2M	N3-C4-N9	4.03	134.01	127.17
4	BB	609	A2M	N3-C4-N9	4.02	134.01	127.17
3	BA	1448	OMU	N3-C2-N1	4.02	120.12	114.89
4	BB	1201	A2M	N3-C4-N9	4.02	134.00	127.17
4	BB	622	A2M	N3-C4-N9	4.01	133.98	127.17
3	BA	1742	OMU	N3-C2-N1	4.00	120.09	114.89
4	BB	545	A2M	N3-C4-N9	3.99	133.95	127.17
3	BA	1181	OMU	N3-C2-N1	3.99	120.09	114.89
4	BB	73	OMU	N3-C2-N1	3.98	120.07	114.89
1	AA	2070	7MG	C4-C5-N7	3.95	110.05	105.38
1	AA	1700	OMG	N9-C8-N7	-3.94	106.09	113.40
3	BA	746	A2M	C1'-N9-C8	3.94	135.84	127.09
3	BA	742	1MA	C2-N3-C4	3.93	120.23	112.53
4	BB	530	PSU	O2-C2-N1	-3.92	118.74	122.79
3	BA	916	OMU	N3-C2-N1	3.91	119.98	114.89
5	BC	163	A2M	N3-C4-N9	3.91	133.82	127.17
1	AA	2054	OMU	N3-C2-N1	3.91	119.97	114.89
5	BC	7	OMU	N3-C2-N1	3.90	119.97	114.89
4	BB	1400	A2M	C1'-N9-C8	3.90	135.76	127.09
4	BB	1093	OMU	N3-C2-N1	3.90	119.97	114.89
1	AA	1531	OMG	C5-C4-N3	-3.88	122.22	128.39
1	AA	2261	MA6	C4-C5-C6	3.88	119.92	115.91
1	AA	714	OMU	C5-C4-N3	3.88	120.23	114.80
4	BB	1375	OMU	C5-C4-N3	3.86	120.21	114.80
4	BB	1435	OMU	C5-C4-N3	3.86	120.20	114.80
4	BB	1400	A2M	N3-C4-N9	3.86	133.73	127.17
3	BA	1181	OMU	C5-C4-N3	3.84	120.18	114.80
3	BA	1267	OMG	N9-C8-N7	-3.84	106.28	113.40
1	AA	36	OMU	C5-C4-N3	3.84	120.18	114.80
1	AA	2153	A2M	N3-C4-N9	3.83	133.67	127.17
1	AA	57	OMU	N3-C2-N1	3.82	119.87	114.89
3	BA	1620	A2M	N3-C4-N9	3.82	133.66	127.17
1	AA	2096	A2M	N3-C4-N9	3.81	133.64	127.17
4	BB	545	A2M	C1'-N9-C8	3.80	135.53	127.09
1	AA	1596	B8N	C1'-C5-C4	3.80	123.37	117.61
5	BC	163	A2M	C1'-N9-C8	3.79	135.50	127.09
4	BB	1093	OMU	C5-C4-N3	3.78	120.10	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BA	46	OMU	C5-C4-N3	3.78	120.09	114.80
3	BA	254	A2M	N3-C4-N9	3.77	133.59	127.17
3	BA	916	OMU	C5-C4-N3	3.77	120.08	114.80
3	BA	1620	A2M	C1'-N9-C8	3.77	135.46	127.09
5	BC	41	A2M	N3-C4-N9	3.77	133.57	127.17
3	BA	746	A2M	N3-C4-N9	3.77	133.57	127.17
1	AA	1652	OMU	N3-C2-N1	3.76	119.79	114.89
4	BB	578	OMU	C5-C4-N3	3.76	120.06	114.80
3	BA	915	OMG	N9-C8-N7	-3.75	106.44	113.40
3	BA	1448	OMU	C5-C4-N3	3.75	120.05	114.80
4	BB	1094	OMG	N9-C8-N7	-3.74	106.46	113.40
1	AA	1899	OMU	N3-C2-N1	3.74	119.76	114.89
1	AA	1531	OMG	N9-C8-N7	-3.74	106.47	113.40
4	BB	622	A2M	C1'-N9-C8	3.73	135.37	127.09
3	BA	1742	OMU	C5-C4-N3	3.73	120.02	114.80
5	BC	7	OMU	C5-C4-N3	3.72	120.02	114.80
3	BA	762	A2M	N3-C4-N9	3.72	133.49	127.17
1	AA	2123	OMU	C5-C4-N3	3.72	120.00	114.80
4	BB	1201	A2M	C1'-N9-C8	3.71	135.33	127.09
4	BB	1388	A2M	N3-C4-N9	3.70	133.47	127.17
4	BB	1245	OMG	N9-C8-N7	-3.69	106.57	113.40
1	AA	2054	OMU	C5-C4-N3	3.68	119.96	114.80
1	AA	131	PSU	C6-N1-C2	-3.67	119.28	122.69
3	BA	1621	OMG	N9-C8-N7	-3.66	106.62	113.40
5	BC	43	A2M	C1'-N9-C8	3.65	135.19	127.09
4	BB	588	A2M	C2'-C1'-N9	-3.65	107.75	113.75
1	AA	1931	OMG	N9-C8-N7	-3.64	106.64	113.40
1	AA	2260	MA6	C2-N1-C6	3.64	120.72	111.83
4	BB	73	OMU	C5-C4-N3	3.63	119.89	114.80
1	AA	2154	OMU	C1'-N1-C2	3.63	124.12	117.59
4	BB	659	OMG	N9-C8-N7	-3.63	106.67	113.40
4	BB	685	OMU	C5-C4-N3	3.63	119.88	114.80
4	BB	1435	OMU	N3-C2-N1	3.62	119.61	114.89
1	AA	57	OMU	C5-C4-N3	3.62	119.87	114.80
4	BB	646	A2M	C1'-N9-C8	3.62	135.12	127.09
1	AA	1899	OMU	C5-C4-N3	3.61	119.86	114.80
1	AA	2227	OMG	N9-C8-N7	-3.61	106.71	113.40
3	BA	1709	OMG	N9-C8-N7	-3.60	106.72	113.40
3	BA	925	OMG	N9-C8-N7	-3.60	106.73	113.40
3	BA	1024	A2M	C1'-N9-C8	3.59	135.07	127.09
3	BA	1605	OMG	N9-C8-N7	-3.57	106.78	113.40
4	BB	609	A2M	C1'-N9-C8	3.57	135.01	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	1062	OMG	N9-C8-N7	-3.57	106.78	113.40
4	BB	1247	OMG	N9-C8-N7	-3.54	106.84	113.40
1	AA	721	A2M	N3-C4-N9	3.53	133.16	127.17
3	BA	927	A2M	C2-N3-C4	3.52	120.44	111.83
3	BA	1086	PSU	C6-N1-C2	-3.52	119.43	122.69
1	AA	56	A2M	C2-N3-C4	3.52	120.42	111.83
4	BB	673	OMG	N9-C8-N7	-3.51	106.88	113.40
4	BB	552	OMG	N9-C8-N7	-3.51	106.90	113.40
1	AA	1652	OMU	C5-C4-N3	3.50	119.70	114.80
4	BB	71	OMG	N9-C8-N7	-3.50	106.92	113.40
4	BB	1201	A2M	C5-N7-C8	3.49	108.94	103.45
3	BA	1024	A2M	C2-N3-C4	3.48	120.33	111.83
3	BA	1614	PSU	C6-N1-C2	-3.48	119.46	122.69
1	AA	1676	OMG	N9-C8-N7	-3.47	106.96	113.40
4	BB	588	A2M	C1'-N9-C8	3.47	134.79	127.09
4	BB	545	A2M	C5-N7-C8	3.47	108.90	103.45
1	AA	1596	B8N	N3-C2-N1	3.46	120.94	116.72
4	BB	1429	PSU	C6-N1-C2	-3.44	119.49	122.69
4	BB	1269	OMG	N9-C8-N7	-3.44	107.02	113.40
1	AA	2154	OMU	C5-C4-N3	3.43	119.60	114.80
1	AA	2096	A2M	C5-N7-C8	3.43	108.84	103.45
1	AA	1619	PSU	C6-N1-C2	-3.42	119.51	122.69
4	BB	1160	PSU	C6-N1-C2	-3.42	119.52	122.69
5	BC	43	A2M	C5-N7-C8	3.42	108.82	103.45
4	BB	455	PSU	C6-N1-C2	-3.41	119.52	122.69
4	BB	1210	PSU	C6-N1-C2	-3.41	119.53	122.69
1	AA	1895	OMG	N9-C8-N7	-3.40	107.09	113.40
4	BB	522	PSU	C6-N1-C2	-3.40	119.54	122.69
4	BB	588	A2M	C2-N3-C4	3.39	120.12	111.83
1	AA	61	PSU	C6-N1-C2	-3.38	119.56	122.69
5	BC	75	OMG	N9-C8-N7	-3.37	107.15	113.40
3	BA	1024	A2M	C5-N7-C8	3.37	108.75	103.45
3	BA	742	1MA	N9-C8-N7	-3.37	107.16	113.40
4	BB	622	A2M	C2-N3-C4	3.36	120.05	111.83
3	BA	1665	A2M	C2-N3-C4	3.36	120.04	111.83
1	AA	2096	A2M	C2-N3-C4	3.36	120.04	111.83
4	BB	524	PSU	C6-N1-C2	-3.35	119.58	122.69
1	AA	2261	MA6	C2-N1-C6	3.35	120.02	111.83
3	BA	743	A2M	C2-N3-C4	3.35	120.00	111.83
4	BB	646	A2M	C2-N3-C4	3.34	119.99	111.83
4	BB	528	PSU	O2-C2-N1	-3.34	119.34	122.79
3	BA	1258	PSU	C6-N1-C2	-3.34	119.59	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	545	A2M	C2-N3-C4	3.34	119.98	111.83
3	BA	927	A2M	C5-N7-C8	3.34	108.69	103.45
5	BC	163	A2M	C2-N3-C4	3.33	119.98	111.83
4	BB	1400	A2M	C5-N7-C8	3.33	108.69	103.45
5	BC	43	A2M	C2-N3-C4	3.33	119.97	111.83
3	BA	746	A2M	C2-N3-C4	3.33	119.96	111.83
1	AA	2260	MA6	N9-C8-N7	-3.33	109.22	113.94
4	BB	400	A2M	C1'-N9-C8	3.33	134.48	127.09
3	BA	996	A2M	C2-N3-C4	3.32	119.95	111.83
4	BB	588	A2M	C5-N7-C8	3.32	108.67	103.45
1	AA	2261	MA6	C2-N3-C4	3.32	119.93	111.83
5	BC	163	A2M	C5-N7-C8	3.31	108.66	103.45
4	BB	1334	PSU	C6-N1-C2	-3.31	119.62	122.69
4	BB	646	A2M	C5-N7-C8	3.31	108.66	103.45
3	BA	996	A2M	C5-N7-C8	3.31	108.66	103.45
4	BB	95	A2M	C1'-N9-C8	3.31	134.44	127.09
3	BA	254	A2M	C2-N3-C4	3.31	119.91	111.83
4	BB	622	A2M	C5-N7-C8	3.30	108.64	103.45
4	BB	611	PSU	C6-N1-C2	-3.30	119.63	122.69
1	AA	56	A2M	C5-N7-C8	3.30	108.63	103.45
3	BA	1129	PSU	C6-N1-C2	-3.29	119.63	122.69
5	BC	41	A2M	C5-N7-C8	3.29	108.62	103.45
3	BA	1609	PSU	C6-N1-C2	-3.29	119.64	122.69
4	BB	95	A2M	C2-N3-C4	3.29	119.86	111.83
4	BB	1388	A2M	C5-N7-C8	3.28	108.61	103.45
4	BB	1319	PSU	C6-N1-C2	-3.28	119.65	122.69
1	AA	2045	PSU	C6-N1-C2	-3.27	119.66	122.69
3	BA	1665	A2M	C5-N7-C8	3.26	108.58	103.45
4	BB	1400	A2M	C2-N3-C4	3.26	119.78	111.83
3	BA	1620	A2M	C2-N3-C4	3.25	119.78	111.83
4	BB	1388	A2M	C2-N3-C4	3.25	119.78	111.83
4	BB	644	PSU	C6-N1-C2	-3.25	119.67	122.69
3	BA	1620	A2M	C5-N7-C8	3.25	108.56	103.45
4	BB	609	A2M	C2-N3-C4	3.24	119.75	111.83
1	AA	2070	7MG	C5-C4-N9	3.24	110.48	106.33
3	BA	746	A2M	C5-N7-C8	3.23	108.53	103.45
4	BB	680	PSU	C6-N1-C2	-3.23	119.69	122.69
1	AA	2260	MA6	C4-C5-C6	3.23	119.25	115.91
4	BB	1201	A2M	C2-N3-C4	3.23	119.71	111.83
4	BB	400	A2M	C2-N3-C4	3.22	119.71	111.83
3	BA	452	PSU	C6-N1-C2	-3.22	119.70	122.69
3	BA	996	A2M	C1'-N9-C8	3.22	134.25	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	95	A2M	C5-N7-C8	3.22	108.51	103.45
3	BA	254	A2M	C5-N7-C8	3.22	108.51	103.45
3	BA	762	A2M	C2-N3-C4	3.21	119.68	111.83
4	BB	615	PSU	C6-N1-C2	-3.21	119.71	122.69
3	BA	743	A2M	C5-N7-C8	3.21	108.49	103.45
1	AA	721	A2M	C5-N7-C8	3.20	108.48	103.45
1	AA	1517	OMG	C2-N1-C6	-3.20	119.31	125.11
4	BB	518	PSU	C6-N1-C2	-3.19	119.73	122.69
5	BC	41	A2M	C2-N3-C4	3.19	119.63	111.83
1	AA	56	A2M	C1'-N9-C8	3.19	134.18	127.09
3	BA	762	A2M	C5-N7-C8	3.19	108.47	103.45
1	AA	1517	OMG	N9-C4-N3	3.19	132.33	125.95
4	BB	1398	PSU	C6-N1-C2	-3.19	119.73	122.69
1	AA	2260	MA6	C2-N3-C4	3.19	119.61	111.83
4	BB	1076	PSU	C6-N1-C2	-3.18	119.74	122.69
3	BA	258	PSU	C6-N1-C2	-3.17	119.75	122.69
1	AA	57	OMU	O4-C4-C5	-3.17	119.70	125.16
3	BA	1665	A2M	C1'-N9-C8	3.16	134.11	127.09
1	AA	1676	OMG	C2-N1-C6	-3.16	119.38	125.11
1	AA	1517	OMG	N9-C8-N7	-3.15	107.55	113.40
1	AA	2153	A2M	C2-N3-C4	3.15	119.53	111.83
1	AA	2153	A2M	C5-N7-C8	3.15	108.40	103.45
5	BC	74	PSU	C6-N1-C2	-3.15	119.77	122.69
3	BA	927	A2M	C1'-N9-C8	3.15	134.08	127.09
4	BB	1229	PSU	C6-N1-C2	-3.14	119.78	122.69
4	BB	1076	PSU	C6-C5-C4	3.14	120.29	118.17
1	AA	131	PSU	O2-C2-N1	-3.14	119.56	122.79
4	BB	400	A2M	C5-N7-C8	3.12	108.36	103.45
4	BB	1435	OMU	O4-C4-C5	-3.11	119.81	125.16
3	BA	1009	PSU	C6-N1-C2	-3.10	119.81	122.69
1	AA	2070	7MG	C2-N1-C6	-3.10	119.49	125.11
4	BB	1409	PSU	C6-N1-C2	-3.09	119.82	122.69
1	AA	721	A2M	C2-N3-C4	3.09	119.38	111.83
4	BB	518	PSU	C6-C5-C4	3.09	120.26	118.17
1	AA	1276	PSU	C6-N1-C2	-3.09	119.83	122.69
4	BB	609	A2M	C5-N7-C8	3.08	108.30	103.45
4	BB	73	OMU	O4-C4-C5	-3.07	119.86	125.16
4	BB	1229	PSU	C6-C5-C4	3.07	120.25	118.17
1	AA	1700	OMG	C2-N1-C6	-3.07	119.55	125.11
1	AA	1592	PSU	C6-N1-C2	-3.06	119.85	122.69
4	BB	542	5MC	C5-C6-N1	-3.06	119.99	123.31
3	BA	1742	OMU	O4-C4-C5	-3.06	119.88	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BA	1028	OMG	N9-C8-N7	-3.06	107.73	113.40
3	BA	1448	OMU	O4-C4-C5	-3.06	119.89	125.16
1	AA	2146	PSU	C6-N1-C2	-3.05	119.86	122.69
3	BA	1709	OMG	C2-N1-C6	-3.04	119.59	125.11
3	BA	1169	PSU	C6-N1-C2	-3.03	119.88	122.69
4	BB	629	PSU	C6-N1-C2	-3.03	119.88	122.69
1	AA	1931	OMG	C2-N1-C6	-3.02	119.64	125.11
5	BC	7	OMU	O4-C4-C5	-3.02	119.96	125.16
1	AA	1899	OMU	O4-C4-C5	-3.01	119.96	125.16
3	BA	743	A2M	C1'-N9-C8	3.01	133.78	127.09
4	BB	1280	PSU	C6-N1-C2	-3.01	119.90	122.69
3	BA	737	PSU	C6-N1-C2	-3.00	119.90	122.69
4	BB	1062	OMG	C2-N1-C6	-2.99	119.68	125.11
4	BB	71	OMG	C2-N1-C6	-2.99	119.69	125.11
3	BA	1028	OMG	C2-N1-C6	-2.99	119.69	125.11
1	AA	1895	OMG	C2-N1-C6	-2.98	119.71	125.11
4	BB	1319	PSU	C6-C5-C4	2.97	120.18	118.17
1	AA	2054	OMU	O4-C4-C5	-2.97	120.03	125.16
3	BA	1181	OMU	O4-C4-C5	-2.96	120.05	125.16
3	BA	1605	OMG	C2-N1-C6	-2.96	119.75	125.11
1	AA	1596	B8N	O4-C4-N3	-2.96	115.19	119.99
4	BB	1398	PSU	C6-C5-C4	2.95	120.17	118.17
1	AA	2227	OMG	C2-N1-C6	-2.95	119.75	125.11
4	BB	673	OMG	C2-N1-C6	-2.95	119.76	125.11
4	BB	1375	OMU	O4-C4-C5	-2.95	120.08	125.16
4	BB	1269	OMG	C2-N1-C6	-2.95	119.77	125.11
1	AA	2261	MA6	C5-N7-C8	2.93	108.06	103.45
1	AA	1676	OMG	N9-C4-N3	2.91	131.78	125.95
4	BB	1247	OMG	C2-N1-C6	-2.91	119.84	125.11
5	BC	75	OMG	C2-N1-C6	-2.90	119.84	125.11
3	BA	1009	PSU	C6-C5-C4	2.90	120.13	118.17
3	BA	1267	OMG	C2-N1-C6	-2.90	119.85	125.11
4	BB	1245	OMG	C2-N1-C6	-2.90	119.85	125.11
3	BA	1614	PSU	O2-C2-N1	-2.89	119.81	122.79
4	BB	1093	OMU	O4-C4-C5	-2.89	120.18	125.16
3	BA	916	OMU	O4-C4-C5	-2.89	120.18	125.16
4	BB	659	OMG	C2-N1-C6	-2.89	119.88	125.11
3	BA	1258	PSU	C6-C5-C4	2.87	120.11	118.17
1	AA	1517	OMG	C5-C6-N1	2.87	120.55	113.25
1	AA	2070	7MG	O6-C6-C5	-2.86	120.61	127.62
4	BB	1076	PSU	O2-C2-N1	-2.85	119.85	122.79
4	BB	1160	PSU	C6-C5-C4	2.85	120.10	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BA	1621	OMG	C2-N1-C6	-2.85	119.94	125.11
1	AA	36	OMU	O4-C4-C5	-2.85	120.25	125.16
4	BB	545	A2M	O4'-C1'-N9	2.84	113.54	108.09
1	AA	2123	OMU	O4-C4-C5	-2.84	120.27	125.16
3	BA	1169	PSU	C6-C5-C4	2.83	120.09	118.17
1	AA	1676	OMG	C5-C6-N1	2.83	120.45	113.25
4	BB	588	A2M	O2'-C2'-C1'	2.82	114.35	108.99
4	BB	578	OMU	O4-C4-C5	-2.82	120.30	125.16
1	AA	1652	OMU	O4-C4-C5	-2.81	120.31	125.16
4	BB	455	PSU	C6-C5-C4	2.81	120.07	118.17
4	BB	644	PSU	O2-C2-N1	-2.80	119.90	122.79
3	BA	258	PSU	O2-C2-N1	-2.80	119.90	122.79
1	AA	1700	OMG	C5-C6-N1	2.80	120.38	113.25
4	BB	680	PSU	C6-C5-C4	2.79	120.06	118.17
4	BB	552	OMG	C2-N1-C6	-2.79	120.05	125.11
3	BA	1709	OMG	C5-C6-N1	2.79	120.35	113.25
3	BA	1614	PSU	C6-C5-C4	2.79	120.05	118.17
3	BA	915	OMG	C2-N1-C6	-2.78	120.06	125.11
4	BB	1062	OMG	C5-C6-N1	2.78	120.33	113.25
3	BA	762	A2M	C2'-C1'-N9	-2.77	109.19	113.75
4	BB	1160	PSU	O2-C2-N1	-2.77	119.93	122.79
1	AA	1931	OMG	C5-C6-N1	2.76	120.29	113.25
3	BA	46	OMU	O4-C4-C5	-2.76	120.40	125.16
4	BB	71	OMG	C5-C6-N1	2.76	120.29	113.25
1	AA	2154	OMU	O4-C4-C5	-2.76	120.40	125.16
1	AA	131	PSU	C6-C5-C4	2.76	120.04	118.17
4	BB	673	OMG	C5-C6-N1	2.76	120.28	113.25
1	AA	61	PSU	O2-C2-N1	-2.75	119.95	122.79
4	BB	524	PSU	O2-C2-N1	-2.75	119.95	122.79
4	BB	1094	OMG	C2-N1-C6	-2.75	120.12	125.11
3	BA	258	PSU	C6-C5-C4	2.75	120.03	118.17
3	BA	1028	OMG	C5-C6-N1	2.75	120.24	113.25
4	BB	1429	PSU	O2-C2-N1	-2.75	119.96	122.79
4	BB	680	PSU	O2-C2-N1	-2.74	119.96	122.79
4	BB	1269	OMG	C5-C6-N1	2.74	120.24	113.25
1	AA	1531	OMG	C2-N1-C6	-2.74	120.14	125.11
1	AA	1895	OMG	C5-C6-N1	2.74	120.22	113.25
1	AA	2045	PSU	O2-C2-N1	-2.73	119.97	122.79
4	BB	530	PSU	C3'-C2'-C1'	2.72	104.90	101.69
4	BB	455	PSU	O2-C2-N1	-2.72	119.99	122.79
4	BB	1247	OMG	C5-C6-N1	2.71	120.16	113.25
1	AA	1531	OMG	C5-C6-N1	2.70	120.13	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BA	925	OMG	C2-N1-C6	-2.70	120.22	125.11
4	BB	1280	PSU	C6-C5-C4	2.70	119.99	118.17
4	BB	1245	OMG	C5-C6-N1	2.70	120.12	113.25
1	AA	2070	7MG	N9-C4-N3	2.69	129.41	125.46
4	BB	518	PSU	O2-C2-N1	-2.69	120.01	122.79
3	BA	1129	PSU	C6-C5-C4	2.69	119.99	118.17
1	AA	714	OMU	O4-C4-C5	-2.68	120.53	125.16
1	AA	2227	OMG	C5-C6-N1	2.68	120.08	113.25
4	BB	1409	PSU	O2-C2-N1	-2.68	120.03	122.79
4	BB	685	OMU	O4-C4-C5	-2.67	120.55	125.16
4	BB	1201	A2M	C2'-C1'-N9	-2.66	109.37	113.75
3	BA	925	OMG	C5-C6-N1	2.66	120.03	113.25
5	BC	74	PSU	C6-C5-C4	2.66	119.97	118.17
4	BB	552	OMG	C5-C6-N1	2.65	120.01	113.25
4	BB	522	PSU	O2-C2-N1	-2.65	120.06	122.79
3	BA	1267	OMG	C5-C6-N1	2.65	120.00	113.25
4	BB	1247	OMG	N9-C4-N3	2.64	131.24	125.95
4	BB	659	OMG	C5-C6-N1	2.64	119.97	113.25
4	BB	1094	OMG	C5-C6-N1	2.64	119.97	113.25
3	BA	915	OMG	C5-C6-N1	2.64	119.97	113.25
3	BA	1621	OMG	C5-C6-N1	2.64	119.96	113.25
3	BA	1086	PSU	C6-C5-C4	2.63	119.95	118.17
5	BC	75	OMG	N9-C4-N3	2.63	131.20	125.95
1	AA	1895	OMG	N9-C4-N3	2.62	131.20	125.95
5	BC	75	OMG	C5-C6-N1	2.62	119.92	113.25
3	BA	1086	PSU	O2-C2-N1	-2.62	120.09	122.79
1	AA	1931	OMG	O6-C6-C5	-2.62	119.62	126.53
4	BB	1319	PSU	O2-C2-N1	-2.61	120.10	122.79
3	BA	1169	PSU	O2-C2-N1	-2.60	120.11	122.79
1	AA	1517	OMG	O6-C6-C5	-2.59	119.69	126.53
3	BA	1605	OMG	C5-C6-N1	2.59	119.85	113.25
3	BA	1609	PSU	C6-C5-C4	2.59	119.92	118.17
4	BB	1334	PSU	C6-C5-C4	2.58	119.92	118.17
1	AA	1931	OMG	N9-C4-N3	2.57	131.09	125.95
1	AA	2261	MA6	N3-C4-N9	2.56	131.52	127.17
3	BA	1129	PSU	O2-C2-N1	-2.56	120.15	122.79
4	BB	615	PSU	C6-C5-C4	2.55	119.90	118.17
4	BB	528	PSU	C5-C6-N1	-2.55	118.60	122.14
4	BB	1280	PSU	O2-C2-N1	-2.54	120.17	122.79
3	BA	452	PSU	O2-C2-N1	-2.53	120.18	122.79
1	AA	1619	PSU	O2-C2-N1	-2.53	120.18	122.79
4	BB	1229	PSU	O2-C2-N1	-2.53	120.18	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	1062	OMG	N9-C4-N3	2.53	131.01	125.95
1	AA	1700	OMG	O6-C6-C5	-2.51	119.90	126.53
1	AA	1592	PSU	O2-C2-N1	-2.51	120.20	122.79
1	AA	61	PSU	C6-C5-C4	2.51	119.87	118.17
4	BB	545	A2M	O4'-C1'-C2'	-2.51	102.27	106.59
3	BA	1267	OMG	C8-N7-C5	2.50	108.72	104.26
3	BA	452	PSU	C6-C5-C4	2.50	119.86	118.17
4	BB	1210	PSU	O2-C2-N1	-2.50	120.21	122.79
1	AA	1531	OMG	O6-C6-C5	-2.50	119.94	126.53
4	BB	629	PSU	O2-C2-N1	-2.49	120.22	122.79
3	BA	1605	OMG	N9-C4-N3	2.49	130.94	125.95
1	AA	2146	PSU	O2-C2-N1	-2.49	120.22	122.79
3	BA	915	OMG	C8-N7-C5	2.49	108.69	104.26
1	AA	1276	PSU	O2-C2-N1	-2.49	120.22	122.79
3	BA	1709	OMG	N9-C4-N3	2.48	130.92	125.95
1	AA	2070	7MG	N9-C8-N7	2.48	106.89	103.37
3	BA	1609	PSU	O2-C2-N1	-2.48	120.23	122.79
1	AA	36	OMU	O2-C2-N1	-2.48	119.57	122.80
4	BB	530	PSU	C5-C6-N1	-2.47	118.71	122.14
3	BA	1605	OMG	C8-N7-C5	2.47	108.66	104.26
5	BC	74	PSU	O2-C2-N1	-2.46	120.25	122.79
3	BA	1620	A2M	C2'-C1'-N9	2.46	117.81	113.75
4	BB	1398	PSU	O2-C2-N1	-2.46	120.25	122.79
4	BB	659	OMG	N9-C4-N3	2.46	130.87	125.95
3	BA	1621	OMG	N9-C4-N3	2.46	130.87	125.95
1	AA	1895	OMG	O6-C6-C5	-2.46	120.05	126.53
4	BB	659	OMG	C8-N7-C5	2.45	108.63	104.26
3	BA	1248	PSU	C6-N1-C2	-2.45	120.42	122.69
4	BB	615	PSU	O2-C2-N1	-2.45	120.26	122.79
4	BB	552	OMG	O6-C6-C5	-2.45	120.07	126.53
4	BB	71	OMG	N9-C4-N3	2.44	130.84	125.95
3	BA	927	A2M	O4'-C1'-N9	2.44	112.78	108.09
3	BA	742	1MA	C8-N7-C5	2.44	108.60	104.26
5	BC	75	OMG	O6-C6-C5	-2.43	120.12	126.53
4	BB	1062	OMG	O6-C6-C5	-2.43	120.13	126.53
3	BA	742	1MA	N9-C4-N3	2.42	132.42	126.90
4	BB	1245	OMG	O6-C6-C5	-2.41	120.17	126.53
1	AA	1700	OMG	C8-N7-C5	2.41	108.55	104.26
3	BA	1709	OMG	O6-C6-C5	-2.40	120.19	126.53
1	AA	2227	OMG	N9-C4-N3	2.40	130.75	125.95
3	BA	1009	PSU	O2-C2-N1	-2.40	120.31	122.79
4	BB	1269	OMG	N9-C4-N3	2.39	130.74	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	673	OMG	N9-C4-N3	2.39	130.73	125.95
3	BA	1621	OMG	C8-N7-C5	2.39	108.51	104.26
4	BB	528	PSU	C3'-C2'-C1'	2.39	104.50	101.69
1	AA	2261	MA6	C4-C5-N7	-2.38	107.86	110.58
1	AA	1592	PSU	C6-C5-C4	2.38	119.78	118.17
1	AA	57	OMU	O2-C2-N1	-2.38	119.70	122.80
4	BB	1094	OMG	O6-C6-C5	-2.38	120.26	126.53
4	BB	611	PSU	O2-C2-N1	-2.37	120.34	122.79
3	BA	927	A2M	C4'-O4'-C1'	-2.37	104.23	109.47
1	AA	1676	OMG	O6-C6-C5	-2.37	120.28	126.53
4	BB	1247	OMG	O6-C6-C5	-2.37	120.28	126.53
4	BB	552	OMG	N9-C4-N3	2.36	130.68	125.95
4	BB	673	OMG	C8-N7-C5	2.36	108.47	104.26
1	AA	1676	OMG	C8-N7-C5	2.36	108.47	104.26
3	BA	1267	OMG	N2-C2-N1	2.36	121.75	116.76
4	BB	1210	PSU	C6-C5-C4	2.36	119.77	118.17
4	BB	71	OMG	O6-C6-C5	-2.36	120.31	126.53
4	BB	1062	OMG	C8-N7-C5	2.36	108.46	104.26
4	BB	1269	OMG	O6-C6-C5	-2.35	120.33	126.53
4	BB	1245	OMG	C8-N7-C5	2.35	108.44	104.26
3	BA	925	OMG	O6-C6-C5	-2.35	120.34	126.53
3	BA	1258	PSU	O2-C2-N1	-2.34	120.37	122.79
4	BB	1334	PSU	O2-C2-N1	-2.34	120.37	122.79
1	AA	1700	OMG	N9-C4-N3	2.32	130.60	125.95
1	AA	2153	A2M	C2'-C1'-N9	-2.32	109.93	113.75
4	BB	71	OMG	C8-N7-C5	2.32	108.40	104.26
3	BA	1181	OMU	O2-C2-N1	-2.32	119.78	122.80
1	AA	2045	PSU	C6-C5-C4	2.31	119.73	118.17
4	BB	1094	OMG	C8-N7-C5	2.31	108.37	104.26
4	BB	1280	PSU	O4'-C1'-C2'	2.31	108.34	105.15
1	AA	2227	OMG	O6-C6-C5	-2.31	120.45	126.53
1	AA	1931	OMG	C8-N7-C5	2.30	108.36	104.26
3	BA	1605	OMG	O6-C6-C5	-2.30	120.46	126.53
1	AA	2227	OMG	C8-N7-C5	2.29	108.35	104.26
3	BA	925	OMG	N2-C2-N1	2.29	121.60	116.76
4	BB	644	PSU	C6-C5-C4	2.29	119.72	118.17
4	BB	1247	OMG	C8-N7-C5	2.29	108.34	104.26
4	BB	1429	PSU	C6-C5-C4	2.29	119.72	118.17
1	AA	2054	OMU	O2-C2-N1	-2.29	119.82	122.80
4	BB	1245	OMG	N9-C4-N3	2.28	130.52	125.95
3	BA	1267	OMG	O6-C6-C5	-2.28	120.51	126.53
3	BA	1028	OMG	N9-C4-N3	2.28	130.51	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	1319	PSU	O4'-C1'-C2'	2.27	108.30	105.15
3	BA	737	PSU	O2-C2-N1	-2.27	120.44	122.79
4	BB	1400	A2M	C2'-C1'-N9	-2.27	110.02	113.75
3	BA	1709	OMG	C8-N7-C5	2.27	108.30	104.26
4	BB	659	OMG	O6-C6-C5	-2.26	120.56	126.53
4	BB	545	A2M	C4'-O4'-C1'	-2.26	104.48	109.47
3	BA	925	OMG	C8-N7-C5	2.26	108.28	104.26
1	AA	2260	MA6	C5-C4-N9	2.26	108.27	105.81
1	AA	2261	MA6	C5-C4-N9	2.25	108.27	105.81
3	BA	1267	OMG	C2'-C1'-N9	-2.25	109.97	114.24
3	BA	1621	OMG	O6-C6-C5	-2.25	120.60	126.53
4	BB	673	OMG	O6-C6-C5	-2.24	120.61	126.53
3	BA	1028	OMG	O6-C6-C5	-2.24	120.62	126.53
4	BB	1094	OMG	N2-C2-N1	2.24	121.49	116.76
4	BB	542	5MC	CM5-C5-C6	-2.22	119.84	122.85
4	BB	1375	OMU	O2-C2-N1	-2.22	119.90	122.80
4	BB	524	PSU	C6-C5-C4	2.22	119.67	118.17
3	BA	915	OMG	O6-C6-C5	-2.21	120.69	126.53
3	BA	1267	OMG	C4-C5-N7	-2.21	107.17	110.67
1	AA	1276	PSU	C6-C5-C4	2.21	119.66	118.17
1	AA	1517	OMG	C8-N7-C5	2.20	108.18	104.26
3	BA	743	A2M	C2'-C1'-N9	2.20	117.36	113.75
3	BA	916	OMU	O2-C2-N1	-2.19	119.95	122.80
4	BB	552	OMG	C8-N7-C5	2.19	108.16	104.26
4	BB	1409	PSU	C6-C5-C4	2.19	119.65	118.17
4	BB	95	A2M	C6-C5-C4	2.19	120.17	117.18
5	BC	75	OMG	C8-N7-C5	2.18	108.15	104.26
3	BA	915	OMG	N9-C4-N3	2.18	130.32	125.95
4	BB	1264	OMC	O2-C2-N3	-2.18	118.89	122.33
3	BA	1248	PSU	O4'-C1'-C2'	2.18	108.16	105.15
1	AA	1531	OMG	N2-C2-N1	2.18	121.35	116.76
1	AA	2261	MA6	C4-N9-C8	2.17	108.02	105.74
3	BA	737	PSU	O4'-C1'-C2'	2.17	108.15	105.15
1	AA	1895	OMG	C8-N7-C5	2.15	108.10	104.26
1	AA	2146	PSU	C6-C5-C4	2.15	119.63	118.17
3	BA	1665	A2M	C6-C5-C4	2.15	120.11	117.18
3	BA	996	A2M	C6-C5-C4	2.15	120.11	117.18
4	BB	578	OMU	C1'-N1-C2	2.15	121.45	117.59
3	BA	1448	OMU	O2-C2-N1	-2.14	120.01	122.80
4	BB	1245	OMG	N2-C2-N1	2.14	121.28	116.76
4	BB	400	A2M	C6-C5-C4	2.14	120.10	117.18
4	BB	1269	OMG	C8-N7-C5	2.14	108.07	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	1398	PSU	O4'-C1'-C2'	2.14	108.11	105.15
4	BB	522	PSU	C6-C5-C4	2.13	119.61	118.17
3	BA	743	A2M	C6-C5-C4	2.13	120.08	117.18
3	BA	1267	OMG	C6-C5-N7	2.12	134.16	130.29
4	BB	400	A2M	C5'-C4'-C3'	-2.12	107.57	115.21
4	BB	1094	OMG	N9-C4-N3	2.12	130.19	125.95
1	AA	1531	OMG	C8-N7-C5	2.11	108.02	104.26
1	AA	1899	OMU	C1'-N1-C2	2.11	121.38	117.59
1	AA	1531	OMG	N9-C4-N3	2.11	130.17	125.95
1	AA	1931	OMG	N2-C2-N1	2.10	121.20	116.76
4	BB	71	OMG	C2'-C1'-N9	-2.09	110.27	114.24
4	BB	588	A2M	C6-C5-C4	2.09	120.03	117.18
3	BA	915	OMG	C4-C5-N7	-2.07	107.38	110.67
3	BA	925	OMG	N1-C2-N3	-2.07	119.53	123.32
1	AA	1596	B8N	O4-C4-C5	-2.07	119.00	122.58
3	BA	1605	OMG	C4-C5-N7	-2.07	107.39	110.67
1	AA	1700	OMG	C8-N9-C4	2.06	109.89	106.03
3	BA	1028	OMG	C8-N7-C5	2.06	107.93	104.26
3	BA	1248	PSU	C5-C4-N3	2.06	121.08	116.55
3	BA	1709	OMG	N2-C2-N1	2.05	121.09	116.76
5	BC	41	A2M	C2'-C1'-N9	-2.05	110.38	113.75
3	BA	737	PSU	C6-C5-C4	2.05	119.56	118.17
1	AA	714	OMU	O2-C2-N1	-2.05	120.13	122.80
1	AA	1596	B8N	O4'-C1'-C2'	2.05	107.98	105.15
3	BA	46	OMU	O2-C2-N1	-2.04	120.14	122.80
4	BB	1201	A2M	C6-C5-C4	2.04	119.96	117.18
1	AA	1531	OMG	N1-C2-N3	-2.03	119.60	123.32
4	BB	609	A2M	C6-C5-C4	2.03	119.95	117.18
3	BA	915	OMG	N2-C2-N1	2.03	121.05	116.76
3	BA	1605	OMG	N2-C2-N1	2.03	121.04	116.76
4	BB	73	OMU	O2-C2-N1	-2.03	120.16	122.80
3	BA	1621	OMG	N2-C2-N1	2.02	121.03	116.76
1	AA	1700	OMG	N2-C2-N1	2.02	121.02	116.76
4	BB	680	PSU	O4'-C1'-C2'	2.02	107.94	105.15
3	BA	1742	OMU	O2-C2-N1	-2.02	120.17	122.80
1	AA	721	A2M	C3'-C2'-C1'	2.00	106.64	102.81
4	BB	552	OMG	N1-C2-N3	-2.00	119.66	123.32

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	BC	43	A2M	C1'-C2'-O2'-CM'
5	BC	75	OMG	O4'-C4'-C5'-O5'
5	BC	163	A2M	C1'-C2'-O2'-CM'
1	AA	46	OMC	O4'-C4'-C5'-O5'
1	AA	57	OMU	C1'-C2'-O2'-CM2
1	AA	721	A2M	O4'-C4'-C5'-O5'
1	AA	721	A2M	C3'-C4'-C5'-O5'
1	AA	1596	B8N	C31-C32-C33-N34
1	AA	1619	PSU	C3'-C4'-C5'-O5'
1	AA	1619	PSU	O4'-C4'-C5'-O5'
1	AA	1652	OMU	C1'-C2'-O2'-CM2
1	AA	1676	OMG	O4'-C4'-C5'-O5'
1	AA	2054	OMU	O4'-C4'-C5'-O5'
1	AA	2096	A2M	C1'-C2'-O2'-CM'
1	AA	2153	A2M	C1'-C2'-O2'-CM'
1	AA	2154	OMU	O4'-C1'-N1-C2
1	AA	2154	OMU	O4'-C1'-N1-C6
1	AA	2154	OMU	C1'-C2'-O2'-CM2
3	BA	737	PSU	C2'-C1'-C5-C4
3	BA	737	PSU	O4'-C1'-C5-C4
3	BA	737	PSU	O4'-C1'-C5-C6
3	BA	742	1MA	O4'-C4'-C5'-O5'
3	BA	743	A2M	C1'-C2'-O2'-CM'
3	BA	1024	A2M	C1'-C2'-O2'-CM'
3	BA	1248	PSU	O4'-C1'-C5-C4
3	BA	1248	PSU	O4'-C1'-C5-C6
3	BA	1608	OMC	C1'-C2'-O2'-CM2
3	BA	1665	A2M	O4'-C4'-C5'-O5'
3	BA	1665	A2M	C1'-C2'-O2'-CM'
4	BB	95	A2M	C1'-C2'-O2'-CM'
4	BB	400	A2M	O4'-C4'-C5'-O5'
4	BB	400	A2M	C3'-C4'-C5'-O5'
4	BB	552	OMG	O4'-C4'-C5'-O5'
4	BB	552	OMG	C3'-C4'-C5'-O5'
4	BB	578	OMU	O4'-C1'-N1-C2
4	BB	588	A2M	C1'-C2'-O2'-CM'
4	BB	609	A2M	C1'-C2'-O2'-CM'
4	BB	629	PSU	O4'-C4'-C5'-O5'
4	BB	1062	OMG	O4'-C4'-C5'-O5'
5	BC	74	PSU	C3'-C4'-C5'-O5'
5	BC	74	PSU	O4'-C4'-C5'-O5'
5	BC	75	OMG	C3'-C4'-C5'-O5'
1	AA	46	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	AA	1676	OMG	C3'-C4'-C5'-O5'
3	BA	742	1MA	C3'-C4'-C5'-O5'
4	BB	522	PSU	C3'-C4'-C5'-O5'
4	BB	522	PSU	O4'-C4'-C5'-O5'
4	BB	629	PSU	C3'-C4'-C5'-O5'
4	BB	1062	OMG	C3'-C4'-C5'-O5'
4	BB	578	OMU	O4'-C1'-N1-C6
4	BB	528	PSU	O4'-C4'-C5'-O5'
4	BB	659	OMG	O4'-C4'-C5'-O5'
1	AA	1899	OMU	O4'-C1'-N1-C2
1	AA	2054	OMU	C3'-C4'-C5'-O5'
3	BA	1614	PSU	C3'-C4'-C5'-O5'
1	AA	36	OMU	C2'-C1'-N1-C6
3	BA	1665	A2M	C3'-C4'-C5'-O5'
1	AA	2260	MA6	O4'-C1'-N9-C4
1	AA	2070	7MG	O4'-C4'-C5'-O5'
3	BA	1258	PSU	C3'-C4'-C5'-O5'
3	BA	1448	OMU	C3'-C4'-C5'-O5'
3	BA	1614	PSU	O4'-C4'-C5'-O5'
4	BB	578	OMU	C3'-C4'-C5'-O5'
1	AA	1899	OMU	O4'-C1'-N1-C6
1	AA	61	PSU	C3'-C4'-C5'-O5'
4	BB	545	A2M	O4'-C4'-C5'-O5'
4	BB	578	OMU	O4'-C4'-C5'-O5'
1	AA	2070	7MG	C3'-C4'-C5'-O5'
4	BB	1201	A2M	C3'-C4'-C5'-O5'
4	BB	1324	5MC	C2'-C1'-N1-C6
1	AA	2146	PSU	O4'-C4'-C5'-O5'
4	BB	545	A2M	C3'-C4'-C5'-O5'
4	BB	588	A2M	C2'-C1'-N9-C8
4	BB	659	OMG	C3'-C4'-C5'-O5'
1	AA	1596	B8N	C31-C32-C33-C34
1	AA	2260	MA6	O4'-C1'-N9-C8
3	BA	1605	OMG	C3'-C4'-C5'-O5'
1	AA	721	A2M	C2'-C1'-N9-C8
1	AA	36	OMU	O4'-C1'-N1-C6
4	BB	1324	5MC	O4'-C1'-N1-C6
1	AA	61	PSU	O4'-C4'-C5'-O5'
3	BA	1448	OMU	O4'-C4'-C5'-O5'
4	BB	524	PSU	O4'-C4'-C5'-O5'
3	BA	742	1MA	C2'-C1'-N9-C8
1	AA	36	OMU	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
3	BA	1329	OMC	C3'-C2'-O2'-CM2
4	BB	588	A2M	C2'-C1'-N9-C4
4	BB	673	OMG	C3'-C2'-O2'-CM2
3	BA	742	1MA	C2'-C1'-N9-C4
1	AA	36	OMU	O4'-C4'-C5'-O5'
1	AA	2134	OMC	O4'-C4'-C5'-O5'
4	BB	528	PSU	C3'-C4'-C5'-O5'
4	BB	578	OMU	C4'-C5'-O5'-P
4	BB	1264	OMC	C4'-C5'-O5'-P
1	AA	36	OMU	O4'-C1'-N1-C2
4	BB	1324	5MC	O4'-C1'-N1-C2
1	AA	36	OMU	C2'-C1'-N1-C2
4	BB	1062	OMG	C1'-C2'-O2'-CM2
3	BA	737	PSU	O4'-C4'-C5'-O5'
3	BA	1258	PSU	O4'-C4'-C5'-O5'
3	BA	254	A2M	C3'-C2'-O2'-CM'
4	BB	588	A2M	C3'-C2'-O2'-CM'
4	BB	1201	A2M	O4'-C4'-C5'-O5'
4	BB	1324	5MC	C2'-C1'-N1-C2
4	BB	588	A2M	O4'-C1'-N9-C8
1	AA	1899	OMU	C4'-C5'-O5'-P
3	BA	927	A2M	O4'-C1'-N9-C8
1	AA	1596	B8N	N34-C33-C34-O36
1	AA	1531	OMG	C4'-C5'-O5'-P
3	BA	1608	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

37 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BB	685	OMU	1	0
1	AA	2045	PSU	2	0
1	AA	2260	MA6	2	0
3	BA	1181	OMU	1	0
1	AA	2261	MA6	1	0
3	BA	1620	A2M	1	0
1	AA	2153	A2M	1	0
4	BB	400	A2M	1	0
1	AA	57	OMU	4	0
1	AA	1596	B8N	2	0
4	BB	609	A2M	3	0
1	AA	2154	OMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BB	1388	A2M	1	0
3	BA	1024	A2M	2	0
5	BC	163	A2M	2	0
4	BB	659	OMG	1	0
4	BB	578	OMU	1	0
4	BB	1324	5MC	1	0
3	BA	743	A2M	1	0
1	AA	2096	A2M	2	0
5	BC	7	OMU	1	0
1	AA	46	OMC	1	0
3	BA	1608	OMC	2	0
1	AA	56	A2M	3	0
4	BB	601	OMC	1	0
4	BB	1076	PSU	1	0
1	AA	1652	OMU	3	0
4	BB	1062	OMG	1	0
3	BA	760	OMC	1	0
4	BB	1429	PSU	1	0
1	AA	2123	OMU	1	0
1	AA	2070	7MG	1	0
3	BA	1614	PSU	1	0
3	BA	254	A2M	2	0
3	BA	1267	OMG	1	0
5	BC	43	A2M	1	0
3	BA	762	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 241 ligands modelled in this entry, 241 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
2	AB	1
1	AA	1
18	Bp	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AB	7:A	O3'	65:G	P	16.40
1	AA	1595:C	O3'	1596:B8N	P	3.15
1	Bp	71:SER	C	72:ARG	N	3.01

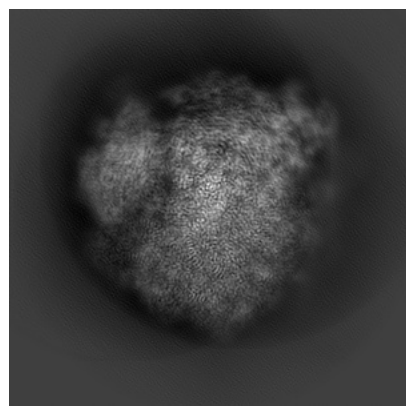
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17212. These allow visual inspection of the internal detail of the map and identification of artifacts.

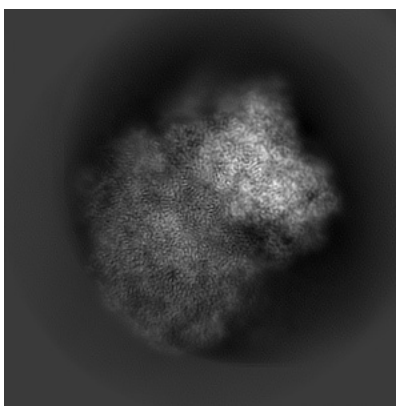
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

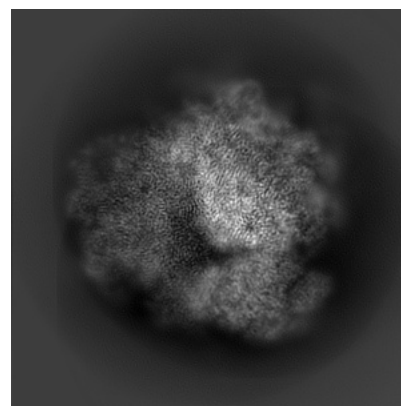
6.1.1 Primary map



X

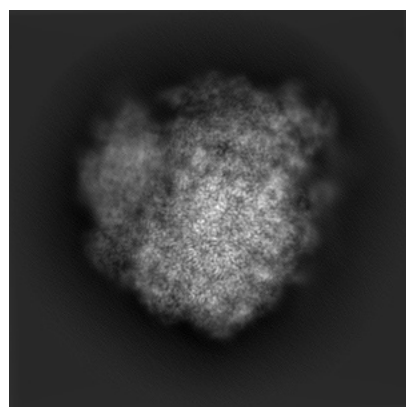


Y

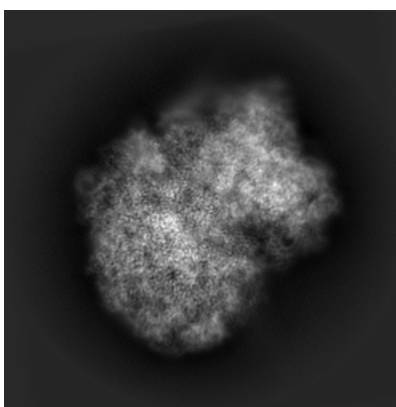


Z

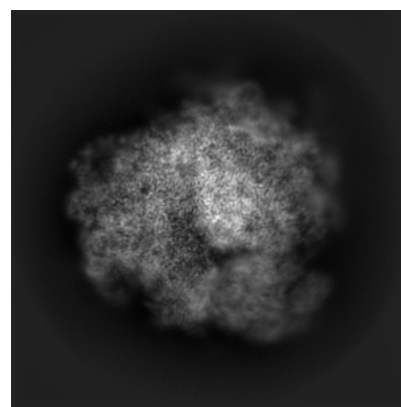
6.1.2 Raw map



X



Y

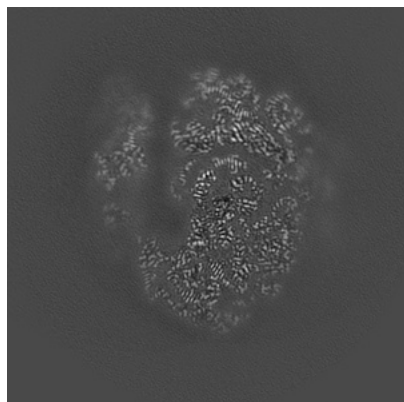


Z

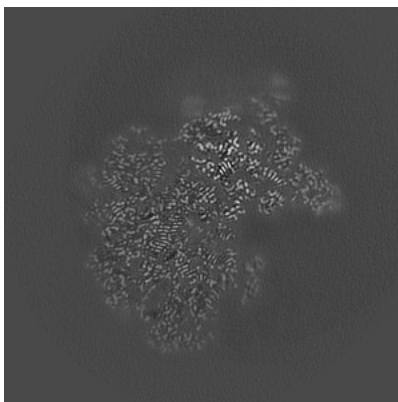
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

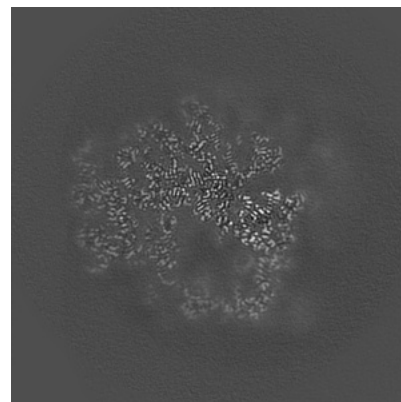
6.2.1 Primary map



X Index: 240

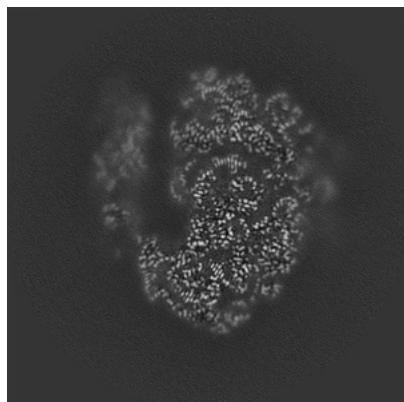


Y Index: 240

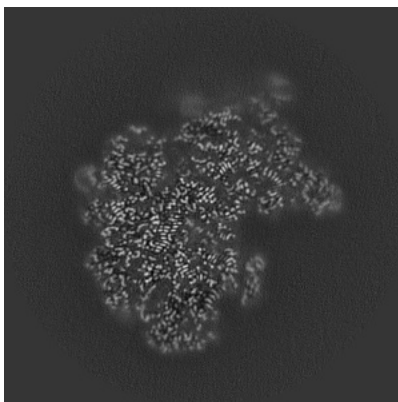


Z Index: 240

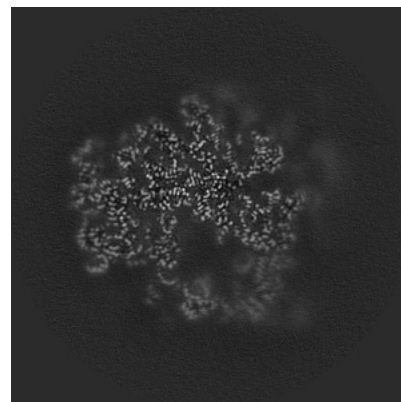
6.2.2 Raw map



X Index: 240



Y Index: 240

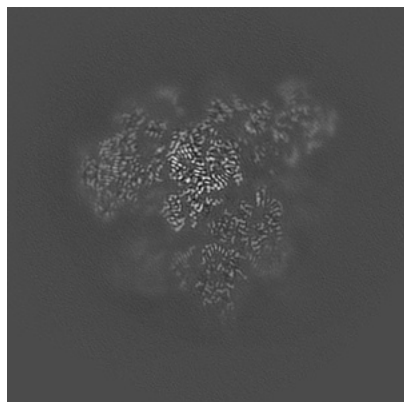


Z Index: 240

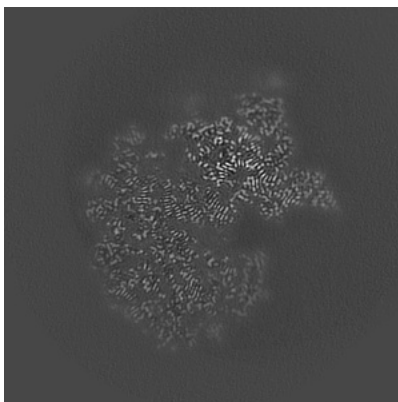
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

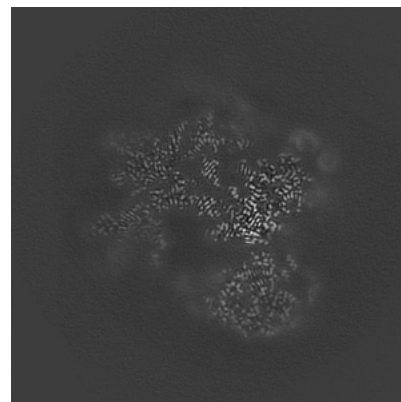
6.3.1 Primary map



X Index: 292

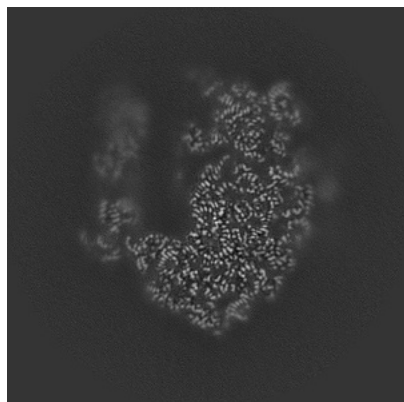


Y Index: 230

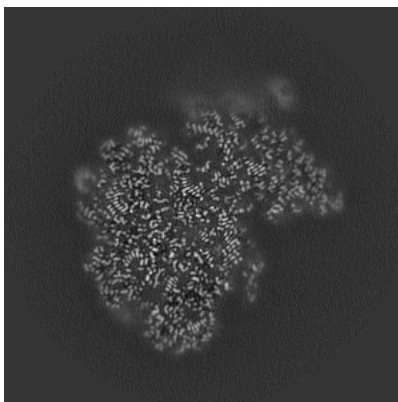


Z Index: 274

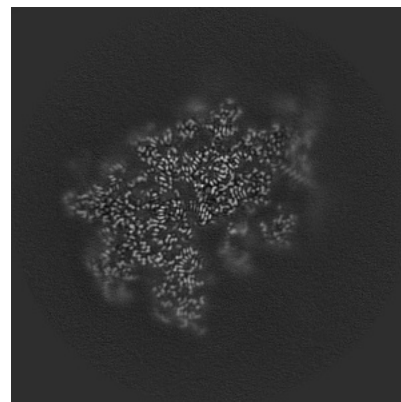
6.3.2 Raw map



X Index: 232



Y Index: 247

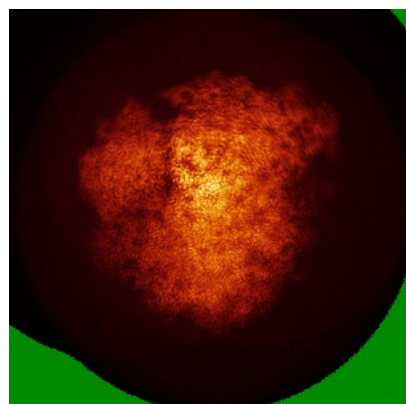


Z Index: 208

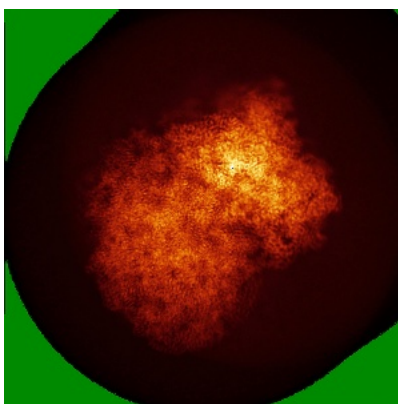
The images above show the largest variance slices of the map in three orthogonal directions.

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

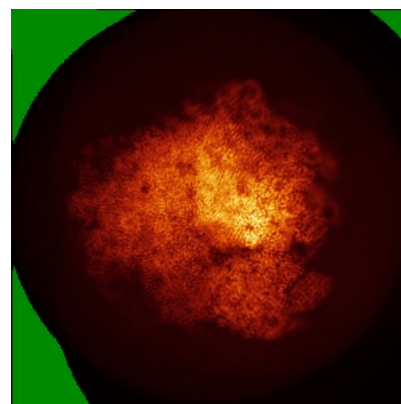
6.4.1 Primary map



X

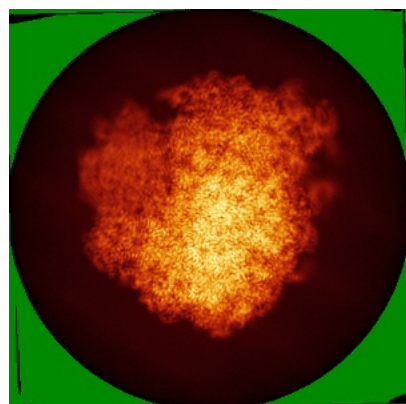


Y

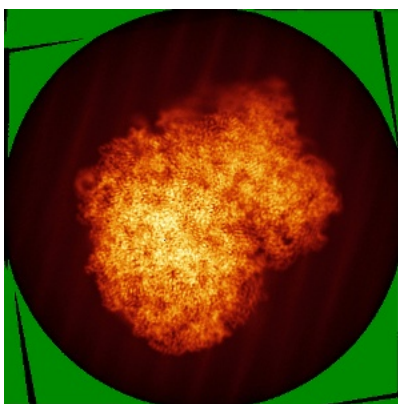


Z

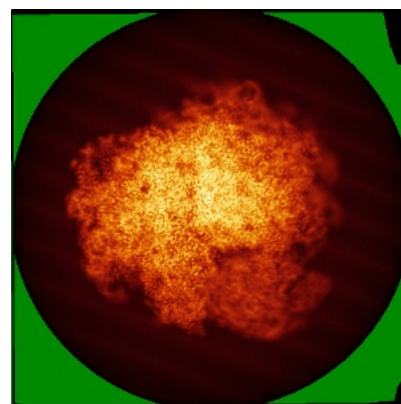
6.4.2 Raw map



X



Y

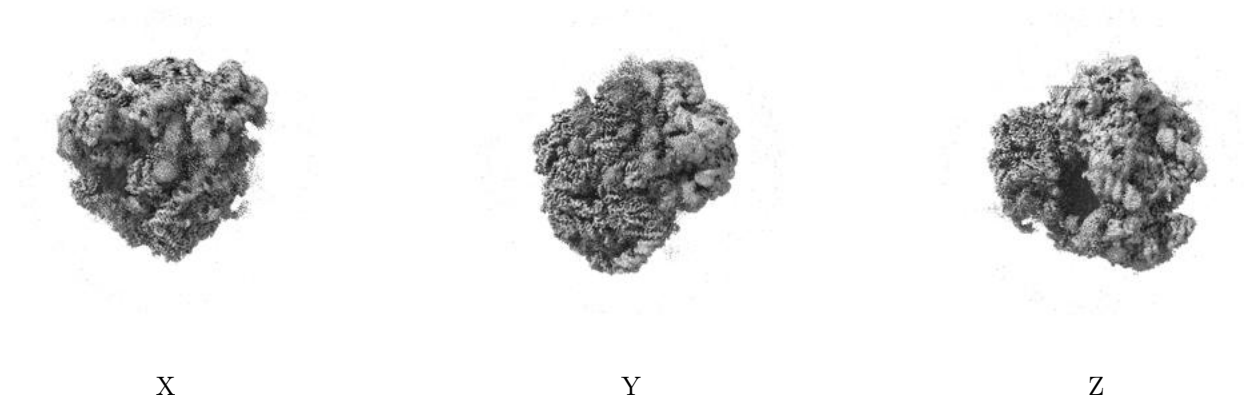


Z

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

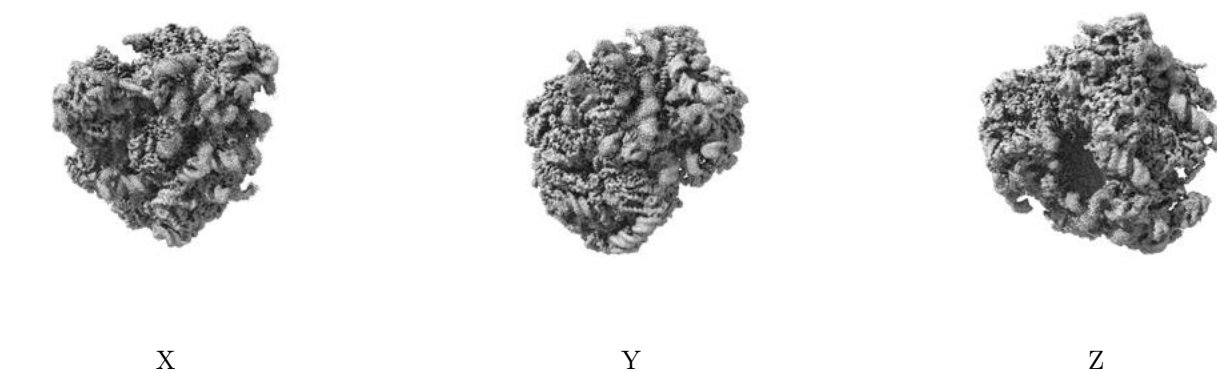
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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.

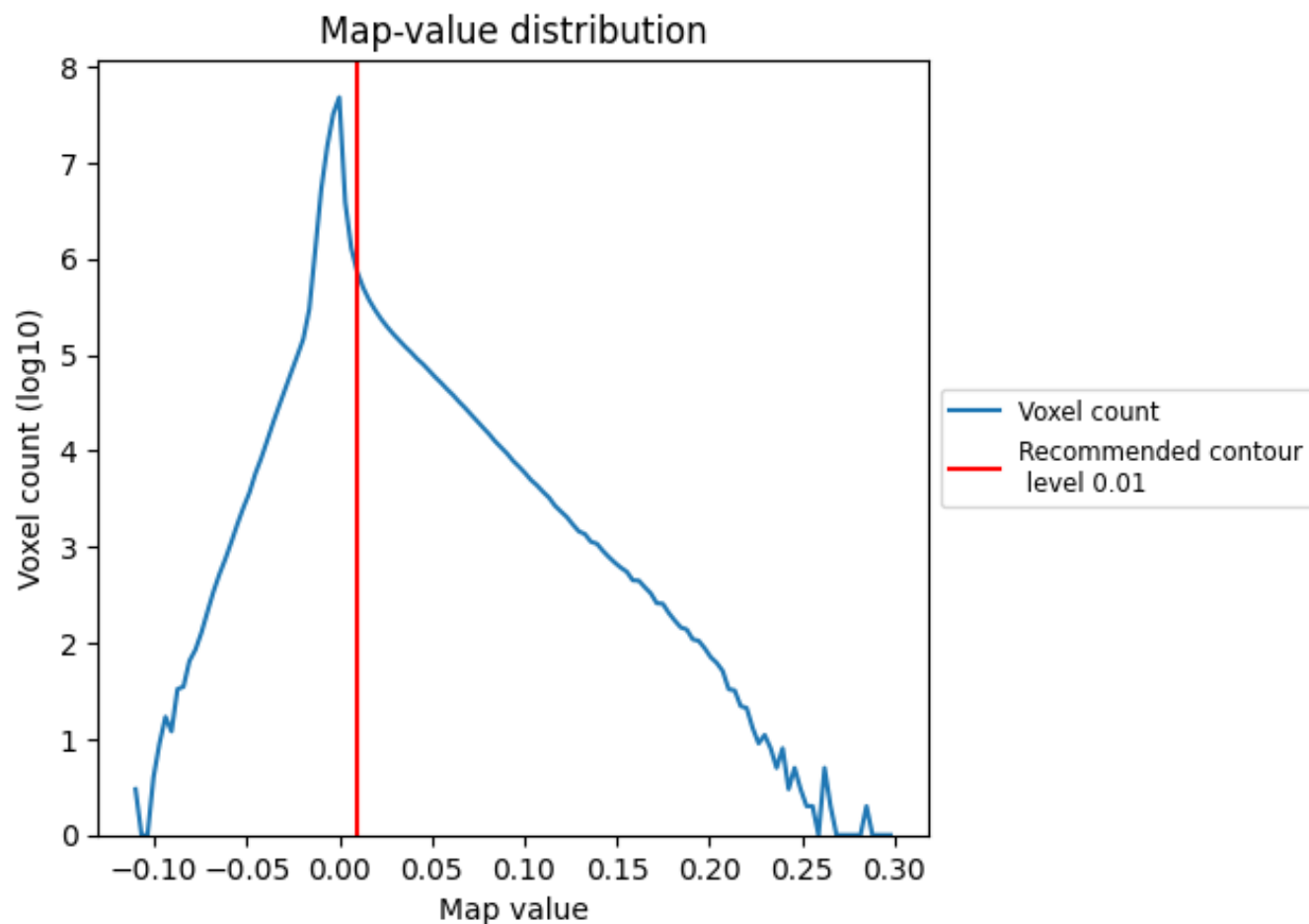
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

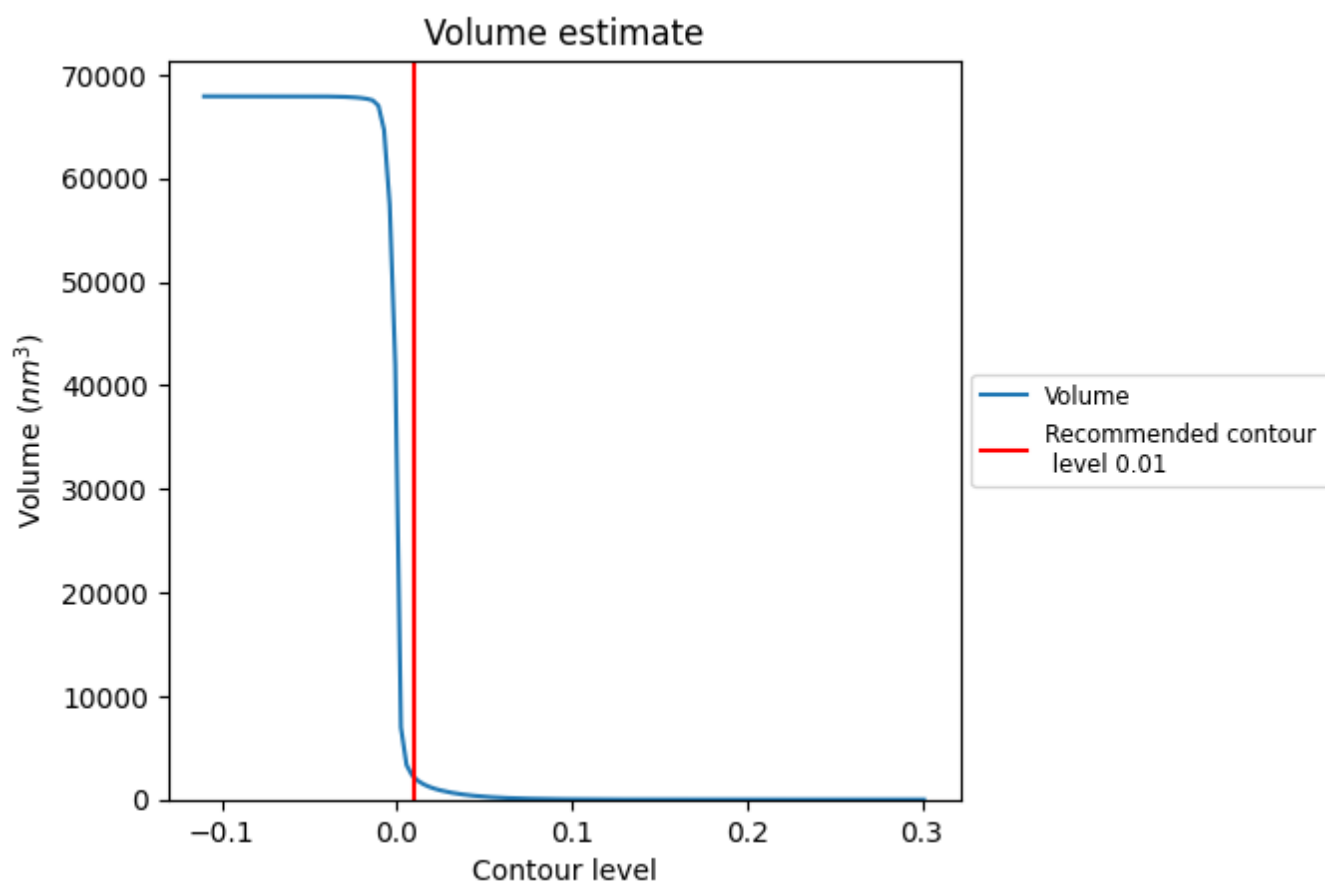
This section contains the results of statistical analysis of the map.

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.

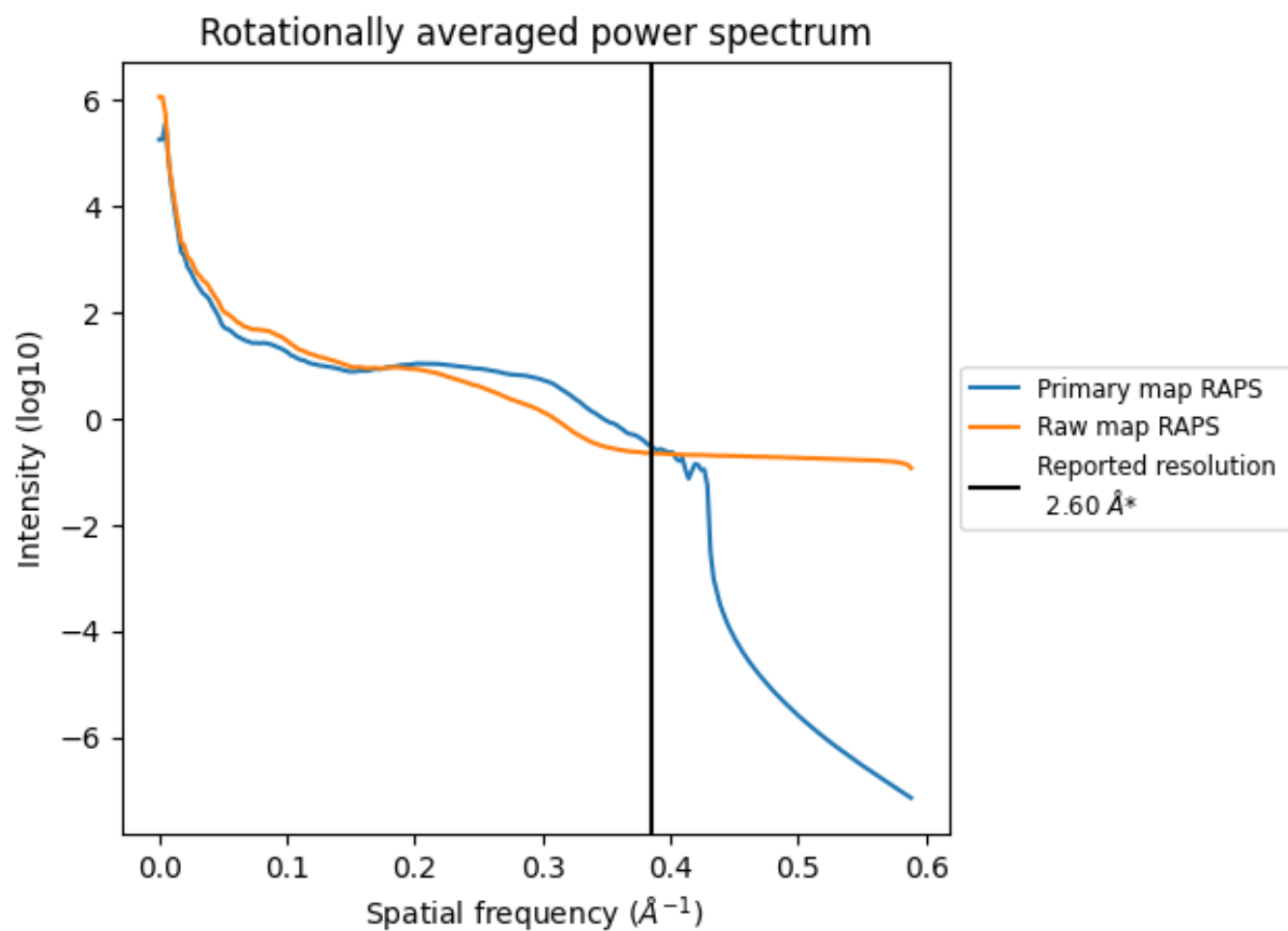
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2123 nm³; this corresponds to an approximate mass of 1918 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 ⓘ

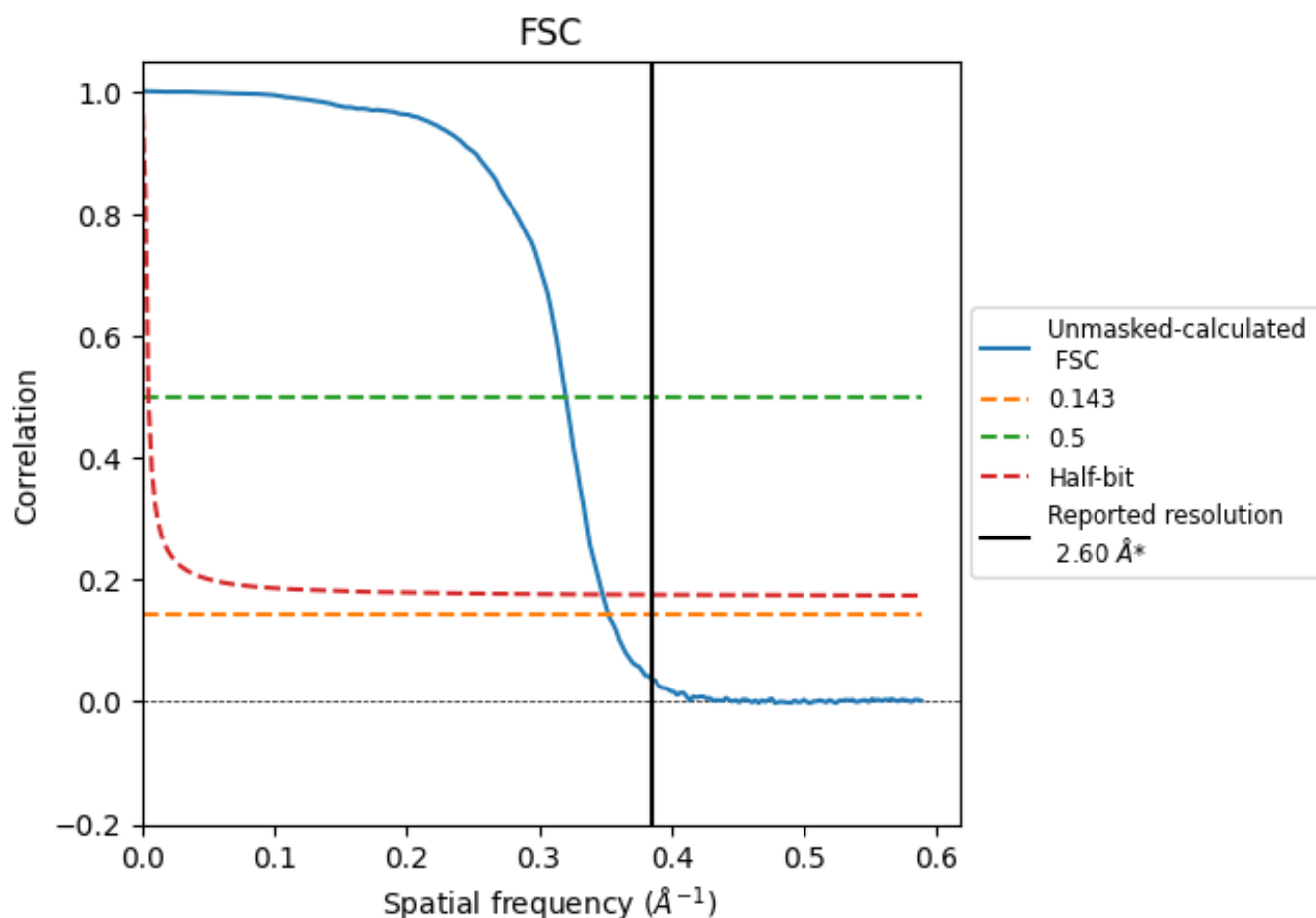


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

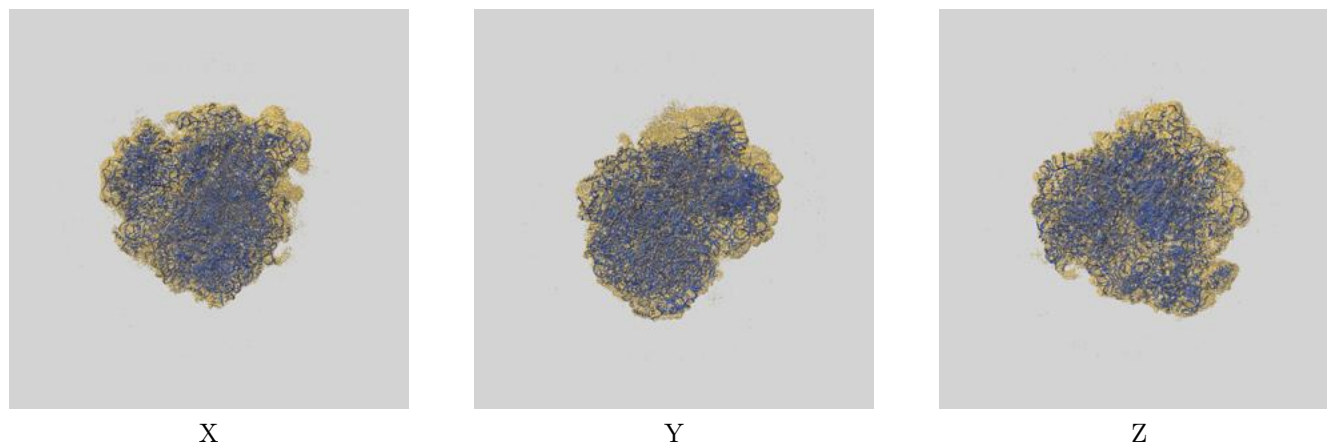
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.84	3.12	2.87

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

9 Map-model fit [i](#)

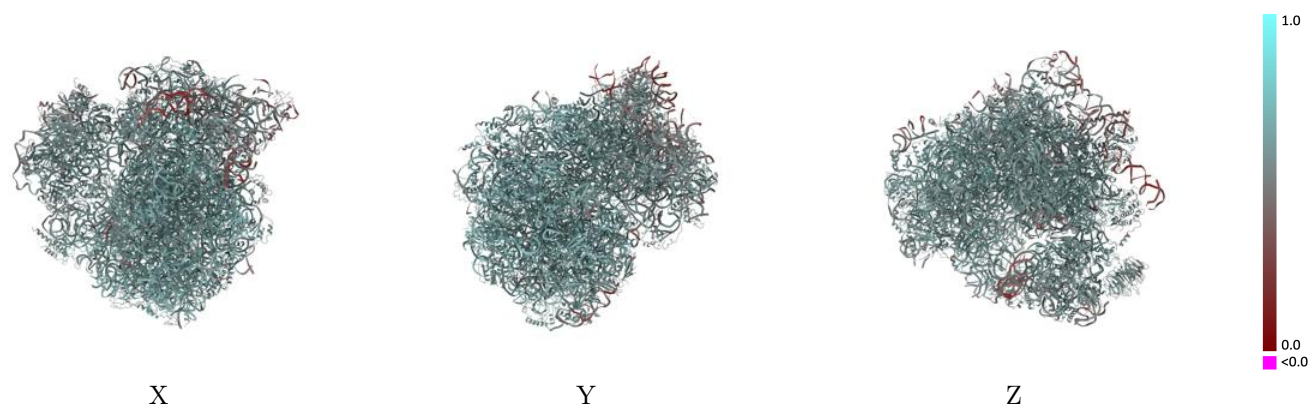
This section contains information regarding the fit between EMDB map EMD-17212 and PDB model 8OVE. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



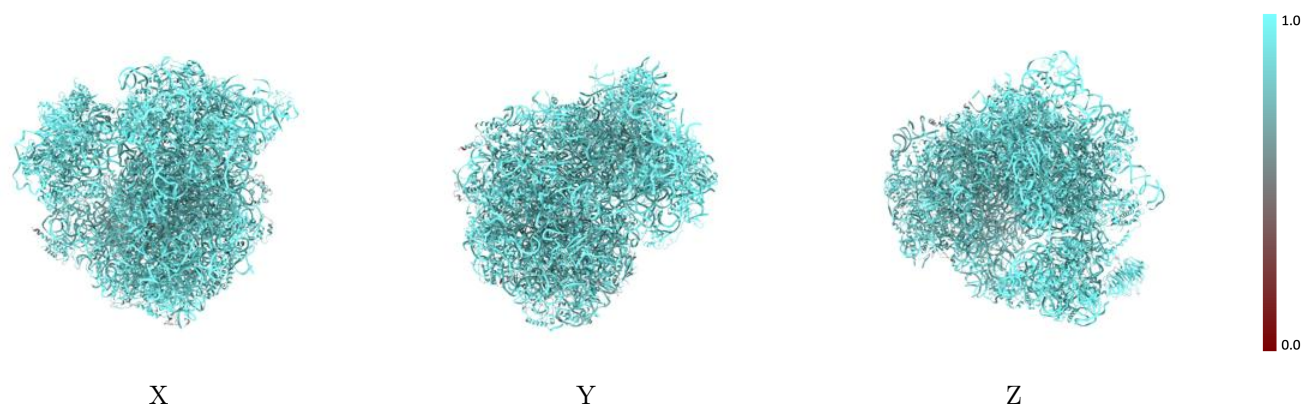
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



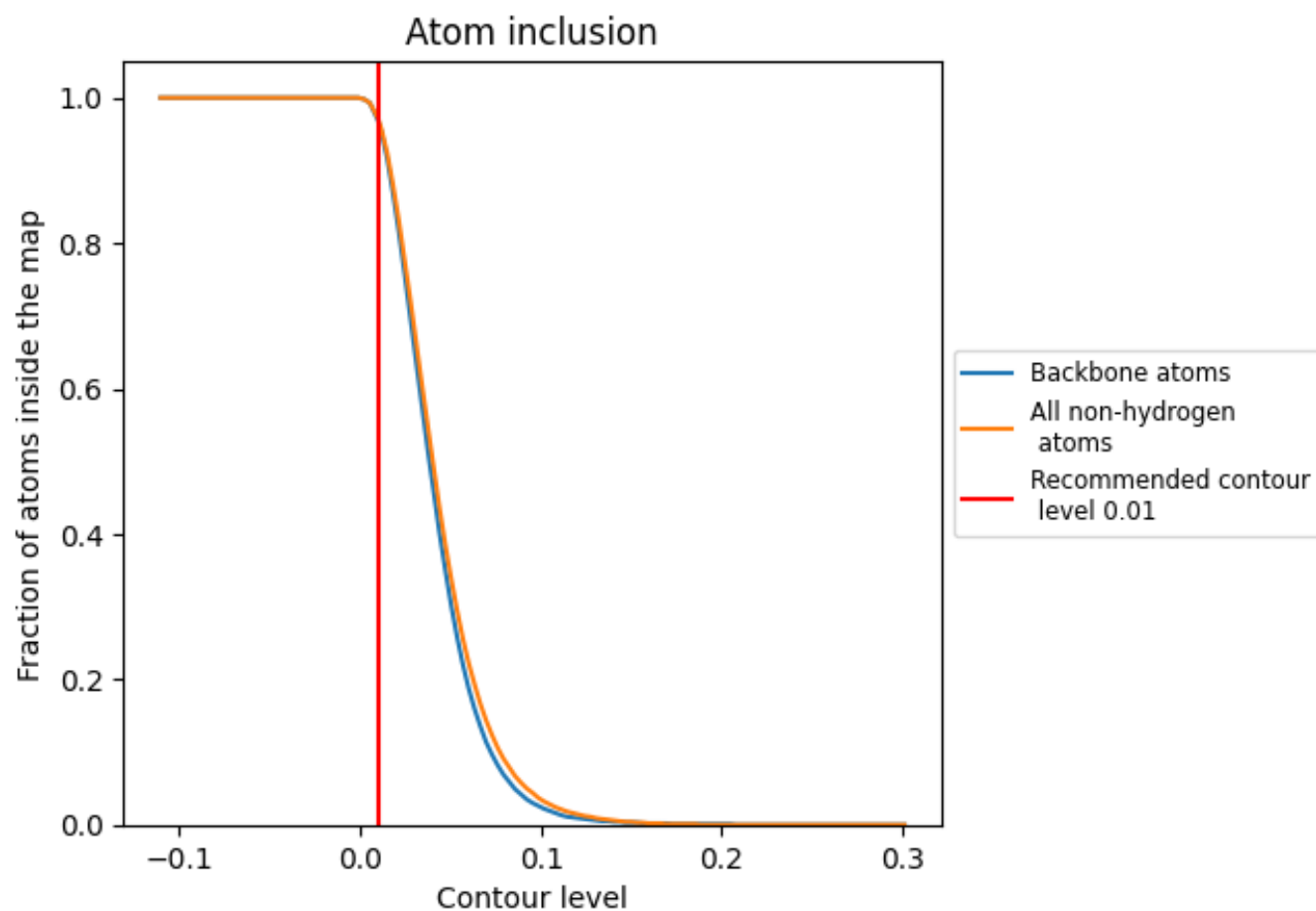
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9720	 0.6050
A	 1.0000	 0.5020
A0	 0.9920	 0.6190
A1	 0.9820	 0.5640
A2	 0.9910	 0.5810
A3	 0.9860	 0.5420
A4	 0.9920	 0.5480
A5	 0.9860	 0.5690
A6	 0.9900	 0.5690
A7	 0.9820	 0.5330
A8	 0.9840	 0.5950
AA	 0.9930	 0.5580
AB	 0.8490	 0.4950
AC	 0.9940	 0.5680
AD	 0.9860	 0.5360
AE	 0.9780	 0.5780
AG	 0.9940	 0.6070
AH	 0.9920	 0.6180
AI	 0.9860	 0.5650
AJ	 0.9890	 0.6010
AK	 0.9930	 0.5810
AL	 0.9950	 0.5400
AM	 0.9900	 0.5610
AO	 0.9940	 0.5780
AP	 0.9900	 0.5850
AQ	 0.9830	 0.5380
AR	 0.9940	 0.5720
AS	 0.9890	 0.6090
AT	 0.9930	 0.5620
AU	 0.9930	 0.5590
AV	 0.9920	 0.6290
AW	 0.9840	 0.5770
AX	 0.9780	 0.5610
AY	 0.9670	 0.5390
AZ	 0.9910	 0.5690



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Chain	Atom inclusion	Q-score
Az	 0.9910	 0.4630
BA	 0.9790	 0.6380
BB	 0.9790	 0.6300
BC	 0.9830	 0.6360
BD	 0.9760	 0.5910
BE	 0.9830	 0.6170
BF	 0.9210	 0.5810
BG	 0.9760	 0.6230
BH	 0.9650	 0.6020
BI	 0.9690	 0.6540
BK	 0.9380	 0.6150
BL	 0.8750	 0.5320
BN	 0.9110	 0.6300
BO	 0.9490	 0.6410
BP	 0.8710	 0.6040
BQ	 0.9930	 0.6710
BR	 0.9860	 0.6710
BS	 0.9440	 0.6320
BT	 0.9520	 0.6030
BU	 0.8920	 0.6150
BV	 0.8260	 0.5330
BW	 0.9800	 0.6550
BX	 0.9680	 0.6470
BY	 0.9840	 0.6460
BZ	 0.9520	 0.6330
Ba	 0.9390	 0.6160
Bb	 0.9540	 0.6570
Bc	 0.9270	 0.6280
Bd	 0.9760	 0.6480
Be	 0.9950	 0.6760
Bf	 0.9620	 0.6510
Bg	 0.9780	 0.6290
Bh	 0.9160	 0.6150
Bi	 0.9430	 0.6570
Bj	 0.9510	 0.6440
Bk	 0.9050	 0.6050
Bl	 0.9620	 0.6510
Bm	 0.9340	 0.6130
Bn	 0.9920	 0.6760
Bo	 0.9870	 0.6640
Bp	 0.8570	 0.5860
Bq	 0.9840	 0.6540

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Chain	Atom inclusion	Q-score
Br	 0.9490	 0.6430
Bs	 0.7090	 0.5470
Bt	 0.9540	 0.6300
Bu	 0.8950	 0.5960
Bv	 0.9150	 0.5940
Bw	 0.9590	 0.6450
Bx	 0.9300	 0.6220
By	 0.9010	 0.5830
Bz	 0.9740	 0.6400