



Full wwPDB EM Validation Report ⓘ

Oct 12, 2026 – 04:22 pm BST

PDB ID : 9SYG / pdb_00009syg
EMDB ID : EMD-55348
Title : CRYO-EM STRUCTURE OF TRYPANOSOMA BRUCEI BLOODSTREAM
FORM 80S RIBOSOME : NATIVE VACANT
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2025-10-12
Resolution : 2.68 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

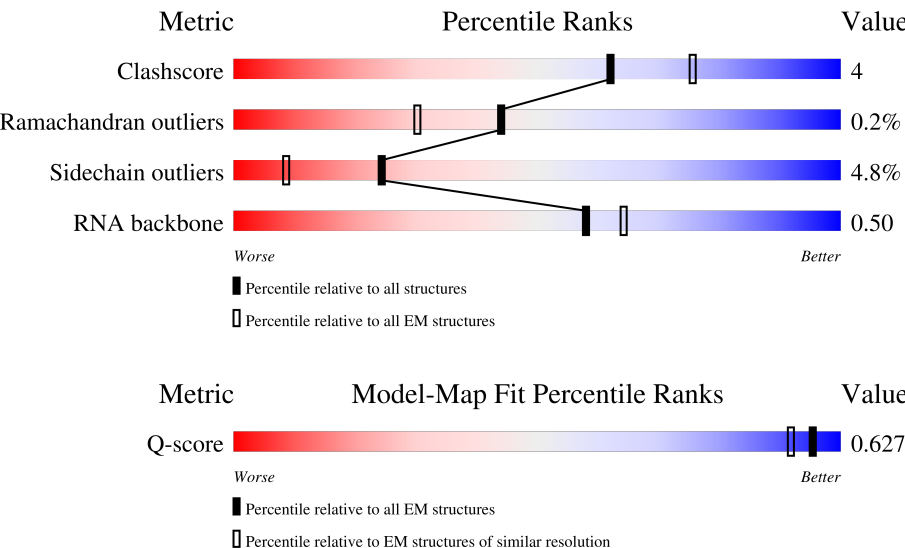
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.68 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	9255 (2.18 - 3.18)

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	A0	256	71% 14% • 13%
2	A1	273	85% 11% •
3	A2	190	88% 8% •

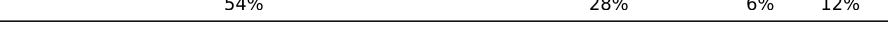
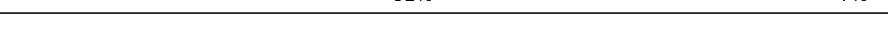
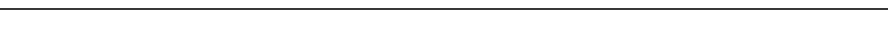
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Mol	Chain	Length	Quality of chain
4	A3	250	
5	A4	202	
6	A5	220	
7	A6	190	
8	A7	318	
9	A8	57	
10	AA	2280	
11	AB	76	
12	AC	277	
13	AD	172	
14	AE	174	
15	AG	151	
16	AH	144	
17	AI	152	
18	AJ	130	
19	AK	149	
20	AL	142	
21	AM	153	
22	AO	167	
23	AP	266	
24	AQ	117	
25	AR	194	
26	AS	143	
27	AT	137	
28	AU	113	

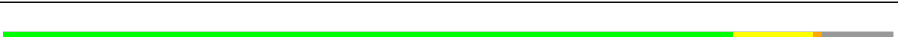
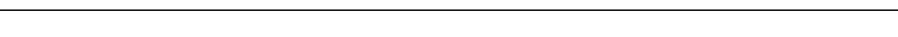
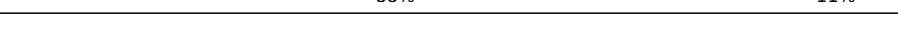
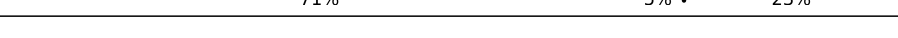
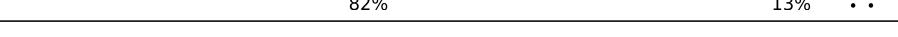
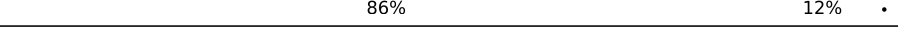
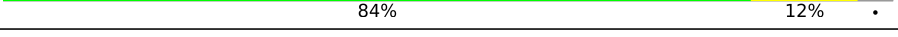
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Mol	Chain	Length	Quality of chain
29	AV	111	 77% 15% 6%
30	AW	86	 77% 21% ..
31	AX	214	 75% 20% ..
32	AY	66	 79% 11% 11%
33	AZ	103	 50% 7% 43%
34	Az	279	 17% 12% 70%
35	BA	1866	 61% 21% 14%
36	BB	1544	 49% 20% 27%
37	BC	209	 52% 22% 23%
38	BD	120	 82% 15% ..
39	BE	216	 54% 20% 6% 19%
40	BF	78	 53% 27% 9% 12%
41	BG	183	 74% 20% 7%
42	BH	136	 54% 28% 6% 12%
43	BI	193	 91% 8% ..
44	BK	213	 79% 16% ..
45	BL	194	 72% 19% 8%
46	BN	218	 87% 11% .
47	BO	222	 92% 7%
48	BP	189	 79% 13% 6%
49	BQ	221	 84% 8% 8%
50	BR	166	 86% 5% 8%
51	BS	179	 85% 13% ..
52	BT	260	 65% 10% 24%
53	BU	159	 82% 15% ..

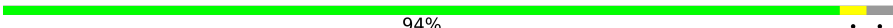
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Mol	Chain	Length	Quality of chain
54	BV	130	
55	BW	139	
56	BX	164	
57	BY	125	
58	BZ	143	
59	Ba	133	
60	Bb	145	
61	Bc	146	
62	Bd	71	
63	Be	260	
64	Bf	429	
65	Bg	105	
66	Bh	188	
67	Bi	132	
68	Bj	170	
69	Bk	127	
70	Bl	149	
71	Bm	109	
72	Bn	84	
73	Bo	93	
74	Bp	82	
75	Bq	51	
76	Br	374	
77	Bs	128	
78	Bt	106	

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Mol	Chain	Length	Quality of chain
79	Bu	308	 83% 15% .
80	Bv	192	 59% 17% 24%
81	Bw	257	 78% 11% 11%
82	Bx	276	 76% 8% . 15%
83	By	189	 71% 26% ..
84	Bz	34	 94% . .

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 207369 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	222	Total	C	N	O	S	0	0
			1801	1136	339	318	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	262	Total	C	N	O	S	0	0
			2062	1306	388	359	9		

- Molecule 3 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	183	Total	C	N	O	S	0	0
			1463	915	282	261	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A3	238	Total	C	N	O	S	0	0
			1885	1170	388	323	4		

- Molecule 5 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A4	198	Total	C	N	O	S	0	0
			1606	1026	309	266	5		

- Molecule 6 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A5	190	Total	C	N	O	S	0	0
			1521	959	303	257	2		

- Molecule 7 is a protein called Probable 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A6	179	Total	C	N	O	S	0	0
			1477	929	297	243	8		

- Molecule 8 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A7	305	Total	C	N	O	S	0	0
			2315	1450	412	442	11		

- Molecule 9 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A8	57	Total	C	N	O	S	0	0
			461	284	96	76	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A8	5	HIS	ASP	conflict	UNP G0UD55
A8	19	SER	ALA	conflict	UNP G0UD55
A8	50	ASN	HIS	conflict	UNP G0UD55

- Molecule 10 is a RNA chain called SSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AA	1829	Total	C	N	O	P	0	0
			39092	17480	7034	12749	1829		

- Molecule 11 is a RNA chain called E-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AB	10	Total	C	N	O	P	0	0
			210	95	40	66	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AC	208	Total	C	N	O	S	0	0
			1647	1049	297	291	10		

- Molecule 13 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AD	99	Total	C	N	O	S	0	0
			814	531	140	139	4		

- Molecule 14 is a protein called 40S ribosomal proteins S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AE	153	Total	C	N	O	S	0	0
			1251	783	253	210	5		

- Molecule 15 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AG	150	Total	C	N	O	S	0	0
			1198	753	234	203	8		

- Molecule 16 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AH	136	Total	C	N	O	S	0	0
			1011	622	195	186	8		

- Molecule 17 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AI	121	Total	C	N	O	S	0	0
			975	619	190	163	3		

- Molecule 18 is a protein called 40S ribosomal protein S15a, putative.

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

- Molecule 19 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AK	143	Total	C	N	O	S	0	0
			1143	731	214	195	3		

- Molecule 20 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AL	122	Total	C	N	O	S	0	0
			969	613	192	159	5		

- Molecule 21 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AM	135	Total	C	N	O	S	0	0
			1098	689	215	190	4		

- Molecule 22 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AO	154	Total	C	N	O	S	0	0
			1220	770	242	199	9		

- Molecule 23 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AP	218	Total	C	N	O	S	0	0
			1688	1078	298	303	9		

- Molecule 24 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 25 is a protein called 40S ribosomal protein S21, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AR	89	Total	C	N	O	S	0	0
			666	415	119	129	3		

- Molecule 26 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AS	139	Total	C	N	O	S	0	0
			1089	692	212	183	2		

- Molecule 27 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AT	130	Total	C	N	O	S	0	0
			1043	665	204	171	3		

- Molecule 28 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AU	74	Total	C	N	O	S	0	0
			582	369	106	102	5		

- Molecule 29 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AV	104	Total	C	N	O	S	0	0
			835	515	176	136	8		

- Molecule 30 is a protein called 40S ribosomal protein S27, putative.

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

- Molecule 31 is a protein called 40S ribosomal protein S3, putative.

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

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AY	59	Total	C	N	O	S	0	0
			474	298	98	77	1		

- Molecule 33 is a protein called 40S ribosomal protein S33, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AZ	59	Total	C	N	O	S	0	0
			454	274	95	81	4		

- Molecule 34 is a protein called RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Az	84	Total	C	N	O	S	0	0
			673	427	124	121	1		

- Molecule 35 is a RNA chain called LSUa rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	1614	Total	C	N	O	P	1	0
			34591	15454	6264	11258	1615		

- Molecule 36 is a RNA chain called LSUb rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	1126	Total	C	N	O	P	0	0
			24057	10763	4299	7869	1126		

- Molecule 37 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	160	Total	C	N	O	P	0	0
			3412	1530	610	1113	159		

- Molecule 38 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BD	120	Total	C	N	O	P	0	0
			2553	1140	452	842	119		

- Molecule 39 is a RNA chain called SrRNA-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	174	Total	C	N	O	P	0	0
			3691	1649	644	1224	174		

- Molecule 40 is a RNA chain called SrRNA-6.

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

- Molecule 41 is a RNA chain called SrRNA-2.

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

- Molecule 42 is a RNA chain called SrRNA-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	119	Total	C	N	O	P	0	0
			2540	1132	453	836	119		

- Molecule 43 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BI	192	Total	C	N	O	S	0	0
			1526	956	315	247	8		

- Molecule 44 is a protein called 60S ribosomal protein L10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BK	204	Total	C	N	O	S	0	0
			1668	1055	327	273	13		

- Molecule 45 is a protein called 60S ribosomal protein L11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BL	178	Total	C	N	O	S	0	0
			1408	889	263	249	7		

- Molecule 46 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BN	215	Total	C	N	O	S	0	0
			1762	1097	365	294	6		

- Molecule 47 is a protein called 60S ribosomal protein L13a, putative.

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

- Molecule 48 is a protein called 40S ribosomal protein L14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BP	177	Total	C	N	O	S	0	0
			1414	892	278	240	4		

- Molecule 49 is a protein called Ribosomal protein L15.

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

- Molecule 50 is a protein called 60S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BR	152	Total	C	N	O	S	0	0
			1228	772	244	204	8		

- Molecule 51 is a protein called 60S ribosomal protein L18a.

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

- Molecule 52 is a protein called 60S ribosomal protein L19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BT	197	Total	C	N	O	S	0	0
			1597	979	350	260	8		

- Molecule 53 is a protein called 60S ribosomal protein L21E, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BU	158	Total	C	N	O	S	0	0
			1253	799	243	205	6		

- Molecule 54 is a protein called 60S ribosomal protein L22, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BV	122	Total	C	N	O	S	0	0
			979	629	179	168	3		

- Molecule 55 is a protein called 60S ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BW	130	Total	C	N	O	S	0	0
			983	623	186	169	5		

- Molecule 56 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BX	118	Total	C	N	O	S	0	0
			966	614	182	168	2		

- Molecule 57 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BY	64	Total	C	N	O	S	0	0
			547	356	108	79	4		

- Molecule 58 is a protein called 60S ribosomal protein L26, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BZ	122	Total	C	N	O	S	0	0
			993	614	210	164	5		

- Molecule 59 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ba	133	Total	C	N	O	S	0	0
			1090	691	220	176	3		

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

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

- Molecule 61 is a protein called 60S ribosomal protein L28, putative.

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

- Molecule 62 is a protein called 60S ribosomal protein L29.

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

- Molecule 63 is a protein called 60S ribosomal protein L2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Be	257	Total	C	N	O	S	1	0
			1962	1223	401	325	13		

- Molecule 64 is a protein called Ribosomal protein L3, mitochondrial, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bf	396	Total	C	N	O	S	0	0
			3174	2001	626	534	13		

- Molecule 65 is a protein called 60S ribosomal protein L30.

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

- Molecule 66 is a protein called 60S ribosomal subunit protein L31, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bh	148	Total	C	N	O	S	0	0
			1160	735	231	190	4		

- Molecule 67 is a protein called 60S ribosomal protein L32, putative.

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

- Molecule 68 is a protein called 60S ribosomal protein L34, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bj	131	Total	C	N	O	S	0	0
			1035	638	229	164	4		

- Molecule 69 is a protein called 60S ribosomal protein L35, putative.

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

- Molecule 70 is a protein called 60S ribosomal protein L35A, putative.

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

- Molecule 71 is a protein called Ribosomal protein L36, putative.

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

- Molecule 72 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bn	82	Total	C	N	O	S	0	0
			693	422	160	105	6		

- Molecule 73 is a protein called 60S ribosomal protein L37a, putative.

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

- Molecule 74 is a protein called 60S ribosomal protein L38, putative.

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

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

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

- Molecule 76 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Br	367	Total	C	N	O	S	0	0
			2882	1802	575	488	17		

- Molecule 77 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bs	50	Total	C	N	O	S	0	0
			400	250	83	60	7		

- Molecule 78 is a protein called 60S ribosomal protein L44.

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

- Molecule 79 is a protein called 60S ribosomal protein L5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bu	303	Total	C	N	O	S	0	0
			2388	1503	458	421	6		

- Molecule 80 is a protein called 60S ribosomal protein L6, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bv	146	Total	C	N	O	S	0	0
			1121	712	206	200	3		

- Molecule 81 is a protein called 60S ribosomal protein L7, putative.

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

- Molecule 82 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Bx	235	Total	C	N	O	S	0	0
			1874	1178	369	321	6		

- Molecule 83 is a protein called 60S ribosomal protein L9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	By	186	Total	C	N	O	S	0	0
			1515	961	281	269	4		

- Molecule 84 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bz	33	Total	C	N	O	S	0	0
			289	175	75	37	2		

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	A0	1	Total	Mg	0
			1	1	
85	A3	1	Total	Mg	0
			1	1	
85	AA	50	Total	Mg	0
			50	50	
85	BA	69	Total	Mg	0
			69	69	
85	BB	61	Total	Mg	0
			61	61	
85	BC	4	Total	Mg	0
			4	4	
85	BD	3	Total	Mg	0
			3	3	
85	BE	3	Total	Mg	0
			3	3	
85	BF	1	Total	Mg	0
			1	1	
85	BG	1	Total	Mg	0
			1	1	
85	BH	1	Total	Mg	0
			1	1	
85	BW	1	Total	Mg	0
			1	1	
85	Bn	1	Total	Mg	0
			1	1	

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	A8	1	Total 1	Zn 1	0
86	AV	1	Total 1	Zn 1	0
86	Bn	1	Total 1	Zn 1	0
86	Bo	1	Total 1	Zn 1	0
86	Bs	1	Total 1	Zn 1	0
86	Bt	1	Total 1	Zn 1	0

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

Mol	Chain	Residues	Atoms		AltConf
87	AA	25	Total 25	K 25	0
87	BA	22	Total 22	K 22	0
87	BB	22	Total 22	K 22	0
87	BC	1	Total 1	K 1	0
87	BE	1	Total 1	K 1	0
87	BG	6	Total 6	K 6	0
87	BH	1	Total 1	K 1	0
87	Be	1	Total 1	K 1	0
87	Bn	1	Total 1	K 1	0

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

Mol	Chain	Residues	Atoms		AltConf
88	AA	5	Total 5	Na 5	0
88	BA	8	Total 8	Na 8	0
88	BB	9	Total 9	Na 9	0

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Mol	Chain	Residues	Atoms		AltConf
88	BR	1	Total 1	Na 1	0
88	BU	1	Total 1	Na 1	0

- Molecule 89 is water.

Mol	Chain	Residues	Atoms		AltConf
89	A1	1	Total 1	O 1	0
89	A2	1	Total 1	O 1	0
89	A5	6	Total 6	O 6	0
89	AA	264	Total 264	O 264	0
89	AC	1	Total 1	O 1	0
89	AE	5	Total 5	O 5	0
89	AG	10	Total 10	O 10	0
89	AH	3	Total 3	O 3	0
89	AO	1	Total 1	O 1	0
89	AP	2	Total 2	O 2	0
89	AV	7	Total 7	O 7	0
89	AX	1	Total 1	O 1	0
89	BA	239	Total 239	O 239	0
89	BB	353	Total 353	O 353	0
89	BC	8	Total 8	O 8	0
89	BE	13	Total 13	O 13	0
89	BG	40	Total 40	O 40	0

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Mol	Chain	Residues	Atoms		AltConf
89	BH	9	Total 9	O 9	0
89	BI	2	Total 2	O 2	0
89	BK	2	Total 2	O 2	0
89	BQ	4	Total 4	O 4	0
89	BR	6	Total 6	O 6	0
89	BT	4	Total 4	O 4	0
89	BU	1	Total 1	O 1	0
89	BV	3	Total 3	O 3	0
89	BW	11	Total 11	O 11	0
89	BY	2	Total 2	O 2	0
89	Bb	3	Total 3	O 3	0
89	Be	6	Total 6	O 6	0
89	Bf	25	Total 25	O 25	0
89	Bi	3	Total 3	O 3	0
89	Bj	1	Total 1	O 1	0
89	Bl	2	Total 2	O 2	0
89	Bn	9	Total 9	O 9	0
89	Bo	6	Total 6	O 6	0
89	Br	4	Total 4	O 4	0
89	Bt	1	Total 1	O 1	0
89	Bx	1	Total 1	O 1	0

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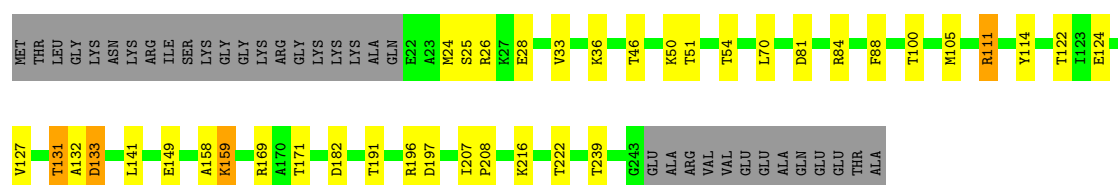
Mol	Chain	Residues	Atoms		AltConf
89	Bz	5	Total	O	0
			5	5	

3 Residue-property plots

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

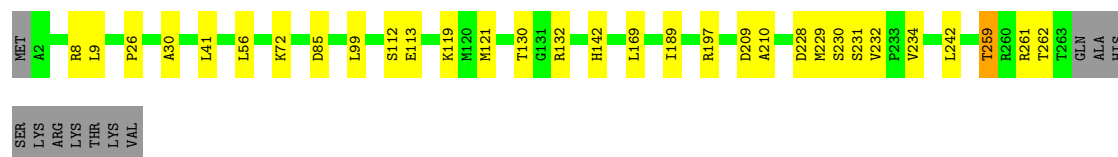
• Molecule 1: 40S ribosomal protein S3a

Chain A0: 



• Molecule 2: 40S ribosomal protein S4

Chain A1: 



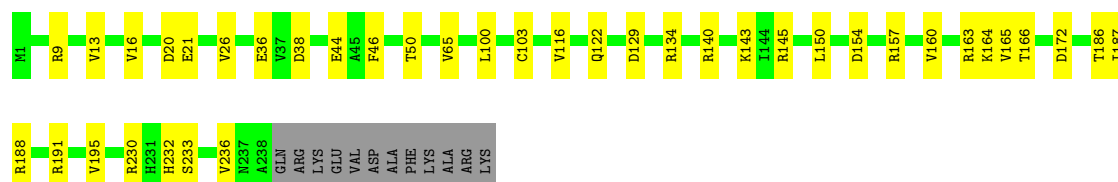
• Molecule 3: 40S ribosomal protein S5, putative

Chain A2: 

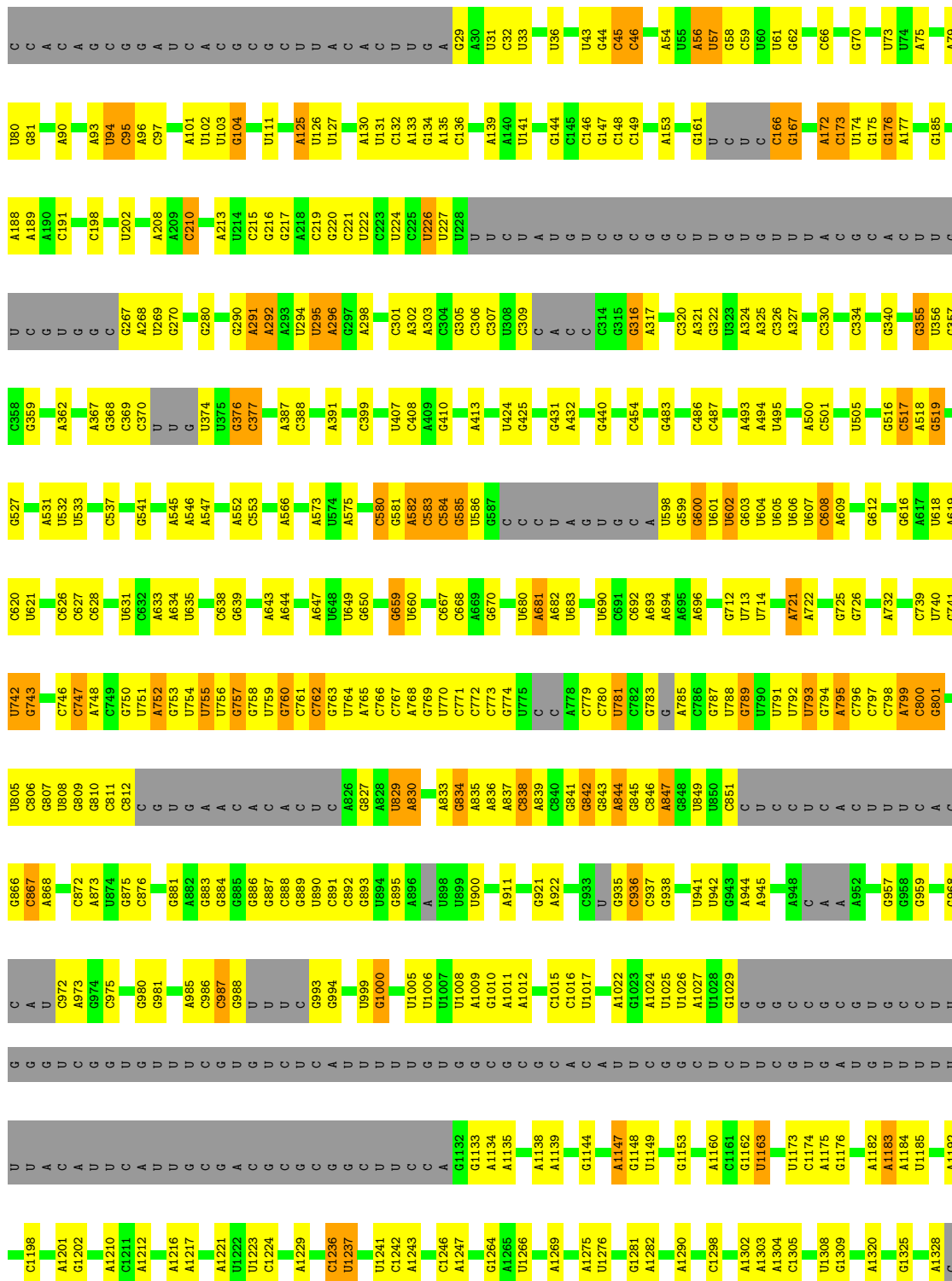


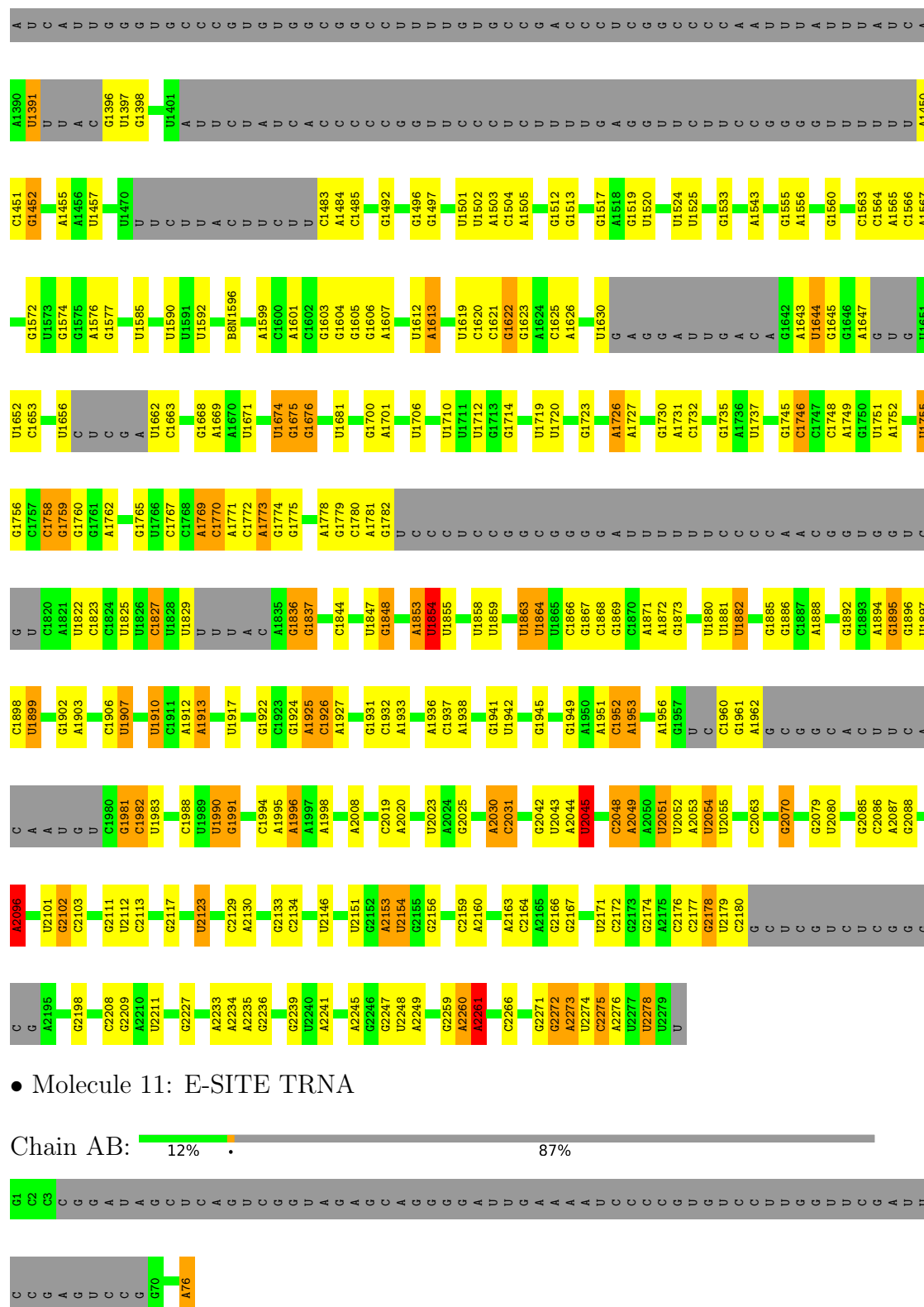
• Molecule 4: 40S ribosomal protein S6

Chain A3: 





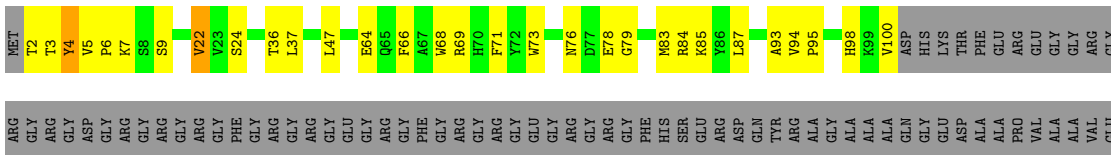




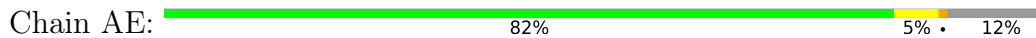
• Molecule 11: E-SITE TRNA

• Molecule 12: 40S ribosomal protein SA

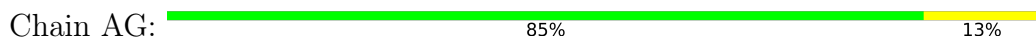
- Molecule 13: 40S ribosomal protein S10, putative



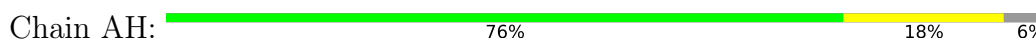
- Molecule 14: 40S ribosomal proteins S11, putative



- Molecule 15: 40S ribosomal protein S13, putative



- Molecule 16: 40S ribosomal protein S14



- Molecule 17: 40S ribosomal protein S15, putative



- Molecule 18: 40S ribosomal protein S15a, putative

ME1	T2	R23	L26	S30	S31	G59	K60	I61	V62	L104	T105	T106	S107	E114	R117	A118	R119	N120	Y130
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------

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|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|
| ME7 | SE7 | GLY | GLU | LYS | THR | H7 | V12 | C33 | R36 | G39 | I42 | I45 | L46 | P47 | E48 | E56 | L69 | G76 | G77 | S78 | V87 | R88 | I91 | K101 | I102 | H103 | N104 | E107 | D119 | S147 | I148 | R149 |
|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ALA | ARG | ARG | GLY | PRO | ALA | ARG | LYS | MET | G2 | T8 | K19 | K23 | L24 | N25 | K26 | K36 | M58 | R63 | R67 | K72 | L73 | E77 | R80 | R81 | M82 | V85 | P86 | E87 | V88 | R100 | V101 | D102 | K103 | Q104 | T105 | L106 | A107 | K110 | R111 | M112 | L121 | P122 | N123 | VAL | VAL | ALA | ALA | PRO | ASN | VAL | SER | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|

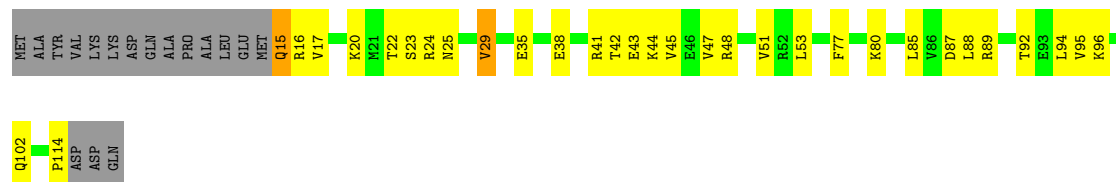
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|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLY | VAL | SER | ARG | THR | LYS | MET | L3 | R15 | T19 | G23 | K33 | T34 | K35 | N44 | A57 | L60 | K67 | L85 | Q88 | R89 | K92 | T93 | T96 | M103 | V104 | D105 | T106 | R107 | D111 | R114 | K117 | R125 | L130 | H136 | T137 | CYS | THR | SER | GLY | ARG | ARG | GLY | LYS | THR |
|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|
| MET | ALA | VAL | ALA | ARG | THR | LYS | ASP | T22 | H27 | R30 | H38 | E42 | G43 | K44 | C50 | A51 | E52 | F53 | K54 | R55 | T56 | S57 | A112 | L127 | C133 | A136 | K142 | D149 | M160 | G161 | ALA | GLU | THR | LYS | ALA | VAL |
|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|

- | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| | G117 | N118 | E130 | V131 | I135 | M139 | L144 | V147 | R151 | R184 | V193 | P194 | V203 | E204 | D205 | C211 | R217 | R229 | T230 | T231 | Y232 | A241 | V245 | S246 | R247 | D248 | E252 | M259 | GLY | ARG | LYS | MET | VAL | ALA | ALA | | | | |
| MET | ALA | ASP | ALA | PRO | ARG | GLY | THR | GLY | GLY | GLU | GLN | ARG | GLY | PHE | GLY | ARG | GLY | ARG | GLY | GLY | GLY | ARG | GLY | GLY | GLY | ASP | GLU | LYS | E242 | T47 | K48 | L49 | I68 | E62 | L66 | I81 | L86 | L92 | F40 |

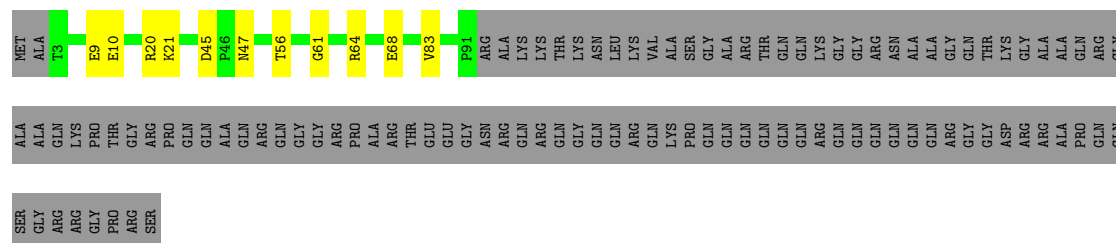
- 

Chain AQ:  58% 26% 15%



- Molecule 25: 40S ribosomal protein S21, putative

Chain AR:  40% 6% 54%



- Molecule 26: 40S ribosomal protein S23, putative

Chain AS:  83% 13% 2%



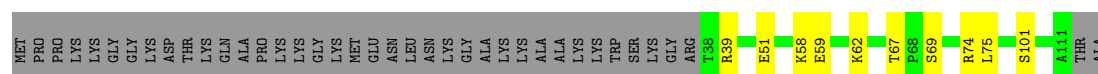
- Molecule 27: 40S ribosomal protein S24

Chain AT:  82% 11% 5%



- Molecule 28: 40S ribosomal protein S25

Chain AU:  57% 9% 35%



- Molecule 29: 40S ribosomal protein S26

Chain AV:  77% 15% 6%



- Molecule 30: 40S ribosomal protein S27, putative

- Molecule 31: 40S ribosomal protein S3, putative

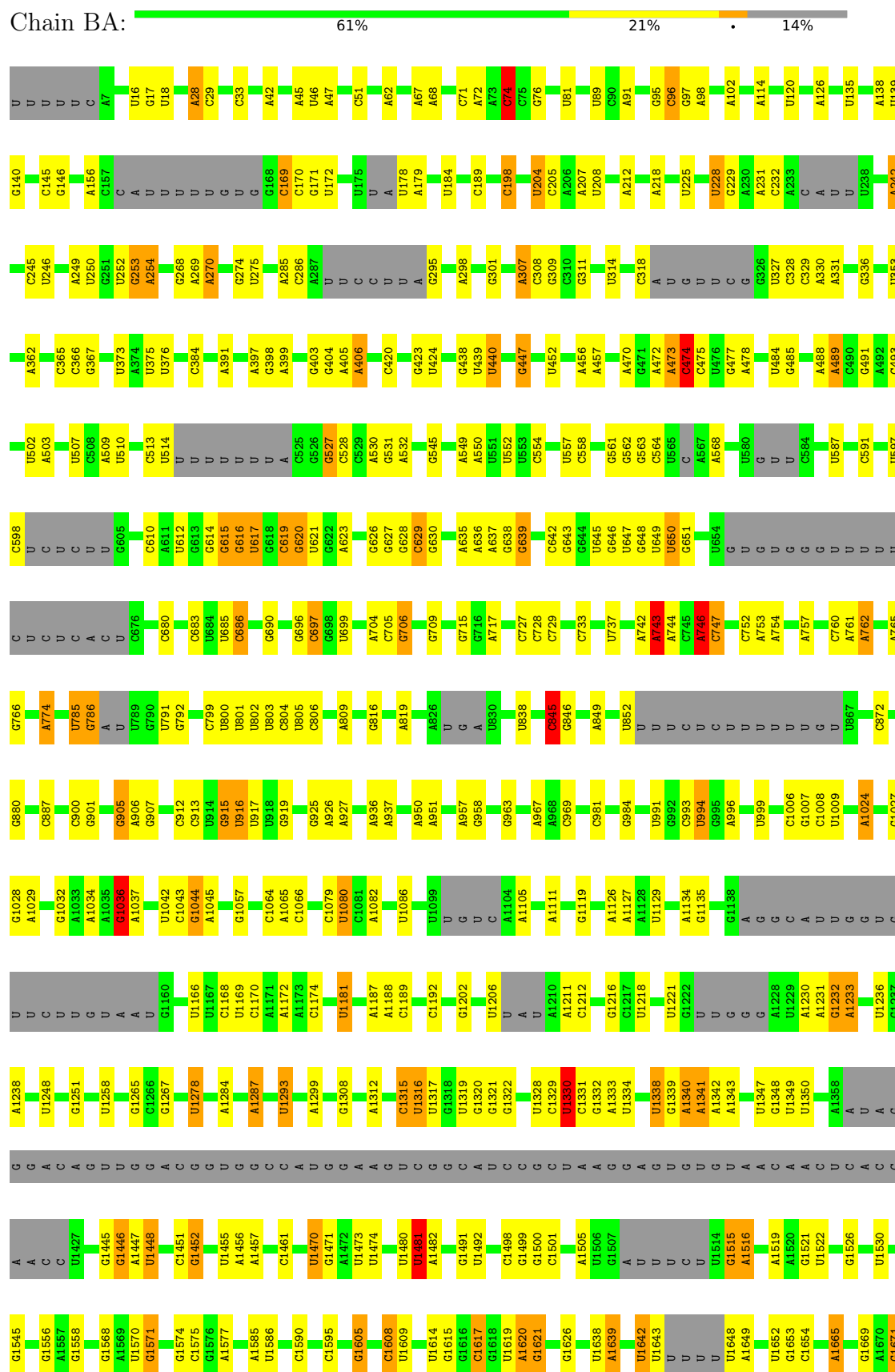
- Molecule 32: 40S ribosomal protein S30

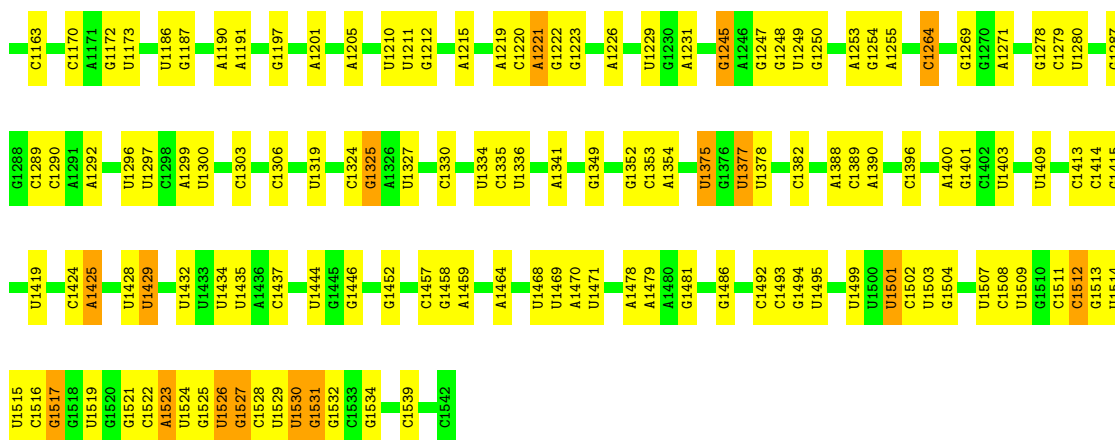
- Molecule 33: 40S ribosomal protein S33, putative

- Molecule 34: RNA-binding protein



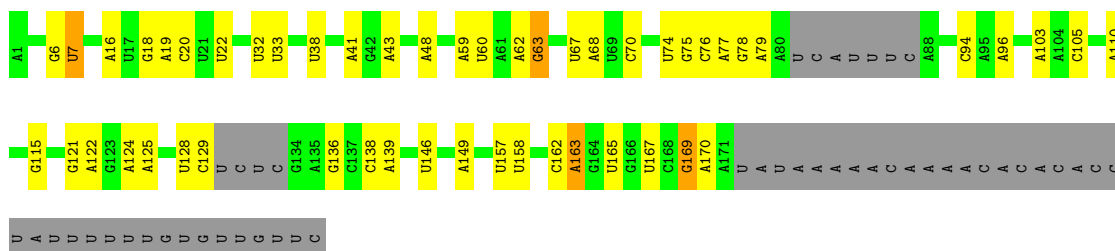
● Molecule 35: LSUa rRNA





• Molecule 37: 5.8S rRNA

Chain BC: 52% 22% 23%



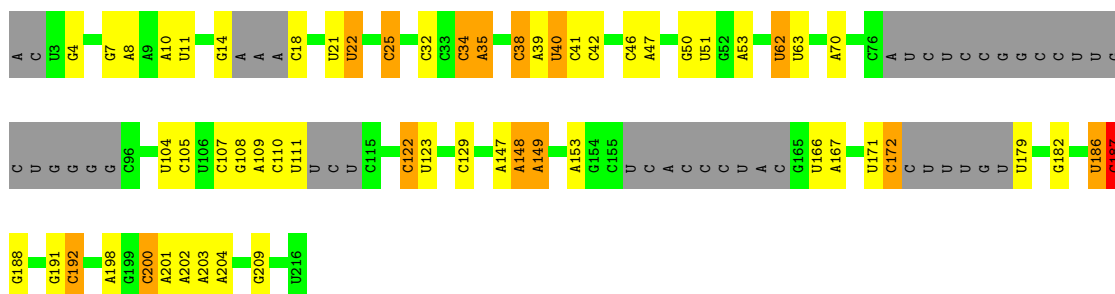
• Molecule 38: 5S rRNA

Chain BD: 82% 15%



• Molecule 39: SrRNA-1

Chain BE: 54% 20% 6% 19%



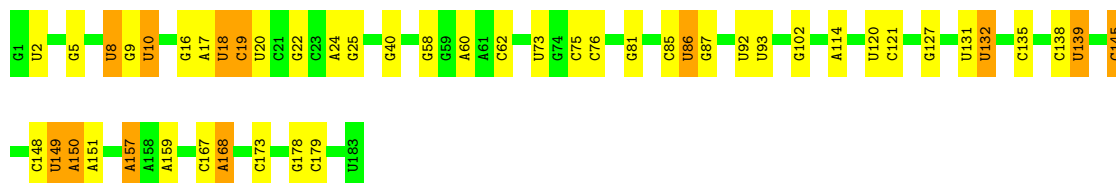
• Molecule 40: SrRNA-6

Chain BF: 53% 27% 9% 12%



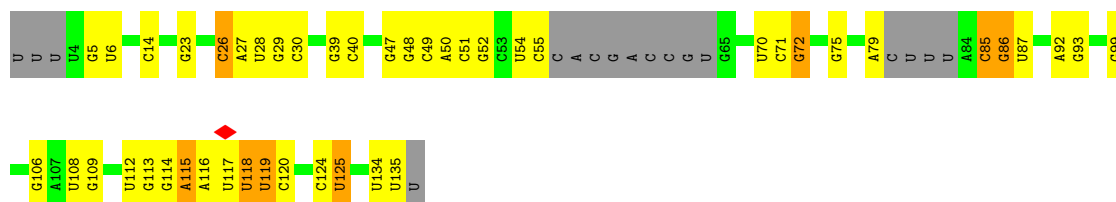
- Molecule 41: SrRNA-2

Chain BG: 74% 20% 7%



- Molecule 42: SrRNA-4

Chain BH: 54% 28% 6% 12%



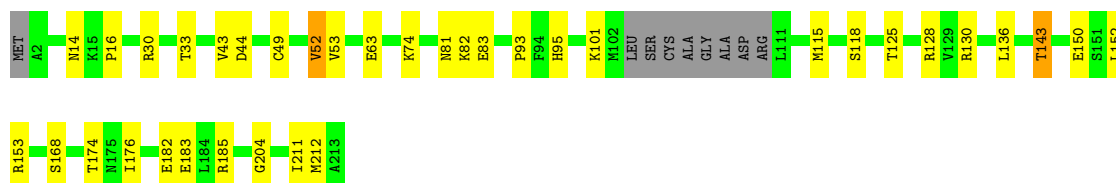
- Molecule 43: 60S ribosomal protein L18

Chain BI: 91% 8% ..



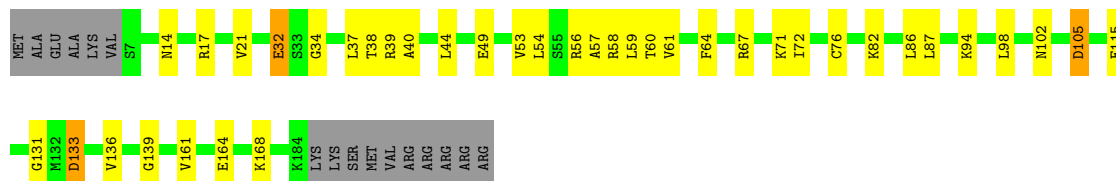
- Molecule 44: 60S ribosomal protein L10, putative

Chain BK: 79% 16% . .



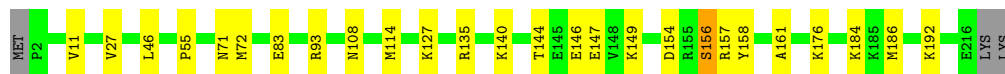
- Molecule 45: 60S ribosomal protein L11, putative

Chain BL: 72% 19% . 8%

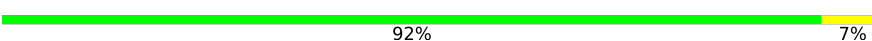


- Molecule 46: 60S ribosomal protein L13

Chain BN:  87% 11%



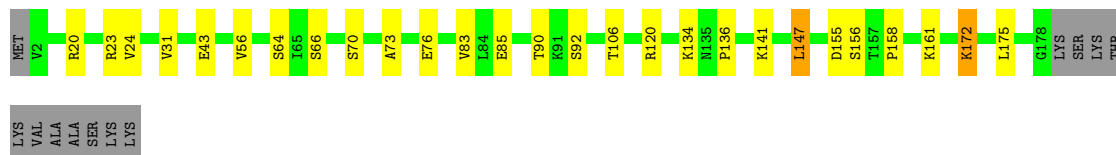
- Molecule 47: 60S ribosomal protein L13a, putative

Chain BO:  92% 7%



- Molecule 48: 40S ribosomal protein L14, putative

Chain BP:  79% 13% 6%



- Molecule 49: Ribosomal protein L15

Chain BQ:  84% 8% 8%



- Molecule 50: 60S ribosomal protein L17, putative

Chain BR:  86% 5% 8%



- Molecule 51: 60S ribosomal protein L18a

Chain BS:  85% 13% ..

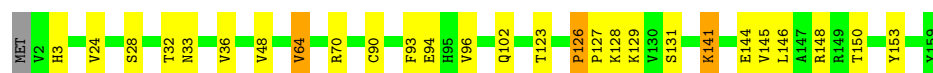


- Molecule 52: 60S ribosomal protein L19, putative

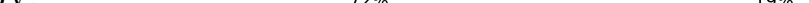
Chain BT:  65% 10% 24%

- Molecule 53: 60S ribosomal protein L21E, putative

Chain BU:  82% 15% 3%

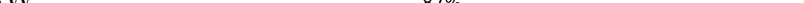


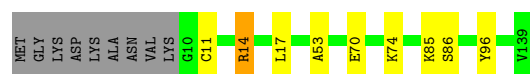
- Molecule 54: 60S ribosomal protein L22, putative

Chain BV:  72% 19% 6%

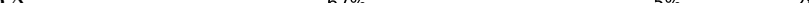


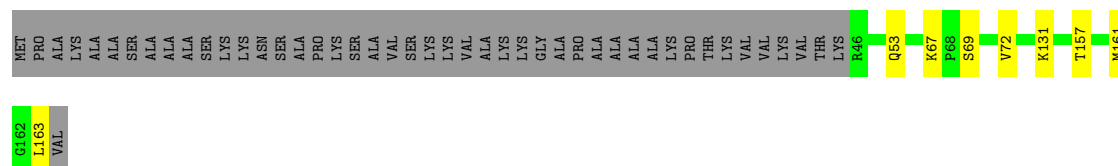
- Molecule 55: 60S ribosomal protein L23, putative

Chain BW:  87% 6% • 6%

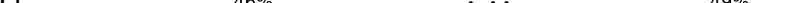


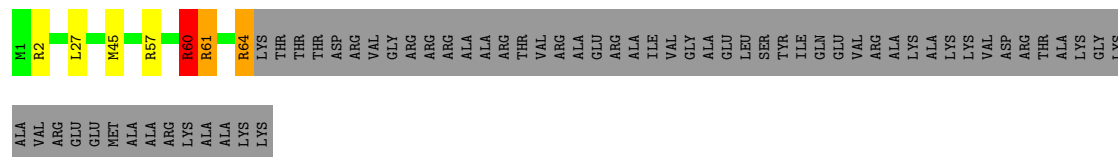
- Molecule 56: 60S ribosomal protein L23a

Chain BX:  67% 5% 28%

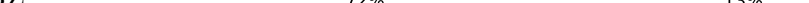


- Molecule 57: Ribosomal protein L24

Chain BY:  46% ... 49%



- Molecule 58: 60S ribosomal protein L26, putative

Chain BZ:  72% 13% 15%



- Molecule 59: 60S ribosomal protein L27

Chain Ba: 82% 17% .



- Molecule 60: 60S ribosomal protein L27a

Chain Bb: 89% 10% ..



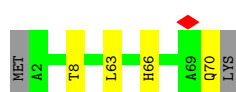
- Molecule 61: 60S ribosomal protein L28, putative

Chain Bc: 82% 17% .



- Molecule 62: 60S ribosomal protein L29

Chain Bd: 92% 6% .



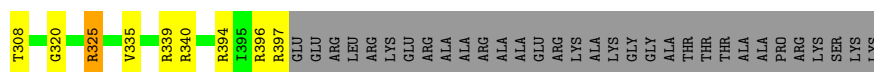
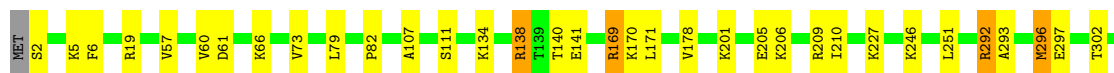
- Molecule 63: 60S ribosomal protein L2, putative

Chain Be: 92% 7% .



- Molecule 64: Ribosomal protein L3, mitochondrial, putative

Chain Bf: 82% 9% 8%



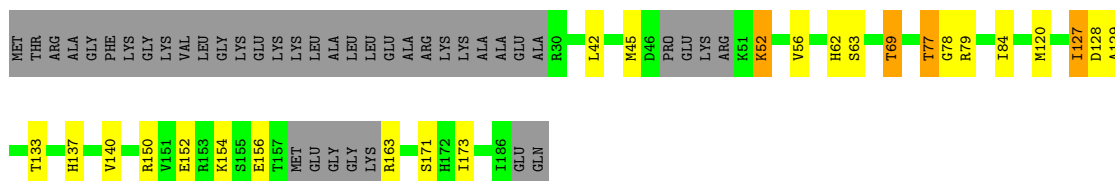
- Molecule 65: 60S ribosomal protein L30

Chain Bg:  76% 11% 12%



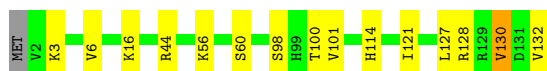
- Molecule 66: 60S ribosomal subunit protein L31, putative

Chain Bh:  65% 11% 21%



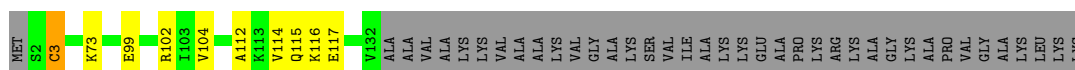
- Molecule 67: 60S ribosomal protein L32, putative

Chain Bi:  88% 11% ..



- Molecule 68: 60S ribosomal protein L34, putative

Chain Bj:  71% 5% 23%



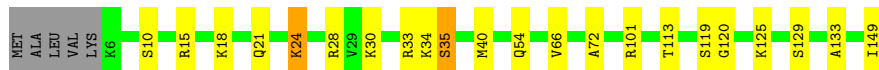
- Molecule 69: 60S ribosomal protein L35, putative

Chain Bk:  83% 13% ..



- Molecule 70: 60S ribosomal protein L35A, putative

Chain Bl:  82% 13% ..



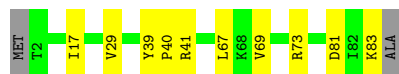
- Molecule 71: Ribosomal protein L36, putative

Chain Bm:  82% 8% 10%



- Molecule 72: Ribosomal protein L37

Chain Bn:  86% 12%



- Molecule 73: 60S ribosomal protein L37a, putative

Chain Bo:  84% 12%



- Molecule 74: 60S ribosomal protein L38, putative

Chain Bp:  68% 21% 9%



- Molecule 75: 60S ribosomal protein L39, putative

Chain Bq:  88% 10%



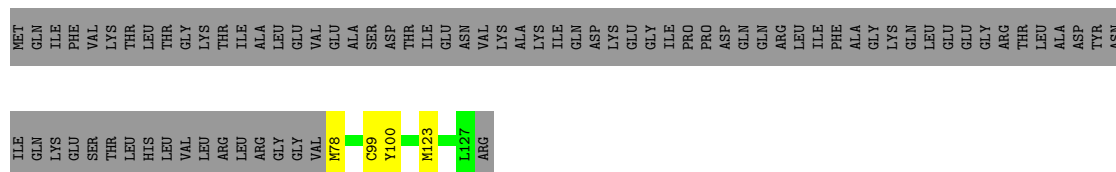
- Molecule 76: 60S ribosomal protein L4

Chain Br:  90% 8%



- Molecule 77: Ubiquitin-60S ribosomal protein L40

Chain Bs:  36% 61%



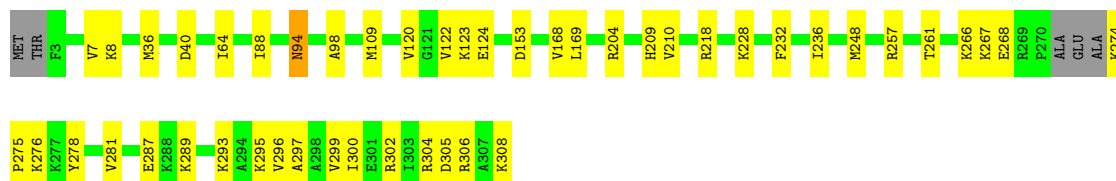
- Molecule 78: 60S ribosomal protein L44

Chain Bt:  87% 5% 8%



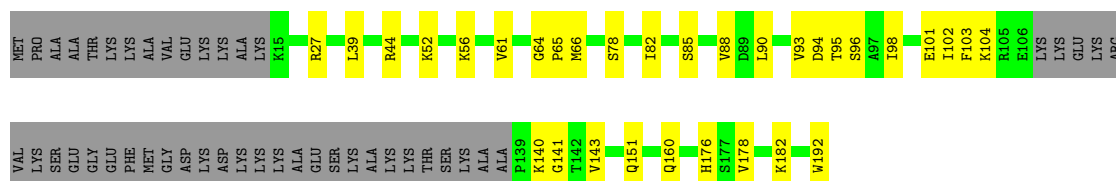
- Molecule 79: 60S ribosomal protein L5, putative

Chain Bu:  83% 15% .



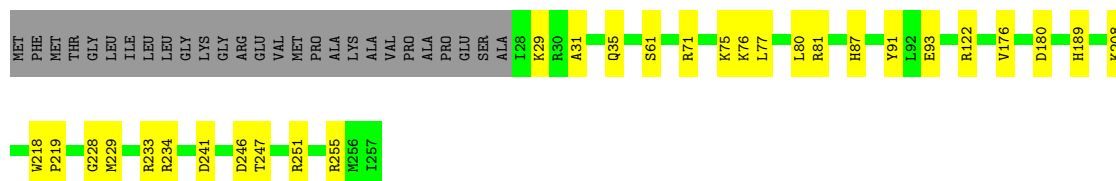
- Molecule 80: 60S ribosomal protein L6, putative

Chain Bv:  59% 17% 24%



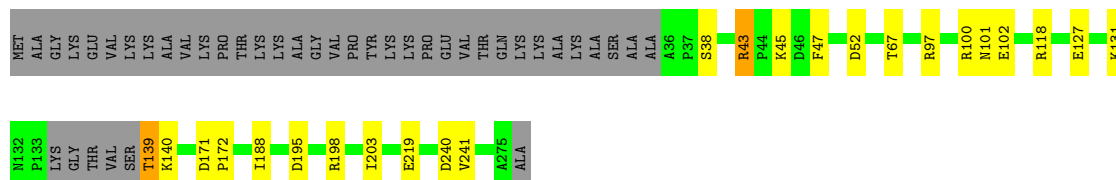
- Molecule 81: 60S ribosomal protein L7, putative

Chain Bw:  78% 11% 11%



- Molecule 82: 60S ribosomal protein L7a

Chain Bx:  76% 8% 15%



- Molecule 83: 60S ribosomal protein L9, putative

Chain By:  71% 26% ..



- Molecule 84: 60S ribosomal protein L41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.309	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.261	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.005	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: SNC, PSU, OMG, 5MC, ZN, 1MA, NA, A2M, B8N, K, MA6, MG, OMC, G7M, OMU

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	A0	0.23	0/1828	0.38	0/2460
2	A1	0.22	0/2096	0.38	0/2819
3	A2	0.21	0/1485	0.32	0/1997
4	A3	0.21	0/1907	0.36	0/2548
5	A4	0.20	0/1638	0.35	0/2212
6	A5	0.26	0/1545	0.39	0/2067
7	A6	0.21	0/1507	0.32	0/2023
8	A7	1.02	0/2360	1.14	0/3216
9	A8	0.40	0/467	0.53	0/618
10	AA	0.67	8/42683 (0.0%)	1.29	45/66469 (0.1%)
11	AB	0.50	0/233	0.85	0/359
12	AC	0.23	0/1681	0.39	0/2274
13	AD	0.20	0/837	0.45	0/1129
14	AE	0.25	0/1276	0.33	0/1717
15	AG	0.33	0/1219	0.42	0/1634
16	AH	0.28	0/1026	0.48	0/1377
17	AI	0.19	0/996	0.35	0/1336
18	AJ	0.25	0/1035	0.41	0/1386
19	AK	0.23	0/1163	0.43	0/1564
20	AL	0.19	0/981	0.36	0/1310
21	AM	0.20	0/1116	0.30	0/1495
22	AO	0.20	0/1245	0.36	0/1665
23	AP	0.24	0/1723	0.35	0/2328
24	AQ	0.23	0/809	0.50	0/1091
25	AR	0.19	0/676	0.36	0/919
26	AS	0.24	0/1110	0.39	0/1485
27	AT	0.21	0/1059	0.44	0/1406
28	AU	0.20	0/588	0.41	0/786
29	AV	0.31	0/851	0.39	0/1139
30	AW	0.21	0/674	0.45	0/904
31	AX	0.19	0/1674	0.36	0/2236
32	AY	0.21	0/480	0.35	0/634

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AZ	0.17	0/453	0.29	0/602
34	Az	0.19	0/685	0.57	0/920
35	BA	0.66	0/37724	0.84	39/58780 (0.1%)
36	BB	0.71	3/25581 (0.0%)	0.85	16/39866 (0.0%)
37	BC	0.61	0/3640	0.75	0/5666
38	BD	0.56	0/2852	0.75	1/4444 (0.0%)
39	BE	0.58	0/4116	0.87	12/6397 (0.2%)
40	BF	0.47	0/1604	0.90	2/2487 (0.1%)
41	BG	0.63	0/4383	0.82	1/6835 (0.0%)
42	BH	0.59	0/2836	0.82	1/4415 (0.0%)
43	BI	0.30	0/1552	0.43	0/2070
44	BK	0.21	0/1702	0.35	0/2281
45	BL	0.22	0/1430	0.41	0/1911
46	BN	0.22	0/1793	0.37	0/2391
47	BO	0.24	0/1832	0.37	0/2446
48	BP	0.26	0/1434	0.42	0/1921
49	BQ	0.27	0/1755	0.36	0/2346
50	BR	0.24	0/1253	0.36	0/1681
51	BS	0.23	0/1500	0.36	0/2018
52	BT	0.24	0/1614	0.37	0/2140
53	BU	0.25	0/1283	0.42	1/1727 (0.1%)
54	BV	0.16	0/995	0.44	0/1329
55	BW	0.32	0/1000	0.43	0/1347
56	BX	0.22	0/983	0.33	0/1322
57	BY	0.37	0/567	0.53	0/763
58	BZ	0.20	0/1006	0.33	0/1340
59	Ba	0.26	0/1110	0.39	0/1479
60	Bb	0.25	0/1165	0.35	0/1554
61	Bc	0.22	0/1179	0.35	0/1573
62	Bd	0.45	0/572	0.66	0/766
63	Be	0.28	0/2007	0.39	0/2700
64	Bf	0.39	0/3244	0.51	0/4360
65	Bg	0.33	0/718	0.44	0/969
66	Bh	0.34	0/1179	0.49	0/1577
67	Bi	0.24	0/1097	0.31	0/1468
68	Bj	0.22	0/1053	0.35	0/1410
69	Bk	0.22	0/1026	0.41	0/1355
70	Bl	0.40	0/1187	0.57	0/1592
71	Bm	0.21	0/796	0.40	0/1057
72	Bn	0.29	0/707	0.40	0/942
73	Bo	0.38	0/711	0.49	0/946
74	Bp	0.20	0/618	0.48	0/822
75	Bq	0.24	0/471	0.31	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Br	0.32	0/2936	0.45	0/3941
77	Bs	0.14	0/406	0.34	0/538
78	Bt	0.25	0/815	0.38	0/1077
79	Bu	0.20	0/2428	0.37	0/3254
80	Bv	0.21	0/1141	0.35	0/1538
81	Bw	0.29	0/1907	0.39	0/2556
82	Bx	0.28	0/1901	0.44	0/2557
83	By	0.19	0/1536	0.36	0/2065
84	Bz	0.39	0/293	0.34	0/381
All	All	0.54	11/217744 (0.0%)	0.84	118/319151 (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
8	A7	0	13
9	A8	0	1
43	BI	0	2
55	BW	0	1
57	BY	0	3
59	Ba	0	1
64	Bf	0	4
70	Bl	0	1
73	Bo	0	1
76	Br	0	1
82	Bx	0	1
All	All	0	29

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AA	1613	A	N9-C4	24.33	1.52	1.37
10	AA	1613	A	N9-C8	-19.16	1.22	1.37
10	AA	1613	A	C8-N7	14.92	1.42	1.31
10	AA	1613	A	C5-C4	-13.90	1.29	1.38
10	AA	1613	A	N3-C4	5.59	1.38	1.34
10	AA	36	OMU	O3'-P	5.36	1.61	1.56
36	BB	1375	OMU	O3'-P	5.34	1.61	1.56
36	BB	590	A2M	O3'-P	5.17	1.61	1.56
36	BB	545	A2M	O3'-P	5.04	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AA	721	A2M	O3'-P	5.02	1.61	1.56
10	AA	2096	A2M	O3'-P	5.01	1.61	1.56

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	1613	A	N7-C8-N9	-158.07	34.76	113.80
10	AA	1613	A	C4-C5-N7	-148.03	36.68	110.70
10	AA	1613	A	C8-N9-C4	-109.12	62.15	105.80
10	AA	1613	A	C5-N7-C8	70.12	138.96	103.90
10	AA	1613	A	C6-C5-N7	25.34	150.04	132.30
10	AA	1613	A	C4-N9-C1'	15.49	154.19	126.30
10	AA	1613	A	C5-C6-N1	11.92	123.66	117.70
10	AA	1613	A	N9-C4-C5	-11.60	101.16	105.80
35	BA	74	C	C2-N1-C1'	9.57	129.33	118.80
10	AA	1613	A	C8-N9-C1'	8.72	143.40	127.70
35	BA	1843	U	C2-N1-C1'	8.38	127.75	117.70
10	AA	936	C	N1-C2-O2	8.32	123.89	118.90
35	BA	74	C	N1-C2-O2	8.22	123.83	118.90
10	AA	1613	A	N1-C2-N3	-8.16	125.22	129.30
10	AA	1613	A	C2-N3-C4	8.14	114.67	110.60
10	AA	936	C	C2-N1-C1'	7.99	127.59	118.80
39	BE	110	C	C2-N1-C1'	7.96	127.55	118.80
35	BA	1315	C	C2-N1-C1'	7.63	127.19	118.80
36	BB	1079	C	C2-N1-C1'	7.34	126.87	118.80
10	AA	1613	A	C4-C5-C6	-7.16	113.42	117.00
35	BA	74	C	C6-N1-C1'	-7.14	112.23	120.80
35	BA	1683	U	C2-N1-C1'	7.09	126.20	117.70
10	AA	936	C	N3-C2-O2	-7.04	116.97	121.90
35	BA	1843	U	N1-C2-O2	6.97	127.68	122.80
35	BA	1315	C	N1-C2-O2	6.92	123.05	118.90
35	BA	1843	U	N3-C2-O2	-6.92	117.36	122.20
35	BA	204	U	C2-N1-C1'	6.82	125.89	117.70
35	BA	74	C	N3-C2-O2	-6.82	117.13	121.90
10	AA	752	A	P-O3'-C3'	6.47	127.46	119.70
38	BD	63	C	P-O3'-C3'	6.31	127.28	119.70
36	BB	462	A	O5'-C5'-C4'	6.31	114.45	109.40
35	BA	1671	G	O4'-C1'-N9	6.31	113.25	108.20
10	AA	683	U	C2-N1-C1'	6.24	125.19	117.70
35	BA	845	C	O4'-C1'-N1	6.16	112.81	108.50
39	BE	110	C	C6-N1-C2	-6.16	117.83	120.30
35	BA	1042	U	C2-N1-C1'	6.15	125.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	1039	C	O5'-C5'-C4'	6.12	114.30	109.40
35	BA	204	U	N3-C2-O2	-6.03	117.98	122.20
10	AA	580	C	N1-C2-O2	5.99	122.50	118.90
10	AA	1613	A	N3-C4-N9	5.94	132.15	127.40
10	AA	1242	C	C2-N1-C1'	5.88	125.27	118.80
36	BB	1531	G	P-O3'-C3'	5.88	126.75	119.70
10	AA	627	C	C2-N1-C1'	5.83	125.22	118.80
35	BA	474	C	O5'-C5'-C4'	5.79	114.03	109.40
36	BB	1079	C	N1-C2-O2	5.79	122.37	118.90
35	BA	1293	U	C2-N1-C1'	5.78	124.63	117.70
10	AA	626	C	C2-N1-C1'	5.72	125.09	118.80
35	BA	204	U	N1-C2-O2	5.72	126.80	122.80
10	AA	628	C	C2-N1-C1'	5.70	125.07	118.80
10	AA	936	C	C6-N1-C2	-5.69	118.02	120.30
39	BE	25	C	C2-N1-C1'	5.69	125.05	118.80
35	BA	1843	U	C6-N1-C1'	-5.65	113.30	121.20
36	BB	780	U	N3-C2-O2	-5.63	118.26	122.20
36	BB	1039	C	C2-N1-C1'	5.62	124.98	118.80
10	AA	620	C	N3-C2-O2	-5.55	118.01	121.90
10	AA	712	G	C4-N9-C1'	5.55	133.72	126.50
39	BE	129	C	C2-N1-C1'	5.53	124.88	118.80
35	BA	1617	C	O5'-C5'-C4'	5.51	113.81	109.40
10	AA	1823	C	C2-N1-C1'	5.50	124.84	118.80
35	BA	1315	C	C6-N1-C1'	-5.48	114.23	120.80
35	BA	649	U	O4'-C1'-N1	5.46	112.33	108.50
35	BA	1481	U	C2-N1-C1'	5.46	124.25	117.70
10	AA	95	C	C2-N1-C1'	5.45	124.79	118.80
40	BF	62	U	C2-N1-C1'	5.44	124.22	117.70
35	BA	1713	U	C2-N1-C1'	5.43	124.22	117.70
35	BA	650	U	O4'-C1'-N1	5.42	112.30	108.50
35	BA	96	C	O5'-C5'-C4'	5.41	113.73	109.40
53	BU	126	PRO	CA-N-CD	-5.41	104.42	112.00
40	BF	61	C	C2-N1-C1'	5.41	124.75	118.80
39	BE	110	C	O4'-C1'-N1	5.38	112.27	108.50
10	AA	79	A	O5'-C5'-C4'	5.38	113.71	109.40
10	AA	936	C	C6-N1-C1'	-5.38	114.34	120.80
35	BA	1315	C	O5'-C5'-C4'	5.38	113.70	109.40
39	BE	25	C	N3-C2-O2	-5.38	118.14	121.90
36	BB	1170	C	O4'-C1'-N1	5.37	112.26	108.50
39	BE	187	C	C2-N1-C1'	5.37	124.71	118.80
10	AA	413	A	O5'-C5'-C4'	5.34	113.67	109.40
10	AA	1823	C	N1-C2-O2	5.34	122.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1315	C	N3-C2-O2	-5.33	118.17	121.90
36	BB	8	U	N3-C2-O2	-5.32	118.47	122.20
39	BE	110	C	C6-N1-C1'	-5.30	114.43	120.80
10	AA	1866	C	N1-C2-O2	5.29	122.07	118.90
39	BE	110	C	N1-C2-O2	5.29	122.07	118.90
35	BA	1206	U	O4'-C1'-N1	5.28	112.20	108.50
35	BA	1287	A	N9-C1'-C2'	5.25	117.78	112.00
39	BE	18	C	C2-N1-C1'	5.25	124.58	118.80
36	BB	1012	C	C2-N1-C1'	5.25	124.58	118.80
10	AA	620	C	N1-C2-O2	5.25	122.05	118.90
10	AA	1866	C	C2-N1-C1'	5.25	124.57	118.80
39	BE	148	A	O5'-C5'-C4'	5.24	113.59	109.40
10	AA	1868	C	C2-N1-C1'	5.24	124.57	118.80
10	AA	683	U	N1-C2-O2	5.24	126.47	122.80
36	BB	780	U	C2-N1-C1'	5.22	123.96	117.70
10	AA	1854	U	C2-N1-C1'	5.21	123.95	117.70
41	BG	86	U	C2-N1-C1'	5.20	123.94	117.70
35	BA	477	G	O4'-C1'-N9	5.19	112.35	108.20
36	BB	25	A	O5'-C5'-C4'	5.19	113.55	109.40
10	AA	210	C	N1-C2-O2	5.16	122.00	118.90
10	AA	1982	C	N1-C2-O2	5.15	121.99	118.90
10	AA	2273	A	O5'-C5'-C4'	5.13	113.51	109.40
36	BB	990	C	O4'-C1'-N1	5.13	112.09	108.50
35	BA	1042	U	N1-C2-O2	5.12	126.38	122.80
35	BA	1684	U	C2-N1-C1'	5.12	123.84	117.70
35	BA	198	C	C2-N1-C1'	5.12	124.43	118.80
35	BA	845	C	C2-N1-C1'	5.11	124.42	118.80
35	BA	1168	C	C2-N1-C1'	5.11	124.42	118.80
36	BB	1079	C	C6-N1-C1'	-5.10	114.68	120.80
36	BB	637	A	O5'-C5'-C4'	5.10	113.48	109.40
36	BB	814	C	N1-C2-O2	5.08	121.95	118.90
35	BA	1860	G	C4-N9-C1'	5.08	133.11	126.50
42	BH	108	U	C2-N1-C1'	5.08	123.79	117.70
10	AA	2031	C	N1-C2-O2	5.07	121.94	118.90
35	BA	423	G	O4'-C1'-N9	5.06	112.25	108.20
35	BA	1036	G	O5'-C5'-C4'	5.05	113.44	109.40
10	AA	1823	C	N3-C2-O2	-5.04	118.37	121.90
39	BE	38	C	C2-N1-C1'	5.03	124.33	118.80
10	AA	2042	G	O5'-C5'-C4'	5.02	113.42	109.40
10	AA	627	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	A7	122	ARG	Sidechain
8	A7	129	ARG	Sidechain
8	A7	134	ARG	Sidechain
8	A7	148	ARG	Sidechain
8	A7	187	ARG	Sidechain
8	A7	221	ARG	Sidechain
8	A7	249	ARG	Sidechain
8	A7	261	ARG	Sidechain
8	A7	310	ARG	Sidechain
8	A7	36	ARG	Sidechain
8	A7	61	ARG	Sidechain
8	A7	62	ARG	Sidechain
8	A7	92	ARG	Sidechain
9	A8	10	ARG	Sidechain
43	BI	13	ARG	Sidechain
43	BI	73	ARG	Sidechain
55	BW	14	ARG	Sidechain
57	BY	60	ARG	Sidechain
57	BY	61	ARG	Sidechain
57	BY	64	ARG	Sidechain
59	Ba	54	ARG	Sidechain
64	Bf	138	ARG	Sidechain
64	Bf	169	ARG	Sidechain
64	Bf	292	ARG	Sidechain
64	Bf	325	ARG	Sidechain
70	Bl	28	ARG	Sidechain
73	Bo	87	ARG	Sidechain
76	Br	309	ARG	Sidechain
82	Bx	43	ARG	Sidechain

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	A0	1801	0	1871	24	0
2	A1	2062	0	2181	17	0
3	A2	1463	0	1524	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A3	1885	0	1994	23	0
5	A4	1606	0	1675	21	0
6	A5	1521	0	1604	14	0
7	A6	1477	0	1536	12	0
8	A7	2315	0	2212	32	0
9	A8	461	0	467	3	0
10	AA	39092	0	19779	285	0
11	AB	210	0	113	1	0
12	AC	1647	0	1684	25	0
13	AD	814	0	819	19	0
14	AE	1251	0	1301	9	0
15	AG	1198	0	1276	11	0
16	AH	1011	0	1021	20	0
17	AI	975	0	1008	22	0
18	AJ	1018	0	1050	8	0
19	AK	1143	0	1204	13	0
20	AL	969	0	1039	21	0
21	AM	1098	0	1146	14	0
22	AO	1220	0	1286	15	0
23	AP	1688	0	1734	19	0
24	AQ	800	0	856	21	0
25	AR	666	0	670	9	0
26	AS	1089	0	1144	9	0
27	AT	1043	0	1130	10	0
28	AU	582	0	629	5	0
29	AV	835	0	869	13	0
30	AW	660	0	664	11	0
31	AX	1652	0	1721	31	0
32	AY	474	0	519	7	0
33	AZ	454	0	488	1	0
34	Az	673	0	689	30	0
35	BA	34591	0	17479	170	0
36	BB	24057	0	12189	140	0
37	BC	3412	0	1738	19	0
38	BD	2553	0	1294	9	0
39	BE	3691	0	1875	22	0
40	BF	1444	0	744	19	0
41	BG	3919	0	1975	25	0
42	BH	2540	0	1286	22	0
43	BI	1526	0	1646	8	0
44	BK	1668	0	1743	22	0
45	BL	1408	0	1440	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	BN	1762	0	1864	16	0
47	BO	1801	0	1952	9	0
48	BP	1414	0	1514	14	0
49	BQ	1716	0	1795	10	0
50	BR	1228	0	1286	2	0
51	BS	1465	0	1500	14	0
52	BT	1597	0	1671	19	0
53	BU	1253	0	1304	15	0
54	BV	979	0	1002	17	0
55	BW	983	0	1040	7	0
56	BX	966	0	1030	6	0
57	BY	547	0	551	4	0
58	BZ	993	0	1072	12	0
59	Ba	1090	0	1156	16	0
60	Bb	1137	0	1174	9	0
61	Bc	1162	0	1246	18	0
62	Bd	561	0	583	2	0
63	Be	1962	0	2024	13	0
64	Bf	3174	0	3300	18	0
65	Bg	708	0	726	6	0
66	Bh	1160	0	1207	18	0
67	Bi	1075	0	1135	11	0
68	Bj	1035	0	1065	6	0
69	Bk	1018	0	1141	13	0
70	Bl	1163	0	1221	15	0
71	Bm	786	0	865	7	0
72	Bn	693	0	708	6	0
73	Bo	699	0	726	6	0
74	Bp	609	0	666	14	0
75	Bq	457	0	495	4	0
76	Br	2882	0	3011	16	0
77	Bs	400	0	428	3	0
78	Bt	801	0	861	5	0
79	Bu	2388	0	2455	33	0
80	Bv	1121	0	1182	19	0
81	Bw	1872	0	1966	16	0
82	Bx	1874	0	2008	12	0
83	By	1515	0	1589	30	0
84	Bz	289	0	325	0	0
85	A0	1	0	0	0	0
85	A3	1	0	0	0	0
85	AA	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	BA	69	0	0	0	0
85	BB	61	0	0	0	0
85	BC	4	0	0	0	0
85	BD	3	0	0	0	0
85	BE	3	0	0	0	0
85	BF	1	0	0	0	0
85	BG	1	0	0	0	0
85	BH	1	0	0	0	0
85	BW	1	0	0	0	0
85	Bn	1	0	0	0	0
86	A8	1	0	0	0	0
86	AV	1	0	0	0	0
86	Bn	1	0	0	0	0
86	Bo	1	0	0	0	0
86	Bs	1	0	0	0	0
86	Bt	1	0	0	0	0
87	AA	25	0	0	0	0
87	BA	22	0	0	0	0
87	BB	22	0	0	0	0
87	BC	1	0	0	0	0
87	BE	1	0	0	0	0
87	BG	6	0	0	0	0
87	BH	1	0	0	0	0
87	Be	1	0	0	0	0
87	Bn	1	0	0	0	0
88	AA	5	0	0	0	0
88	BA	8	0	0	0	0
88	BB	9	0	0	0	0
88	BR	1	0	0	0	0
88	BU	1	0	0	0	0
89	A1	1	0	0	0	0
89	A2	1	0	0	0	0
89	A5	6	0	0	0	0
89	AA	264	0	0	2	0
89	AC	1	0	0	0	0
89	AE	5	0	0	1	0
89	AG	10	0	0	1	0
89	AH	3	0	0	0	0
89	AO	1	0	0	0	0
89	AP	2	0	0	0	0
89	AV	7	0	0	0	0
89	AX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	BA	239	0	0	1	0
89	BB	353	0	0	2	0
89	BC	8	0	0	0	0
89	BE	13	0	0	0	0
89	BG	40	0	0	1	0
89	BH	9	0	0	0	0
89	BI	2	0	0	0	0
89	BK	2	0	0	0	0
89	BQ	4	0	0	0	0
89	BR	6	0	0	0	0
89	BT	4	0	0	0	0
89	BU	1	0	0	0	0
89	BV	3	0	0	0	0
89	BW	11	0	0	1	0
89	BY	2	0	0	0	0
89	Bb	3	0	0	0	0
89	Be	6	0	0	1	0
89	Bf	25	0	0	1	0
89	Bi	3	0	0	0	0
89	Bj	1	0	0	0	0
89	Bl	2	0	0	0	0
89	Bn	9	0	0	0	0
89	Bo	6	0	0	0	0
89	Br	4	0	0	0	0
89	Bt	1	0	0	0	0
89	Bx	1	0	0	0	0
89	Bz	5	0	0	0	0
All	All	207369	0	153156	1510	0

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

All (1510) 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)
36:BB:1424:C:H4'	36:BB:1425:A:C6	1.88	1.07
10:AA:837:A:H2	10:AA:893:G:N1	1.58	1.01
10:AA:837:A:C2	10:AA:893:G:N1	2.30	0.99
35:BA:1864:G:H1	36:BB:6:A:H61	1.10	0.97
36:BB:1424:C:H4'	36:BB:1425:A:C5	1.99	0.97
42:BH:79:A:H2	42:BH:86:G:H1	0.99	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BB:1424:C:H4'	36:BB:1425:A:N6	1.81	0.95
35:BA:198:C:H5	35:BA:295:G:H1	1.18	0.91
35:BA:169:C:H42	35:BA:327:U:H3	1.16	0.91
35:BA:169:C:N4	35:BA:327:U:H3	1.70	0.88
35:BA:1760:G:H1	35:BA:1811:U:H3	1.16	0.88
24:AQ:43:GLU:O	24:AQ:44:LYS:NZ	2.10	0.84
28:AU:58:LYS:O	28:AU:62:LYS:NZ	2.10	0.84
36:BB:469:U:H3	36:BB:501:C:H42	1.26	0.83
10:AA:747:C:N4	10:AA:800:C:O2	2.11	0.82
10:AA:999:U:H5'	10:AA:1000:G:H5''	1.60	0.81
44:BK:211:ILE:HD13	79:Bu:300:ILE:HG22	1.60	0.81
35:BA:1111:A:H61	35:BA:1233:A:H8	1.28	0.81
10:AA:1827:C:N4	22:AO:133:CYS:SG	2.54	0.81
83:By:180:GLN:HG3	83:By:181:THR:HG23	1.63	0.81
35:BA:615:G:N3	35:BA:619:C:N4	2.30	0.80
36:BB:1424:C:C4'	36:BB:1425:A:N6	2.43	0.80
39:BE:34:C:O2'	39:BE:192:C:N4	2.15	0.80
10:AA:1483:C:N4	10:AA:1492:G:N7	2.28	0.80
34:Az:177:PHE:HD1	34:Az:178:THR:H	1.30	0.80
10:AA:1613:A:H61	10:AA:1922:G:H22	1.30	0.80
10:AA:770:U:H3	10:AA:780:C:H42	1.26	0.79
10:AA:1391:U:O3'	30:AW:14:ARG:NH1	2.16	0.79
20:AL:77:GLU:HA	20:AL:80:ARG:HE	1.47	0.79
42:BH:52:G:H1	42:BH:70:U:H3	1.26	0.79
35:BA:1498:C:H5	35:BA:1521:G:H1	1.30	0.78
35:BA:1864:G:H1	36:BB:6:A:N6	1.82	0.77
42:BH:79:A:N1	42:BH:86:G:O6	2.18	0.77
15:AG:142:GLU:OE1	15:AG:142:GLU:N	2.17	0.77
35:BA:984:G:N7	89:BA:2101:HOH:O	2.16	0.77
10:AA:1712:U:H3	10:AA:1723:G:H22	1.31	0.77
15:AG:38:CYS:HB2	15:AG:78:LYS:HE3	1.66	0.76
42:BH:79:A:C2	42:BH:86:G:N1	2.48	0.76
44:BK:16:PRO:O	44:BK:95:HIS:ND1	2.16	0.76
10:AA:1398:G:H22	10:AA:1455:A:H2	1.30	0.76
26:AS:28:LYS:O	26:AS:32:THR:OG1	2.02	0.76
42:BH:26:C:N3	42:BH:125:U:O2'	2.19	0.76
10:AA:1643:A:H3'	10:AA:1644:U:H5''	1.67	0.76
28:AU:51:GLU:OE2	28:AU:51:GLU:N	2.19	0.75
31:AX:91:GLU:HG2	31:AX:92:VAL:HG23	1.67	0.75
42:BH:79:A:H2	42:BH:86:G:N1	1.82	0.75
10:AA:732:A:N6	10:AA:1246:C:O2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BF:55:C:H42	40:BF:60:C:H5	1.34	0.74
10:AA:616:G:H1	10:AA:631:U:H3	1.36	0.74
36:BB:990:C:H5'	36:BB:991:A:H5''	1.69	0.74
12:AC:48:GLU:N	12:AC:48:GLU:OE1	2.20	0.74
8:A7:177:LEU:HD11	8:A7:191:ASP:HB2	1.70	0.74
10:AA:835:A:H2	10:AA:895:G:H22	1.36	0.74
10:AA:580:C:N4	10:AA:604:U:O4	2.15	0.74
10:AA:1622:G:OP1	13:AD:3:THR:OG1	2.06	0.73
39:BE:38:C:H5	39:BE:188:G:H1	1.36	0.73
35:BA:1671:G:O2'	35:BA:1673:G:OP2	2.07	0.73
82:Bx:219:GLU:N	82:Bx:219:GLU:OE2	2.22	0.73
10:AA:837:A:N1	10:AA:893:G:O6	2.21	0.73
37:BC:70:C:OP2	58:BZ:111:ARG:NH1	2.21	0.73
36:BB:1296:U:OP1	36:BB:1352:G:N2	2.22	0.72
8:A7:119:PRO:HB2	8:A7:164:LEU:HD13	1.69	0.72
34:Az:180:MET:SD	34:Az:180:MET:N	2.62	0.72
61:Bc:34:ASN:O	61:Bc:35:ASN:ND2	2.23	0.72
35:BA:743:A2M:H5'	35:BA:743:A2M:H8	1.71	0.72
30:AW:57:CYS:SG	30:AW:60:CYS:N	2.63	0.71
59:Ba:34:GLU:OE1	59:Ba:34:GLU:N	2.23	0.71
10:AA:585:G:H1	10:AA:599:G:H22	1.35	0.71
20:AL:72:LYS:HZ2	20:AL:73:LEU:HD22	1.54	0.71
45:BL:105:ASP:OD1	45:BL:105:ASP:N	2.15	0.71
17:AI:117:GLU:OE1	17:AI:117:GLU:N	2.21	0.71
89:BB:1708:HOH:O	68:Bj:3:CYS:SG	2.48	0.70
10:AA:1264:G:O6	63:Be:250:ARG:NH1	2.24	0.70
54:BV:83:MET:HE3	54:BV:83:MET:HA	1.73	0.70
21:AM:103:MET:HE2	21:AM:107:ARG:HH21	1.56	0.70
35:BA:513:C:H5	35:BA:715:G:H1	1.40	0.70
25:AR:10:GLU:OE2	25:AR:10:GLU:N	2.23	0.70
35:BA:1760:G:N2	35:BA:1811:U:O2	2.22	0.70
10:AA:340:G:H21	14:AE:55:GLY:HA3	1.54	0.70
45:BL:32:GLU:HG2	45:BL:34:GLY:H	1.55	0.70
81:Bw:246:ASP:OD1	81:Bw:247:THR:N	2.25	0.70
52:BT:179:LYS:HA	52:BT:182:GLU:HB2	1.72	0.70
10:AA:756:U:H2'	10:AA:757:G:C8	2.27	0.69
10:AA:837:A:H2	10:AA:893:G:H1	0.78	0.69
39:BE:25:C:H5	39:BE:209:G:H1	1.40	0.69
10:AA:794:G:H2'	10:AA:795:A:C8	2.27	0.69
17:AI:59:ARG:O	17:AI:59:ARG:NH1	2.25	0.69
62:Bd:66:HIS:O	62:Bd:70:GLN:HB3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AL:82:MET:HE3	20:AL:82:MET:HA	1.74	0.69
44:BK:212:MET:HE3	44:BK:212:MET:HA	1.74	0.69
51:BS:10:CYS:SG	51:BS:28:LYS:NZ	2.65	0.69
35:BA:212:A:N6	35:BA:228:U:O2'	2.25	0.69
74:Bp:28:ASN:HB2	74:Bp:31:VAL:HG12	1.75	0.69
42:BH:115:A:OP1	66:Bh:62:HIS:NE2	2.26	0.69
51:BS:133:ASN:O	51:BS:134:HIS:ND1	2.26	0.69
12:AC:232:GLU:OE1	12:AC:232:GLU:N	2.25	0.69
16:AH:90:MET:HE1	16:AH:105:ALA:HB1	1.74	0.68
12:AC:116:ARG:NH1	12:AC:162:ASP:OD2	2.26	0.68
40:BF:4:C:H5	47:BO:11:ARG:HE	1.42	0.68
44:BK:183:GLU:OE1	44:BK:183:GLU:N	2.19	0.68
46:BN:184:LYS:HD3	46:BN:186:MET:HE1	1.74	0.68
74:Bp:10:GLU:OE1	74:Bp:10:GLU:N	2.18	0.68
35:BA:761:A:H2'	35:BA:762:A2M:H8	1.76	0.68
40:BF:23:U:OP1	83:By:22:ARG:NH1	2.26	0.68
74:Bp:52:LYS:HA	74:Bp:55:LYS:HB3	1.75	0.68
55:BW:70:GLU:OE1	55:BW:70:GLU:N	2.22	0.68
52:BT:191:ASP:OD1	52:BT:192:ASP:N	2.26	0.68
21:AM:15:ARG:NH1	45:BL:115:GLU:OE1	2.27	0.68
63:Be:250:ARG:H	63:Be:250:ARG:HD3	1.59	0.67
82:Bx:139:THR:OG1	82:Bx:140:LYS:N	2.26	0.67
10:AA:2096:A2M:H8	10:AA:2096:A2M:H5''	1.77	0.67
7:A6:63:GLU:OE2	7:A6:64:ASN:N	2.27	0.67
10:AA:770:U:H3	10:AA:780:C:N4	1.91	0.67
10:AA:2235:A:H3'	36:BB:520:A:H62	1.59	0.67
83:By:13:GLU:OE2	83:By:13:GLU:N	2.24	0.67
8:A7:108:HIS:HA	8:A7:134:ARG:HH12	1.58	0.67
10:AA:841:G:H4'	10:AA:842:G:H5'	1.76	0.67
36:BB:837:C:H5	36:BB:970:G:H1	1.42	0.67
5:A4:119:ARG:NH2	10:AA:739:C:O2	2.27	0.67
9:A8:53:PHE:HB3	24:AQ:77:PHE:HB3	1.77	0.67
20:AL:87:GLU:HG2	20:AL:88:VAL:HG13	1.74	0.67
7:A6:21:GLU:OE1	7:A6:21:GLU:N	2.24	0.66
25:AR:68:GLU:OE1	25:AR:68:GLU:N	2.28	0.66
80:Bv:101:GLU:N	80:Bv:101:GLU:OE2	2.26	0.66
23:AP:130:GLU:OE1	31:AX:115:ARG:NH1	2.28	0.66
41:BG:138:C:O2'	83:By:153:SER:OG	2.14	0.66
69:Bk:76:ASP:OD1	69:Bk:77:LYS:N	2.28	0.66
35:BA:178:U:O4	35:BA:318:C:N3	2.29	0.66
51:BS:70:LYS:O	51:BS:74:ARG:NH2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Bk:24:GLU:OE2	69:Bk:24:GLU:N	2.27	0.66
5:A4:74:MET:HE3	10:AA:1134:A:H61	1.60	0.66
9:A8:7:TRP:O	10:AA:1917:U:O2'	2.12	0.66
46:BN:140:LYS:HE3	46:BN:140:LYS:HA	1.78	0.66
24:AQ:38:GLU:O	24:AQ:42:THR:HG23	1.95	0.66
14:AE:126:HIS:ND1	89:AE:201:HOH:O	2.29	0.65
36:BB:1424:C:C4'	36:BB:1425:A:H62	2.09	0.65
1:A0:149:GLU:OE2	1:A0:149:GLU:N	2.21	0.65
10:AA:1162:G:H2'	10:AA:1163:U:C6	2.31	0.65
34:Az:172:GLN:HA	34:Az:175:GLU:HG3	1.78	0.65
54:BV:103:LEU:HB3	54:BV:107:ILE:HG12	1.79	0.65
35:BA:169:C:H2'	35:BA:170:C:C6	2.31	0.65
44:BK:14:ASN:O	44:BK:128:ARG:NH2	2.30	0.65
10:AA:603:G:OP2	10:AA:603:G:N2	2.27	0.65
35:BA:1470:U:OP1	48:BP:20:ARG:NH2	2.30	0.65
53:BU:128:LYS:HD3	53:BU:128:LYS:N	2.11	0.65
10:AA:1483:C:H5'	10:AA:1484:A:H5''	1.78	0.65
10:AA:2276:A:O2'	29:AV:99:ARG:O	2.12	0.65
20:AL:102:ASP:OD1	20:AL:103:LYS:N	2.29	0.65
35:BA:331:A:N7	71:Bm:37:ARG:NH2	2.44	0.65
79:Bu:124:GLU:OE1	79:Bu:124:GLU:N	2.28	0.65
53:BU:48:VAL:HG21	53:BU:94:GLU:HG2	1.79	0.64
34:Az:205:LYS:O	34:Az:209:GLU:HG3	1.97	0.64
35:BA:619:C:H1'	35:BA:620:G:H2'	1.79	0.64
73:Bo:8:MET:HE3	73:Bo:12:GLY:HA2	1.79	0.64
1:A0:158:ALA:O	1:A0:159:LYS:HB2	1.96	0.64
4:A3:150:LEU:HD23	4:A3:150:LEU:H	1.63	0.64
27:AT:11:THR:OG1	27:AT:33:ASN:OD1	2.13	0.64
10:AA:1396:G:H1	10:AA:1457:U:H3	1.46	0.63
17:AI:38:GLU:OE2	17:AI:38:GLU:N	2.20	0.63
23:AP:66:LEU:O	25:AR:20:ARG:NH1	2.31	0.63
24:AQ:48:ARG:HB2	24:AQ:87:ASP:HB3	1.79	0.63
29:AV:29:SER:OG	29:AV:29:SER:O	2.16	0.63
58:BZ:54:ARG:NH1	58:BZ:64:GLU:OE2	2.32	0.63
22:AO:52:GLU:OE1	22:AO:52:GLU:N	2.20	0.63
21:AM:111:ASP:OD1	21:AM:114:ARG:NH2	2.28	0.63
31:AX:37:GLU:OE2	31:AX:50:ARG:NH1	2.31	0.63
39:BE:148:A:H5''	74:Bp:26:LYS:HE3	1.80	0.62
10:AA:1701:A:N7	89:AA:2402:HOH:O	2.31	0.62
24:AQ:16:ARG:HB2	24:AQ:89:ARG:HA	1.81	0.62
34:Az:163:ILE:N	34:Az:191:ASN:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BP:136:PRO:HB3	48:BP:141:LYS:HB3	1.80	0.62
36:BB:449:C:O2'	36:BB:578:OMU:OP2	2.17	0.62
56:BX:157:THR:O	56:BX:161:MET:HG3	2.00	0.62
79:Bu:7:VAL:HG13	79:Bu:8:LYS:HG2	1.81	0.62
10:AA:227:U:O2	10:AA:267:G:O6	2.18	0.62
35:BA:169:C:N4	35:BA:327:U:N3	2.37	0.62
40:BF:15:U:O2'	51:BS:170:LYS:NZ	2.32	0.62
22:AO:44:LYS:H	22:AO:44:LYS:HE2	1.63	0.62
30:AW:20:HIS:ND1	30:AW:21:LYS:O	2.33	0.62
79:Bu:274:LYS:NZ	79:Bu:275:PRO:O	2.33	0.62
12:AC:63:THR:O	12:AC:83:ASN:ND2	2.33	0.62
43:BI:80:LYS:NZ	62:Bd:70:GLN:O	2.31	0.62
4:A3:129:ASP:OD1	4:A3:129:ASP:N	2.31	0.61
7:A6:90:ASP:OD1	7:A6:90:ASP:N	2.33	0.61
75:Bq:13:TYR:OH	75:Bq:50:HIS:O	2.17	0.61
80:Bv:140:LYS:NZ	80:Bv:141:GLY:O	2.27	0.61
48:BP:158:PRO:HA	48:BP:161:LYS:HE2	1.82	0.61
16:AH:16:LYS:N	16:AH:16:LYS:HE2	2.15	0.61
36:BB:1014:U:H2'	36:BB:1015:C:C6	2.36	0.61
1:A0:88:PHE:HB3	1:A0:100:THR:HB	1.81	0.61
8:A7:224:ASP:HB2	8:A7:231:LEU:HD21	1.82	0.61
10:AA:1981:G:OP2	10:AA:1981:G:N2	2.30	0.61
66:Bh:84:ILE:HD11	66:Bh:120:MET:HE1	1.82	0.61
20:AL:72:LYS:NZ	20:AL:73:LEU:HD22	2.15	0.61
24:AQ:23:SER:HB3	24:AQ:29:VAL:HG13	1.83	0.61
10:AA:844:A:H61	10:AA:888:C:H42	1.48	0.61
13:AD:84:ARG:NH1	13:AD:93:ALA:O	2.33	0.61
35:BA:905:G:OP2	43:BI:63:SER:OG	2.16	0.61
10:AA:585:G:H1	10:AA:599:G:H1	1.48	0.61
7:A6:16:ARG:NH2	10:AA:31:U:O2	2.31	0.61
41:BG:132:U:H3	41:BG:157:A:H2	1.47	0.61
79:Bu:267:LYS:NZ	79:Bu:268:GLU:O	2.26	0.61
44:BK:81:ASN:OD1	44:BK:82:LYS:N	2.33	0.61
46:BN:144:THR:OG1	46:BN:147:GLU:OE1	2.17	0.61
10:AA:585:G:H1	10:AA:599:G:N2	1.99	0.61
34:Az:208:LYS:HZ2	34:Az:209:GLU:HB3	1.65	0.61
81:Bw:81:ARG:NH1	81:Bw:93:GLU:OE2	2.32	0.61
30:AW:85:ASP:N	30:AW:85:ASP:OD1	2.34	0.60
36:BB:477:A:H2'	36:BB:478:A:C8	2.35	0.60
31:AX:197:ASP:N	31:AX:197:ASP:OD1	2.33	0.60
30:AW:66:ARG:NH1	30:AW:73:MET:SD	2.75	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BB:1424:C:H4'	36:BB:1425:A:H62	1.65	0.60
45:BL:133:ASP:N	45:BL:133:ASP:OD1	2.33	0.60
58:BZ:33:SER:OG	58:BZ:35:GLU:OE1	2.19	0.60
12:AC:57:MET:HE2	12:AC:57:MET:HA	1.84	0.60
60:Bb:72:THR:HG22	60:Bb:108:LYS:HB3	1.82	0.60
64:Bf:320:GLY:O	64:Bf:340:ARG:NH1	2.35	0.60
10:AA:172:A:O2'	10:AA:173:C:OP1	2.18	0.60
10:AA:763:G:H2'	10:AA:764:U:C6	2.36	0.60
35:BA:384:C:OP2	71:Bm:35:ASN:ND2	2.35	0.60
64:Bf:396:ARG:NH2	64:Bf:397:ARG:HB2	2.16	0.60
80:Bv:27:ARG:NH2	80:Bv:78:SER:O	2.35	0.60
54:BV:42:ASP:O	54:BV:46:ASN:ND2	2.35	0.60
31:AX:141:ILE:O	31:AX:142:LYS:HG3	2.02	0.60
35:BA:1036:G:N2	35:BA:1045[B]:A:N7	2.49	0.60
79:Bu:293:LYS:HA	79:Bu:296:VAL:HG12	1.82	0.60
79:Bu:299:VAL:HG22	79:Bu:302:ARG:HH22	1.67	0.60
10:AA:1625:C:H2'	10:AA:1626:A:H8	1.65	0.60
52:BT:136:ARG:O	52:BT:140:GLU:HG2	2.01	0.60
12:AC:224:THR:HG22	12:AC:225:ILE:HG23	1.83	0.59
15:AG:87:ASP:OD1	15:AG:87:ASP:N	2.31	0.59
45:BL:82:LYS:HD2	45:BL:86:LEU:HD23	1.84	0.59
10:AA:788:U:H2'	10:AA:789:G:H8	1.67	0.59
13:AD:22:VAL:O	31:AX:74:GLN:NE2	2.33	0.59
35:BA:761:A:H2'	35:BA:762:A2M:C8	2.32	0.59
36:BB:1013:U:H5''	59:Ba:55:GLY:HA2	1.84	0.59
10:AA:793:U:H2'	10:AA:794:G:C8	2.37	0.59
24:AQ:17:VAL:HG21	24:AQ:95:VAL:HG11	1.84	0.59
40:BF:72:C:OP1	70:Bl:101:ARG:NH2	2.35	0.59
1:A0:111:ARG:HA	1:A0:114:TYR:HB3	1.83	0.59
19:AK:45:ILE:O	19:AK:46:LEU:HB2	2.03	0.59
35:BA:447:G:O2'	35:BA:472:A:N1	2.34	0.59
10:AA:635:U:OP2	27:AT:5:LYS:NZ	2.35	0.59
35:BA:254:A2M:O5'	35:BA:254:A2M:H8	2.03	0.59
56:BX:163:LEU:HA	69:Bk:38:MET:HE2	1.85	0.59
79:Bu:88:ILE:HA	79:Bu:248:MET:HE2	1.84	0.59
35:BA:229:G:H5''	61:Bc:127:ARG:HD2	1.85	0.59
35:BA:1570:U:H2'	35:BA:1571:G:C8	2.38	0.59
36:BB:838:U:H2'	36:BB:839:G:C8	2.38	0.59
41:BG:149:U:H5	41:BG:151:A:N7	2.01	0.59
5:A4:21:GLU:OE1	5:A4:21:GLU:N	2.21	0.58
12:AC:49:SER:O	12:AC:53:LYS:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:958:G:O2'	39:BE:122:C:O2'	2.18	0.58
49:BQ:162:ASP:HB3	49:BQ:165:ILE:HG22	1.84	0.58
54:BV:18:GLN:HG2	54:BV:83:MET:HE1	1.84	0.58
36:BB:400:A2M:O5'	36:BB:400:A2M:H8	2.03	0.58
35:BA:120:U:OP1	49:BQ:19:GLY:N	2.36	0.58
35:BA:563:G:H2'	35:BA:564:C:C6	2.38	0.58
35:BA:1170:C:OP1	44:BK:130:ARG:NH2	2.36	0.58
36:BB:1424:C:H4'	36:BB:1425:A:N7	2.18	0.58
82:Bx:171:ASP:HB2	82:Bx:172:PRO:HD3	1.85	0.58
83:By:129:LYS:HG2	83:By:145:GLU:HG2	1.86	0.58
27:AT:34:HIS:HB2	27:AT:37:TRP:HB2	1.84	0.58
10:AA:829:U:H2'	10:AA:830:A:C8	2.39	0.58
10:AA:834:G:N2	10:AA:834:G:OP1	2.37	0.58
36:BB:996:G:H1	36:BB:1016:U:H3	1.51	0.58
42:BH:118:U:O2'	42:BH:119:U:O2	2.21	0.58
48:BP:155:ASP:O	48:BP:156:SER:OG	2.22	0.58
51:BS:79:ASP:OD1	51:BS:91:HIS:NE2	2.36	0.58
10:AA:290:G:OP2	14:AE:40:LYS:NZ	2.31	0.58
10:AA:2151:U:O2'	36:BB:556:U:O2'	2.21	0.58
10:AA:1450:A:O2'	10:AA:1452:G:OP2	2.16	0.58
35:BA:612:U:O2	76:Br:314:ARG:NH2	2.36	0.58
35:BA:189:C:H5	35:BA:309:G:H1	1.49	0.58
35:BA:1847:C:OP1	56:BX:131:LYS:NZ	2.31	0.58
45:BL:60:THR:HG22	45:BL:67:ARG:HA	1.85	0.58
10:AA:788:U:H2'	10:AA:789:G:C8	2.39	0.58
39:BE:186:U:O2'	39:BE:187:C:O2	2.20	0.58
10:AA:291:A:O2'	10:AA:292:A:OP1	2.22	0.57
10:AA:2044:A:H2'	10:AA:2045:PSU:H6	1.68	0.57
59:Ba:49:PRO:HD3	59:Ba:67:VAL:HG12	1.86	0.57
16:AH:109:LEU:HD23	29:AV:47:LEU:HD21	1.86	0.57
20:AL:106:LEU:HD22	20:AL:110:LYS:HE3	1.85	0.57
35:BA:650:U:H2'	35:BA:651:G:C8	2.39	0.57
10:AA:758:G:H1	10:AA:791:U:H3	1.51	0.57
10:AA:837:A:N1	10:AA:893:G:C6	2.72	0.57
36:BB:789:G:OP2	63:Be:37:ARG:NH2	2.37	0.57
10:AA:769:G:H22	10:AA:781:U:H3	1.50	0.57
17:AI:30:ASP:OD2	17:AI:31:PRO:HD3	2.04	0.57
22:AO:38:HIS:NE2	22:AO:42:GLU:OE2	2.37	0.57
38:BD:48:G:OP1	79:Bu:94:ASN:ND2	2.36	0.57
46:BN:146:GLU:HA	46:BN:149:LYS:HD2	1.85	0.57
35:BA:1863:U:H2'	35:BA:1864:G:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:By:87:ARG:HD3	83:By:89:LYS:HE3	1.86	0.57
34:Az:176:LEU:O	34:Az:178:THR:N	2.37	0.57
35:BA:1332:G:H2'	35:BA:1333:A:C8	2.40	0.57
28:AU:59:GLU:N	28:AU:59:GLU:OE1	2.37	0.57
36:BB:1501:U:H1'	70:Bl:21:GLN:HG2	1.87	0.57
8:A7:161:SER:HB3	8:A7:168:VAL:HG22	1.86	0.57
22:AO:57:SER:HB2	22:AO:112:ALA:HA	1.87	0.57
36:BB:769:U:H2'	36:BB:770:G:C8	2.40	0.57
49:BQ:104:ALA:O	49:BQ:109:ARG:NH1	2.37	0.57
8:A7:3:VAL:HA	8:A7:314:VAL:HA	1.86	0.57
35:BA:1642:U:H4'	35:BA:1643:U:H5'	1.87	0.56
35:BA:1648:U:H3	66:Bh:79:ARG:NH2	2.02	0.56
42:BH:5:G:H2'	42:BH:6:U:C6	2.40	0.56
36:BB:1424:C:H5''	36:BB:1425:A:N7	2.20	0.56
51:BS:153:LEU:HB3	51:BS:156:ARG:HD3	1.87	0.56
64:Bf:107:ALA:HB1	64:Bf:205:GLU:HG3	1.87	0.56
79:Bu:305:ASP:HA	79:Bu:308:LYS:HD3	1.87	0.56
8:A7:91:LEU:HB2	8:A7:105:PHE:HB2	1.87	0.56
10:AA:598:U:H2'	10:AA:599:G:C8	2.40	0.56
10:AA:1881:U:H3'	10:AA:1882:U:H5''	1.87	0.56
19:AK:101:LYS:HE2	19:AK:102:TYR:CZ	2.40	0.56
35:BA:74:C:O2'	46:BN:71:ASN:OD1	2.22	0.56
51:BS:46:MET:HG3	53:BU:146:LEU:HD12	1.87	0.56
34:Az:161:SER:OG	34:Az:162:PRO:HD3	2.05	0.56
34:Az:214:GLU:OE1	34:Az:218:LYS:N	2.34	0.56
52:BT:186:GLU:HA	52:BT:189:ARG:HH21	1.69	0.56
66:Bh:77:THR:OG1	66:Bh:78:GLY:N	2.39	0.56
10:AA:763:G:H2'	10:AA:764:U:H6	1.70	0.56
10:AA:1647:A:OP1	17:Al:66:ARG:NH1	2.39	0.56
64:Bf:141:GLU:OE2	64:Bf:141:GLU:N	2.31	0.56
20:AL:106:LEU:O	20:AL:110:LYS:HG3	2.06	0.56
35:BA:81:U:H5''	49:BQ:203:PRO:HG3	1.86	0.56
57:BY:45:MET:HE2	57:BY:45:MET:HA	1.88	0.56
80:Bv:61:VAL:HG11	80:Bv:98:ILE:HG21	1.86	0.56
10:AA:767:C:H2'	10:AA:768:A:H8	1.71	0.56
10:AA:843:G:H21	10:AA:889:G:H1	1.54	0.56
34:Az:176:LEU:HD12	34:Az:177:PHE:H	1.69	0.56
54:BV:100:LYS:O	54:BV:101:LYS:HG2	2.06	0.56
41:BG:18:U:H2'	41:BG:19:C:C6	2.40	0.56
58:BZ:63:ARG:NH2	58:BZ:81:LYS:O	2.37	0.56
53:BU:144:GLU:N	53:BU:144:GLU:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Bk:92:THR:HG22	69:Bk:94:ARG:H	1.71	0.56
73:Bo:84:ARG:HG2	73:Bo:84:ARG:HH11	1.70	0.56
4:A3:150:LEU:HD12	4:A3:154:ASP:HB3	1.87	0.56
55:BW:17:LEU:HD13	55:BW:53:ALA:HB3	1.88	0.55
5:A4:101:GLN:NE2	10:AA:808:U:O2	2.35	0.55
8:A7:164:LEU:O	8:A7:165:ASP:C	2.48	0.55
10:AA:771:C:H2'	10:AA:772:C:H6	1.72	0.55
25:AR:45:ASP:OD1	25:AR:47:ASN:N	2.36	0.55
5:A4:33:GLU:HG3	5:A4:43:LEU:HB3	1.87	0.55
21:AM:88:GLN:HA	21:AM:96:THR:HG23	1.87	0.55
35:BA:1316:U:OP1	47:BO:141:LYS:NZ	2.25	0.55
35:BA:1278:U:OP2	67:Bi:44:ARG:NH2	2.39	0.55
42:BH:79:A:N1	42:BH:86:G:C6	2.74	0.55
46:BN:72:MET:HE2	60:Bb:102:LEU:HD22	1.88	0.55
48:BP:85:GLU:H	48:BP:85:GLU:CD	2.13	0.55
60:Bb:86:GLU:HA	60:Bb:89:LYS:HE2	1.89	0.55
35:BA:232:C:H2'	61:Bc:134:MET:HE3	1.88	0.55
36:BB:781:C:O2'	36:BB:1038:U:O2	2.24	0.55
10:AA:2177:C:H2'	10:AA:2178:G:C8	2.42	0.55
10:AA:2177:C:H2'	10:AA:2178:G:H8	1.72	0.55
45:BL:49:GLU:OE1	45:BL:82:LYS:NZ	2.38	0.55
10:AA:2030:A:OP1	28:AU:39:ARG:NH2	2.38	0.55
11:AB:76:A:H62	36:BB:1248:G:H5'	1.72	0.55
13:AD:2:THR:HG23	13:AD:47:LEU:HB3	1.88	0.55
35:BA:1187:A:H2'	35:BA:1233:A:C2	2.42	0.55
36:BB:1117:A:N6	45:BL:131:GLY:O	2.40	0.55
41:BG:92:U:H2'	41:BG:93:U:C6	2.41	0.55
10:AA:355:G:O2'	10:AA:357:G:OP2	2.18	0.55
35:BA:1639:A:N6	66:Bh:156:GLU:OE1	2.40	0.55
8:A7:267:ASN:HD21	8:A7:269:ASP:HB3	1.71	0.55
21:AM:35:LYS:HG2	21:AM:104:VAL:HG21	1.89	0.55
55:BW:85:LYS:NZ	89:BW:301:HOH:O	2.34	0.55
61:Bc:9:TRP:CG	61:Bc:40:LYS:HG3	2.42	0.55
4:A3:230:ARG:NH2	10:AA:847:A:O2'	2.37	0.54
10:AA:500:A:H2'	10:AA:501:C:C6	2.42	0.54
36:BB:1511:C:H2'	36:BB:1512:C:C6	2.42	0.54
73:Bo:36:LYS:HD2	73:Bo:48:ARG:HE	1.72	0.54
44:BK:44:ASP:OD2	44:BK:185:ARG:NH1	2.41	0.54
35:BA:438:G:O2'	35:BA:440:U:OP1	2.25	0.54
45:BL:58:ARG:HG2	45:BL:59:LEU:HG	1.89	0.54
60:Bb:131:ASP:OD2	60:Bb:135:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Bl:149:ILE:OXT	80:Bv:27:ARG:NH1	2.41	0.54
2:A1:85:ASP:N	2:A1:85:ASP:OD1	2.40	0.54
22:AO:42:GLU:C	22:AO:44:LYS:HZ3	2.14	0.54
10:AA:1613:A:H61	10:AA:1922:G:N2	2.03	0.54
36:BB:571:G:O2'	36:BB:574:U:OP2	2.26	0.54
52:BT:89:MET:HE3	52:BT:90:PRO:HD2	1.88	0.54
79:Bu:295:LYS:O	79:Bu:299:VAL:HG23	2.07	0.54
2:A1:228:ASP:OD2	2:A1:231:SER:OG	2.25	0.54
24:AQ:15:GLN:HB2	24:AQ:114:PRO:HG2	1.90	0.54
35:BA:1236:U:H5''	81:Bw:122:ARG:HD2	1.89	0.54
52:BT:92:LYS:HE3	52:BT:96:MET:HE2	1.88	0.54
76:Br:264:THR:HG22	76:Br:265:PHE:H	1.73	0.54
13:AD:78:GLU:H	13:AD:78:GLU:CD	2.15	0.54
21:AM:23:GLY:HA2	21:AM:57:ALA:HB3	1.90	0.54
35:BA:212:A:N1	61:Bc:139:LYS:NZ	2.54	0.54
36:BB:633:G:H2'	36:BB:634:G:C8	2.42	0.54
52:BT:183:LYS:O	52:BT:183:LYS:NZ	2.40	0.54
12:AC:60:HIS:HB3	12:AC:87:ILE:HD11	1.90	0.54
16:AH:49:VAL:HG13	16:AH:53:MET:HE2	1.89	0.54
41:BG:149:U:H1'	41:BG:150:A:H5''	1.89	0.54
79:Bu:289:LYS:HD2	79:Bu:289:LYS:C	2.33	0.54
3:A2:51:ARG:HG3	3:A2:51:ARG:HH11	1.71	0.54
36:BB:1039:C:H2'	36:BB:1040:U:O2	2.07	0.54
43:BI:23:ASN:HB3	43:BI:26:ILE:HB	1.89	0.54
44:BK:93:PRO:HB2	44:BK:125:THR:HG22	1.89	0.54
53:BU:32:THR:O	53:BU:33:ASN:ND2	2.40	0.54
83:By:133:THR:OG1	83:By:141:GLU:OE2	2.19	0.54
13:AD:76:ASN:O	13:AD:79:GLY:N	2.41	0.54
35:BA:727:C:H2'	35:BA:728:C:H6	1.72	0.54
36:BB:608:U:H2'	36:BB:609:A2M:H8	1.89	0.54
2:A1:8:ARG:O	2:A1:9:LEU:HB2	2.07	0.53
10:AA:1668:G:H2'	10:AA:1669:A:O4'	2.07	0.53
1:A0:196:ARG:NH2	1:A0:197:ASP:OD1	2.41	0.53
2:A1:30:ALA:HB3	10:AA:146:C:H1'	1.90	0.53
16:AH:27:TYR:HB3	16:AH:34:PHE:HB2	1.90	0.53
37:BC:67:U:H2'	37:BC:68:A:C8	2.43	0.53
8:A7:146:LEU:HD23	8:A7:181:TRP:CE3	2.43	0.53
10:AA:1748:C:H2'	10:AA:1749:A:C8	2.43	0.53
36:BB:1517:G:H4'	64:Bf:138:ARG:HB3	1.90	0.53
39:BE:35:A:H62	39:BE:192:C:H5	1.55	0.53
59:Ba:100:ASP:HB3	59:Ba:103:LYS:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:Bm:99:GLU:OE1	71:Bm:103:ARG:NH2	2.41	0.53
13:AD:83:MET:O	13:AD:87:LEU:HD12	2.09	0.53
34:Az:161:SER:HG	34:Az:221:ARG:HB3	1.74	0.53
37:BC:20:C:OP1	76:Br:194:LYS:NZ	2.42	0.53
83:By:92:PHE:HD2	83:By:140:ASP:HB3	1.73	0.53
6:A5:21:HIS:HB2	10:AA:126:U:O2	2.08	0.53
31:AX:136:THR:HG23	31:AX:184:ASN:HB3	1.90	0.53
61:Bc:9:TRP:CE2	61:Bc:40:LYS:HB2	2.43	0.53
63:Be:250:ARG:H	63:Be:250:ARG:CD	2.22	0.53
10:AA:302:A:H2'	10:AA:303:A:C8	2.44	0.53
10:AA:424:U:H2'	10:AA:425:G:C8	2.43	0.53
10:AA:1015:C:H2'	10:AA:1016:C:C6	2.44	0.53
35:BA:642:C:H2'	35:BA:643:G:C8	2.43	0.53
58:BZ:80:ASP:OD1	58:BZ:81:LYS:HG2	2.09	0.53
74:Bp:47:MET:HE1	74:Bp:52:LYS:HE3	1.91	0.53
10:AA:762:C:H41	10:AA:788:U:H3	1.57	0.53
55:BW:70:GLU:H	55:BW:70:GLU:CD	2.15	0.53
12:AC:58:HIS:HB3	12:AC:61:LEU:HD23	1.90	0.53
25:AR:61:GLY:HA2	25:AR:64:ARG:HG3	1.91	0.53
36:BB:5:A:H2'	36:BB:6:A:C8	2.44	0.53
53:BU:141:LYS:HZ3	53:BU:141:LYS:H	1.55	0.53
79:Bu:297:ALA:O	79:Bu:300:ILE:HG13	2.08	0.53
80:Bv:160:GLN:HA	80:Bv:160:GLN:OE1	2.08	0.53
1:A0:25:SER:O	1:A0:26:ARG:HG2	2.09	0.53
10:AA:751:U:H3	10:AA:797:C:H42	1.57	0.53
35:BA:1188:A:H2	35:BA:1192:C:H1'	1.73	0.53
36:BB:1020:G:H3'	36:BB:1021:A:H2'	1.91	0.53
53:BU:141:LYS:H	53:BU:141:LYS:NZ	2.06	0.53
79:Bu:304:ARG:HA	79:Bu:304:ARG:NE	2.24	0.53
10:AA:1144:G:H1	10:AA:1237:U:H3	1.56	0.53
10:AA:1853:A:H4'	10:AA:1854:U:O5'	2.09	0.53
35:BA:1007:G:H2'	35:BA:1008:C:C6	2.44	0.53
36:BB:768:U:H1'	71:Bm:67:GLU:OE2	2.09	0.53
36:BB:1530:U:H3	66:Bh:52:LYS:HB2	1.74	0.52
49:BQ:157:ARG:HG3	49:BQ:161:ARG:HD2	1.90	0.52
10:AA:1988:C:H4'	22:AO:136:ALA:HB1	1.91	0.52
16:AH:47:CYS:SG	16:AH:77:ARG:HD2	2.49	0.52
26:AS:124:LYS:HE2	26:AS:127:SER:HA	1.92	0.52
32:AY:25:GLU:HA	32:AY:25:GLU:OE2	2.10	0.52
34:Az:230:GLN:H	34:Az:230:GLN:CD	2.17	0.52
68:Bj:114:VAL:O	68:Bj:117:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:By:185:ILE:HG13	83:By:186:GLU:HG2	1.92	0.52
36:BB:576:A:OP1	36:BB:578:OMU:H5	2.10	0.52
12:AC:140:ILE:O	12:AC:143:THR:OG1	2.24	0.52
19:AK:76:ARG:NH1	19:AK:76:ARG:HB3	2.25	0.52
23:AP:92:LEU:HD22	23:AP:217:ARG:HB3	1.91	0.52
37:BC:6:G:H2'	37:BC:7:OMU:H6	1.91	0.52
10:AA:1863:U:O2'	10:AA:1864:U:OP1	2.23	0.52
35:BA:727:C:H2'	35:BA:728:C:C6	2.45	0.52
54:BV:34:ALA:HA	54:BV:39:PHE:HB2	1.92	0.52
65:Bg:43:LYS:O	65:Bg:47:GLN:HG3	2.09	0.52
76:Br:11:SER:OG	76:Br:14:GLU:O	2.28	0.52
10:AA:320:C:H1'	10:AA:321:A:H2	1.74	0.52
10:AA:1926:C:H5'	21:AM:130:LEU:HD22	1.91	0.52
14:AE:56:LEU:HD22	14:AE:56:LEU:H	1.75	0.52
39:BE:21:U:H5''	39:BE:22:U:H5'	1.90	0.52
74:Bp:50:LYS:H	74:Bp:50:LYS:HD2	1.73	0.52
10:AA:584:C:N4	10:AA:601:U:O4	2.43	0.52
12:AC:43:VAL:HG13	12:AC:44:LEU:HD13	1.92	0.52
17:AI:28:GLU:OE1	17:AI:28:GLU:HA	2.10	0.52
19:AK:104:ASN:ND2	19:AK:107:GLU:OE2	2.43	0.52
36:BB:1011:U:C2	36:BB:1012:C:H5	2.28	0.52
1:A0:207:ILE:HG13	1:A0:208:PRO:HD2	1.91	0.52
10:AA:693:A:H2'	10:AA:694:A:C8	2.45	0.52
16:AH:54:LYS:NZ	16:AH:73:ASP:OD2	2.34	0.52
35:BA:805:U:H2'	35:BA:806:C:C6	2.45	0.52
6:A5:41:ARG:HA	6:A5:59:ARG:O	2.11	0.51
10:AA:95:C:O2'	10:AA:97:C:OP1	2.24	0.51
19:AK:33:CYS:HA	19:AK:69:LEU:O	2.10	0.51
35:BA:746:A2M:H2'	35:BA:747:OMC:C6	2.44	0.51
35:BA:1036:G:N2	35:BA:1045[B]:A:H62	2.08	0.51
37:BC:121:G:H2'	37:BC:122:A:C8	2.45	0.51
1:A0:46:THR:OG1	16:AH:39:ASP:OD2	2.24	0.51
10:AA:839:A:H61	10:AA:891:C:H42	1.57	0.51
10:AA:1184:A:H2'	10:AA:1185:U:H6	1.76	0.51
42:BH:72:G:H8	42:BH:93:G:H22	1.56	0.51
10:AA:892:C:H2'	10:AA:893:G:H8	1.74	0.51
39:BE:148:A:H4'	39:BE:149:A:H5'	1.91	0.51
61:Bc:8:GLN:HB3	61:Bc:46:LEU:HD11	1.91	0.51
4:A3:134:ARG:NH1	10:AA:198:C:OP1	2.36	0.51
10:AA:1990:U:O2'	10:AA:1991:G:OP1	2.26	0.51
17:AI:75:LYS:HD2	17:AI:76:ALA:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AK:56:GLU:OE2	19:AK:88:ARG:NH1	2.44	0.51
34:Az:212:GLY:HA2	34:Az:219:LYS:NZ	2.25	0.51
35:BA:502:U:H2'	35:BA:503:A:C8	2.45	0.51
36:BB:1040:U:H2'	36:BB:1041:G:C8	2.46	0.51
41:BG:148:C:O2'	41:BG:149:U:O2	2.22	0.51
34:Az:161:SER:OG	34:Az:221:ARG:HB3	2.10	0.51
35:BA:765:A:H2'	35:BA:766:G:C8	2.45	0.51
45:BL:98:LEU:O	45:BL:102:ASN:ND2	2.43	0.51
15:AG:56:ASP:OD2	30:AW:53:SER:OG	2.25	0.51
26:AS:109:GLY:O	26:AS:119:ARG:NH1	2.41	0.51
35:BA:1575:C:OP2	67:Bi:60:SER:OG	2.24	0.51
65:Bg:85:ASN:OD1	65:Bg:85:ASN:N	2.43	0.51
1:A0:169:ARG:C	1:A0:171:THR:H	2.19	0.51
10:AA:759:U:H2'	10:AA:760:G:C4	2.45	0.51
10:AA:1962:A:H2	10:AA:1981:G:H1	1.54	0.51
23:AP:184:ARG:HA	23:AP:205:ASP:OD2	2.10	0.51
74:Bp:76:ASN:OD1	74:Bp:76:ASN:N	2.41	0.51
66:Bh:128:ASP:OD1	66:Bh:129:ALA:N	2.44	0.51
10:AA:582:A:O2'	10:AA:583:C:O5'	2.29	0.51
23:AP:147:VAL:HG21	23:AP:229:ARG:HG3	1.92	0.51
36:BB:1428:U:H2'	36:BB:1429:PSU:C6	2.46	0.51
44:BK:52:VAL:HG12	44:BK:152:LEU:HD13	1.93	0.51
70:Bl:113:THR:HG21	70:Bl:125:LYS:HG3	1.92	0.51
8:A7:255:ALA:HB2	8:A7:291:ILE:HG12	1.91	0.51
16:AH:135:ARG:HH21	29:AV:29:SER:HB2	1.75	0.51
35:BA:1316:U:H5	35:BA:1457:A:N7	2.09	0.51
35:BA:1574:G:N2	35:BA:1577:A:OP2	2.40	0.51
45:BL:38:THR:O	45:BL:39:ARG:HG2	2.11	0.51
8:A7:261:ARG:HA	8:A7:273:GLU:HA	1.93	0.50
12:AC:162:ASP:O	12:AC:166:ASP:HB2	2.11	0.50
17:AI:41:LYS:HG3	17:AI:52:MET:HE2	1.92	0.50
35:BA:1342:A:H2'	35:BA:1343:A:C8	2.46	0.50
61:Bc:2:THR:OG1	61:Bc:3:HIS:N	2.39	0.50
10:AA:585:G:H22	10:AA:599:G:N2	2.10	0.50
13:AD:6:PRO:HG2	13:AD:9:SER:HB2	1.93	0.50
7:A6:125:ARG:HD3	32:AY:33:ARG:HD3	1.93	0.50
44:BK:82:LYS:HG3	44:BK:83:GLU:OE1	2.11	0.50
61:Bc:30:ASP:HB3	61:Bc:33:ASN:HB2	1.94	0.50
10:AA:771:C:H2'	10:AA:772:C:C6	2.46	0.50
10:AA:986:C:H2'	10:AA:987:C:C6	2.46	0.50
10:AA:1574:G:N1	10:AA:2070:G7M:OP2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BB:980:A:H3'	36:BB:981:C:C6	2.46	0.50
20:AL:25:ASN:OD1	20:AL:26:LYS:N	2.42	0.50
22:AO:44:LYS:HE2	22:AO:44:LYS:N	2.26	0.50
24:AQ:23:SER:OG	24:AQ:24:ARG:N	2.43	0.50
60:Bb:100:ASP:O	60:Bb:104:ASN:ND2	2.40	0.50
10:AA:1201:A:H2'	10:AA:1202:G:C8	2.46	0.50
10:AA:1524:U:H2'	10:AA:1525:U:C6	2.47	0.50
13:AD:94:VAL:HG22	13:AD:95:PRO:HD2	1.94	0.50
31:AX:32:GLY:O	31:AX:51:SER:OG	2.15	0.50
36:BB:487:G:H2'	36:BB:488:A:C8	2.47	0.50
42:BH:79:A:OP1	54:BV:15:ARG:NH2	2.45	0.50
35:BA:1595:C:OP1	61:Bc:21:LYS:NZ	2.45	0.50
10:AA:1585:U:H5'	17:AI:138:PRO:HA	1.93	0.50
12:AC:204:ARG:O	12:AC:208:SER:OG	2.28	0.50
35:BA:762:A2M:N1	35:BA:917:U:H5	2.10	0.50
35:BA:1032:G:N7	63:Be:9:ARG:NH2	2.59	0.50
36:BB:97:A:O2'	36:BB:384:C:O2	2.29	0.50
36:BB:814:C:H5	36:BB:819:G:H1	1.60	0.50
4:A3:232:HIS:O	4:A3:236:VAL:HG13	2.12	0.50
10:AA:2261:MA6:H5''	10:AA:2261:MA6:H8	1.94	0.50
13:AD:98:HIS:CE1	31:AX:63:ARG:HH21	2.30	0.50
43:BI:16:ARG:NH2	43:BI:53:LEU:O	2.44	0.50
59:Ba:82:THR:HG22	59:Ba:84:TYR:H	1.77	0.50
1:A0:24:MET:HE3	16:AH:77:ARG:HH22	1.77	0.49
5:A4:164:ARG:O	5:A4:168:GLU:HB2	2.12	0.49
10:AA:1847:U:O2'	10:AA:1848:G:N7	2.44	0.49
35:BA:804:C:H2'	35:BA:805:U:C6	2.47	0.49
35:BA:1473:U:H1'	81:Bw:251:ARG:HE	1.76	0.49
36:BB:671:C:H2'	36:BB:672:U:H6	1.76	0.49
63:Be:109:GLU:OE1	63:Be:109:GLU:N	2.35	0.49
7:A6:15:ARG:HD3	10:AA:29:G:C6	2.46	0.49
10:AA:2123:OMU:H5	89:AA:2502:HOH:O	2.11	0.49
40:BF:73:A:N3	70:Bl:35:SER:OG	2.45	0.49
45:BL:61:VAL:HB	45:BL:64:PHE:HB2	1.94	0.49
83:By:135:ALA:HB1	83:By:139:LYS:HD3	1.93	0.49
10:AA:883:G:H2'	10:AA:884:G:C8	2.47	0.49
59:Ba:93:ARG:CZ	59:Ba:93:ARG:HA	2.41	0.49
73:Bo:56:ARG:HH11	73:Bo:56:ARG:HG2	1.77	0.49
5:A4:155:MET:HE3	5:A4:186:VAL:HG23	1.94	0.49
6:A5:153:LYS:HE2	10:AA:221:C:C4	2.47	0.49
47:BO:3:LEU:HD23	47:BO:4:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A1:72:LYS:NZ	10:AA:148:C:OP1	2.43	0.49
10:AA:797:C:H2'	10:AA:798:C:C6	2.48	0.49
17:AI:64:LEU:HD22	17:AI:64:LEU:H	1.76	0.49
24:AQ:25:ASN:O	24:AQ:29:VAL:HG22	2.13	0.49
36:BB:1013:U:H4'	36:BB:1014:U:OP1	2.13	0.49
44:BK:174:THR:HG22	44:BK:176:ILE:H	1.77	0.49
57:BY:57:ARG:HG2	57:BY:61:ARG:HE	1.77	0.49
66:Bh:163:ARG:N	66:Bh:163:ARG:HD3	2.26	0.49
68:Bj:112:ALA:O	68:Bj:115:GLN:HG3	2.13	0.49
78:Bt:6:LYS:HG3	78:Bt:95:ASP:HB2	1.93	0.49
83:By:137:LEU:HD12	83:By:137:LEU:H	1.77	0.49
10:AA:742:U:H3'	10:AA:743:G:H5'	1.95	0.49
10:AA:750:G:H2'	10:AA:751:U:O4'	2.12	0.49
10:AA:849:U:H3	10:AA:886:G:H1	1.60	0.49
10:AA:1576:A:H2'	10:AA:1577:G:C8	2.47	0.49
10:AA:1936:A:H2'	10:AA:1937:C:C6	2.47	0.49
31:AX:53:LYS:HA	31:AX:55:ARG:NH2	2.27	0.49
35:BA:531:G:H2'	35:BA:532:A:C8	2.47	0.49
40:BF:62:U:O4	80:Bv:176:HIS:NE2	2.42	0.49
41:BG:2:U:H5	41:BG:22:G:H1	1.60	0.49
7:A6:170:ARG:HH21	10:AA:639:G:H2'	1.77	0.49
10:AA:301:C:H2'	10:AA:302:A:H8	1.78	0.49
35:BA:774:A:OP1	43:BI:115:SER:OG	2.29	0.49
35:BA:785:U:H4'	35:BA:786:G:O5'	2.13	0.49
35:BA:1862:A:N1	36:BB:8:U:H5	2.11	0.49
36:BB:1289:C:H2'	36:BB:1290:C:O2	2.13	0.49
36:BB:1352:G:OP2	83:By:171:ARG:NH2	2.41	0.49
76:Br:246:ARG:HG3	76:Br:247:PHE:N	2.27	0.49
13:AD:78:GLU:OE1	13:AD:78:GLU:N	2.31	0.49
34:Az:203:ALA:O	34:Az:207:VAL:HG12	2.13	0.49
35:BA:994:U:OP2	36:BB:91:C:O2'	2.27	0.49
35:BA:1558:G:O2'	67:Bi:100:THR:HG22	2.13	0.49
36:BB:1527:G:H2'	36:BB:1528:C:C6	2.48	0.49
45:BL:56:ARG:NH1	45:BL:71:LYS:HE3	2.27	0.49
59:Ba:67:VAL:O	59:Ba:112:LYS:NZ	2.46	0.49
63:Be:247:ARG:NE	89:Be:401:HOH:O	2.45	0.49
10:AA:306:C:H2'	10:AA:307:C:H6	1.76	0.49
10:AA:583:C:O2'	10:AA:584:C:H5''	2.13	0.49
10:AA:1745:G:H2'	10:AA:1746:C:C6	2.47	0.49
10:AA:2101:U:H2'	10:AA:2102:G:C8	2.48	0.49
18:AJ:23:ARG:HG3	18:AJ:23:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AQ:95:VAL:HG23	24:AQ:96:LYS:HD2	1.95	0.49
35:BA:488:A:H2'	35:BA:489:A:O4'	2.13	0.49
35:BA:562:G:H2'	35:BA:563:G:C8	2.48	0.49
66:Bh:152:GLU:HG2	66:Bh:154:LYS:HE2	1.95	0.49
17:Al:48:ALA:O	17:Al:52:MET:HG3	2.12	0.49
19:AK:48:GLU:OE2	19:AK:48:GLU:HA	2.13	0.49
35:BA:126:A:OP1	82:Bx:118:ARG:NH2	2.39	0.49
36:BB:496:A:H2'	36:BB:497:C:C6	2.47	0.49
66:Bh:150:ARG:HB2	66:Bh:173:ILE:HD11	1.95	0.49
79:Bu:64:ILE:HD13	79:Bu:109:MET:HG2	1.93	0.49
10:AA:1147:A:H2'	10:AA:1148:G:C8	2.48	0.48
36:BB:671:C:H2'	36:BB:672:U:C6	2.48	0.48
10:AA:959:G:OP2	10:AA:959:G:N2	2.33	0.48
39:BE:34:C:O2	39:BE:192:C:N4	2.44	0.48
53:BU:70:ARG:NH1	79:Bu:40:ASP:OD1	2.46	0.48
81:Bw:229:MET:HB3	81:Bw:241:ASP:OD2	2.13	0.48
36:BB:637:A:N3	36:BB:1278:G:O2'	2.39	0.48
39:BE:203:A:H2'	39:BE:204:A:C8	2.48	0.48
42:BH:124:C:H2'	42:BH:125:U:H5''	1.96	0.48
53:BU:148:ARG:O	53:BU:148:ARG:HG3	2.14	0.48
79:Bu:232:PHE:O	79:Bu:236:ILE:HD12	2.13	0.48
2:A1:209:ASP:OD1	2:A1:210:ALA:N	2.46	0.48
10:AA:1236:C:OP2	30:AW:21:LYS:NZ	2.45	0.48
27:AT:10:VAL:HG22	27:AT:34:HIS:HB3	1.95	0.48
35:BA:651:G:H21	81:Bw:87:HIS:CE1	2.32	0.48
35:BA:1680:G:O6	75:Bq:2:GLY:N	2.47	0.48
36:BB:1414:C:H2'	36:BB:1415:G:C8	2.47	0.48
74:Bp:54:ASP:N	74:Bp:54:ASP:OD1	2.42	0.48
79:Bu:204:ARG:HD3	79:Bu:209:HIS:CE1	2.49	0.48
10:AA:1735:G:H22	31:AX:202:ASP:HB2	1.78	0.48
10:AA:1772:C:O2'	10:AA:1773:A:OP1	2.30	0.48
13:AD:66:PHE:CZ	13:AD:69:ARG:HA	2.47	0.48
44:BK:182:GLU:OE1	44:BK:185:ARG:NH2	2.46	0.48
46:BN:157:ARG:O	46:BN:157:ARG:HG3	2.13	0.48
68:Bj:99:GLU:OE1	68:Bj:102:ARG:NH1	2.44	0.48
16:AH:17:ASP:N	16:AH:17:ASP:OD1	2.46	0.48
35:BA:1861:C:O2'	37:BC:139:A:N3	2.42	0.48
36:BB:424:G:H2'	36:BB:425:C:C6	2.49	0.48
58:BZ:48:ARG:HH11	58:BZ:107:LYS:HG2	1.78	0.48
3:A2:50:ALA:HB2	3:A2:130:MET:HE1	1.96	0.48
34:Az:177:PHE:HD1	34:Az:178:THR:N	2.05	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BB:1038:U:H2'	36:BB:1039:C:H5'	1.95	0.48
79:Bu:287:GLU:OE2	79:Bu:287:GLU:N	2.21	0.48
10:AA:601:U:O2'	10:AA:602:U:O2	2.18	0.48
36:BB:1424:C:C5'	36:BB:1425:A:H62	2.26	0.48
36:BB:1507:U:H2'	36:BB:1508:C:C6	2.49	0.48
38:BD:92:G:H2'	38:BD:93:G:C8	2.49	0.48
47:BO:203:GLU:OE1	47:BO:207:LYS:NZ	2.47	0.48
10:AA:2112:U:H2'	10:AA:2113:C:C6	2.49	0.48
23:AP:248:ASP:OD1	23:AP:248:ASP:N	2.45	0.48
27:AT:58:ASP:O	27:AT:61:GLN:HB2	2.13	0.48
35:BA:71:C:OP1	49:BQ:196:HIS:ND1	2.38	0.48
36:BB:810:C:H2'	36:BB:811:A:H8	1.77	0.48
10:AA:585:G:H22	10:AA:599:G:H22	1.60	0.48
10:AA:835:A:H2'	10:AA:836:A:H8	1.79	0.48
36:BB:980:A:H3'	36:BB:981:C:H6	1.77	0.48
57:BY:2:ARG:HD2	57:BY:2:ARG:HA	1.61	0.48
5:A4:164:ARG:NH1	5:A4:168:GLU:OE2	2.42	0.47
31:AX:177:ARG:NH2	32:AY:63:GLY:O	2.47	0.47
35:BA:728:C:O2	70:Bl:133:ALA:HB3	2.15	0.47
36:BB:996:G:H2'	36:BB:997:G:C8	2.49	0.47
42:BH:54:U:H2'	42:BH:55:C:C6	2.49	0.47
48:BP:147:LEU:HD21	70:Bl:18:LYS:HG2	1.95	0.47
31:AX:135:VAL:HG22	31:AX:185:VAL:HG22	1.96	0.47
82:Bx:240:ASP:N	82:Bx:240:ASP:OD1	2.48	0.47
10:AA:762:C:H2'	10:AA:763:G:C8	2.49	0.47
10:AA:1016:C:H2'	10:AA:1017:U:O4'	2.15	0.47
10:AA:1183:A:H2'	10:AA:1184:A:C8	2.49	0.47
23:AP:116:ASP:OD1	23:AP:117:GLY:N	2.46	0.47
35:BA:1044:G:H4'	35:BA:1045[B]:A:C8	2.48	0.47
1:A0:131:THR:OG1	1:A0:132:ALA:O	2.32	0.47
1:A0:133:ASP:OD1	1:A0:133:ASP:N	2.47	0.47
8:A7:3:VAL:HB	8:A7:314:VAL:HG23	1.96	0.47
10:AA:746:C:H2'	10:AA:747:C:H4'	1.96	0.47
10:AA:2163:A:H2'	10:AA:2164:C:O4'	2.14	0.47
36:BB:1290:C:H5	36:BB:1306:C:H42	1.61	0.47
38:BD:63:C:H3'	44:BK:204:GLY:O	2.14	0.47
49:BQ:22:MET:O	49:BQ:26:GLU:HG2	2.15	0.47
10:AA:295:U:O2'	10:AA:296:A:O5'	2.28	0.47
10:AA:1302:A:H2'	10:AA:1304:A:H5''	1.97	0.47
10:AA:1512:G:O2'	10:AA:1513:G:H5'	2.14	0.47
13:AD:100:VAL:HG13	31:AX:61:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:958:G:O6	73:Bo:4:ARG:NH2	2.48	0.47
36:BB:1292:A:H4'	44:BK:74:LYS:HG2	1.96	0.47
45:BL:164:GLU:OE1	45:BL:164:GLU:N	2.36	0.47
58:BZ:8:ASN:HB3	58:BZ:11:LYS:HB3	1.97	0.47
83:By:151:GLN:O	83:By:155:GLU:HG2	2.13	0.47
2:A1:189:ILE:HG21	2:A1:229:MET:HE1	1.96	0.47
10:AA:1216:A:H2'	10:AA:1217:A:C8	2.49	0.47
18:AJ:26:LEU:HD12	18:AJ:62:VAL:HG22	1.95	0.47
35:BA:16:U:H2'	35:BA:17:G:H8	1.80	0.47
35:BA:502:U:H2'	35:BA:503:A:H8	1.79	0.47
35:BA:639:G:OP1	81:Bw:71:ARG:NH2	2.47	0.47
36:BB:359:A:O2'	36:BB:360:U:OP1	2.27	0.47
36:BB:1022:G:H2'	36:BB:1023:U:C6	2.50	0.47
64:Bf:201:LYS:HE3	64:Bf:201:LYS:HB3	1.60	0.47
81:Bw:80:LEU:HD23	81:Bw:91:TYR:CE1	2.50	0.47
6:A5:116:HIS:O	6:A5:165:ARG:NH1	2.46	0.47
12:AC:241:ARG:HB2	20:AL:82:MET:HE1	1.97	0.47
22:AO:50:CYS:O	22:AO:54:VAL:HG13	2.15	0.47
31:AX:153:ASP:C	31:AX:153:ASP:OD1	2.58	0.47
54:BV:81:THR:OG1	54:BV:83:MET:N	2.43	0.47
78:Bt:95:ASP:HB3	78:Bt:96:LYS:NZ	2.30	0.47
79:Bu:302:ARG:HG2	79:Bu:306:ARG:NH2	2.29	0.47
2:A1:119:LYS:HD3	2:A1:121:MET:HE3	1.96	0.47
10:AA:837:A:H2	10:AA:893:G:C2	2.30	0.47
12:AC:232:GLU:H	12:AC:232:GLU:CD	2.17	0.47
23:AP:241:ALA:O	25:AR:21:LYS:NZ	2.48	0.47
29:AV:35:ASP:OD1	29:AV:35:ASP:N	2.45	0.47
35:BA:456:A:H2'	35:BA:457:A:C8	2.50	0.47
35:BA:1830:G:O2'	35:BA:1831:A:OP1	2.31	0.47
36:BB:477:A:H2'	36:BB:478:A:H8	1.78	0.47
36:BB:1335:C:H2'	36:BB:1336:U:C6	2.50	0.47
36:BB:1377:U:H2'	36:BB:1378:U:C6	2.50	0.47
36:BB:1424:C:H5'	36:BB:1425:A:H62	1.80	0.47
63:Be:140:ASN:OD1	63:Be:143:THR:OG1	2.30	0.47
70:Bl:33:ARG:C	70:Bl:34:LYS:HG2	2.39	0.47
4:A3:44:GLU:OE2	4:A3:44:GLU:HA	2.15	0.47
10:AA:80:U:H2'	10:AA:81:G:C8	2.50	0.47
10:AA:486:C:H2'	10:AA:487:C:C6	2.50	0.47
21:AM:92:LYS:HB3	21:AM:92:LYS:HE3	1.58	0.47
35:BA:557:U:H2'	35:BA:558:C:C6	2.50	0.47
35:BA:906:A:H4'	35:BA:907:G:H5'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BW:86:SER:HA	55:BW:96:TYR:HB3	1.97	0.47
2:A1:130:THR:C	2:A1:132:ARG:H	2.23	0.46
12:AC:74:ILE:HD11	12:AC:186:THR:HG23	1.96	0.46
24:AQ:47:VAL:HG12	24:AQ:88:LEU:HB3	1.97	0.46
74:Bp:7:ASN:ND2	74:Bp:10:GLU:OE2	2.48	0.46
79:Bu:98:ALA:HB1	79:Bu:168:VAL:HG23	1.97	0.46
83:By:43:ASP:HB3	83:By:56:VAL:HB	1.97	0.46
83:By:107:LEU:HD23	83:By:123:VAL:HG22	1.97	0.46
20:AL:104:GLN:OE1	20:AL:104:GLN:N	2.42	0.46
39:BE:38:C:H2'	39:BE:39:A:O4'	2.15	0.46
45:BL:38:THR:C	45:BL:40:ALA:H	2.23	0.46
59:Ba:66:GLN:OE1	59:Ba:66:GLN:HA	2.16	0.46
69:Bk:99:LEU:HD22	69:Bk:103:GLU:HB3	1.97	0.46
73:Bo:56:ARG:HG2	73:Bo:56:ARG:NH1	2.29	0.46
76:Br:8:SER:HB3	76:Br:17:VAL:HG13	1.97	0.46
3:A2:87:HIS:HB2	3:A2:94:PRO:HG3	1.98	0.46
10:AA:56:A2M:HM'3	10:AA:56:A2M:H1'	1.74	0.46
10:AA:216:G:O2'	10:AA:217:G:H5''	2.15	0.46
10:AA:890:U:H2'	10:AA:891:C:C6	2.51	0.46
10:AA:2044:A:H2'	10:AA:2045:PSU:C6	2.49	0.46
20:AL:36:MET:HE3	20:AL:36:MET:HB3	1.80	0.46
27:AT:9:GLU:OE1	27:AT:9:GLU:HA	2.15	0.46
35:BA:747:OMC:HM21	36:BB:1325:G:C6	2.50	0.46
36:BB:362:G:H2'	36:BB:363:C:C6	2.51	0.46
42:BH:47:G:H2'	42:BH:48:G:N3	2.30	0.46
81:Bw:31:ALA:O	81:Bw:35:GLN:HG3	2.16	0.46
2:A1:26:PRO:HD3	10:AA:541:G:OP1	2.15	0.46
4:A3:188:ARG:NH1	10:AA:173:C:OP2	2.48	0.46
10:AA:376:G:H3'	10:AA:377:C:H5''	1.97	0.46
10:AA:1644:U:H2'	10:AA:1645:G:C8	2.51	0.46
31:AX:192:SER:OG	31:AX:195:GLU:O	2.24	0.46
35:BA:915:OMG:H2'	35:BA:916:OMU:H6	1.96	0.46
61:Bc:119:ARG:NH1	67:Bi:114:HIS:O	2.49	0.46
63:Be:54:ARG:HG2	63:Be:56:ALA:H	1.81	0.46
66:Bh:127:ILE:HD13	66:Bh:127:ILE:HA	1.81	0.46
69:Bk:77:LYS:HD2	69:Bk:77:LYS:HA	1.69	0.46
72:Bn:83:LYS:HB3	72:Bn:83:LYS:HE3	1.57	0.46
81:Bw:218:TRP:CD1	81:Bw:219:PRO:HD2	2.51	0.46
12:AC:112:VAL:HG12	12:AC:159:VAL:HB	1.98	0.46
36:BB:683:A:H2'	36:BB:684:C:C6	2.49	0.46
10:AA:1662:U:N3	13:AD:4:TYR:HE1	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AD:64:GLU:HB2	13:AD:73:TRP:CD1	2.50	0.46
26:AS:39:ASN:ND2	26:AS:41:PHE:O	2.49	0.46
31:AX:156:MET:HE2	31:AX:156:MET:HB2	1.80	0.46
35:BA:1330:OMU:HM23	35:BA:1330:OMU:H1'	1.65	0.46
38:BD:23:A:H2'	38:BD:24:U:C6	2.50	0.46
5:A4:12:LYS:HB2	10:AA:1022:A:OP2	2.16	0.46
18:AJ:60:LYS:HE3	18:AJ:60:LYS:HB2	1.68	0.46
35:BA:912:C:H2'	35:BA:913:C:C6	2.51	0.46
54:BV:101:LYS:HG3	54:BV:103:LEU:HD22	1.97	0.46
57:BY:60:ARG:HA	57:BY:60:ARG:HD2	1.70	0.46
69:Bk:125:VAL:HG13	69:Bk:126:LYS:HG2	1.97	0.46
10:AA:1737:U:H3	10:AA:1886:G:H22	1.62	0.46
10:AA:2275:C:OP2	29:AV:5:ARG:NH1	2.48	0.46
20:AL:58:MET:HE3	20:AL:58:MET:HB3	1.76	0.46
24:AQ:102:GLN:OE1	31:AX:39:ARG:NH1	2.49	0.46
35:BA:743:A2M:H5'	35:BA:743:A2M:C8	2.44	0.46
35:BA:1864:G:H2'	35:BA:1865:U:H6	1.80	0.46
36:BB:1140:A:H2'	36:BB:1141:G:C8	2.50	0.46
48:BP:23:ARG:HE	48:BP:43:GLU:CD	2.24	0.46
53:BU:36:VAL:HA	53:BU:64:VAL:HG22	1.98	0.46
54:BV:40:SER:O	54:BV:43:ILE:N	2.48	0.46
55:BW:11:CYS:O	64:Bf:66:LYS:NZ	2.26	0.46
72:Bn:39:TYR:CD1	72:Bn:40:PRO:HA	2.51	0.46
80:Bv:95:THR:OG1	80:Bv:96:SER:N	2.44	0.46
83:By:159:MET:HE3	83:By:159:MET:HB2	1.88	0.46
30:AW:11:PRO:HB2	30:AW:16:GLU:HG2	1.98	0.46
35:BA:1648:U:H3	66:Bh:79:ARG:CZ	2.29	0.46
36:BB:29:C:OP1	36:BB:32:C:N4	2.48	0.46
40:BF:56:A:H4'	40:BF:57:G:O5'	2.15	0.46
41:BG:62:C:O2'	83:By:118:ARG:HD3	2.16	0.46
42:BH:27:A:OP2	66:Bh:69:THR:HG21	2.16	0.46
52:BT:178:LEU:O	52:BT:179:LYS:NZ	2.41	0.46
7:A6:63:GLU:CD	7:A6:64:ASN:H	2.24	0.46
8:A7:198:TYR:HE1	20:AL:23:LYS:HA	1.80	0.46
10:AA:1960:C:H42	10:AA:1983:U:H5	1.64	0.46
12:AC:148:ILE:HG22	12:AC:149:GLN:NE2	2.31	0.46
17:AI:72:LYS:HB2	17:AI:72:LYS:HE2	1.69	0.46
22:AO:27:HIS:HB3	22:AO:30:ARG:HG3	1.98	0.46
35:BA:616:G:H5''	35:BA:706:G:H1'	1.98	0.46
36:BB:1221:A:OP2	46:BN:192:LYS:NZ	2.49	0.46
2:A1:197:ARG:HD3	2:A1:197:ARG:HA	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A7:148:ARG:HA	8:A7:148:ARG:HD3	1.60	0.45
10:AA:608:C:O2'	10:AA:609:A:H8	1.99	0.45
10:AA:972:C:H2'	10:AA:973:A:O4'	2.16	0.45
10:AA:1762:A:O2'	22:AO:149:ASP:OD2	2.25	0.45
29:AV:7:ASN:HB3	29:AV:10:ARG:O	2.16	0.45
35:BA:753:A:H2'	35:BA:754:A:C8	2.50	0.45
35:BA:1181:OMU:H6	35:BA:1181:OMU:O5'	2.16	0.45
52:BT:165:LYS:HB3	52:BT:165:LYS:HE3	1.54	0.45
4:A3:140:ARG:HB3	4:A3:143:LYS:HG3	1.98	0.45
26:AS:101:LEU:HB3	26:AS:124:LYS:HG2	1.98	0.45
36:BB:473:U:H3	36:BB:500:G:H1	1.64	0.45
59:Ba:46:LYS:N	59:Ba:68:GLY:O	2.31	0.45
60:Bb:132:LYS:HB3	60:Bb:132:LYS:HE2	1.62	0.45
64:Bf:296:MET:HA	66:Bh:52:LYS:HD3	1.98	0.45
10:AA:302:A:H2'	10:AA:303:A:H8	1.80	0.45
17:AI:28:GLU:C	17:AI:31:PRO:HD2	2.41	0.45
19:AK:88:ARG:NH2	19:AK:119:ASP:OD2	2.50	0.45
26:AS:41:PHE:O	26:AS:43:GLY:N	2.46	0.45
35:BA:1024:A2M:HM'3	35:BA:1024:A2M:H1'	1.72	0.45
41:BG:19:C:H2'	41:BG:20:U:C6	2.51	0.45
52:BT:89:MET:HE3	52:BT:89:MET:HA	1.99	0.45
78:Bt:6:LYS:H	78:Bt:95:ASP:CG	2.25	0.45
10:AA:1008:U:H2'	10:AA:1009:A:C8	2.52	0.45
10:AA:1625:C:H2'	10:AA:1626:A:C8	2.49	0.45
16:AH:87:HIS:HA	16:AH:120:GLY:O	2.17	0.45
17:AI:62:VAL:O	17:AI:66:ARG:HG2	2.16	0.45
36:BB:95:A2M:HM'3	36:BB:95:A2M:H1'	1.75	0.45
39:BE:202:A:H2'	39:BE:203:A:C8	2.51	0.45
42:BH:5:G:H2'	42:BH:6:U:H6	1.81	0.45
47:BO:191:GLU:OE2	47:BO:194:ARG:NH2	2.45	0.45
52:BT:173:ALA:C	52:BT:175:LYS:H	2.25	0.45
2:A1:112:SER:OG	2:A1:113:GLU:N	2.49	0.45
10:AA:43:U:H2'	10:AA:44:G:O4'	2.16	0.45
10:AA:188:A:H2'	10:AA:189:A:O4'	2.16	0.45
10:AA:267:G:N3	10:AA:267:G:H2'	2.31	0.45
10:AA:500:A:H2'	10:AA:501:C:H6	1.81	0.45
10:AA:2272:G:O2'	29:AV:5:ARG:NH2	2.49	0.45
31:AX:57:VAL:HG12	31:AX:58:LEU:HD12	1.97	0.45
31:AX:159:SER:OG	31:AX:160:GLY:N	2.50	0.45
34:Az:177:PHE:CD1	34:Az:178:THR:N	2.76	0.45
35:BA:97:G:H2'	35:BA:98:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:1187:A:H5''	35:BA:1188:A:H5'	1.98	0.45
36:BB:1414:C:H2'	36:BB:1415:G:H8	1.81	0.45
39:BE:104:U:H2'	39:BE:105:C:C6	2.52	0.45
44:BK:30:ARG:HG3	44:BK:63:GLU:HG3	1.98	0.45
45:BL:139:GLY:HA2	45:BL:161:VAL:HG21	1.98	0.45
82:Bx:100:ARG:NH1	82:Bx:101:ASN:OD1	2.49	0.45
10:AA:320:C:H1'	10:AA:321:A:C2	2.50	0.45
10:AA:968:G:OP2	10:AA:968:G:N2	2.33	0.45
20:AL:19:LYS:NZ	31:AX:208:GLU:HA	2.32	0.45
35:BA:478:A:C2	37:BC:16:A:H1'	2.52	0.45
35:BA:1299:A:OP1	70:Bl:125:LYS:NZ	2.50	0.45
35:BA:1643:U:H5''	50:BR:42:ARG:HG3	1.99	0.45
41:BG:145:C:P	41:BG:145:C:H6	2.40	0.45
64:Bf:394:ARG:NH1	64:Bf:394:ARG:HB3	2.31	0.45
10:AA:517:C:O2'	10:AA:519:G:OP1	2.29	0.45
10:AA:2153:A2M:H1'	10:AA:2153:A2M:HM'3	1.57	0.45
23:AP:118:ASN:HB2	23:AP:151:ARG:NH2	2.32	0.45
27:AT:68:LYS:HE2	27:AT:68:LYS:HB3	1.57	0.45
36:BB:996:G:H22	36:BB:1016:U:H3	1.63	0.45
36:BB:1424:C:C5'	36:BB:1425:A:N7	2.79	0.45
44:BK:150:GLU:OE2	44:BK:153:ARG:NH1	2.49	0.45
76:Br:303:LYS:HA	76:Br:303:LYS:HD2	1.79	0.45
3:A2:37:HIS:CD2	3:A2:72:LYS:HG2	2.52	0.45
10:AA:1982:C:N4	10:AA:1983:U:O4	2.50	0.45
16:AH:77:ARG:HD3	16:AH:77:ARG:C	2.42	0.45
23:AP:139:MET:HE3	23:AP:139:MET:HB2	1.81	0.45
35:BA:615:G:H1'	35:BA:619:C:N4	2.32	0.45
48:BP:90:THR:HG22	48:BP:92:SER:H	1.82	0.45
76:Br:362:LYS:HB2	76:Br:362:LYS:HE2	1.72	0.45
79:Bu:94:ASN:HD22	79:Bu:210:VAL:HG21	1.81	0.45
4:A3:163:ARG:HH11	10:AA:94:U:H6	1.65	0.45
18:AJ:118:ALA:C	18:AJ:120:ASN:H	2.25	0.45
34:Az:209:GLU:CD	34:Az:210:LYS:HD3	2.42	0.45
35:BA:697:C:H6	35:BA:697:C:H5'	1.82	0.45
35:BA:1349:U:H2'	35:BA:1350:U:C6	2.52	0.45
40:BF:66:U:H4'	40:BF:67:U:H3'	1.99	0.45
46:BN:146:GLU:OE1	46:BN:146:GLU:N	2.50	0.45
6:A5:155:SER:OG	10:AA:220:G:OP2	2.34	0.45
16:AH:99:LYS:HE3	16:AH:99:LYS:HB2	1.60	0.45
26:AS:6:GLY:O	26:AS:7:GLN:HB3	2.17	0.45
27:AT:2:VAL:HB	27:AT:3:PHE:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:484:U:H2'	35:BA:485:G:C8	2.51	0.45
37:BC:169:G:OP1	82:Bx:100:ARG:NH2	2.50	0.45
39:BE:7:G:N2	39:BE:10:A:OP2	2.41	0.45
41:BG:73:U:OP1	64:Bf:19:ARG:NH2	2.47	0.45
83:By:183:THR:OG1	83:By:184:ASN:N	2.49	0.45
6:A5:207:GLU:HG3	14:AE:24:TYR:CD2	2.52	0.44
17:AI:100:VAL:HG22	17:AI:113:GLU:HG2	1.99	0.44
20:AL:24:LEU:HD22	20:AL:24:LEU:HA	1.84	0.44
24:AQ:43:GLU:OE1	24:AQ:45:VAL:HG23	2.17	0.44
35:BA:530:A:O2'	40:BF:70:C:H5	2.00	0.44
36:BB:469:U:H3	36:BB:501:C:N4	2.04	0.44
36:BB:1354:A:O2'	83:By:172:LYS:NZ	2.37	0.44
37:BC:7:OMU:HM23	37:BC:7:OMU:H1'	1.71	0.44
37:BC:96:A:OP1	69:Bk:71:ARG:NH2	2.50	0.44
41:BG:24:A:O2'	47:BO:6:ARG:HD2	2.17	0.44
69:Bk:104:LYS:HB2	69:Bk:104:LYS:HE3	1.76	0.44
80:Bv:39:LEU:HD11	80:Bv:82:ILE:HG13	1.99	0.44
80:Bv:102:ILE:HG13	80:Bv:103:PHE:N	2.31	0.44
2:A1:228:ASP:OD1	2:A1:230:SER:OG	2.33	0.44
6:A5:178:GLN:HB3	6:A5:184:LEU:HD23	1.98	0.44
10:AA:1726:A:H4'	10:AA:1727:A:O5'	2.17	0.44
10:AA:1760:G:H1	10:AA:1825:U:H3	1.64	0.44
20:AL:107:ALA:HA	20:AL:110:LYS:HD2	1.99	0.44
24:AQ:35:GLU:HA	24:AQ:38:GLU:HG3	1.99	0.44
35:BA:375:U:H2'	35:BA:376:U:C6	2.51	0.44
35:BA:1338:U:H5''	35:BA:1339:G:H3'	1.99	0.44
36:BB:412:U:H2'	36:BB:413:A:C8	2.52	0.44
36:BB:643:U:H2'	36:BB:644:PSU:C6	2.52	0.44
36:BB:799:G:O2'	36:BB:800:U:H6	1.98	0.44
40:BF:73:A:H5''	80:Bv:44:ARG:CZ	2.48	0.44
77:Bs:123:MET:HE3	77:Bs:123:MET:HB3	1.86	0.44
1:A0:182:ASP:C	1:A0:182:ASP:OD1	2.61	0.44
8:A7:5:TYR:HE1	8:A7:310:ARG:HB3	1.83	0.44
8:A7:258:LYS:H	8:A7:258:LYS:HG2	1.52	0.44
10:AA:680:U:O2'	10:AA:681:A:OP2	2.32	0.44
10:AA:766:C:H2'	10:AA:767:C:C6	2.52	0.44
17:AI:30:ASP:CG	17:AI:31:PRO:HD3	2.42	0.44
35:BA:245:C:H2'	35:BA:246:U:C6	2.53	0.44
36:BB:1013:U:OP1	59:Ba:55:GLY:N	2.39	0.44
44:BK:49:CYS:HB3	44:BK:168:SER:OG	2.18	0.44
45:BL:37:LEU:HD21	45:BL:54:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BL:87:LEU:HD13	45:BL:136:VAL:HG21	1.98	0.44
83:By:74:HIS:O	83:By:78:MET:HG3	2.18	0.44
10:AA:1995:A:H2'	10:AA:1996:A:C8	2.52	0.44
10:AA:2048:C:H2'	10:AA:2049:A:C8	2.52	0.44
12:AC:46:MET:HE3	20:AL:112:MET:HE1	1.99	0.44
15:AG:29:SER:HB3	15:AG:32:ASP:OD1	2.16	0.44
35:BA:145:C:H4'	35:BA:146:G:H5''	1.98	0.44
35:BA:1864:G:H2'	35:BA:1865:U:C6	2.52	0.44
37:BC:60:U:O4	69:Bk:63:ASN:ND2	2.42	0.44
41:BG:138:C:H2'	41:BG:139:U:C6	2.53	0.44
52:BT:178:LEU:C	52:BT:180:LYS:H	2.25	0.44
64:Bf:5:LYS:HG2	64:Bf:6:PHE:CE2	2.53	0.44
3:A2:44:LYS:HE3	3:A2:44:LYS:HB3	1.81	0.44
4:A3:16:VAL:HG11	4:A3:46:PHE:HZ	1.82	0.44
4:A3:157:ARG:HH22	10:AA:374:U:H5'	1.82	0.44
5:A4:82:THR:O	5:A4:86:GLU:HG2	2.18	0.44
10:AA:1173:U:H2'	10:AA:1174:C:O4'	2.17	0.44
10:AA:1566:C:C2	10:AA:1567:A:C8	3.06	0.44
10:AA:2233:A:H2'	10:AA:2234:A:C8	2.51	0.44
17:AI:59:ARG:H	17:AI:59:ARG:HD3	1.82	0.44
30:AW:5:ASP:OD1	30:AW:5:ASP:N	2.41	0.44
30:AW:22:ARG:HA	30:AW:27:GLN:HB3	2.00	0.44
35:BA:626:G:H2'	35:BA:629:C:C5	2.53	0.44
36:BB:1526:U:H3	36:BB:1534:G:H1	1.64	0.44
40:BF:64:C:H5''	80:Bv:66:MET:CE	2.48	0.44
41:BG:139:U:O2'	83:By:150:GLU:OE2	2.35	0.44
58:BZ:81:LYS:HB3	58:BZ:81:LYS:HE2	1.73	0.44
81:Bw:77:LEU:HD23	81:Bw:77:LEU:HA	1.70	0.44
8:A7:284:ILE:H	8:A7:284:ILE:HG13	1.30	0.44
10:AA:1829:U:N3	10:AA:1836:G:OP1	2.40	0.44
10:AA:1941:G:H2'	10:AA:1942:U:C6	2.53	0.44
10:AA:2208:C:H2'	10:AA:2209:G:O4'	2.18	0.44
21:AM:33:MET:HE2	21:AM:33:MET:HB3	1.82	0.44
36:BB:646:A2M:HM'3	36:BB:646:A2M:H1'	1.73	0.44
36:BB:1132:G:N3	36:BB:1132:G:H2'	2.33	0.44
45:BL:57:ALA:HB2	45:BL:72:ILE:HG13	2.00	0.44
46:BN:93:ARG:HA	46:BN:93:ARG:HD2	1.76	0.44
52:BT:176:GLN:O	52:BT:179:LYS:NZ	2.39	0.44
76:Br:294:GLU:O	76:Br:298:ARG:HG3	2.17	0.44
1:A0:216:LYS:NZ	10:AA:1163:U:OP1	2.51	0.44
6:A5:105:ASP:OD2	42:BH:85:C:N4	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A6:93:ASP:N	7:A6:93:ASP:OD1	2.50	0.44
8:A7:234:MET:HE3	8:A7:234:MET:HB3	1.80	0.44
10:AA:133:A:H2'	10:AA:134:G:C8	2.52	0.44
10:AA:773:C:C2	10:AA:774:G:C8	3.06	0.44
32:AY:39:LYS:HA	32:AY:39:LYS:HD3	1.80	0.44
35:BA:617:U:O4	76:Br:313:TYR:OH	2.35	0.44
35:BA:845:C:H3'	35:BA:846:G:H8	1.83	0.44
41:BG:167:C:H2'	41:BG:168:A:O4'	2.17	0.44
41:BG:178:G:H2'	41:BG:179:C:C6	2.53	0.44
47:BO:192:LYS:HE3	47:BO:192:LYS:HB3	1.84	0.44
51:BS:124:GLU:OE2	53:BU:153:TYR:OH	2.33	0.44
58:BZ:39:LYS:HE3	58:BZ:40:TYR:CZ	2.53	0.44
59:Ba:67:VAL:HG22	59:Ba:116:GLN:HG2	1.99	0.44
63:Be:92:VAL:HG12	63:Be:103:PRO:HG2	2.00	0.44
66:Bh:154:LYS:HE3	66:Bh:154:LYS:HB2	1.81	0.44
1:A0:70:LEU:HD23	1:A0:81:ASP:HB2	2.00	0.44
10:AA:608:C:HO2'	10:AA:609:A:H8	1.66	0.44
10:AA:2051:U:O2'	10:AA:2052:U:H2'	2.18	0.44
15:AG:127:ARG:NH1	89:AG:201:HOH:O	2.32	0.44
19:AK:87:VAL:O	19:AK:91:ILE:HG12	2.18	0.44
31:AX:142:LYS:C	31:AX:142:LYS:HD2	2.42	0.44
36:BB:361:U:H2'	36:BB:362:G:H8	1.83	0.44
36:BB:793:C:H2'	36:BB:832:C:C5	2.53	0.44
38:BD:120:C:H4'	79:Bu:275:PRO:HA	2.00	0.44
48:BP:106:THR:O	48:BP:106:THR:OG1	2.35	0.44
78:Bt:6:LYS:NZ	78:Bt:94:ASN:O	2.51	0.44
5:A4:182:THR:HG22	5:A4:184:ARG:HG2	1.99	0.44
10:AA:599:G:H2'	10:AA:600:G:H8	1.83	0.44
14:AE:62:LYS:HA	14:AE:62:LYS:HD3	1.90	0.44
34:Az:177:PHE:O	34:Az:178:THR:HG22	2.18	0.44
35:BA:728:C:H2'	35:BA:729:C:C6	2.53	0.44
35:BA:951:A:O2'	36:BB:47:C:O2	2.33	0.44
36:BB:1508:C:H2'	36:BB:1509:U:C6	2.53	0.44
61:Bc:74:LYS:HE2	61:Bc:74:LYS:HB2	1.71	0.44
3:A2:65:LYS:HA	3:A2:65:LYS:HD3	1.53	0.43
10:AA:1010:G:C4	10:AA:1011:A:C8	3.06	0.43
10:AA:1745:G:H2'	10:AA:1746:C:H6	1.83	0.43
10:AA:2154:OMU:HM23	10:AA:2154:OMU:H1'	1.50	0.43
17:AI:88:ARG:NH2	17:AI:127:SER:O	2.51	0.43
18:AJ:30:SER:HB3	18:AJ:59:GLY:HA3	2.00	0.43
19:AK:46:LEU:HA	19:AK:46:LEU:HD13	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AM:44:MET:HE3	21:AM:44:MET:HB3	1.69	0.43
36:BB:379:U:H4'	36:BB:380:A:O5'	2.17	0.43
36:BB:769:U:H2'	36:BB:770:G:H8	1.81	0.43
39:BE:172:C:H2'	39:BE:179:U:C6	2.53	0.43
45:BL:71:LYS:HD2	45:BL:71:LYS:N	2.33	0.43
53:BU:148:ARG:HD2	53:BU:153:TYR:CZ	2.53	0.43
61:Bc:101:ASP:OD1	61:Bc:101:ASP:N	2.50	0.43
78:Bt:9:LYS:HE2	78:Bt:9:LYS:HB3	1.71	0.43
8:A7:174:TRP:HA	8:A7:198:TYR:HB2	2.00	0.43
10:AA:692:C:OP2	32:AY:39:LYS:NZ	2.50	0.43
10:AA:1871:A:H2'	10:AA:1872:A:C8	2.53	0.43
12:AC:173:ALA:HB1	12:AC:178:ILE:HB	2.00	0.43
14:AE:115:ARG:HG2	26:AS:7:GLN:HA	1.99	0.43
35:BA:405:A:H2'	35:BA:406:A:O4'	2.17	0.43
35:BA:1065:A:H2'	35:BA:1066:C:C6	2.52	0.43
36:BB:79:C:O2'	41:BG:81:G:H4'	2.18	0.43
48:BP:141:LYS:HD3	48:BP:141:LYS:HA	1.65	0.43
65:Bg:85:ASN:HB2	65:Bg:97:ARG:HB3	2.00	0.43
10:AA:1325:G:H5''	30:AW:69:GLY:O	2.18	0.43
10:AA:1771:A:C5	22:AO:160:MET:HE3	2.52	0.43
31:AX:82:LYS:HA	31:AX:82:LYS:HD2	1.80	0.43
34:Az:210:LYS:HA	34:Az:210:LYS:HD2	1.78	0.43
36:BB:811:A:H2'	36:BB:812:G:C8	2.53	0.43
39:BE:8:A:C2	39:BE:104:U:H4'	2.53	0.43
50:BR:3:HIS:HB3	50:BR:4:TYR:H	1.45	0.43
81:Bw:29:LYS:HD3	81:Bw:29:LYS:HA	1.82	0.43
5:A4:42:GLN:HG3	5:A4:75:LEU:HB2	2.01	0.43
5:A4:60:LYS:HE3	5:A4:60:LYS:HB3	1.90	0.43
8:A7:137:ASN:HD21	8:A7:141:GLU:HB3	1.83	0.43
8:A7:143:MET:SD	8:A7:143:MET:N	2.92	0.43
13:AD:7:LYS:HE2	13:AD:7:LYS:HA	2.01	0.43
35:BA:18:U:OP1	56:BX:67:LYS:NZ	2.51	0.43
36:BB:55:C:N3	89:BB:1708:HOH:O	2.36	0.43
39:BE:62:U:H2'	39:BE:63:U:O2	2.18	0.43
70:Bl:24:LYS:HB2	70:Bl:24:LYS:HE3	1.49	0.43
80:Bv:90:LEU:HD22	80:Bv:93:VAL:HG21	2.01	0.43
83:By:103:VAL:HG22	83:By:108:VAL:HG22	2.00	0.43
1:A0:33:VAL:O	1:A0:100:THR:OG1	2.25	0.43
8:A7:178:VAL:HB	8:A7:192:LEU:HD12	1.99	0.43
10:AA:306:C:H2'	10:AA:307:C:C6	2.52	0.43
10:AA:1990:U:HO2'	10:AA:1991:G:P	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AA:2043:U:OP1	21:AM:89:ARG:NH2	2.43	0.43
29:AV:46:MET:HE3	29:AV:69:PRO:HB2	2.00	0.43
31:AX:210:LYS:O	31:AX:210:LYS:NZ	2.42	0.43
35:BA:1515:G:O2'	35:BA:1516:A:H5''	2.18	0.43
35:BA:1556:G:OP2	76:Br:203:ARG:HD3	2.18	0.43
35:BA:1568:G:O2'	35:BA:1570:U:OP1	2.24	0.43
36:BB:670:C:H2'	36:BB:671:C:C6	2.52	0.43
36:BB:1349:G:O2'	77:Bs:100:TYR:O	2.36	0.43
37:BC:163:A2M:H1'	37:BC:163:A2M:HM'3	1.72	0.43
41:BG:17:A:H2'	41:BG:18:U:C6	2.53	0.43
46:BN:83:GLU:CD	71:Bm:28:ARG:HH22	2.25	0.43
51:BS:14:ARG:HD2	51:BS:15:GLU:O	2.18	0.43
52:BT:183:LYS:HA	52:BT:183:LYS:HD2	1.92	0.43
54:BV:98:LEU:HB3	54:BV:104:ARG:HA	2.00	0.43
59:Ba:33:LYS:HA	59:Ba:33:LYS:HE2	2.00	0.43
61:Bc:4:SER:HB3	76:Br:285:THR:HG23	2.01	0.43
74:Bp:40:ARG:HG3	74:Bp:40:ARG:O	2.19	0.43
79:Bu:296:VAL:O	79:Bu:300:ILE:HG23	2.18	0.43
83:By:92:PHE:CD2	83:By:140:ASP:HB3	2.51	0.43
1:A0:81:ASP:OD1	1:A0:81:ASP:C	2.61	0.43
10:AA:132:C:H2'	10:AA:133:A:H8	1.83	0.43
10:AA:546:A:H2'	10:AA:546:A:N3	2.34	0.43
10:AA:1397:U:H2'	10:AA:1398:G:C8	2.53	0.43
10:AA:1676:OMG:HM23	10:AA:1676:OMG:H1'	1.73	0.43
10:AA:1952:C:H5'	10:AA:1953:A:OP2	2.19	0.43
17:AI:79:LYS:NZ	17:AI:79:LYS:H	2.16	0.43
18:AJ:30:SER:CB	18:AJ:59:GLY:HA3	2.49	0.43
23:AP:247:ARG:HH21	23:AP:252:GLU:HA	1.82	0.43
35:BA:1834:C:H2'	35:BA:1835:U:C6	2.54	0.43
36:BB:135:A:H2'	36:BB:136:A:C8	2.54	0.43
36:BB:685:OMU:H1'	36:BB:685:OMU:HM23	1.59	0.43
36:BB:1022:G:H2'	36:BB:1023:U:H6	1.83	0.43
37:BC:63:G:H22	37:BC:96:A:H2	1.65	0.43
59:Ba:75:ASN:OD1	59:Ba:76:HIS:N	2.51	0.43
59:Ba:104:LYS:HB3	59:Ba:104:LYS:HE3	1.73	0.43
66:Bh:133:THR:O	66:Bh:137:HIS:HB3	2.19	0.43
70:Bl:40:MET:HE3	70:Bl:40:MET:HB3	1.93	0.43
72:Bn:17:ILE:HG12	72:Bn:29:VAL:HG22	1.98	0.43
79:Bu:122:VAL:O	79:Bu:257:ARG:NH2	2.52	0.43
4:A3:65:VAL:O	4:A3:103:CYS:HB3	2.18	0.43
5:A4:103:LYS:HB3	5:A4:103:LYS:HE3	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A6:57:LEU:O	7:A6:60:THR:HG22	2.19	0.43
10:AA:147:G:H2'	10:AA:148:C:C6	2.54	0.43
10:AA:759:U:H2'	10:AA:760:G:C5	2.54	0.43
26:AS:32:THR:HG22	26:AS:34:VAL:HB	1.99	0.43
27:AT:20:ASN:C	27:AT:22:LEU:H	2.26	0.43
35:BA:253:G:H8	35:BA:253:G:OP2	2.02	0.43
35:BA:270:A:C6	58:BZ:7:ARG:HD2	2.54	0.43
35:BA:729:C:O2	70:Bl:54:GLN:NE2	2.51	0.43
35:BA:765:A:H2'	35:BA:766:G:H8	1.83	0.43
35:BA:1134:A:H2'	35:BA:1135:G:C8	2.54	0.43
36:BB:133:G:OP1	52:BT:104:ARG:NH1	2.52	0.43
36:BB:810:C:H2'	36:BB:811:A:C8	2.54	0.43
36:BB:1522:C:H2'	36:BB:1523:A:O4'	2.18	0.43
39:BE:40:U:H1'	39:BE:187:C:N4	2.34	0.43
59:Ba:53:VAL:HG22	59:Ba:56:MET:HE3	2.01	0.43
74:Bp:9:LYS:HE3	74:Bp:9:LYS:HB2	1.60	0.43
82:Bx:195:ASP:OD2	82:Bx:198:ARG:NH1	2.52	0.43
3:A2:88:LEU:HD23	3:A2:88:LEU:HA	1.88	0.43
10:AA:175:G:H2'	10:AA:176:G:C8	2.53	0.43
10:AA:757:G:H2'	10:AA:758:G:C8	2.54	0.43
10:AA:944:A:H5''	10:AA:945:A:H5'	2.01	0.43
23:AP:131:VAL:O	23:AP:135:ILE:HG12	2.17	0.43
23:AP:245:VAL:HG21	25:AR:56:THR:HB	2.00	0.43
24:AQ:15:GLN:N	24:AQ:15:GLN:CD	2.76	0.43
36:BB:804:U:OP1	82:Bx:97:ARG:NH1	2.50	0.43
36:BB:998:U:H2'	36:BB:999:G:C8	2.54	0.43
54:BV:99:LYS:HA	54:BV:104:ARG:HB2	2.00	0.43
64:Bf:302:THR:OG1	64:Bf:308:THR:O	2.33	0.43
67:Bi:127:LEU:HD23	67:Bi:127:LEU:HA	1.81	0.43
5:A4:90:ARG:HG2	5:A4:90:ARG:HH11	1.84	0.43
10:AA:301:C:H2'	10:AA:302:A:C8	2.54	0.43
10:AA:800:C:H1'	10:AA:801:G:C8	2.54	0.43
10:AA:1836:G:O2'	10:AA:1837:G:H8	2.02	0.43
10:AA:1910:U:H4'	10:AA:1913:A:H1'	2.01	0.43
10:AA:2266:C:OP1	16:AH:134:ARG:NH1	2.51	0.43
43:BI:35:PHE:CD2	76:Br:291:MET:HG2	2.54	0.43
44:BK:52:VAL:HG11	44:BK:136:LEU:HD12	2.00	0.43
46:BN:156:SER:C	46:BN:158:TYR:H	2.27	0.43
51:BS:19:GLU:N	51:BS:19:GLU:OE1	2.50	0.43
54:BV:10:SER:O	54:BV:10:SER:OG	2.29	0.43
64:Bf:246:LYS:HB3	64:Bf:246:LYS:HE3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:24:MET:HE3	16:AH:77:ARG:NH2	2.33	0.43
2:A1:41:LEU:HD12	2:A1:41:LEU:HA	1.78	0.43
10:AA:750:G:H1	10:AA:798:C:H42	1.66	0.43
10:AA:866:G:O2'	10:AA:867:C:O5'	2.35	0.43
10:AA:2260:MA6:O5'	10:AA:2260:MA6:H8	2.19	0.43
12:AC:114:SER:HB3	12:AC:123:ILE:HD13	2.01	0.43
12:AC:204:ARG:H	12:AC:204:ARG:HG2	1.63	0.43
13:AD:24:SER:HA	13:AD:71:PHE:O	2.19	0.43
15:AG:30:SER:HA	15:AG:67:THR:HG22	1.99	0.43
23:AP:144:LEU:HD23	23:AP:144:LEU:HA	1.86	0.43
35:BA:1445:G:O2'	35:BA:1446:G:H5''	2.19	0.43
36:BB:1375:OMU:O5'	36:BB:1375:OMU:H6	2.19	0.43
36:BB:1515:U:H2'	36:BB:1516:C:C6	2.54	0.43
65:Bg:58:ASN:O	65:Bg:59:CYS:C	2.62	0.43
77:Bs:78:MET:HE2	83:By:93:ALA:HB1	2.00	0.43
83:By:9:ILE:HG23	83:By:72:LEU:HD13	2.00	0.43
4:A3:38:ASP:OD1	4:A3:38:ASP:C	2.61	0.42
8:A7:111:ASP:OD1	8:A7:111:ASP:N	2.51	0.42
10:AA:58:G:H2'	10:AA:59:C:C6	2.54	0.42
10:AA:309:C:N4	10:AA:316:G:O6	2.52	0.42
10:AA:887:G:H2'	10:AA:888:C:O4'	2.19	0.42
31:AX:27:GLU:HG2	31:AX:68:LEU:HD21	2.01	0.42
35:BA:1126:A:N1	38:BD:102:C:O2'	2.50	0.42
35:BA:1232:G:O2'	35:BA:1233:A:OP1	2.36	0.42
35:BA:1745:G:H4'	35:BA:1746:U:OP1	2.19	0.42
60:Bb:30:SER:O	60:Bb:30:SER:OG	2.36	0.42
61:Bc:58:ASP:OD1	61:Bc:58:ASP:N	2.51	0.42
67:Bi:98:SER:HB3	67:Bi:101:VAL:HG23	2.01	0.42
79:Bu:36:MET:HE1	79:Bu:153:ASP:OD1	2.18	0.42
79:Bu:289:LYS:HD3	79:Bu:293:LYS:NZ	2.34	0.42
4:A3:122:GLN:HA	4:A3:122:GLN:OE1	2.17	0.42
4:A3:145:ARG:HG2	4:A3:150:LEU:HG	2.00	0.42
8:A7:97:GLN:CD	8:A7:97:GLN:H	2.26	0.42
10:AA:1758:C:O2'	10:AA:1759:G:O5'	2.37	0.42
16:AH:57:ALA:HB3	16:AH:60:ASP:OD2	2.19	0.42
23:AP:118:ASN:OD1	23:AP:118:ASN:N	2.51	0.42
35:BA:242:A:N7	41:BG:10:U:H5	2.17	0.42
35:BA:1738:C:H5'	72:Bn:41:ARG:HD2	2.00	0.42
35:BA:1811:U:H2'	35:BA:1812:C:C6	2.53	0.42
36:BB:1058:G:H2'	36:BB:1059:C:H6	1.83	0.42
36:BB:1278:G:H2'	36:BB:1279:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BH:29:G:H2'	42:BH:30:C:C6	2.54	0.42
45:BL:168:LYS:HA	45:BL:168:LYS:HD2	1.76	0.42
53:BU:126:PRO:HD2	53:BU:126:PRO:O	2.18	0.42
63:Be:242:ARG:NH2	63:Be:244:GLY:O	2.52	0.42
72:Bn:67:LEU:HD23	72:Bn:67:LEU:HA	1.89	0.42
1:A0:105:MET:HE1	1:A0:191:THR:HG22	2.01	0.42
8:A7:245:PHE:O	8:A7:246:SER:C	2.62	0.42
10:AA:44:G:H2'	10:AA:45:C:C6	2.55	0.42
10:AA:838:C:H2'	10:AA:839:A:O4'	2.20	0.42
10:AA:1566:C:H2'	10:AA:1567:A:H8	1.84	0.42
13:AD:68:TRP:O	13:AD:69:ARG:HG2	2.19	0.42
34:Az:209:GLU:OE2	34:Az:210:LYS:HD3	2.18	0.42
35:BA:527:G:O6	67:Bi:3:LYS:NZ	2.44	0.42
35:BA:846:G:H5'	43:Bi:43:PRO:HB2	2.00	0.42
45:BL:14:ASN:HB3	45:BL:17:ARG:HG2	2.01	0.42
52:BT:105:LEU:HD12	52:BT:138:LEU:HD23	2.01	0.42
55:BW:74:LYS:HB3	55:BW:74:LYS:HE3	1.70	0.42
82:Bx:127:GLU:OE1	82:Bx:127:GLU:C	2.62	0.42
2:A1:259:THR:O	2:A1:262:THR:OG1	2.34	0.42
4:A3:145:ARG:HA	4:A3:150:LEU:HD21	2.01	0.42
4:A3:157:ARG:NH2	10:AA:374:U:H5'	2.35	0.42
4:A3:164:LYS:HE2	4:A3:172:ASP:OD2	2.19	0.42
5:A4:77:ARG:NH1	5:A4:133:ASP:OD1	2.23	0.42
10:AA:668:C:O2	32:AY:13:LYS:NZ	2.43	0.42
10:AA:1138:A:H8	10:AA:1138:A:OP2	2.02	0.42
35:BA:1619:U:H2'	35:BA:1620:A2M:H8	2.00	0.42
37:BC:67:U:H2'	37:BC:68:A:H8	1.83	0.42
37:BC:128:U:H2'	37:BC:129:C:C6	2.54	0.42
47:BO:208:MET:HE1	48:BP:120:ARG:HB2	2.02	0.42
48:BP:172:LYS:HZ2	48:BP:172:LYS:HG2	1.75	0.42
58:BZ:35:GLU:H	58:BZ:35:GLU:CD	2.24	0.42
61:Bc:2:THR:HG1	61:Bc:3:HIS:H	1.65	0.42
83:By:139:LYS:HD3	83:By:139:LYS:HA	1.80	0.42
3:A2:77:ARG:NH2	10:AA:2020:A:OP1	2.53	0.42
10:AA:46:OMC:HM23	10:AA:46:OMC:H1'	1.81	0.42
10:AA:659:G:H4'	32:AY:58:ASN:O	2.19	0.42
10:AA:1565:A:H2'	10:AA:1566:C:C6	2.55	0.42
10:AA:1867:G:OP1	20:AL:63:ARG:NH2	2.52	0.42
22:AO:127:LEU:HD23	22:AO:127:LEU:HA	1.87	0.42
29:AV:48:ASP:OD1	29:AV:48:ASP:N	2.49	0.42
35:BA:527:G:N7	67:Bi:3:LYS:NZ	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BF:36:G:O2'	40:BF:37:C:O5'	2.36	0.42
51:BS:12:VAL:HG22	51:BS:28:LYS:HG3	2.01	0.42
68:Bj:73:LYS:HE2	68:Bj:73:LYS:HB2	1.94	0.42
70:Bl:149:ILE:HG21	80:Bv:192:TRP:CD1	2.54	0.42
83:By:13:GLU:H	83:By:13:GLU:CD	2.19	0.42
1:A0:81:ASP:HA	1:A0:84:ARG:HG3	2.01	0.42
10:AA:764:U:C2	10:AA:765:A:C8	3.07	0.42
10:AA:2087:A:H2'	10:AA:2088:G:H8	1.84	0.42
18:AJ:106:THR:OG1	18:AJ:107:SER:O	2.21	0.42
38:BD:22:A:C5	79:Bu:278:TYR:HD2	2.37	0.42
40:BF:72:C:N4	70:Bl:101:ARG:O	2.46	0.42
41:BG:87:G:N3	89:BG:302:HOH:O	2.36	0.42
49:BQ:97:THR:HG21	49:BQ:104:ALA:HA	2.00	0.42
67:Bi:127:LEU:O	67:Bi:130:VAL:HG12	2.20	0.42
4:A3:20:ASP:OD1	4:A3:21:GLU:N	2.53	0.42
6:A5:42:ARG:HB3	6:A5:58:LEU:O	2.20	0.42
10:AA:1778:A:H3'	10:AA:1779:G:N2	2.35	0.42
10:AA:2171:U:H2'	10:AA:2172:C:C6	2.54	0.42
21:AM:60:LEU:HD23	21:AM:60:LEU:HA	1.86	0.42
22:AO:142:LYS:HB3	22:AO:142:LYS:HE2	1.73	0.42
23:AP:81:ILE:HG21	23:AP:86:LEU:HG	2.01	0.42
34:Az:230:GLN:OE1	34:Az:230:GLN:N	2.31	0.42
36:BB:1377:U:H2'	36:BB:1378:U:H6	1.84	0.42
37:BC:78:G:H2'	37:BC:79:A:H8	1.85	0.42
49:BQ:26:GLU:HB2	71:Bm:52:ILE:HG13	2.02	0.42
66:Bh:127:ILE:O	66:Bh:128:ASP:HB3	2.19	0.42
2:A1:242:LEU:HA	2:A1:242:LEU:HD23	1.77	0.42
5:A4:4:GLN:HA	5:A4:4:GLN:OE1	2.20	0.42
6:A5:106:ALA:HB2	6:A5:184:LEU:HG	2.02	0.42
7:A6:114:LYS:HA	7:A6:114:LYS:HD2	1.76	0.42
10:AA:226:U:OP1	34:Az:172:GLN:NE2	2.52	0.42
10:AA:755:U:H2'	10:AA:756:U:C6	2.54	0.42
10:AA:765:A:H2'	10:AA:766:C:H6	1.85	0.42
10:AA:1896:G:H2'	10:AA:1897:U:C6	2.55	0.42
10:AA:2234:A:H2'	36:BB:520:A:N6	2.35	0.42
12:AC:43:VAL:O	12:AC:44:LEU:HB2	2.20	0.42
18:AJ:114:GLU:OE1	18:AJ:117:ARG:NH2	2.48	0.42
35:BA:685:U:H2'	35:BA:686:C:C6	2.54	0.42
36:BB:1211:U:H2'	36:BB:1212:G:H8	1.85	0.42
47:BO:22:PRO:HG2	47:BO:24:ILE:HD11	2.01	0.42
74:Bp:55:LYS:HB2	74:Bp:55:LYS:HE2	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Bu:276:LYS:H	79:Bu:276:LYS:HG3	1.65	0.42
81:Bw:228:GLY:O	81:Bw:255:ARG:NH2	2.53	0.42
1:A0:149:GLU:H	1:A0:149:GLU:CD	2.19	0.42
4:A3:65:VAL:HG21	4:A3:100:LEU:HD13	2.02	0.42
8:A7:204:VAL:HG13	8:A7:225:LEU:HD11	2.01	0.42
10:AA:1769:A:H5''	10:AA:1770:C:H5	1.84	0.42
10:AA:1836:G:O2'	10:AA:1837:G:O5'	2.38	0.42
15:AG:72:LEU:HD12	15:AG:72:LEU:HA	1.82	0.42
36:BB:1105:A:H2'	36:BB:1106:G:C8	2.54	0.42
36:BB:1248:G:O2'	36:BB:1249:U:OP2	2.32	0.42
39:BE:53:A:OP1	54:BV:108:ARG:NH2	2.52	0.42
48:BP:73:ALA:HA	48:BP:76:GLU:HG3	2.02	0.42
51:BS:145:HIS:N	51:BS:146:PRO:HD2	2.34	0.42
53:BU:127:PRO:HB2	53:BU:129:LYS:NZ	2.35	0.42
74:Bp:50:LYS:HD2	74:Bp:50:LYS:N	2.34	0.42
81:Bw:233:ARG:O	81:Bw:234:ARG:HB2	2.20	0.42
4:A3:187:ILE:O	4:A3:191:ARG:HG3	2.20	0.42
10:AA:1960:C:H3'	10:AA:1961:G:H8	1.85	0.42
31:AX:189:ARG:HG2	31:AX:190:PRO:O	2.19	0.42
36:BB:137:A:N6	36:BB:358:A:OP1	2.53	0.42
5:A4:43:LEU:N	5:A4:44:PRO:HD2	2.35	0.41
5:A4:59:HIS:CE1	5:A4:172:PRO:HB2	2.55	0.41
10:AA:799:A:H3'	10:AA:800:C:C6	2.55	0.41
10:AA:808:U:H2'	10:AA:809:G:O4'	2.20	0.41
13:AD:85:LYS:HB2	13:AD:85:LYS:NZ	2.34	0.41
14:AE:68:LYS:HB2	14:AE:68:LYS:HE2	1.71	0.41
31:AX:176:LEU:HD12	31:AX:181:ILE:HG13	2.02	0.41
34:Az:156:SER:OG	34:Az:197:LEU:O	2.33	0.41
34:Az:188:TYR:C	34:Az:190:GLN:H	2.27	0.41
36:BB:545:A2M:H8	36:BB:545:A2M:H2'	1.91	0.41
40:BF:55:C:N4	40:BF:60:C:H5	2.11	0.41
44:BK:101:LYS:HA	44:BK:101:LYS:HD2	1.81	0.41
44:BK:143:THR:O	44:BK:143:THR:OG1	2.37	0.41
68:Bj:116:LYS:HA	68:Bj:116:LYS:HD3	1.66	0.41
3:A2:190:ARG:O	33:AZ:97:ARG:NH2	2.52	0.41
7:A6:106:ARG:HA	7:A6:106:ARG:HD2	1.72	0.41
10:AA:1652:U:H2'	10:AA:1653:C:C6	2.55	0.41
16:AH:90:MET:HB3	16:AH:90:MET:HE2	1.66	0.41
24:AQ:43:GLU:OE1	24:AQ:43:GLU:C	2.63	0.41
24:AQ:80:LYS:HE2	24:AQ:80:LYS:HB3	1.78	0.41
34:Az:177:PHE:HD2	34:Az:206:PHE:CZ	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:509:A:H2'	35:BA:510:U:C6	2.56	0.41
35:BA:1342:A:H2'	35:BA:1343:A:H8	1.83	0.41
35:BA:1451:C:H2'	35:BA:1452:G:O4'	2.20	0.41
36:BB:1511:C:H2'	36:BB:1512:C:H6	1.85	0.41
37:BC:76:C:H2'	37:BC:77:A:O4'	2.20	0.41
48:BP:85:GLU:CD	48:BP:85:GLU:N	2.78	0.41
59:Ba:99:SER:OG	59:Ba:100:ASP:N	2.53	0.41
79:Bu:123:LYS:HA	79:Bu:123:LYS:HD2	1.82	0.41
79:Bu:299:VAL:HG22	79:Bu:302:ARG:NH2	2.32	0.41
6:A5:61:ASP:OD1	6:A5:62:THR:HG22	2.20	0.41
8:A7:137:ASN:HB3	8:A7:143:MET:SD	2.60	0.41
10:AA:387:A:H2'	10:AA:388:C:C6	2.55	0.41
10:AA:798:C:C4	10:AA:799:A:C5	3.07	0.41
10:AA:798:C:H2'	10:AA:799:A:O4'	2.21	0.41
17:AI:36:THR:OG1	17:AI:37:GLU:N	2.53	0.41
17:AI:130:TYR:OH	21:AM:125:ARG:NH1	2.51	0.41
24:AQ:41:ARG:HB2	24:AQ:41:ARG:HH11	1.85	0.41
28:AU:74:ARG:HH11	28:AU:74:ARG:HG3	1.86	0.41
29:AV:27:ASN:ND2	29:AV:81:CYS:SG	2.83	0.41
34:Az:231:LYS:HE3	34:Az:231:LYS:HB3	1.61	0.41
35:BA:1340:A:O2'	35:BA:1341:A:O5'	2.32	0.41
38:BD:74:A:O2'	51:BS:52:LYS:NZ	2.53	0.41
44:BK:115:MET:HE3	44:BK:115:MET:HB3	1.95	0.41
49:BQ:64:LYS:HD2	49:BQ:67:MET:HE2	2.03	0.41
58:BZ:33:SER:OG	58:BZ:34:LYS:N	2.51	0.41
67:Bi:128:ARG:HE	67:Bi:128:ARG:HB3	1.65	0.41
10:AA:773:C:H2'	10:AA:774:G:C8	2.55	0.41
10:AA:1681:U:H5'	31:AX:146:ALA:HB2	2.01	0.41
31:AX:142:LYS:HD2	31:AX:142:LYS:O	2.20	0.41
36:BB:640:G:H2'	36:BB:641:A:C8	2.55	0.41
39:BE:200:C:O2'	39:BE:201:A:H5'	2.20	0.41
60:Bb:22:VAL:O	60:Bb:24:LYS:N	2.50	0.41
61:Bc:56:LYS:HE2	61:Bc:56:LYS:HB2	1.95	0.41
75:Bq:21:ARG:HE	75:Bq:21:ARG:HB3	1.55	0.41
76:Br:296:VAL:O	76:Br:300:LEU:HG	2.20	0.41
1:A0:36:LYS:HE2	1:A0:36:LYS:HB3	1.59	0.41
20:AL:77:GLU:N	20:AL:80:ARG:HH21	2.19	0.41
23:AP:62:GLU:N	23:AP:62:GLU:OE1	2.53	0.41
24:AQ:20:LYS:HG3	24:AQ:85:LEU:HD13	2.02	0.41
25:AR:9:GLU:HG3	25:AR:10:GLU:OE2	2.20	0.41
40:BF:53:C:C2	80:Bv:182:LYS:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:Be:117:GLU:HG2	63:Be:124:GLY:H	1.84	0.41
4:A3:36:GLU:OE2	4:A3:50:THR:HB	2.20	0.41
9:A8:4:LEU:HD23	9:A8:4:LEU:HA	1.89	0.41
10:AA:1925:A:N3	10:AA:1925:A:H2'	2.36	0.41
19:AK:101:LYS:HG3	19:AK:102:TYR:CD2	2.56	0.41
24:AQ:92:THR:O	24:AQ:96:LYS:HG2	2.21	0.41
35:BA:253:G:H2'	35:BA:254:A2M:C8	2.50	0.41
35:BA:307:A:N3	46:BN:135:ARG:NH2	2.68	0.41
35:BA:752:C:H2'	35:BA:753:A:H8	1.84	0.41
35:BA:1864:G:N2	36:BB:6:A:N1	2.55	0.41
36:BB:1011:U:C2	36:BB:1012:C:C5	3.07	0.41
56:BX:72:VAL:HG12	69:Bk:70:LEU:HD13	2.02	0.41
64:Bf:82:PRO:HG2	64:Bf:171:LEU:HB2	2.03	0.41
67:Bi:16:LYS:HE3	67:Bi:16:LYS:HB2	1.82	0.41
75:Bq:16:LYS:HD3	75:Bq:16:LYS:HA	1.91	0.41
80:Bv:56:LYS:HE2	80:Bv:56:LYS:HB2	1.78	0.41
80:Bv:104:LYS:HB3	80:Bv:104:LYS:HE3	1.52	0.41
6:A5:216:ASP:OD1	6:A5:216:ASP:C	2.63	0.41
8:A7:238:ALA:O	8:A7:239:PRO:C	2.62	0.41
10:AA:935:G:N2	27:AT:13:ARG:HB3	2.35	0.41
15:AG:110:ASP:O	15:AG:114:ARG:HG2	2.21	0.41
22:AO:160:MET:HB3	22:AO:161:GLY:H	1.55	0.41
23:AP:193:VAL:HB	23:AP:194:PRO:HD3	2.03	0.41
35:BA:178:U:H2'	35:BA:179:A:O4'	2.21	0.41
40:BF:19:C:H2'	40:BF:20:U:C6	2.55	0.41
41:BG:75:C:OP1	64:Bf:227:LYS:HG3	2.21	0.41
52:BT:24:LEU:HD23	52:BT:50:VAL:HG22	2.03	0.41
54:BV:30:CYS:C	54:BV:33:PRO:HD2	2.46	0.41
72:Bn:69:VAL:O	72:Bn:73:ARG:HG2	2.20	0.41
74:Bp:18:LYS:NZ	74:Bp:19:ASP:H	2.18	0.41
79:Bu:266:LYS:H	79:Bu:266:LYS:HD2	1.86	0.41
79:Bu:287:GLU:H	79:Bu:287:GLU:CD	2.14	0.41
2:A1:121:MET:HE1	2:A1:142:HIS:CG	2.55	0.41
8:A7:176:ASN:OD1	8:A7:176:ASN:N	2.54	0.41
17:AI:29:ILE:O	17:AI:32:LEU:HB2	2.20	0.41
35:BA:1849:A:H2	35:BA:1850:A:H62	1.66	0.41
36:BB:608:U:H2'	36:BB:609:A2M:C8	2.51	0.41
36:BB:1424:C:C4'	36:BB:1425:A:N7	2.83	0.41
39:BE:35:A:H2'	39:BE:35:A:N3	2.35	0.41
52:BT:111:GLU:C	52:BT:111:GLU:OE2	2.64	0.41
1:A0:111:ARG:HE	1:A0:111:ARG:HB2	1.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A5:21:HIS:O	6:A5:22:ARG:HB3	2.21	0.41
10:AA:57:OMU:H6	10:AA:57:OMU:O5'	2.21	0.41
10:AA:166:C:O2'	10:AA:167:G:OP1	2.34	0.41
10:AA:172:A:HO2'	10:AA:173:C:P	2.44	0.41
10:AA:756:U:H2'	10:AA:757:G:H8	1.78	0.41
10:AA:1755:U:H5'	10:AA:1756:G:OP2	2.21	0.41
19:AK:36:ARG:NH1	19:AK:39:GLY:O	2.53	0.41
20:AL:100:ARG:HA	20:AL:121:LEU:O	2.21	0.41
31:AX:6:LYS:HA	31:AX:6:LYS:HD3	1.66	0.41
34:Az:152:HIS:O	34:Az:155:SER:HB3	2.21	0.41
35:BA:28:A:H2'	35:BA:29:C:H6	1.86	0.41
35:BA:743:A2M:HM'3	35:BA:743:A2M:H1'	1.82	0.41
35:BA:1481:U:H2'	35:BA:1482:A:H8	1.86	0.41
36:BB:578:OMU:H1'	36:BB:578:OMU:HM23	1.64	0.41
36:BB:798:G:O2'	36:BB:799:G:H5'	2.21	0.41
36:BB:1024:C:O2'	36:BB:1025:U:H5'	2.21	0.41
38:BD:69:U:H2'	38:BD:70:C:C6	2.56	0.41
40:BF:72:C:H5''	40:BF:73:A:OP2	2.20	0.41
40:BF:72:C:H6	40:BF:72:C:H2'	1.75	0.41
42:BH:92:A:H2'	42:BH:93:G:O4'	2.20	0.41
42:BH:118:U:O2'	42:BH:119:U:H5''	2.20	0.41
46:BN:154:ASP:OD1	46:BN:161:ALA:HB3	2.21	0.41
65:Bg:105:ASP:OD1	65:Bg:105:ASP:C	2.63	0.41
10:AA:1758:C:O2'	10:AA:1759:G:H8	2.04	0.41
23:AP:47:THR:HG22	23:AP:49:LEU:H	1.86	0.41
29:AV:53:ARG:O	29:AV:57:GLU:HG2	2.21	0.41
35:BA:473:A:O2'	35:BA:474:C:OP1	2.33	0.41
36:BB:768:U:H2'	36:BB:769:U:C6	2.56	0.41
36:BB:1296:U:H6	36:BB:1296:U:H2'	1.73	0.41
60:Bb:27:LYS:H	60:Bb:27:LYS:HG2	1.59	0.41
64:Bf:57:VAL:HG22	64:Bf:73:VAL:HG22	2.03	0.41
64:Bf:293:ALA:HB3	64:Bf:296:MET:HG3	2.03	0.41
64:Bf:339:ARG:NE	89:Bf:502:HOH:O	2.38	0.41
66:Bh:63:SER:O	66:Bh:63:SER:OG	2.36	0.41
69:Bk:23:SER:OG	69:Bk:24:GLU:OE2	2.34	0.41
82:Bx:131:LYS:HE3	82:Bx:131:LYS:HB3	1.63	0.41
8:A7:282:LYS:O	8:A7:283:LYS:C	2.63	0.40
10:AA:837:A:H2'	10:AA:838:C:H5''	2.01	0.40
10:AA:2103:C:H5''	19:AK:78:SER:OG	2.21	0.40
12:AC:92:GLU:HG2	25:AR:83:VAL:HG13	2.03	0.40
16:AH:12:SER:O	16:AH:12:SER:OG	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BB:1245:OMG:HM23	36:BB:1245:OMG:H1'	1.91	0.40
37:BC:18:G:H2'	37:BC:19:A:C8	2.56	0.40
45:BL:44:LEU:HD12	45:BL:44:LEU:HA	1.79	0.40
52:BT:163:ARG:CZ	52:BT:163:ARG:HB2	2.51	0.40
61:Bc:2:THR:HG1	61:Bc:3:HIS:CE1	2.36	0.40
5:A4:87:LEU:HD23	5:A4:96:VAL:HG11	2.03	0.40
10:AA:215:C:O2'	10:AA:216:G:H5'	2.22	0.40
10:AA:1858:U:H2'	10:AA:1859:U:C6	2.57	0.40
15:AG:38:CYS:SG	15:AG:42:LYS:NZ	2.90	0.40
35:BA:367:G:N7	71:Bm:39:ALA:HB2	2.36	0.40
35:BA:1665:A2M:HM'3	35:BA:1665:A2M:H1'	1.95	0.40
36:BB:766:C:O2'	36:BB:767:G:H8	2.04	0.40
36:BB:1186:U:H2'	36:BB:1187:G:H8	1.86	0.40
42:BH:39:G:H2'	42:BH:40:C:C6	2.56	0.40
46:BN:108:ASN:CG	46:BN:114:MET:HG3	2.47	0.40
54:BV:33:PRO:HB2	54:BV:39:PHE:CD1	2.56	0.40
63:Be:129:ALA:HB3	63:Be:132:ASP:OD2	2.21	0.40
80:Bv:66:MET:HB2	80:Bv:151:GLN:NE2	2.36	0.40
82:Bx:102:GLU:OE2	82:Bx:102:GLU:HA	2.21	0.40
6:A5:55:LEU:HD12	6:A5:55:LEU:HA	1.85	0.40
10:AA:172:A:O2'	10:AA:173:C:P	2.79	0.40
10:AA:849:U:C2	10:AA:887:G:N2	2.90	0.40
10:AA:972:C:H2'	10:AA:973:A:C8	2.56	0.40
10:AA:1827:C:H6	10:AA:1827:C:H2'	1.74	0.40
10:AA:2096:A2M:H5''	10:AA:2096:A2M:C8	2.48	0.40
31:AX:141:ILE:H	31:AX:141:ILE:HG12	1.61	0.40
34:Az:158:VAL:HG13	34:Az:222:VAL:HG23	2.03	0.40
34:Az:197:LEU:HD22	34:Az:203:ALA:HB2	2.04	0.40
35:BA:72:A:O2'	35:BA:74:C:H5	2.04	0.40
35:BA:485:G:H1'	41:BG:8:U:H5	1.86	0.40
35:BA:1321:G:N2	51:BS:114:SER:HB2	2.36	0.40
36:BB:1400:A2M:H1'	36:BB:1400:A2M:HM'3	1.67	0.40
41:BG:131:U:H2'	41:BG:132:U:O4'	2.21	0.40
45:BL:94:LYS:HD3	45:BL:94:LYS:HA	1.85	0.40
46:BN:55:PRO:HB3	46:BN:154:ASP:HB3	2.04	0.40
53:BU:93:PHE:HA	53:BU:96:VAL:HG12	2.04	0.40
69:Bk:126:LYS:HE2	69:Bk:126:LYS:HB2	1.93	0.40
81:Bw:180:ASP:OD1	81:Bw:180:ASP:N	2.54	0.40
81:Bw:208:LYS:HE2	81:Bw:208:LYS:HB2	1.70	0.40
83:By:11:PHE:HB3	83:By:79:ILE:HD13	2.03	0.40
83:By:40:LEU:HD23	83:By:40:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:By:138:VAL:HB	83:By:141:GLU:HG2	2.02	0.40
5:A4:36:HIS:HB3	5:A4:39:LEU:HB2	2.04	0.40
10:AA:2086:C:H2'	10:AA:2087:A:H8	1.87	0.40
12:AC:95:ILE:HD13	12:AC:217:GLU:HG2	2.04	0.40
16:AH:57:ALA:C	16:AH:59:ARG:H	2.30	0.40
29:AV:103:LYS:HZ3	29:AV:103:LYS:HB2	1.87	0.40
35:BA:1556:G:OP2	76:Br:203:ARG:NH1	2.54	0.40
35:BA:1837:G:H2'	35:BA:1839:A:N7	2.37	0.40
36:BB:1152:U:H2'	36:BB:1153:G:C8	2.56	0.40
37:BC:146:U:H4'	56:BX:69:SER:O	2.21	0.40
65:Bg:60:PRO:HA	65:Bg:61:PRO:HD3	1.96	0.40
76:Br:252:LYS:O	76:Br:256:GLU:HG3	2.22	0.40
80:Bv:64:GLY:O	80:Bv:65:PRO:C	2.64	0.40
1:A0:28:GLU:OE1	1:A0:50:LYS:NZ	2.52	0.40
8:A7:95:ASN:O	8:A7:96:LEU:C	2.64	0.40
10:AA:101:A:C2	10:AA:104:G:C6	3.10	0.40
10:AA:440:G:H5'	14:AE:95:LYS:HD2	2.03	0.40
10:AA:585:G:N2	10:AA:599:G:H22	2.20	0.40
10:AA:993:G:H2'	10:AA:994:G:C8	2.56	0.40
10:AA:1223:U:H2'	10:AA:1224:C:C6	2.56	0.40
10:AA:1674:OMU:H4'	10:AA:1675:G:C5'	2.52	0.40
15:AG:66:VAL:HG22	15:AG:67:THR:HG23	2.02	0.40
21:AM:117:LYS:HD2	21:AM:117:LYS:HA	1.92	0.40
36:BB:1139:A:H2'	36:BB:1140:A:C8	2.56	0.40
41:BG:75:C:O2'	41:BG:76:C:H5'	2.22	0.40
43:BI:79:LYS:HZ2	43:BI:79:LYS:HG2	1.63	0.40
54:BV:106:TRP:C	54:BV:107:ILE:HD13	2.47	0.40
70:Bl:72:ALA:HB2	70:Bl:120:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	220/256 (86%)	209 (95%)	9 (4%)	2 (1%)	14	31
2	A1	260/273 (95%)	241 (93%)	19 (7%)	0	100	100
3	A2	179/190 (94%)	177 (99%)	2 (1%)	0	100	100
4	A3	236/250 (94%)	231 (98%)	5 (2%)	0	100	100
5	A4	196/202 (97%)	190 (97%)	6 (3%)	0	100	100
6	A5	186/220 (84%)	178 (96%)	8 (4%)	0	100	100
7	A6	177/190 (93%)	171 (97%)	6 (3%)	0	100	100
8	A7	298/318 (94%)	257 (86%)	33 (11%)	8 (3%)	4	9
9	A8	55/57 (96%)	52 (94%)	3 (6%)	0	100	100
12	AC	206/277 (74%)	196 (95%)	10 (5%)	0	100	100
13	AD	97/172 (56%)	95 (98%)	2 (2%)	0	100	100
14	AE	151/174 (87%)	146 (97%)	5 (3%)	0	100	100
15	AG	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
16	AH	134/144 (93%)	123 (92%)	11 (8%)	0	100	100
17	AI	119/152 (78%)	114 (96%)	5 (4%)	0	100	100
18	AJ	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
19	AK	141/149 (95%)	131 (93%)	9 (6%)	1 (1%)	18	37
20	AL	120/142 (84%)	115 (96%)	5 (4%)	0	100	100
21	AM	133/153 (87%)	131 (98%)	2 (2%)	0	100	100
22	AO	152/167 (91%)	150 (99%)	2 (1%)	0	100	100
23	AP	216/266 (81%)	208 (96%)	7 (3%)	1 (0%)	24	45
24	AQ	98/117 (84%)	97 (99%)	1 (1%)	0	100	100
25	AR	87/194 (45%)	84 (97%)	3 (3%)	0	100	100
26	AS	137/143 (96%)	125 (91%)	12 (9%)	0	100	100
27	AT	128/137 (93%)	120 (94%)	7 (6%)	1 (1%)	16	34
28	AU	72/113 (64%)	68 (94%)	4 (6%)	0	100	100
29	AV	102/111 (92%)	94 (92%)	8 (8%)	0	100	100
30	AW	83/86 (96%)	75 (90%)	8 (10%)	0	100	100
31	AX	206/214 (96%)	198 (96%)	7 (3%)	1 (0%)	24	45
32	AY	55/66 (83%)	52 (94%)	3 (6%)	0	100	100
33	AZ	55/103 (53%)	54 (98%)	1 (2%)	0	100	100
34	Az	82/279 (29%)	70 (85%)	11 (13%)	1 (1%)	10	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BI	190/193 (98%)	181 (95%)	9 (5%)	0	100	100
44	BK	200/213 (94%)	193 (96%)	7 (4%)	0	100	100
45	BL	176/194 (91%)	170 (97%)	6 (3%)	0	100	100
46	BN	213/218 (98%)	204 (96%)	9 (4%)	0	100	100
47	BO	219/222 (99%)	215 (98%)	4 (2%)	0	100	100
48	BP	175/189 (93%)	170 (97%)	5 (3%)	0	100	100
49	BQ	201/221 (91%)	198 (98%)	3 (2%)	0	100	100
50	BR	150/166 (90%)	145 (97%)	5 (3%)	0	100	100
51	BS	176/179 (98%)	170 (97%)	6 (3%)	0	100	100
52	BT	195/260 (75%)	191 (98%)	4 (2%)	0	100	100
53	BU	156/159 (98%)	145 (93%)	11 (7%)	0	100	100
54	BV	120/130 (92%)	112 (93%)	8 (7%)	0	100	100
55	BW	128/139 (92%)	126 (98%)	2 (2%)	0	100	100
56	BX	116/164 (71%)	112 (97%)	4 (3%)	0	100	100
57	BY	62/125 (50%)	61 (98%)	1 (2%)	0	100	100
58	BZ	120/143 (84%)	116 (97%)	4 (3%)	0	100	100
59	Ba	131/133 (98%)	128 (98%)	3 (2%)	0	100	100
60	Bb	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
61	Bc	142/146 (97%)	138 (97%)	4 (3%)	0	100	100
62	Bd	67/71 (94%)	64 (96%)	3 (4%)	0	100	100
63	Be	256/260 (98%)	250 (98%)	6 (2%)	0	100	100
64	Bf	394/429 (92%)	381 (97%)	13 (3%)	0	100	100
65	Bg	90/105 (86%)	87 (97%)	3 (3%)	0	100	100
66	Bh	142/188 (76%)	134 (94%)	8 (6%)	0	100	100
67	Bi	129/132 (98%)	127 (98%)	2 (2%)	0	100	100
68	Bj	129/170 (76%)	125 (97%)	4 (3%)	0	100	100
69	Bk	121/127 (95%)	116 (96%)	4 (3%)	1 (1%)	16	34
70	Bl	142/149 (95%)	138 (97%)	4 (3%)	0	100	100
71	Bm	96/109 (88%)	94 (98%)	2 (2%)	0	100	100
72	Bn	80/84 (95%)	76 (95%)	4 (5%)	0	100	100
73	Bo	87/93 (94%)	84 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	Bp	73/82 (89%)	70 (96%)	3 (4%)	0	100	100
75	Bq	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
76	Br	365/374 (98%)	358 (98%)	7 (2%)	0	100	100
77	Bs	48/128 (38%)	47 (98%)	1 (2%)	0	100	100
78	Bt	95/106 (90%)	89 (94%)	6 (6%)	0	100	100
79	Bu	299/308 (97%)	288 (96%)	11 (4%)	0	100	100
80	Bv	142/192 (74%)	134 (94%)	8 (6%)	0	100	100
81	Bw	228/257 (89%)	218 (96%)	10 (4%)	0	100	100
82	Bx	231/276 (84%)	221 (96%)	9 (4%)	1 (0%)	30	51
83	By	184/189 (97%)	173 (94%)	11 (6%)	0	100	100
84	Bz	31/34 (91%)	31 (100%)	0	0	100	100
All	All	11145/12849 (87%)	10678 (96%)	450 (4%)	17 (0%)	44	65

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A0	159	LYS
8	A7	284	ILE
19	AK	46	LEU
34	Az	177	PHE
8	A7	165	ASP
1	A0	124	GLU
8	A7	140	GLY
8	A7	201	SER
8	A7	276	PRO
8	A7	277	GLU
27	AT	107	LYS
69	Bk	6	LYS
23	AP	58	ILE
31	AX	61	LYS
82	Bx	52	ASP
8	A7	65	GLY
8	A7	239	PRO

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	191/218 (88%)	181 (95%)	10 (5%)	21	43
2	A1	221/231 (96%)	214 (97%)	7 (3%)	34	61
3	A2	157/160 (98%)	153 (98%)	4 (2%)	42	69
4	A3	194/207 (94%)	184 (95%)	10 (5%)	21	43
5	A4	174/187 (93%)	165 (95%)	9 (5%)	21	43
6	A5	154/180 (86%)	150 (97%)	4 (3%)	40	68
7	A6	159/166 (96%)	156 (98%)	3 (2%)	50	75
8	A7	247/266 (93%)	164 (66%)	83 (34%)	0	0
9	A8	48/50 (96%)	45 (94%)	3 (6%)	16	35
12	AC	182/243 (75%)	175 (96%)	7 (4%)	29	55
13	AD	87/131 (66%)	82 (94%)	5 (6%)	18	40
14	AE	138/156 (88%)	134 (97%)	4 (3%)	37	64
15	AG	129/131 (98%)	121 (94%)	8 (6%)	16	36
16	AH	102/112 (91%)	99 (97%)	3 (3%)	37	64
17	AI	100/128 (78%)	98 (98%)	2 (2%)	48	74
18	AJ	108/109 (99%)	106 (98%)	2 (2%)	50	75
19	AK	117/124 (94%)	113 (97%)	4 (3%)	32	59
20	AL	101/122 (83%)	95 (94%)	6 (6%)	18	38
21	AM	118/133 (89%)	112 (95%)	6 (5%)	21	44
22	AO	127/137 (93%)	122 (96%)	5 (4%)	28	54
23	AP	181/204 (89%)	174 (96%)	7 (4%)	28	54
24	AQ	90/104 (86%)	84 (93%)	6 (7%)	15	32
25	AR	73/150 (49%)	73 (100%)	0	100	100
26	AS	114/118 (97%)	106 (93%)	8 (7%)	14	31
27	AT	109/116 (94%)	104 (95%)	5 (5%)	24	48
28	AU	65/94 (69%)	61 (94%)	4 (6%)	16	36
29	AV	90/97 (93%)	86 (96%)	4 (4%)	25	50
30	AW	74/75 (99%)	69 (93%)	5 (7%)	14	32
31	AX	176/180 (98%)	167 (95%)	9 (5%)	21	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	AY	49/53 (92%)	48 (98%)	1 (2%)	48	74
33	AZ	49/84 (58%)	43 (88%)	6 (12%)	5	10
34	Az	72/216 (33%)	66 (92%)	6 (8%)	10	24
43	BI	164/165 (99%)	159 (97%)	5 (3%)	36	63
44	BK	178/185 (96%)	172 (97%)	6 (3%)	32	59
45	BL	148/167 (89%)	142 (96%)	6 (4%)	27	52
46	BN	185/188 (98%)	179 (97%)	6 (3%)	34	61
47	BO	194/195 (100%)	191 (98%)	3 (2%)	57	79
48	BP	147/158 (93%)	136 (92%)	11 (8%)	12	28
49	BQ	176/193 (91%)	172 (98%)	4 (2%)	44	71
50	BR	130/144 (90%)	124 (95%)	6 (5%)	24	48
51	BS	159/160 (99%)	153 (96%)	6 (4%)	29	55
52	BT	154/198 (78%)	151 (98%)	3 (2%)	50	75
53	BU	132/134 (98%)	121 (92%)	11 (8%)	10	24
54	BV	100/116 (86%)	89 (89%)	11 (11%)	6	13
55	BW	101/108 (94%)	100 (99%)	1 (1%)	68	84
56	BX	105/136 (77%)	104 (99%)	1 (1%)	68	84
57	BY	56/102 (55%)	53 (95%)	3 (5%)	20	42
58	BZ	108/125 (86%)	105 (97%)	3 (3%)	38	65
59	Ba	115/117 (98%)	112 (97%)	3 (3%)	40	68
60	Bb	115/116 (99%)	113 (98%)	2 (2%)	53	77
61	Bc	128/130 (98%)	123 (96%)	5 (4%)	28	54
62	Bd	57/59 (97%)	55 (96%)	2 (4%)	32	58
63	Be	201/204 (98%)	199 (99%)	2 (1%)	68	84
64	Bf	337/360 (94%)	318 (94%)	19 (6%)	19	40
65	Bg	81/92 (88%)	78 (96%)	3 (4%)	30	56
66	Bh	121/162 (75%)	112 (93%)	9 (7%)	13	28
67	Bi	116/117 (99%)	111 (96%)	5 (4%)	26	51
68	Bj	100/137 (73%)	98 (98%)	2 (2%)	48	74
69	Bk	106/114 (93%)	103 (97%)	3 (3%)	38	65
70	Bl	122/126 (97%)	114 (93%)	8 (7%)	15	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	Bm	81/90 (90%)	80 (99%)	1 (1%)	63	82
72	Bn	70/71 (99%)	69 (99%)	1 (1%)	59	80
73	Bo	72/76 (95%)	69 (96%)	3 (4%)	26	52
74	Bp	70/77 (91%)	64 (91%)	6 (9%)	10	22
75	Bq	46/47 (98%)	46 (100%)	0	100	100
76	Br	304/310 (98%)	296 (97%)	8 (3%)	40	68
77	Bs	42/111 (38%)	41 (98%)	1 (2%)	43	70
78	Bt	87/95 (92%)	87 (100%)	0	100	100
79	Bu	239/247 (97%)	232 (97%)	7 (3%)	37	64
80	Bv	121/160 (76%)	115 (95%)	6 (5%)	22	45
81	Bw	193/213 (91%)	188 (97%)	5 (3%)	40	68
82	Bx	199/229 (87%)	190 (96%)	9 (4%)	24	49
83	By	169/172 (98%)	158 (94%)	11 (6%)	15	34
84	Bz	29/31 (94%)	28 (97%)	1 (3%)	32	59
All	All	9554/10819 (88%)	9100 (95%)	454 (5%)	24	46

All (454) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	51	THR
1	A0	54	THR
1	A0	111	ARG
1	A0	122	THR
1	A0	127	VAL
1	A0	131	THR
1	A0	133	ASP
1	A0	141	LEU
1	A0	222	THR
1	A0	239	THR
2	A1	56	LEU
2	A1	99	LEU
2	A1	169	LEU
2	A1	232	VAL
2	A1	234	VAL
2	A1	259	THR
2	A1	261	ARG
3	A2	18	GLN

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Mol	Chain	Res	Type
3	A2	35	VAL
3	A2	64	PHE
3	A2	155	LEU
4	A3	9	ARG
4	A3	13	VAL
4	A3	26	VAL
4	A3	116	VAL
4	A3	160	VAL
4	A3	165	VAL
4	A3	166	THR
4	A3	186	THR
4	A3	195	VAL
4	A3	233	SER
5	A4	51	VAL
5	A4	53	THR
5	A4	75	LEU
5	A4	84	THR
5	A4	109	ASN
5	A4	140	VAL
5	A4	167	VAL
5	A4	187	THR
5	A4	201	SER
6	A5	18	THR
6	A5	58	LEU
6	A5	62	THR
6	A5	93	THR
7	A6	49	SER
7	A6	60	THR
7	A6	90	ASP
8	A7	3	VAL
8	A7	6	GLU
8	A7	13	ARG
8	A7	18	SER
8	A7	19	LEU
8	A7	30	LYS
8	A7	34	THR
8	A7	38	LYS
8	A7	42	SER
8	A7	55	SER
8	A7	61	ARG
8	A7	66	HIS
8	A7	77	ASN

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Mol	Chain	Res	Type
8	A7	78	ASN
8	A7	80	ASN
8	A7	83	VAL
8	A7	89	HIS
8	A7	90	SER
8	A7	109	THR
8	A7	110	LYS
8	A7	111	ASP
8	A7	112	VAL
8	A7	121	ASN
8	A7	122	ARG
8	A7	131	ASN
8	A7	134	ARG
8	A7	139	LYS
8	A7	142	CYS
8	A7	143	MET
8	A7	145	THR
8	A7	148	ARG
8	A7	158	VAL
8	A7	160	PHE
8	A7	164	LEU
8	A7	165	ASP
8	A7	168	VAL
8	A7	169	ILE
8	A7	170	VAL
8	A7	176	ASN
8	A7	178	VAL
8	A7	187	ARG
8	A7	192	LEU
8	A7	193	LYS
8	A7	196	THR
8	A7	199	VAL
8	A7	207	ASP
8	A7	210	LEU
8	A7	211	CYS
8	A7	214	SER
8	A7	216	LYS
8	A7	219	VAL
8	A7	221	ARG
8	A7	223	TRP
8	A7	226	THR
8	A7	227	LYS

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Mol	Chain	Res	Type
8	A7	232	SER
8	A7	233	GLU
8	A7	234	MET
8	A7	243	ILE
8	A7	244	CYS
8	A7	245	PHE
8	A7	248	ASN
8	A7	249	ARG
8	A7	252	MET
8	A7	253	CYS
8	A7	258	LYS
8	A7	260	ILE
8	A7	261	ARG
8	A7	265	LEU
8	A7	267	ASN
8	A7	269	ASP
8	A7	270	ILE
8	A7	274	LEU
8	A7	284	ILE
8	A7	285	VAL
8	A7	287	GLU
8	A7	289	VAL
8	A7	290	SER
8	A7	291	ILE
8	A7	300	LEU
8	A7	307	ASN
8	A7	308	VAL
8	A7	311	VAL
9	A8	9	SER
9	A8	26	SER
9	A8	54	VAL
12	AC	63	THR
12	AC	78	THR
12	AC	82	THR
12	AC	113	CYS
12	AC	148	ILE
12	AC	206	SER
12	AC	208	SER
13	AD	4	TYR
13	AD	5	VAL
13	AD	22	VAL
13	AD	36	THR

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Mol	Chain	Res	Type
13	AD	37	LEU
14	AE	14	VAL
14	AE	56	LEU
14	AE	68	LYS
14	AE	124	THR
15	AG	48	SER
15	AG	66	VAL
15	AG	87	ASP
15	AG	132	VAL
15	AG	143	SER
15	AG	144	SER
15	AG	147	SER
15	AG	149	MET
16	AH	29	SER
16	AH	74	VAL
16	AH	98	THR
17	AI	22	PHE
17	AI	112	VAL
18	AJ	31	SER
18	AJ	104	LEU
19	AK	12	VAL
19	AK	42	ILE
19	AK	46	LEU
19	AK	147	SER
20	AL	8	THR
20	AL	24	LEU
20	AL	67	ARG
20	AL	85	VAL
20	AL	105	THR
20	AL	121	LEU
21	AM	19	THR
21	AM	67	LYS
21	AM	85	LEU
21	AM	93	THR
21	AM	105	ASP
21	AM	136	HIS
22	AO	22	THR
22	AO	56	THR
22	AO	57	SER
22	AO	133	CYS
22	AO	142	LYS
23	AP	86	LEU

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Mol	Chain	Res	Type
23	AP	203	VAL
23	AP	205	ASP
23	AP	211	CYS
23	AP	231	THR
23	AP	232	TYR
23	AP	248	ASP
24	AQ	15	GLN
24	AQ	22	THR
24	AQ	29	VAL
24	AQ	51	VAL
24	AQ	53	LEU
24	AQ	94	LEU
26	AS	34	VAL
26	AS	55	ILE
26	AS	70	VAL
26	AS	91	LEU
26	AS	99	GLU
26	AS	112	VAL
26	AS	115	ILE
26	AS	125	VAL
27	AT	2	VAL
27	AT	33	ASN
27	AT	90	LYS
27	AT	107	LYS
27	AT	108	LEU
28	AU	67	THR
28	AU	69	SER
28	AU	75	LEU
28	AU	101	SER
29	AV	29	SER
29	AV	32	VAL
29	AV	102	SER
29	AV	104	VAL
30	AW	9	SER
30	AW	36	VAL
30	AW	64	LEU
30	AW	68	THR
30	AW	85	ASP
31	AX	41	THR
31	AX	53	LYS
31	AX	136	THR
31	AX	141	ILE

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Mol	Chain	Res	Type
31	AX	158	LYS
31	AX	171	THR
31	AX	183	VAL
31	AX	199	VAL
31	AX	205	THR
32	AY	22	SER
33	AZ	50	THR
33	AZ	52	SER
33	AZ	61	VAL
33	AZ	75	THR
33	AZ	76	ILE
33	AZ	91	SER
34	Az	160	LEU
34	Az	178	THR
34	Az	182	VAL
34	Az	205	LYS
34	Az	220	LEU
34	Az	225	SER
43	BI	21	SER
43	BI	26	ILE
43	BI	47	LEU
43	BI	121	THR
43	BI	192	HIS
44	BK	33	THR
44	BK	43	VAL
44	BK	52	VAL
44	BK	53	VAL
44	BK	118	SER
44	BK	143	THR
45	BL	21	VAL
45	BL	32	GLU
45	BL	53	VAL
45	BL	76	CYS
45	BL	105	ASP
45	BL	133	ASP
46	BN	11	VAL
46	BN	27	VAL
46	BN	46	LEU
46	BN	127	LYS
46	BN	156	SER
46	BN	176	LYS
47	BO	169	SER

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Mol	Chain	Res	Type
47	BO	170	ASP
47	BO	193	VAL
48	BP	24	VAL
48	BP	31	VAL
48	BP	56	VAL
48	BP	64	SER
48	BP	66	SER
48	BP	70	SER
48	BP	83	VAL
48	BP	134	LYS
48	BP	147	LEU
48	BP	172	LYS
48	BP	175	LEU
49	BQ	83	VAL
49	BQ	117	VAL
49	BQ	143	THR
49	BQ	219	ARG
50	BR	5	SER
50	BR	12	SER
50	BR	16	LYS
50	BR	54	LYS
50	BR	78	GLN
50	BR	93	SER
51	BS	2	VAL
51	BS	10	CYS
51	BS	14	ARG
51	BS	59	ASP
51	BS	84	SER
51	BS	131	ILE
52	BT	72	MET
52	BT	86	GLU
52	BT	179	LYS
53	BU	3	HIS
53	BU	24	VAL
53	BU	28	SER
53	BU	64	VAL
53	BU	90	CYS
53	BU	102	GLN
53	BU	123	THR
53	BU	131	SER
53	BU	141	LYS
53	BU	145	VAL

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Mol	Chain	Res	Type
53	BU	150	THR
54	BV	4	VAL
54	BV	10	SER
54	BV	19	LEU
54	BV	30	CYS
54	BV	43	ILE
54	BV	56	LYS
54	BV	64	LEU
54	BV	76	THR
54	BV	77	LEU
54	BV	81	THR
54	BV	116	THR
55	BW	14	ARG
56	BX	53	GLN
57	BY	27	LEU
57	BY	60	ARG
57	BY	64	ARG
58	BZ	98	THR
58	BZ	120	ASP
58	BZ	123	THR
59	Ba	57	SER
59	Ba	60	SER
59	Ba	93	ARG
60	Bb	27	LYS
60	Bb	60	HIS
61	Bc	6	ASP
61	Bc	15	ASN
61	Bc	48	THR
61	Bc	111	ARG
61	Bc	133	LYS
62	Bd	8	THR
62	Bd	63	LEU
63	Be	18	VAL
63	Be	126	LEU
64	Bf	2	SER
64	Bf	60	VAL
64	Bf	61	ASP
64	Bf	79	LEU
64	Bf	111	SER
64	Bf	134	LYS
64	Bf	140	THR
64	Bf	169	ARG

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Mol	Chain	Res	Type
64	Bf	170	LYS
64	Bf	178	VAL
64	Bf	206	LYS
64	Bf	209	ARG
64	Bf	210	ILE
64	Bf	251	LEU
64	Bf	292	ARG
64	Bf	296	MET
64	Bf	297	GLU
64	Bf	325	ARG
64	Bf	335	VAL
65	Bg	23	THR
65	Bg	73	LEU
65	Bg	82	SER
66	Bh	42	LEU
66	Bh	45	MET
66	Bh	52	LYS
66	Bh	56	VAL
66	Bh	69	THR
66	Bh	77	THR
66	Bh	127	ILE
66	Bh	140	VAL
66	Bh	171	SER
67	Bi	6	VAL
67	Bi	56	LYS
67	Bi	121	ILE
67	Bi	130	VAL
67	Bi	132	VAL
68	Bj	3	CYS
68	Bj	104	VAL
69	Bk	7	ILE
69	Bk	59	MET
69	Bk	125	VAL
70	Bl	10	SER
70	Bl	15	ARG
70	Bl	24	LYS
70	Bl	30	LYS
70	Bl	35	SER
70	Bl	66	VAL
70	Bl	119	SER
70	Bl	129	SER
71	Bm	53	SER

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Mol	Chain	Res	Type
72	Bn	81	ASP
73	Bo	50	LYS
73	Bo	77	THR
73	Bo	88	GLU
74	Bp	16	SER
74	Bp	31	VAL
74	Bp	59	SER
74	Bp	61	HIS
74	Bp	63	SER
74	Bp	76	ASN
76	Br	86	SER
76	Br	179	VAL
76	Br	270	THR
76	Br	287	VAL
76	Br	317	THR
76	Br	347	LYS
76	Br	367	VAL
76	Br	369	LYS
77	Bs	99	CYS
79	Bu	94	ASN
79	Bu	120	VAL
79	Bu	169	LEU
79	Bu	218	ARG
79	Bu	228	LYS
79	Bu	261	THR
79	Bu	281	VAL
80	Bv	52	LYS
80	Bv	85	SER
80	Bv	88	VAL
80	Bv	94	ASP
80	Bv	143	VAL
80	Bv	178	VAL
81	Bw	61	SER
81	Bw	75	LYS
81	Bw	76	LYS
81	Bw	176	VAL
81	Bw	189	HIS
82	Bx	38	SER
82	Bx	43	ARG
82	Bx	45	LYS
82	Bx	47	PHE
82	Bx	67	THR

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Mol	Chain	Res	Type
82	Bx	139	THR
82	Bx	188	ILE
82	Bx	203	ILE
82	Bx	241	VAL
83	By	5	SER
83	By	10	THR
83	By	25	THR
83	By	83	THR
83	By	102	THR
83	By	124	VAL
83	By	128	VAL
83	By	130	VAL
83	By	134	ASP
83	By	183	THR
83	By	185	ILE
84	Bz	11	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	69	ASN
2	A1	47	ASN
2	A1	54	ASN
2	A1	198	HIS
4	A3	10	ASN
5	A4	36	HIS
5	A4	42	GLN
5	A4	198	GLN
6	A5	52	ASN
8	A7	12	HIS
8	A7	97	GLN
8	A7	100	GLN
8	A7	102	GLN
8	A7	241	ASN
8	A7	267	ASN
9	A8	21	HIS
9	A8	27	ASN
9	A8	28	GLN
13	AD	51	GLN
13	AD	70	HIS
14	AE	105	ASN
14	AE	114	GLN

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Mol	Chain	Res	Type
15	AG	134	GLN
19	AK	11	GLN
20	AL	74	GLN
20	AL	90	HIS
21	AM	12	HIS
21	AM	18	ASN
22	AO	27	HIS
23	AP	162	HIS
25	AR	34	HIS
26	AS	7	GLN
26	AS	36	GLN
29	AV	84	HIS
31	AX	144	GLN
31	AX	175	HIS
43	BI	142	ASN
45	BL	69	ASN
46	BN	26	ASN
46	BN	108	ASN
46	BN	193	ASN
47	BO	150	ASN
48	BP	51	GLN
48	BP	55	ASN
50	BR	78	GLN
50	BR	97	ASN
50	BR	152	GLN
51	BS	35	ASN
51	BS	121	HIS
52	BT	134	ASN
52	BT	143	HIS
53	BU	33	ASN
53	BU	107	GLN
54	BV	46	ASN
54	BV	75	ASN
56	BX	77	ASN
57	BY	10	HIS
58	BZ	78	HIS
59	Ba	27	ASN
59	Ba	85	ASN
59	Ba	116	GLN
60	Bb	34	ASN
61	Bc	15	ASN
61	Bc	34	ASN

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Mol	Chain	Res	Type
61	Bc	42	GLN
62	Bd	6	ASN
62	Bd	17	HIS
62	Bd	70	GLN
64	Bf	94	GLN
64	Bf	121	ASN
64	Bf	187	GLN
66	Bh	83	ASN
67	Bi	21	HIS
67	Bi	79	ASN
68	Bj	101	GLN
69	Bk	37	GLN
71	Bm	104	GLN
72	Bn	76	ASN
73	Bo	34	HIS
74	Bp	27	HIS
74	Bp	61	HIS
76	Br	40	HIS
76	Br	49	GLN
76	Br	237	HIS
76	Br	243	HIS
76	Br	333	GLN
76	Br	348	ASN
77	Bs	109	ASN
78	Bt	82	GLN
79	Bu	139	GLN
81	Bw	35	GLN
81	Bw	250	ASN
83	By	106	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	AA	1803/2280 (79%)	406 (22%)	14 (0%)
11	AB	8/76 (10%)	1 (12%)	0
35	BA	1591/1866 (85%)	294 (18%)	13 (0%)
36	BB	1120/1544 (72%)	208 (18%)	13 (1%)
37	BC	157/209 (75%)	24 (15%)	0
38	BD	119/120 (99%)	11 (9%)	1 (0%)
39	BE	168/216 (77%)	36 (21%)	0
40	BF	66/78 (84%)	13 (19%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
41	BG	182/183 (99%)	26 (14%)	2 (1%)
42	BH	116/136 (85%)	28 (24%)	1 (0%)
All	All	5330/6708 (79%)	1047 (19%)	45 (0%)

All (1047) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	AA	32	C
10	AA	33	U
10	AA	45	C
10	AA	54	A
10	AA	62	G
10	AA	70	G
10	AA	73	U
10	AA	75	A
10	AA	90	A
10	AA	93	A
10	AA	94	U
10	AA	96	A
10	AA	102	U
10	AA	103	U
10	AA	104	G
10	AA	111	U
10	AA	125	A2M
10	AA	127	U
10	AA	130	A
10	AA	135	A
10	AA	136	C
10	AA	139	A
10	AA	141	U
10	AA	144	G
10	AA	149	C
10	AA	153	A
10	AA	161	G
10	AA	167	G
10	AA	173	C
10	AA	174	U
10	AA	176	G
10	AA	177	A
10	AA	185	G
10	AA	191	C
10	AA	202	U

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Mol	Chain	Res	Type
10	AA	208	A
10	AA	210	C
10	AA	213	A
10	AA	219	C
10	AA	222	U
10	AA	224	U
10	AA	226	U
10	AA	268	A
10	AA	269	U
10	AA	270	G
10	AA	280	G
10	AA	291	A
10	AA	292	A
10	AA	294	U
10	AA	295	U
10	AA	296	A
10	AA	298	A
10	AA	305	G
10	AA	316	G
10	AA	317	A
10	AA	322	G
10	AA	324	A
10	AA	325	A
10	AA	326	C
10	AA	327	A
10	AA	330	C
10	AA	334	C
10	AA	355	G
10	AA	356	U
10	AA	359	G
10	AA	362	A
10	AA	367	A
10	AA	368	G
10	AA	369	C
10	AA	370	C
10	AA	376	G
10	AA	377	C
10	AA	391	A
10	AA	399	C
10	AA	407	U
10	AA	408	C
10	AA	410	G

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Mol	Chain	Res	Type
10	AA	431	G
10	AA	432	A
10	AA	454	C
10	AA	483	G
10	AA	493	A
10	AA	494	A
10	AA	495	U
10	AA	516	G
10	AA	517	C
10	AA	518	A
10	AA	519	G
10	AA	527	G
10	AA	531	A
10	AA	532	U
10	AA	533	U
10	AA	537	C
10	AA	545	A
10	AA	547	A
10	AA	552	A
10	AA	553	C
10	AA	566	A
10	AA	573	A
10	AA	575	A
10	AA	581	G
10	AA	582	A
10	AA	583	C
10	AA	584	C
10	AA	585	G
10	AA	586	U
10	AA	600	G
10	AA	602	U
10	AA	605	U
10	AA	606	U
10	AA	607	U
10	AA	608	C
10	AA	612	G
10	AA	618	U
10	AA	619	A
10	AA	621	U
10	AA	633	A
10	AA	634	A
10	AA	638	C

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Mol	Chain	Res	Type
10	AA	643	A
10	AA	644	A
10	AA	647	A
10	AA	649	U
10	AA	650	G
10	AA	659	G
10	AA	660	U
10	AA	667	C
10	AA	670	G
10	AA	681	A
10	AA	682	A
10	AA	690	U
10	AA	696	A
10	AA	713	U
10	AA	721	A2M
10	AA	722	A
10	AA	725	G
10	AA	726	G
10	AA	740	U
10	AA	742	U
10	AA	743	G
10	AA	747	C
10	AA	748	A
10	AA	752	A
10	AA	753	G
10	AA	754	U
10	AA	755	U
10	AA	757	G
10	AA	760	G
10	AA	761	C
10	AA	762	C
10	AA	779	C
10	AA	781	U
10	AA	783	G
10	AA	785	A
10	AA	787	G
10	AA	789	G
10	AA	792	U
10	AA	793	U
10	AA	795	A
10	AA	796	C
10	AA	800	C

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Mol	Chain	Res	Type
10	AA	801	G
10	AA	805	U
10	AA	806	C
10	AA	807	G
10	AA	810	G
10	AA	811	C
10	AA	812	C
10	AA	827	G
10	AA	829	U
10	AA	830	A
10	AA	833	A
10	AA	834	G
10	AA	838	C
10	AA	842	G
10	AA	844	A
10	AA	845	G
10	AA	846	C
10	AA	847	A
10	AA	851	C
10	AA	867	C
10	AA	868	A
10	AA	872	C
10	AA	873	A
10	AA	875	G
10	AA	876	C
10	AA	881	G
10	AA	900	U
10	AA	911	A
10	AA	921	G
10	AA	922	A
10	AA	936	C
10	AA	937	C
10	AA	938	G
10	AA	941	U
10	AA	942	U
10	AA	957	G
10	AA	975	C
10	AA	980	G
10	AA	981	G
10	AA	985	A
10	AA	987	C
10	AA	988	G

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Mol	Chain	Res	Type
10	AA	1000	G
10	AA	1005	U
10	AA	1006	U
10	AA	1012	A
10	AA	1024	A
10	AA	1025	U
10	AA	1026	U
10	AA	1027	A
10	AA	1029	G
10	AA	1133	G
10	AA	1135	A
10	AA	1139	A
10	AA	1147	A
10	AA	1149	U
10	AA	1153	G
10	AA	1160	A
10	AA	1163	U
10	AA	1175	A
10	AA	1176	G
10	AA	1182	A
10	AA	1183	A
10	AA	1192	A
10	AA	1198	C
10	AA	1210	A
10	AA	1212	A
10	AA	1221	A
10	AA	1229	A
10	AA	1236	C
10	AA	1237	U
10	AA	1241	U
10	AA	1243	A
10	AA	1247	A
10	AA	1266	U
10	AA	1269	A
10	AA	1275	A
10	AA	1281	G
10	AA	1282	A
10	AA	1290	A
10	AA	1298	C
10	AA	1303	A
10	AA	1305	C
10	AA	1308	U

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Mol	Chain	Res	Type
10	AA	1309	G
10	AA	1320	A
10	AA	1328	A
10	AA	1391	U
10	AA	1451	C
10	AA	1452	G
10	AA	1485	C
10	AA	1496	G
10	AA	1497	G
10	AA	1501	U
10	AA	1502	U
10	AA	1503	A
10	AA	1504	C
10	AA	1505	A
10	AA	1519	G
10	AA	1520	U
10	AA	1533	G
10	AA	1543	A
10	AA	1555	G
10	AA	1556	A
10	AA	1560	G
10	AA	1563	C
10	AA	1564	C
10	AA	1572	G
10	AA	1590	U
10	AA	1599	A
10	AA	1601	A
10	AA	1604	G
10	AA	1605	G
10	AA	1606	G
10	AA	1607	A
10	AA	1620	C
10	AA	1621	C
10	AA	1622	G
10	AA	1623	G
10	AA	1630	U
10	AA	1644	U
10	AA	1656	U
10	AA	1663	C
10	AA	1671	U
10	AA	1675	G
10	AA	1706	U

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Mol	Chain	Res	Type
10	AA	1714	G
10	AA	1719	U
10	AA	1720	U
10	AA	1726	A
10	AA	1730	G
10	AA	1731	A
10	AA	1732	C
10	AA	1746	C
10	AA	1751	U
10	AA	1752	A
10	AA	1755	U
10	AA	1758	C
10	AA	1759	G
10	AA	1765	G
10	AA	1767	C
10	AA	1769	A
10	AA	1770	C
10	AA	1773	A
10	AA	1774	G
10	AA	1775	G
10	AA	1780	C
10	AA	1781	A
10	AA	1782	G
10	AA	1822	U
10	AA	1827	C
10	AA	1836	G
10	AA	1837	G
10	AA	1848	G
10	AA	1853	A
10	AA	1854	U
10	AA	1855	U
10	AA	1863	U
10	AA	1864	U
10	AA	1869	G
10	AA	1873	G
10	AA	1880	U
10	AA	1882	U
10	AA	1885	G
10	AA	1888	A
10	AA	1892	G
10	AA	1894	A
10	AA	1895	OMG

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Mol	Chain	Res	Type
10	AA	1898	C
10	AA	1899	OMU
10	AA	1902	G
10	AA	1903	A
10	AA	1906	C
10	AA	1907	PSU
10	AA	1910	U
10	AA	1912	A
10	AA	1913	A
10	AA	1925	A
10	AA	1926	C
10	AA	1927	A
10	AA	1933	A
10	AA	1938	A
10	AA	1945	G
10	AA	1949	G
10	AA	1951	A
10	AA	1952	C
10	AA	1953	A
10	AA	1956	A
10	AA	1981	G
10	AA	1991	G
10	AA	1994	C
10	AA	1996	A
10	AA	1998	A
10	AA	2008	A
10	AA	2019	C
10	AA	2023	U
10	AA	2025	G
10	AA	2030	A
10	AA	2031	C
10	AA	2045	PSU
10	AA	2048	C
10	AA	2049	A
10	AA	2051	U
10	AA	2053	A
10	AA	2054	OMU
10	AA	2055	U
10	AA	2063	C
10	AA	2079	G
10	AA	2080	U
10	AA	2085	G

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Mol	Chain	Res	Type
10	AA	2096	A2M
10	AA	2102	G
10	AA	2111	G
10	AA	2117	G
10	AA	2129	C
10	AA	2130	A
10	AA	2133	G
10	AA	2134	OMC
10	AA	2156	G
10	AA	2159	C
10	AA	2160	A
10	AA	2166	G
10	AA	2167	G
10	AA	2174	G
10	AA	2176	C
10	AA	2178	G
10	AA	2179	U
10	AA	2180	C
10	AA	2198	G
10	AA	2211	U
10	AA	2236	G
10	AA	2239	G
10	AA	2241	A
10	AA	2245	A
10	AA	2247	G
10	AA	2248	U
10	AA	2249	A
10	AA	2259	G
10	AA	2261	MA6
10	AA	2271	G
10	AA	2272	G
10	AA	2273	A
10	AA	2274	U
10	AA	2275	C
10	AA	2278	PSU
11	AB	76	A
35	BA	28	A
35	BA	33	C
35	BA	42	A
35	BA	45	A
35	BA	47	A
35	BA	51	C

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Mol	Chain	Res	Type
35	BA	62	A
35	BA	67	A
35	BA	68	A
35	BA	74	C
35	BA	76	G
35	BA	89	U
35	BA	91	A
35	BA	95	G
35	BA	96	C
35	BA	102	A
35	BA	114	A
35	BA	135	U
35	BA	138	A
35	BA	139	U
35	BA	140	G
35	BA	156	A
35	BA	169	C
35	BA	171	G
35	BA	172	U
35	BA	184	U
35	BA	204	U
35	BA	205	C
35	BA	207	A
35	BA	208	U
35	BA	218	A
35	BA	225	U
35	BA	228	U
35	BA	231	A
35	BA	242	A
35	BA	249	A
35	BA	250	U
35	BA	252	U
35	BA	253	G
35	BA	268	G
35	BA	269	A
35	BA	270	A
35	BA	274	G
35	BA	275	U
35	BA	285	A
35	BA	286	C
35	BA	298	A
35	BA	301	G

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Mol	Chain	Res	Type
35	BA	307	A
35	BA	308	C
35	BA	311	G
35	BA	314	U
35	BA	328	C
35	BA	329	C
35	BA	330	A
35	BA	336	G
35	BA	353	U
35	BA	362	A
35	BA	365	C
35	BA	366	C
35	BA	373	U
35	BA	391	A
35	BA	397	A
35	BA	398	G
35	BA	399	A
35	BA	403	G
35	BA	404	G
35	BA	406	A
35	BA	420	C
35	BA	424	U
35	BA	439	U
35	BA	440	U
35	BA	447	G
35	BA	470	A
35	BA	473	A
35	BA	474	C
35	BA	475	C
35	BA	489	A
35	BA	491	G
35	BA	493	C
35	BA	507	U
35	BA	514	U
35	BA	527	G
35	BA	528	C
35	BA	545	G
35	BA	549	A
35	BA	550	A
35	BA	552	U
35	BA	554	C
35	BA	561	G

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Mol	Chain	Res	Type
35	BA	568	A
35	BA	587	U
35	BA	591	C
35	BA	597	U
35	BA	598	C
35	BA	610	C
35	BA	614	G
35	BA	615	G
35	BA	616	G
35	BA	617	U
35	BA	619	C
35	BA	620	G
35	BA	621	U
35	BA	623	A
35	BA	627	G
35	BA	628	G
35	BA	629	C
35	BA	630	G
35	BA	635	A
35	BA	636	A
35	BA	637	A
35	BA	638	G
35	BA	639	G
35	BA	645	U
35	BA	646	G
35	BA	647	U
35	BA	648	G
35	BA	680	C
35	BA	683	C
35	BA	686	C
35	BA	690	G
35	BA	696	G
35	BA	697	C
35	BA	699	U
35	BA	704	A
35	BA	705	C
35	BA	706	G
35	BA	709	G
35	BA	717	A
35	BA	733	C
35	BA	743	A2M
35	BA	744	A

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Mol	Chain	Res	Type
35	BA	746	A2M
35	BA	757	A
35	BA	774	A
35	BA	785	U
35	BA	786	G
35	BA	791	U
35	BA	792	G
35	BA	799	C
35	BA	800	U
35	BA	801	U
35	BA	802	U
35	BA	803	U
35	BA	809	A
35	BA	816	G
35	BA	819	A
35	BA	838	U
35	BA	845	C
35	BA	849	A
35	BA	852	U
35	BA	872	C
35	BA	880	G
35	BA	887	C
35	BA	900	C
35	BA	901	G
35	BA	905	G
35	BA	919	G
35	BA	926	A
35	BA	936	A
35	BA	937	A
35	BA	950	A
35	BA	957	A
35	BA	963	G
35	BA	967	A
35	BA	969	C
35	BA	981	C
35	BA	991	U
35	BA	994	U
35	BA	999	U
35	BA	1027	G
35	BA	1029	A
35	BA	1034	A
35	BA	1036	G

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Mol	Chain	Res	Type
35	BA	1037	A
35	BA	1043	C
35	BA	1044	G
35	BA	1057	G
35	BA	1064	C
35	BA	1079	C
35	BA	1080	PSU
35	BA	1082	A
35	BA	1105	A
35	BA	1119	G
35	BA	1127	A
35	BA	1172	A
35	BA	1174	C
35	BA	1189	C
35	BA	1202	G
35	BA	1211	A
35	BA	1212	C
35	BA	1216	G
35	BA	1218	U
35	BA	1221	U
35	BA	1230	A
35	BA	1231	A
35	BA	1232	G
35	BA	1233	A
35	BA	1238	A
35	BA	1251	G
35	BA	1265	G
35	BA	1278	U
35	BA	1284	A
35	BA	1287	A
35	BA	1293	U
35	BA	1308	G
35	BA	1312	A
35	BA	1315	C
35	BA	1316	U
35	BA	1317	U
35	BA	1319	U
35	BA	1320	G
35	BA	1322	G
35	BA	1328	U
35	BA	1330	OMU
35	BA	1331	C

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Mol	Chain	Res	Type
35	BA	1334	U
35	BA	1338	U
35	BA	1340	A
35	BA	1341	A
35	BA	1347	U
35	BA	1348	G
35	BA	1446	G
35	BA	1447	A
35	BA	1448	OMU
35	BA	1452	G
35	BA	1455	U
35	BA	1456	A
35	BA	1461	C
35	BA	1470	U
35	BA	1471	G
35	BA	1474	U
35	BA	1480	U
35	BA	1481	U
35	BA	1491	G
35	BA	1492	U
35	BA	1499	G
35	BA	1500	G
35	BA	1501	C
35	BA	1505	A
35	BA	1515	G
35	BA	1516	A
35	BA	1519	A
35	BA	1522	U
35	BA	1526	G
35	BA	1530	U
35	BA	1545	G
35	BA	1571	G
35	BA	1585	A
35	BA	1586	U
35	BA	1590	C
35	BA	1605	OMG
35	BA	1608	OMC
35	BA	1615	G
35	BA	1617	C
35	BA	1621	OMG
35	BA	1626	G
35	BA	1638	U

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Mol	Chain	Res	Type
35	BA	1639	A
35	BA	1642	U
35	BA	1649	A
35	BA	1652	U
35	BA	1653	G
35	BA	1654	C
35	BA	1669	G
35	BA	1672	C
35	BA	1673	G
35	BA	1696	C
35	BA	1722	U
35	BA	1728	C
35	BA	1737	A
35	BA	1738	C
35	BA	1744	U
35	BA	1746	U
35	BA	1749	G
35	BA	1750	G
35	BA	1754	G
35	BA	1755	U
35	BA	1757	A
35	BA	1758	A
35	BA	1814	G
35	BA	1818	A
35	BA	1827	A
35	BA	1831	A
35	BA	1832	A
35	BA	1835	U
35	BA	1839	A
35	BA	1854	G
35	BA	1861	C
35	BA	1862	A
35	BA	1866	G
35	BA	1867	G
35	BA	1868	G
35	BA	1869	A
36	BB	12	G
36	BB	18	A
36	BB	22	A
36	BB	25	A
36	BB	29	C
36	BB	54	U

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Mol	Chain	Res	Type
36	BB	61	C
36	BB	62	A
36	BB	63	U
36	BB	68	A
36	BB	69	A
36	BB	75	C
36	BB	76	A
36	BB	90	G
36	BB	136	A
36	BB	359	A
36	BB	360	U
36	BB	380	A
36	BB	381	C
36	BB	386	G
36	BB	395	A
36	BB	398	G
36	BB	404	U
36	BB	408	A
36	BB	422	A
36	BB	452	A
36	BB	469	U
36	BB	470	G
36	BB	474	G
36	BB	482	G
36	BB	487	G
36	BB	513	G
36	BB	518	PSU
36	BB	520	A
36	BB	521	C
36	BB	523	A
36	BB	536	G
36	BB	537	G
36	BB	545	A2M
36	BB	548	C
36	BB	552	OMG
36	BB	562	U
36	BB	571	G
36	BB	572	C
36	BB	574	U
36	BB	577	A
36	BB	578	OMU
36	BB	579	G

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Mol	Chain	Res	Type
36	BB	598	U
36	BB	599	G
36	BB	600	U
36	BB	629	PSU
36	BB	637	A
36	BB	638	C
36	BB	639	G
36	BB	657	G
36	BB	661	A
36	BB	666	A
36	BB	667	G
36	BB	668	A
36	BB	675	U
36	BB	676	G
36	BB	683	A
36	BB	699	G
36	BB	710	U
36	BB	766	C
36	BB	767	G
36	BB	772	U
36	BB	778	U
36	BB	779	A
36	BB	786	G
36	BB	787	A
36	BB	789	G
36	BB	790	A
36	BB	798	G
36	BB	799	G
36	BB	800	U
36	BB	801	U
36	BB	803	U
36	BB	804	U
36	BB	807	G
36	BB	817	C
36	BB	818	G
36	BB	819	G
36	BB	831	U
36	BB	832	C
36	BB	837	C
36	BB	970	G
36	BB	971	C
36	BB	972	C

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Mol	Chain	Res	Type
36	BB	974	U
36	BB	975	G
36	BB	976	C
36	BB	977	G
36	BB	978	G
36	BB	979	A
36	BB	980	A
36	BB	983	A
36	BB	991	A
36	BB	992	A
36	BB	993	C
36	BB	1012	C
36	BB	1013	U
36	BB	1014	U
36	BB	1016	U
36	BB	1023	U
36	BB	1027	G
36	BB	1028	U
36	BB	1035	A
36	BB	1037	A
36	BB	1038	U
36	BB	1039	C
36	BB	1049	G
36	BB	1050	G
36	BB	1057	G
36	BB	1062	OMG
36	BB	1069	A
36	BB	1091	G
36	BB	1095	U
36	BB	1099	A
36	BB	1119	A
36	BB	1120	G
36	BB	1124	U
36	BB	1132	G
36	BB	1134	A
36	BB	1137	A
36	BB	1139	A
36	BB	1147	A
36	BB	1157	G
36	BB	1163	C
36	BB	1172	G
36	BB	1173	U

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Mol	Chain	Res	Type
36	BB	1190	A
36	BB	1191	A
36	BB	1197	G
36	BB	1205	A
36	BB	1215	A
36	BB	1219	A
36	BB	1220	C
36	BB	1221	A
36	BB	1222	G
36	BB	1223	G
36	BB	1226	A
36	BB	1231	A
36	BB	1250	G
36	BB	1253	A
36	BB	1254	G
36	BB	1255	A
36	BB	1264	OMC
36	BB	1271	A
36	BB	1287	G
36	BB	1297	U
36	BB	1299	A
36	BB	1300	U
36	BB	1303	C
36	BB	1325	G
36	BB	1327	U
36	BB	1330	C
36	BB	1341	A
36	BB	1353	C
36	BB	1377	U
36	BB	1382	C
36	BB	1389	C
36	BB	1390	A
36	BB	1396	C
36	BB	1401	G
36	BB	1425	A
36	BB	1432	U
36	BB	1437	C
36	BB	1444	U
36	BB	1446	G
36	BB	1452	G
36	BB	1457	C
36	BB	1458	G

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Mol	Chain	Res	Type
36	BB	1459	A
36	BB	1464	A
36	BB	1468	U
36	BB	1469	U
36	BB	1470	A
36	BB	1471	U
36	BB	1478	A
36	BB	1479	A
36	BB	1481	G
36	BB	1486	G
36	BB	1492	C
36	BB	1493	C
36	BB	1494	G
36	BB	1495	U
36	BB	1499	U
36	BB	1501	U
36	BB	1502	C
36	BB	1503	U
36	BB	1504	G
36	BB	1512	C
36	BB	1513	G
36	BB	1514	U
36	BB	1517	G
36	BB	1519	U
36	BB	1521	G
36	BB	1523	A
36	BB	1525	G
36	BB	1526	U
36	BB	1527	G
36	BB	1529	U
36	BB	1530	U
36	BB	1531	G
36	BB	1532	G
36	BB	1539	C
37	BC	22	U
37	BC	32	U
37	BC	33	U
37	BC	38	U
37	BC	48	A
37	BC	59	A
37	BC	62	A
37	BC	63	G

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Mol	Chain	Res	Type
37	BC	94	C
37	BC	103	A
37	BC	105	C
37	BC	110	A
37	BC	115	G
37	BC	124	A
37	BC	125	A
37	BC	136	G
37	BC	138	C
37	BC	149	A
37	BC	157	U
37	BC	158	U
37	BC	162	C
37	BC	165	U
37	BC	169	G
37	BC	170	A
38	BD	12	U
38	BD	23	A
38	BD	40	C
38	BD	48	G
38	BD	53	U
38	BD	64	A
38	BD	97	U
38	BD	100	A
38	BD	110	G
38	BD	117	U
38	BD	119	U
39	BE	4	G
39	BE	11	U
39	BE	14	G
39	BE	22	U
39	BE	32	C
39	BE	34	C
39	BE	35	A
39	BE	40	U
39	BE	41	C
39	BE	42	C
39	BE	46	C
39	BE	47	A
39	BE	50	G
39	BE	51	U
39	BE	62	U

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Mol	Chain	Res	Type
39	BE	70	A
39	BE	107	C
39	BE	108	G
39	BE	109	A
39	BE	111	U
39	BE	122	C
39	BE	123	U
39	BE	147	A
39	BE	149	A
39	BE	153	A
39	BE	166	U
39	BE	167	A
39	BE	171	U
39	BE	172	C
39	BE	182	G
39	BE	186	U
39	BE	187	C
39	BE	191	G
39	BE	192	C
39	BE	198	A
39	BE	200	C
40	BF	10	G
40	BF	11	C
40	BF	14	C
40	BF	24	C
40	BF	25	C
40	BF	36	G
40	BF	57	G
40	BF	58	U
40	BF	63	U
40	BF	69	U
40	BF	70	C
40	BF	72	C
40	BF	73	A
41	BG	5	G
41	BG	8	U
41	BG	9	G
41	BG	10	U
41	BG	16	G
41	BG	19	C
41	BG	25	G
41	BG	40	G

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Mol	Chain	Res	Type
41	BG	58	G
41	BG	60	A
41	BG	85	C
41	BG	86	U
41	BG	102	G
41	BG	114	A
41	BG	120	U
41	BG	121	C
41	BG	127	G
41	BG	132	U
41	BG	135	C
41	BG	139	U
41	BG	145	C
41	BG	150	A
41	BG	157	A
41	BG	159	A
41	BG	168	A
41	BG	173	C
42	BH	14	C
42	BH	23	G
42	BH	26	C
42	BH	28	U
42	BH	49	C
42	BH	50	A
42	BH	51	C
42	BH	71	C
42	BH	72	G
42	BH	75	G
42	BH	85	C
42	BH	86	G
42	BH	87	U
42	BH	99	G
42	BH	106	G
42	BH	109	G
42	BH	112	U
42	BH	113	G
42	BH	114	G
42	BH	115	A
42	BH	116	A
42	BH	117	U
42	BH	118	U
42	BH	119	U

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Mol	Chain	Res	Type
42	BH	120	C
42	BH	125	U
42	BH	134	U
42	BH	135	U

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	AA	166	C
10	AA	172	A
10	AA	291	A
10	AA	376	G
10	AA	741	G
10	AA	752	A
10	AA	792	U
10	AA	799	A
10	AA	1769	A
10	AA	1853	A
10	AA	1863	U
10	AA	1924	G
10	AA	1990	U
10	AA	2247	G
35	BA	67	A
35	BA	268	G
35	BA	627	G
35	BA	635	A
35	BA	637	A
35	BA	638	G
35	BA	704	A
35	BA	785	U
35	BA	800	U
35	BA	993	C
35	BA	1036	G
35	BA	1745	G
35	BA	1830	G
36	BB	379	U
36	BB	636	A
36	BB	817	C
36	BB	974	U
36	BB	977	G
36	BB	982	U
36	BB	1013	U

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Mol	Chain	Res	Type
36	BB	1038	U
36	BB	1172	G
36	BB	1470	A
36	BB	1524	U
36	BB	1530	U
36	BB	1531	G
38	BD	63	C
40	BF	56	A
41	BG	18	U
41	BG	149	U
42	BH	112	U

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

145 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	$\# Z > 2$
36	PSU	BB	1403	85,36	18,21,22	4.27	8 (44%)	22,30,33	1.92	6 (27%)
36	OMG	BB	673	36	23,26,27	2.36	9 (39%)	33,38,41	2.56	10 (30%)
10	A2M	AA	125	85,10	22,25,26	3.48	10 (45%)	31,36,39	2.41	10 (32%)
10	MA6	AA	2261	10	23,26,27	1.60	5 (21%)	34,38,41	3.02	11 (32%)
36	PSU	BB	1229	36	18,21,22	4.34	7 (38%)	22,30,33	1.83	5 (22%)
35	PSU	BA	1609	35	18,21,22	4.32	7 (38%)	22,30,33	1.77	5 (22%)
36	PSU	BB	518	36	18,21,22	4.42	8 (44%)	22,30,33	1.74	4 (18%)
10	OMG	AA	1676	10	23,26,27	2.37	9 (39%)	33,38,41	2.61	10 (30%)
35	A2M	BA	996	35	22,25,26	3.46	10 (45%)	31,36,39	2.40	10 (32%)
10	B8N	AA	1596	10	24,29,30	3.01	6 (25%)	29,42,45	1.72	5 (17%)
10	PSU	AA	1592	10	18,21,22	4.39	7 (38%)	22,30,33	1.82	5 (22%)
36	PSU	BB	680	85,36	18,21,22	0.87	1 (5%)	22,30,33	0.63	0
10	A2M	AA	2153	10	22,25,26	3.50	11 (50%)	31,36,39	2.44	11 (35%)
36	PSU	BB	1210	36	18,21,22	4.33	7 (38%)	22,30,33	1.82	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	PSU	BA	1169	35	18,21,22	4.36	7 (38%)	22,30,33	1.88	5 (22%)
35	PSU	BA	1086	35,87	18,21,22	4.29	7 (38%)	22,30,33	1.82	5 (22%)
8	SNC	A7	157	8	4,7,8	0.71	0	1,7,9	0.33	0
36	PSU	BB	1434	36	18,21,22	4.35	7 (38%)	22,30,33	1.77	5 (22%)
10	PSU	AA	2045	10	18,21,22	4.35	7 (38%)	22,30,33	1.75	4 (18%)
10	OMG	AA	1517	10	23,26,27	2.39	9 (39%)	33,38,41	2.57	10 (30%)
36	OMU	BB	1435	36	19,22,23	2.87	8 (42%)	26,31,34	1.73	4 (15%)
36	PSU	BB	1409	36	18,21,22	4.39	7 (38%)	22,30,33	1.74	5 (22%)
35	PSU	BA	1129	35,87	18,21,22	4.33	7 (38%)	22,30,33	1.81	5 (22%)
36	OMC	BB	1264	36	19,22,23	2.88	8 (42%)	26,31,34	0.82	0
35	OMG	BA	1709	35	23,26,27	2.36	9 (39%)	33,38,41	2.43	11 (33%)
10	OMC	AA	66	10	19,22,23	2.90	8 (42%)	26,31,34	0.76	0
36	OMG	BB	1245	36	23,26,27	2.35	9 (39%)	33,38,41	2.52	10 (30%)
10	OMC	AA	1844	10	19,22,23	2.91	8 (42%)	26,31,34	0.69	0
36	PSU	BB	1419	36	18,21,22	4.35	8 (44%)	22,30,33	1.91	6 (27%)
35	OMU	BA	1742	85,35	19,22,23	2.88	8 (42%)	26,31,34	1.78	5 (19%)
10	PSU	AA	1907	10	18,21,22	4.38	8 (44%)	22,30,33	1.78	5 (22%)
36	A2M	BB	646	36	22,25,26	3.47	10 (45%)	31,36,39	2.40	9 (29%)
35	A2M	BA	1620	85,35,36	22,25,26	3.49	10 (45%)	31,36,39	2.37	9 (29%)
36	OMU	BB	1093	36	19,22,23	2.94	8 (42%)	26,31,34	1.77	5 (19%)
36	OMG	BB	1269	36	23,26,27	2.33	8 (34%)	33,38,41	2.53	10 (30%)
36	A2M	BB	545	85,36	22,25,26	3.40	10 (45%)	31,36,39	2.56	14 (45%)
36	OMU	BB	1375	36	19,22,23	0.21	0	26,31,34	0.47	0
10	OMC	AA	2134	10	19,22,23	0.27	0	26,31,34	0.46	0
10	PSU	AA	131	10	18,21,22	4.41	7 (38%)	22,30,33	1.86	5 (22%)
36	PSU	BB	644	36	18,21,22	4.30	7 (38%)	22,30,33	1.82	5 (22%)
37	A2M	BC	43	37	22,25,26	3.46	10 (45%)	31,36,39	2.39	9 (29%)
36	A2M	BB	588	35,36	22,25,26	0.19	0	31,36,39	0.31	0
35	A2M	BA	1665	35,36	22,25,26	3.44	10 (45%)	31,36,39	2.43	10 (32%)
36	PSU	BB	455	36,87	18,21,22	0.88	1 (5%)	22,30,33	0.63	0
35	OMC	BA	1329	35	19,22,23	2.97	8 (42%)	26,31,34	0.70	0
35	OMG	BA	1621	85,35,36	23,26,27	2.34	9 (39%)	33,38,41	2.49	11 (33%)
37	PSU	BC	74	37	18,21,22	4.42	7 (38%)	22,30,33	1.86	5 (22%)
10	PSU	AA	1710	10	18,21,22	4.33	7 (38%)	22,30,33	1.74	4 (18%)
35	A2M	BA	927	35	22,25,26	3.45	10 (45%)	31,36,39	2.41	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	OMG	BB	1094	36	23,26,27	2.34	9 (39%)	33,38,41	2.44	12 (36%)
35	OMU	BA	916	35	19,22,23	2.89	8 (42%)	26,31,34	1.79	5 (19%)
36	PSU	BB	1334	36	18,21,22	4.31	7 (38%)	22,30,33	1.88	5 (22%)
35	OMG	BA	1605	35	23,26,27	2.36	9 (39%)	33,38,41	2.57	10 (30%)
10	OMG	AA	1931	10	23,26,27	2.38	9 (39%)	33,38,41	2.54	10 (30%)
35	A2M	BA	254	35	22,25,26	3.45	9 (40%)	31,36,39	2.38	11 (35%)
36	OMU	BB	685	36	19,22,23	2.91	8 (42%)	26,31,34	1.78	5 (19%)
36	A2M	BB	590	36	22,25,26	3.45	10 (45%)	31,36,39	2.37	10 (32%)
35	OMG	BA	915	35	23,26,27	2.39	9 (39%)	33,38,41	2.52	10 (30%)
37	OMU	BC	7	37,35	19,22,23	2.90	8 (42%)	26,31,34	1.74	5 (19%)
10	OMG	AA	1603	10	23,26,27	2.40	9 (39%)	33,38,41	2.51	10 (30%)
36	OMG	BB	72	36	23,26,27	2.34	8 (34%)	33,38,41	2.50	10 (30%)
10	OMU	AA	714	10	19,22,23	2.89	8 (42%)	26,31,34	1.78	5 (19%)
36	PSU	BB	1429	36,87	18,21,22	4.24	7 (38%)	22,30,33	1.78	5 (22%)
35	PSU	BA	1614	35,36	18,21,22	4.33	7 (38%)	22,30,33	1.85	5 (22%)
36	OMC	BB	377	36	19,22,23	2.95	8 (42%)	26,31,34	0.72	0
35	OMG	BA	1267	35	23,26,27	2.35	9 (39%)	33,38,41	2.43	12 (36%)
10	OMU	AA	2123	10	19,22,23	2.73	7 (36%)	26,31,34	1.81	5 (19%)
36	OMU	BB	578	36,87	19,22,23	2.89	8 (42%)	26,31,34	1.73	4 (15%)
35	A2M	BA	762	35	22,25,26	3.52	11 (50%)	31,36,39	2.37	10 (32%)
36	A2M	BB	95	36	22,25,26	3.51	10 (45%)	31,36,39	2.40	11 (35%)
10	PSU	AA	1276	10	18,21,22	4.35	7 (38%)	22,30,33	1.83	5 (22%)
36	A2M	BB	1388	36	22,25,26	3.48	9 (40%)	31,36,39	2.39	11 (35%)
10	A2M	AA	2096	10	22,25,26	3.44	9 (40%)	31,36,39	2.40	11 (35%)
10	A2M	AA	721	85,10	22,25,26	3.43	10 (45%)	31,36,39	2.45	11 (35%)
10	OMU	AA	1899	10	19,22,23	2.98	8 (42%)	26,31,34	1.78	5 (19%)
35	PSU	BA	1080	35,36	18,21,22	4.43	7 (38%)	22,30,33	1.88	6 (27%)
36	PSU	BB	490	36	18,21,22	4.45	7 (38%)	22,30,33	1.89	5 (22%)
35	1MA	BA	742	85,35	21,25,26	2.83	6 (28%)	31,37,40	2.94	8 (25%)
10	OMU	AA	36	10	19,22,23	0.22	0	26,31,34	0.50	0
36	OMC	BB	601	36	19,22,23	2.76	7 (36%)	26,31,34	0.70	0
35	PSU	BA	737	85,35	18,21,22	4.31	7 (38%)	22,30,33	1.76	6 (27%)
10	MA6	AA	2260	10	23,26,27	1.50	5 (21%)	34,38,41	3.01	12 (35%)
36	OMG	BB	1247	36	23,26,27	2.37	9 (39%)	33,38,41	2.52	10 (30%)
36	PSU	BB	611	36	18,21,22	4.32	7 (38%)	22,30,33	1.65	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	5MC	BB	1324	36,87	18,22,23	3.41	7 (38%)	26,32,35	1.18	1 (3%)
37	OMG	BC	75	37	23,26,27	2.38	9 (39%)	33,38,41	2.50	10 (30%)
36	OMC	BB	1413	36	19,22,23	2.80	8 (42%)	26,31,34	0.78	0
10	OMU	AA	57	10	19,22,23	2.91	8 (42%)	26,31,34	1.71	5 (19%)
10	PSU	AA	505	10	18,21,22	4.31	7 (38%)	22,30,33	1.94	5 (22%)
36	OMG	BB	552	36	23,26,27	2.34	9 (39%)	33,38,41	2.49	10 (30%)
37	A2M	BC	41	37	22,25,26	3.47	10 (45%)	31,36,39	2.40	10 (32%)
10	OMG	AA	1895	85,10	23,26,27	2.36	9 (39%)	33,38,41	2.51	10 (30%)
36	A2M	BB	609	36	22,25,26	3.48	10 (45%)	31,36,39	2.36	11 (35%)
35	PSU	BA	1248	35,87	18,21,22	4.30	8 (44%)	22,30,33	1.86	6 (27%)
36	PSU	BB	629	36	18,21,22	4.31	7 (38%)	22,30,33	1.77	5 (22%)
10	OMU	AA	2154	10	19,22,23	2.93	8 (42%)	26,31,34	1.80	5 (19%)
35	OMC	BA	1006	35	19,22,23	2.83	8 (42%)	26,31,34	0.75	0
36	PSU	BB	1160	36	18,21,22	4.36	7 (38%)	22,30,33	1.85	5 (22%)
35	PSU	BA	1009	35	18,21,22	4.28	7 (38%)	22,30,33	1.83	4 (18%)
10	OMG	AA	1531	10	23,26,27	0.30	0	33,38,41	0.36	0
35	OMU	BA	46	35	19,22,23	2.92	8 (42%)	26,31,34	1.83	5 (19%)
10	G7M	AA	2070	10	23,26,27	3.70	11 (47%)	35,39,42	1.68	7 (20%)
36	5MC	BB	542	85,36	18,22,23	3.34	7 (38%)	26,32,35	1.08	2 (7%)
37	OMU	BC	167	37,35	19,22,23	2.94	8 (42%)	26,31,34	1.78	5 (19%)
36	OMG	BB	659	85,36	23,26,27	2.31	9 (39%)	33,38,41	2.38	12 (36%)
35	OMU	BA	1181	35	19,22,23	2.90	8 (42%)	26,31,34	1.82	5 (19%)
36	OMU	BB	73	36	19,22,23	2.90	8 (42%)	26,31,34	1.76	5 (19%)
35	OMG	BA	1028	85,35	23,26,27	2.35	9 (39%)	33,38,41	2.29	9 (27%)
10	OMC	AA	1932	10	19,22,23	2.89	8 (42%)	26,31,34	0.75	0
10	PSU	AA	2146	10	18,21,22	4.21	7 (38%)	22,30,33	1.83	4 (18%)
10	PSU	AA	61	10	18,21,22	4.42	7 (38%)	22,30,33	1.87	5 (22%)
35	PSU	BA	1258	35	18,21,22	4.37	7 (38%)	22,30,33	1.85	5 (22%)
36	OMG	BB	71	36	23,26,27	2.37	8 (34%)	33,38,41	2.44	12 (36%)
36	A2M	BB	400	36	22,25,26	3.45	10 (45%)	31,36,39	2.33	9 (29%)
35	OMC	BA	1608	35	19,22,23	2.84	8 (42%)	26,31,34	0.82	1 (3%)
37	A2M	BC	163	37,35	22,25,26	3.47	10 (45%)	31,36,39	2.36	11 (35%)
10	OMU	AA	2054	10	19,22,23	2.92	8 (42%)	26,31,34	1.78	5 (19%)
36	PSU	BB	1076	36	18,21,22	4.34	7 (38%)	22,30,33	1.98	5 (22%)
10	OMG	AA	1700	10	23,26,27	2.32	9 (39%)	33,38,41	2.47	11 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	A2M	BA	743	35,36	22,25,26	3.49	10 (45%)	31,36,39	2.48	12 (38%)
10	OMG	AA	2227	10	23,26,27	2.30	8 (34%)	33,38,41	2.45	10 (30%)
10	PSU	AA	1619	10	18,21,22	4.40	8 (44%)	22,30,33	1.67	4 (18%)
35	OMC	BA	747	85,35	19,22,23	2.82	7 (36%)	26,31,34	0.86	0
36	OMG	BB	1062	36	23,26,27	2.36	9 (39%)	33,38,41	2.54	10 (30%)
10	OMU	AA	1674	10	19,22,23	2.97	8 (42%)	26,31,34	1.71	5 (19%)
35	A2M	BA	746	35	22,25,26	3.41	9 (40%)	31,36,39	2.40	9 (29%)
10	PSU	AA	2278	10	18,21,22	4.37	7 (38%)	22,30,33	1.75	5 (22%)
36	PSU	BB	1280	36	18,21,22	4.29	8 (44%)	22,30,33	1.90	6 (27%)
35	PSU	BA	1166	35	18,21,22	4.37	7 (38%)	22,30,33	1.76	5 (22%)
36	A2M	BB	1400	88,36	22,25,26	0.17	0	31,36,39	0.55	0
35	OMU	BA	1448	35	19,22,23	2.92	8 (42%)	26,31,34	1.77	4 (15%)
10	A2M	AA	56	85,10	22,25,26	3.47	10 (45%)	31,36,39	2.39	9 (29%)
36	OMC	BB	1175	36	19,22,23	0.28	0	26,31,34	0.41	0
35	OMC	BA	760	35	19,22,23	2.86	8 (42%)	26,31,34	0.73	0
36	PSU	BB	1319	36	18,21,22	4.36	8 (44%)	22,30,33	1.90	6 (27%)
36	PSU	BB	615	36	18,21,22	4.30	7 (38%)	22,30,33	1.81	5 (22%)
36	A2M	BB	622	35,36	22,25,26	3.46	9 (40%)	31,36,39	2.38	10 (32%)
35	A2M	BA	1024	35	22,25,26	3.50	10 (45%)	31,36,39	2.42	10 (32%)
10	PSU	AA	1612	10	18,21,22	0.86	1 (5%)	22,30,33	0.64	0
35	OMG	BA	925	35	23,26,27	2.34	9 (39%)	33,38,41	2.44	10 (30%)
10	OMC	AA	46	10	19,22,23	2.85	8 (42%)	26,31,34	0.75	0
35	OMU	BA	1330	35	19,22,23	3.05	8 (42%)	26,31,34	1.84	5 (19%)
35	PSU	BA	452	35	18,21,22	4.37	7 (38%)	22,30,33	1.87	5 (22%)
36	PSU	BB	528	36	18,21,22	4.37	7 (38%)	22,30,33	1.84	5 (22%)
36	A2M	BB	1201	36	22,25,26	3.44	10 (45%)	31,36,39	2.48	12 (38%)

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
36	PSU	BB	1403	85,36	-	0/7/25/26	0/2/2/2
36	OMG	BB	673	36	-	0/9/27/28	0/3/3/3
10	A2M	AA	125	85,10	-	2/9/27/28	0/3/3/3
10	MA6	AA	2261	10	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	PSU	BB	1229	36	-	0/7/25/26	0/2/2/2
35	PSU	BA	1609	35	-	0/7/25/26	0/2/2/2
36	PSU	BB	518	36	-	2/7/25/26	0/2/2/2
10	OMG	AA	1676	10	-	1/9/27/28	0/3/3/3
35	A2M	BA	996	35	-	0/9/27/28	0/3/3/3
10	B8N	AA	1596	10	-	1/16/34/35	0/2/2/2
10	PSU	AA	1592	10	-	1/7/25/26	0/2/2/2
36	PSU	BB	680	85,36	-	0/7/25/26	0/2/2/2
10	A2M	AA	2153	10	-	1/9/27/28	0/3/3/3
36	PSU	BB	1210	36	-	0/7/25/26	0/2/2/2
35	PSU	BA	1169	35	-	0/7/25/26	0/2/2/2
35	PSU	BA	1086	35,87	-	0/7/25/26	0/2/2/2
8	SNC	A7	157	8	-	0/0/6/8	-
36	PSU	BB	1434	36	-	2/7/25/26	0/2/2/2
10	PSU	AA	2045	10	-	2/7/25/26	0/2/2/2
10	OMG	AA	1517	10	-	0/9/27/28	0/3/3/3
36	OMU	BB	1435	36	-	0/9/27/28	0/2/2/2
36	PSU	BB	1409	36	-	0/7/25/26	0/2/2/2
35	PSU	BA	1129	35,87	-	0/7/25/26	0/2/2/2
36	OMC	BB	1264	36	-	1/9/27/28	0/2/2/2
35	OMG	BA	1709	35	-	0/9/27/28	0/3/3/3
10	OMC	AA	66	10	-	0/9/27/28	0/2/2/2
36	OMG	BB	1245	36	-	0/9/27/28	0/3/3/3
10	OMC	AA	1844	10	-	0/9/27/28	0/2/2/2
36	PSU	BB	1419	36	-	0/7/25/26	0/2/2/2
35	OMU	BA	1742	85,35	-	0/9/27/28	0/2/2/2
10	PSU	AA	1907	10	-	1/7/25/26	0/2/2/2
36	A2M	BB	646	36	-	1/9/27/28	0/3/3/3
35	A2M	BA	1620	85,35,36	-	0/9/27/28	0/3/3/3
36	OMU	BB	1093	36	-	0/9/27/28	0/2/2/2
36	OMG	BB	1269	36	-	0/9/27/28	0/3/3/3
36	A2M	BB	545	85,36	-	2/9/27/28	0/3/3/3
36	OMU	BB	1375	36	-	0/9/27/28	0/2/2/2
10	OMC	AA	2134	10	-	2/9/27/28	0/2/2/2
10	PSU	AA	131	10	-	0/7/25/26	0/2/2/2
36	PSU	BB	644	36	-	0/7/25/26	0/2/2/2
37	A2M	BC	43	37	-	0/9/27/28	0/3/3/3
36	A2M	BB	588	35,36	-	3/9/27/28	0/3/3/3
35	A2M	BA	1665	35,36	-	0/9/27/28	0/3/3/3
36	PSU	BB	455	36,87	-	0/7/25/26	0/2/2/2
35	OMC	BA	1329	35	-	3/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	OMG	BA	1621	85,35,36	-	1/9/27/28	0/3/3/3
37	PSU	BC	74	37	-	0/7/25/26	0/2/2/2
10	PSU	AA	1710	10	-	2/7/25/26	0/2/2/2
35	A2M	BA	927	35	-	0/9/27/28	0/3/3/3
36	OMG	BB	1094	36	-	0/9/27/28	0/3/3/3
35	OMU	BA	916	35	-	0/9/27/28	0/2/2/2
36	PSU	BB	1334	36	-	0/7/25/26	0/2/2/2
35	OMG	BA	1605	35	-	2/9/27/28	0/3/3/3
10	OMG	AA	1931	10	-	2/9/27/28	0/3/3/3
35	A2M	BA	254	35	-	0/9/27/28	0/3/3/3
36	OMU	BB	685	36	-	1/9/27/28	0/2/2/2
36	A2M	BB	590	36	-	0/9/27/28	0/3/3/3
35	OMG	BA	915	35	-	0/9/27/28	0/3/3/3
37	OMU	BC	7	37,35	-	1/9/27/28	0/2/2/2
10	OMG	AA	1603	10	-	2/9/27/28	0/3/3/3
36	OMG	BB	72	36	-	0/9/27/28	0/3/3/3
10	OMU	AA	714	10	-	0/9/27/28	0/2/2/2
36	PSU	BB	1429	36,87	-	0/7/25/26	0/2/2/2
35	PSU	BA	1614	35,36	-	2/7/25/26	0/2/2/2
36	OMC	BB	377	36	-	0/9/27/28	0/2/2/2
35	OMG	BA	1267	35	-	0/9/27/28	0/3/3/3
10	OMU	AA	2123	10	-	0/9/27/28	0/2/2/2
36	OMU	BB	578	36,87	-	4/9/27/28	0/2/2/2
35	A2M	BA	762	35	-	1/9/27/28	0/3/3/3
36	A2M	BB	95	36	-	1/9/27/28	0/3/3/3
10	PSU	AA	1276	10	-	0/7/25/26	0/2/2/2
36	A2M	BB	1388	36	-	0/9/27/28	0/3/3/3
10	A2M	AA	2096	10	-	1/9/27/28	0/3/3/3
10	A2M	AA	721	85,10	-	3/9/27/28	0/3/3/3
10	OMU	AA	1899	10	-	1/9/27/28	0/2/2/2
35	PSU	BA	1080	35,36	-	3/7/25/26	0/2/2/2
36	PSU	BB	490	36	-	0/7/25/26	0/2/2/2
35	1MA	BA	742	85,35	-	0/7/25/26	0/3/3/3
10	OMU	AA	36	10	-	5/9/27/28	0/2/2/2
36	OMC	BB	601	36	-	0/9/27/28	0/2/2/2
35	PSU	BA	737	85,35	-	0/7/25/26	0/2/2/2
10	MA6	AA	2260	10	-	0/11/29/30	0/3/3/3
36	OMG	BB	1247	36	-	0/9/27/28	0/3/3/3
36	PSU	BB	611	36	-	0/7/25/26	0/2/2/2
36	5MC	BB	1324	36,87	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	OMG	BC	75	37	-	0/9/27/28	0/3/3/3
36	OMC	BB	1413	36	-	0/9/27/28	0/2/2/2
10	OMU	AA	57	10	-	1/9/27/28	0/2/2/2
10	PSU	AA	505	10	-	0/7/25/26	0/2/2/2
36	OMG	BB	552	36	-	2/9/27/28	0/3/3/3
37	A2M	BC	41	37	-	0/9/27/28	0/3/3/3
10	OMG	AA	1895	85,10	-	1/9/27/28	0/3/3/3
36	A2M	BB	609	36	-	0/9/27/28	0/3/3/3
35	PSU	BA	1248	35,87	-	0/7/25/26	0/2/2/2
36	PSU	BB	629	36	-	2/7/25/26	0/2/2/2
10	OMU	AA	2154	10	-	1/9/27/28	0/2/2/2
35	OMC	BA	1006	35	-	1/9/27/28	0/2/2/2
36	PSU	BB	1160	36	-	0/7/25/26	0/2/2/2
35	PSU	BA	1009	35	-	0/7/25/26	0/2/2/2
10	OMG	AA	1531	10	-	2/9/27/28	0/3/3/3
35	OMU	BA	46	35	-	0/9/27/28	0/2/2/2
10	G7M	AA	2070	10	-	0/7/25/26	0/3/3/3
36	5MC	BB	542	85,36	-	1/7/25/26	0/2/2/2
37	OMU	BC	167	37,35	-	0/9/27/28	0/2/2/2
36	OMG	BB	659	85,36	-	1/9/27/28	0/3/3/3
35	OMU	BA	1181	35	-	0/9/27/28	0/2/2/2
36	OMU	BB	73	36	-	1/9/27/28	0/2/2/2
35	OMG	BA	1028	85,35	-	0/9/27/28	0/3/3/3
10	OMC	AA	1932	10	-	0/9/27/28	0/2/2/2
10	PSU	AA	2146	10	-	0/7/25/26	0/2/2/2
10	PSU	AA	61	10	-	0/7/25/26	0/2/2/2
35	PSU	BA	1258	35	-	2/7/25/26	0/2/2/2
36	OMG	BB	71	36	-	0/9/27/28	0/3/3/3
36	A2M	BB	400	36	-	0/9/27/28	0/3/3/3
35	OMC	BA	1608	35	-	4/9/27/28	0/2/2/2
37	A2M	BC	163	37,35	-	1/9/27/28	0/3/3/3
10	OMU	AA	2054	10	-	2/9/27/28	0/2/2/2
36	PSU	BB	1076	36	-	0/7/25/26	0/2/2/2
10	OMG	AA	1700	10	-	0/9/27/28	0/3/3/3
35	A2M	BA	743	35,36	-	1/9/27/28	0/3/3/3
10	OMG	AA	2227	10	-	0/9/27/28	0/3/3/3
10	PSU	AA	1619	10	-	4/7/25/26	0/2/2/2
35	OMC	BA	747	85,35	-	0/9/27/28	0/2/2/2
36	OMG	BB	1062	36	-	2/9/27/28	0/3/3/3
10	OMU	AA	1674	10	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A2M	BA	746	35	-	1/9/27/28	0/3/3/3
10	PSU	AA	2278	10	-	1/7/25/26	0/2/2/2
36	PSU	BB	1280	36	-	0/7/25/26	0/2/2/2
35	PSU	BA	1166	35	-	0/7/25/26	0/2/2/2
36	A2M	BB	1400	88,36	-	1/9/27/28	0/3/3/3
35	OMU	BA	1448	35	-	2/9/27/28	0/2/2/2
10	A2M	AA	56	85,10	-	1/9/27/28	0/3/3/3
36	OMC	BB	1175	36	-	0/9/27/28	0/2/2/2
35	OMC	BA	760	35	-	0/9/27/28	0/2/2/2
36	PSU	BB	1319	36	-	0/7/25/26	0/2/2/2
36	PSU	BB	615	36	-	0/7/25/26	0/2/2/2
36	A2M	BB	622	35,36	-	0/9/27/28	0/3/3/3
35	A2M	BA	1024	35	-	1/9/27/28	0/3/3/3
10	PSU	AA	1612	10	-	1/7/25/26	0/2/2/2
35	OMG	BA	925	35	-	0/9/27/28	0/3/3/3
10	OMC	AA	46	10	-	0/9/27/28	0/2/2/2
35	OMU	BA	1330	35	-	3/9/27/28	0/2/2/2
35	PSU	BA	452	35	-	0/7/25/26	0/2/2/2
36	PSU	BB	528	36	-	0/7/25/26	0/2/2/2
36	A2M	BB	1201	36	-	1/9/27/28	0/3/3/3

All (1098) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1080	PSU	C6-C5	11.60	1.48	1.35
36	BB	1409	PSU	C6-C5	11.50	1.48	1.35
10	AA	1619	PSU	C6-C5	11.47	1.48	1.35
37	BC	74	PSU	C6-C5	11.44	1.48	1.35
36	BB	518	PSU	C6-C5	11.42	1.48	1.35
36	BB	490	PSU	C6-C5	11.42	1.48	1.35
10	AA	61	PSU	C6-C5	11.41	1.48	1.35
35	BA	1258	PSU	C6-C5	11.35	1.48	1.35
10	AA	1592	PSU	C6-C5	11.33	1.48	1.35
36	BB	1160	PSU	C6-C5	11.31	1.48	1.35
10	AA	131	PSU	C6-C5	11.30	1.48	1.35
35	BA	1129	PSU	C6-C5	11.29	1.48	1.35
10	AA	1907	PSU	C6-C5	11.29	1.48	1.35
36	BB	611	PSU	C6-C5	11.28	1.48	1.35
35	BA	452	PSU	C6-C5	11.28	1.48	1.35
36	BB	1434	PSU	C6-C5	11.23	1.48	1.35
10	AA	2045	PSU	C6-C5	11.23	1.48	1.35
35	BA	1166	PSU	C6-C5	11.22	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	1319	PSU	C6-C5	11.22	1.48	1.35
36	BB	1334	PSU	C6-C5	11.19	1.48	1.35
10	AA	2278	PSU	C6-C5	11.19	1.48	1.35
36	BB	1229	PSU	C6-C5	11.18	1.48	1.35
35	BA	1609	PSU	C6-C5	11.17	1.48	1.35
36	BB	528	PSU	C6-C5	11.17	1.48	1.35
35	BA	1169	PSU	C6-C5	11.16	1.48	1.35
36	BB	1076	PSU	C6-C5	11.16	1.48	1.35
36	BB	1210	PSU	C6-C5	11.16	1.48	1.35
10	AA	505	PSU	C6-C5	11.15	1.48	1.35
10	AA	1710	PSU	C6-C5	11.14	1.48	1.35
36	BB	1419	PSU	C6-C5	11.12	1.48	1.35
10	AA	1276	PSU	C6-C5	11.12	1.48	1.35
35	BA	1086	PSU	C6-C5	11.11	1.48	1.35
35	BA	1614	PSU	C6-C5	11.08	1.48	1.35
36	BB	644	PSU	C6-C5	11.07	1.48	1.35
36	BB	629	PSU	C6-C5	11.06	1.48	1.35
36	BB	615	PSU	C6-C5	11.05	1.48	1.35
35	BA	1009	PSU	C6-C5	11.04	1.48	1.35
35	BA	737	PSU	C6-C5	10.99	1.48	1.35
36	BB	1280	PSU	C6-C5	10.95	1.48	1.35
36	BB	1429	PSU	C6-C5	10.95	1.48	1.35
35	BA	1248	PSU	C6-C5	10.94	1.48	1.35
36	BB	1403	PSU	C6-C5	10.88	1.48	1.35
10	AA	2146	PSU	C6-C5	10.85	1.47	1.35
10	AA	2070	G7M	C8-N7	10.47	1.51	1.33
10	AA	1710	PSU	C2-N1	9.53	1.49	1.36
36	BB	490	PSU	C2-N1	9.51	1.49	1.36
10	AA	131	PSU	C2-N1	9.50	1.49	1.36
37	BC	74	PSU	C2-N1	9.49	1.49	1.36
10	AA	61	PSU	C2-N1	9.45	1.49	1.36
10	AA	1276	PSU	C2-N1	9.43	1.49	1.36
36	BB	518	PSU	C2-N1	9.42	1.49	1.36
35	BA	1080	PSU	C2-N1	9.40	1.49	1.36
10	AA	2278	PSU	C2-N1	9.37	1.49	1.36
35	BA	1169	PSU	C2-N1	9.36	1.49	1.36
10	AA	1619	PSU	C2-N1	9.33	1.49	1.36
10	AA	1592	PSU	C2-N1	9.32	1.49	1.36
35	BA	452	PSU	C2-N1	9.31	1.49	1.36
35	BA	1258	PSU	C2-N1	9.30	1.49	1.36
10	AA	505	PSU	C2-N1	9.30	1.49	1.36
36	BB	1229	PSU	C2-N1	9.30	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	1419	PSU	C2-N1	9.29	1.49	1.36
35	BA	1166	PSU	C2-N1	9.29	1.49	1.36
36	BB	1076	PSU	C2-N1	9.26	1.49	1.36
36	BB	1434	PSU	C2-N1	9.26	1.49	1.36
36	BB	1160	PSU	C2-N1	9.25	1.49	1.36
10	AA	1907	PSU	C2-N1	9.23	1.49	1.36
36	BB	528	PSU	C2-N1	9.21	1.49	1.36
35	BA	1129	PSU	C2-N1	9.21	1.49	1.36
35	BA	1614	PSU	C2-N1	9.20	1.49	1.36
36	BB	1319	PSU	C2-N1	9.20	1.49	1.36
36	BB	1409	PSU	C2-N1	9.19	1.49	1.36
35	BA	737	PSU	C2-N1	9.19	1.49	1.36
36	BB	1210	PSU	C2-N1	9.18	1.49	1.36
35	BA	1248	PSU	C2-N1	9.16	1.49	1.36
36	BB	1334	PSU	C2-N1	9.13	1.49	1.36
36	BB	615	PSU	C2-N1	9.12	1.49	1.36
36	BB	644	PSU	C2-N1	9.12	1.49	1.36
10	AA	2045	PSU	C2-N1	9.12	1.49	1.36
36	BB	629	PSU	C2-N1	9.12	1.49	1.36
35	BA	743	A2M	C2'-C1'	-9.11	1.29	1.53
35	BA	1609	PSU	C2-N1	9.08	1.49	1.36
36	BB	1403	PSU	C2-N1	9.08	1.49	1.36
35	BA	1009	PSU	C2-N1	9.07	1.49	1.36
36	BB	611	PSU	C2-N1	9.06	1.49	1.36
36	BB	1280	PSU	C2-N1	9.02	1.48	1.36
36	BB	1429	PSU	C2-N1	9.02	1.48	1.36
35	BA	1086	PSU	C2-N1	9.00	1.48	1.36
36	BB	1324	5MC	C6-C5	8.99	1.49	1.34
10	AA	2153	A2M	C2'-C1'	-8.98	1.30	1.53
36	BB	95	A2M	C2'-C1'	-8.94	1.30	1.53
35	BA	1024	A2M	C2'-C1'	-8.90	1.30	1.53
37	BC	163	A2M	C2'-C1'	-8.89	1.30	1.53
10	AA	2146	PSU	C2-N1	8.86	1.48	1.36
35	BA	762	A2M	C2'-C1'	-8.85	1.30	1.53
37	BC	43	A2M	C2'-C1'	-8.85	1.30	1.53
10	AA	125	A2M	C2'-C1'	-8.84	1.30	1.53
35	BA	746	A2M	C2'-C1'	-8.84	1.30	1.53
35	BA	1620	A2M	C2'-C1'	-8.84	1.30	1.53
36	BB	1388	A2M	C2'-C1'	-8.82	1.30	1.53
36	BB	609	A2M	C2'-C1'	-8.82	1.30	1.53
10	AA	56	A2M	C2'-C1'	-8.81	1.30	1.53
36	BB	545	A2M	C2'-C1'	-8.81	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	590	A2M	C2'-C1'	-8.80	1.30	1.53
36	BB	622	A2M	C2'-C1'	-8.80	1.30	1.53
36	BB	646	A2M	C2'-C1'	-8.79	1.30	1.53
37	BC	41	A2M	C2'-C1'	-8.77	1.30	1.53
35	BA	1665	A2M	C2'-C1'	-8.74	1.30	1.53
35	BA	996	A2M	C2'-C1'	-8.72	1.30	1.53
36	BB	400	A2M	C2'-C1'	-8.72	1.30	1.53
35	BA	254	A2M	C2'-C1'	-8.64	1.30	1.53
35	BA	927	A2M	C2'-C1'	-8.58	1.31	1.53
10	AA	125	A2M	O4'-C1'	8.58	1.62	1.42
36	BB	542	5MC	C6-C5	8.57	1.48	1.34
36	BB	1201	A2M	C2'-C1'	-8.55	1.31	1.53
35	BA	254	A2M	O4'-C1'	8.53	1.62	1.42
10	AA	2096	A2M	C2'-C1'	-8.53	1.31	1.53
36	BB	590	A2M	O4'-C1'	8.51	1.62	1.42
10	AA	2096	A2M	O4'-C1'	8.49	1.62	1.42
36	BB	609	A2M	O4'-C1'	8.48	1.62	1.42
36	BB	95	A2M	O4'-C1'	8.47	1.62	1.42
36	BB	400	A2M	O4'-C1'	8.46	1.62	1.42
35	BA	762	A2M	O4'-C1'	8.45	1.62	1.42
10	AA	56	A2M	O4'-C1'	8.45	1.62	1.42
35	BA	1024	A2M	O4'-C1'	8.43	1.62	1.42
10	AA	721	A2M	C2'-C1'	-8.43	1.31	1.53
36	BB	646	A2M	O4'-C1'	8.41	1.61	1.42
36	BB	622	A2M	O4'-C1'	8.41	1.61	1.42
37	BC	41	A2M	O4'-C1'	8.40	1.61	1.42
37	BC	163	A2M	O4'-C1'	8.39	1.61	1.42
35	BA	996	A2M	O4'-C1'	8.39	1.61	1.42
35	BA	1620	A2M	O4'-C1'	8.37	1.61	1.42
35	BA	1665	A2M	O4'-C1'	8.36	1.61	1.42
36	BB	1388	A2M	O4'-C1'	8.35	1.61	1.42
37	BC	43	A2M	O4'-C1'	8.35	1.61	1.42
35	BA	743	A2M	O4'-C1'	8.29	1.61	1.42
35	BA	927	A2M	O4'-C1'	8.27	1.61	1.42
36	BB	1201	A2M	O4'-C1'	8.27	1.61	1.42
10	AA	2153	A2M	O4'-C1'	8.25	1.61	1.42
10	AA	1596	B8N	C6-N1	8.17	1.56	1.36
10	AA	721	A2M	O4'-C1'	8.09	1.61	1.42
35	BA	746	A2M	O4'-C1'	8.07	1.61	1.42
36	BB	545	A2M	O4'-C1'	7.96	1.60	1.42
35	BA	742	1MA	C2-N3	7.68	1.44	1.30
36	BB	490	PSU	C2-N3	7.48	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1330	OMU	C2-N1	7.45	1.50	1.38
36	BB	528	PSU	C2-N3	7.42	1.50	1.37
36	BB	518	PSU	C2-N3	7.41	1.50	1.37
10	AA	61	PSU	C2-N3	7.35	1.50	1.37
10	AA	1596	B8N	C4-N3	-7.35	1.26	1.40
10	AA	1619	PSU	C2-N3	7.34	1.50	1.37
35	BA	742	1MA	C4-N3	7.34	1.50	1.35
10	AA	2045	PSU	C2-N3	7.34	1.50	1.37
35	BA	1080	PSU	C2-N3	7.31	1.50	1.37
10	AA	1907	PSU	C2-N3	7.30	1.50	1.37
10	AA	131	PSU	C2-N3	7.30	1.50	1.37
10	AA	1592	PSU	C2-N3	7.30	1.50	1.37
36	BB	1409	PSU	C2-N3	7.29	1.50	1.37
36	BB	1319	PSU	C2-N3	7.28	1.50	1.37
35	BA	1166	PSU	C2-N3	7.26	1.49	1.37
36	BB	1419	PSU	C2-N3	7.26	1.49	1.37
35	BA	737	PSU	C2-N3	7.22	1.49	1.37
35	BA	1169	PSU	C2-N3	7.19	1.49	1.37
35	BA	1609	PSU	C2-N3	7.19	1.49	1.37
35	BA	1614	PSU	C2-N3	7.19	1.49	1.37
36	BB	644	PSU	C2-N3	7.19	1.49	1.37
36	BB	1229	PSU	C2-N3	7.18	1.49	1.37
35	BA	452	PSU	C2-N3	7.17	1.49	1.37
36	BB	629	PSU	C2-N3	7.17	1.49	1.37
36	BB	1280	PSU	C2-N3	7.17	1.49	1.37
10	AA	2278	PSU	C2-N3	7.17	1.49	1.37
37	BC	74	PSU	C2-N3	7.17	1.49	1.37
36	BB	1076	PSU	C2-N3	7.16	1.49	1.37
36	BB	1210	PSU	C2-N3	7.15	1.49	1.37
36	BB	615	PSU	C2-N3	7.15	1.49	1.37
36	BB	611	PSU	C2-N3	7.15	1.49	1.37
36	BB	1160	PSU	C2-N3	7.14	1.49	1.37
36	BB	1434	PSU	C2-N3	7.13	1.49	1.37
10	AA	1276	PSU	C2-N3	7.13	1.49	1.37
35	BA	1258	PSU	C2-N3	7.08	1.49	1.37
35	BA	1129	PSU	C2-N3	7.07	1.49	1.37
35	BA	1086	PSU	C2-N3	7.07	1.49	1.37
36	BB	1403	PSU	C2-N3	7.06	1.49	1.37
36	BB	1334	PSU	C2-N3	7.03	1.49	1.37
35	BA	1248	PSU	C2-N3	7.01	1.49	1.37
35	BA	1009	PSU	C2-N3	6.98	1.49	1.37
36	BB	1429	PSU	C2-N3	6.97	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AA	505	PSU	C2-N3	6.88	1.49	1.37
10	AA	1674	OMU	C2-N1	6.88	1.49	1.38
10	AA	721	A2M	O4'-C4'	-6.87	1.29	1.45
10	AA	1899	OMU	C2-N1	6.85	1.49	1.38
10	AA	2146	PSU	C2-N3	6.82	1.49	1.37
35	BA	1330	OMU	C2-N3	6.73	1.50	1.38
35	BA	927	A2M	O4'-C4'	-6.73	1.30	1.45
35	BA	46	OMU	C2-N1	6.72	1.49	1.38
36	BB	685	OMU	C2-N1	6.71	1.49	1.38
37	BC	167	OMU	C2-N1	6.71	1.49	1.38
35	BA	1620	A2M	O4'-C4'	-6.70	1.30	1.45
36	BB	1093	OMU	C2-N1	6.69	1.49	1.38
10	AA	1710	PSU	C2-N3	6.69	1.49	1.37
35	BA	1448	OMU	C2-N1	6.68	1.49	1.38
36	BB	578	OMU	C2-N1	6.68	1.49	1.38
10	AA	2153	A2M	O4'-C4'	-6.68	1.30	1.45
36	BB	1201	A2M	O4'-C4'	-6.65	1.30	1.45
10	AA	1899	OMU	C2-N3	6.64	1.49	1.38
10	AA	1674	OMU	C2-N3	6.63	1.49	1.38
36	BB	73	OMU	C2-N1	6.63	1.49	1.38
35	BA	1024	A2M	O4'-C4'	-6.62	1.30	1.45
10	AA	2054	OMU	C2-N1	6.61	1.49	1.38
36	BB	646	A2M	O4'-C4'	-6.60	1.30	1.45
36	BB	1388	A2M	O4'-C4'	-6.60	1.30	1.45
10	AA	57	OMU	C2-N1	6.60	1.49	1.38
37	BC	7	OMU	C2-N1	6.59	1.49	1.38
36	BB	1093	OMU	C2-N3	6.59	1.49	1.38
35	BA	996	A2M	O4'-C4'	-6.58	1.30	1.45
10	AA	2154	OMU	C2-N1	6.57	1.49	1.38
37	BC	167	OMU	C2-N3	6.55	1.49	1.38
10	AA	2154	OMU	C2-N3	6.55	1.49	1.38
35	BA	1181	OMU	C2-N1	6.55	1.49	1.38
35	BA	743	A2M	O4'-C4'	-6.54	1.30	1.45
10	AA	2054	OMU	C2-N3	6.54	1.49	1.38
37	BC	7	OMU	C2-N3	6.51	1.49	1.38
35	BA	1742	OMU	C2-N1	6.51	1.48	1.38
35	BA	762	A2M	O4'-C4'	-6.51	1.30	1.45
36	BB	95	A2M	O4'-C4'	-6.49	1.30	1.45
10	AA	714	OMU	C2-N1	6.49	1.48	1.38
36	BB	609	A2M	O4'-C4'	-6.48	1.30	1.45
37	BC	163	A2M	O4'-C4'	-6.48	1.30	1.45
36	BB	622	A2M	O4'-C4'	-6.48	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	BC	43	A2M	O4'-C4'	-6.47	1.30	1.45
36	BB	1435	OMU	C2-N1	6.47	1.48	1.38
35	BA	1665	A2M	O4'-C4'	-6.47	1.30	1.45
35	BA	916	OMU	C2-N1	6.46	1.48	1.38
36	BB	685	OMU	C2-N3	6.46	1.49	1.38
10	AA	57	OMU	C2-N3	6.46	1.49	1.38
37	BC	41	A2M	O4'-C4'	-6.45	1.30	1.45
10	AA	56	A2M	O4'-C4'	-6.45	1.30	1.45
35	BA	1448	OMU	C2-N3	6.45	1.49	1.38
35	BA	254	A2M	O4'-C4'	-6.44	1.30	1.45
35	BA	746	A2M	O4'-C4'	-6.44	1.30	1.45
36	BB	578	OMU	C2-N3	6.43	1.49	1.38
10	AA	714	OMU	C2-N3	6.43	1.49	1.38
35	BA	46	OMU	C2-N3	6.43	1.49	1.38
10	AA	2096	A2M	O4'-C4'	-6.43	1.30	1.45
35	BA	916	OMU	C2-N3	6.42	1.49	1.38
35	BA	1181	OMU	C2-N3	6.42	1.49	1.38
35	BA	1742	OMU	C2-N3	6.42	1.49	1.38
36	BB	1435	OMU	C2-N3	6.41	1.49	1.38
36	BB	73	OMU	C2-N3	6.41	1.49	1.38
36	BB	400	A2M	O4'-C4'	-6.40	1.30	1.45
10	AA	125	A2M	O4'-C4'	-6.35	1.30	1.45
36	BB	590	A2M	O4'-C4'	-6.31	1.30	1.45
36	BB	545	A2M	O4'-C4'	-6.30	1.30	1.45
36	BB	377	OMC	C2-N3	6.29	1.49	1.36
10	AA	2070	G7M	C2-N3	6.26	1.48	1.33
35	BA	1329	OMC	C2-N3	6.21	1.48	1.36
35	BA	915	OMG	C4-N3	6.20	1.49	1.34
10	AA	1517	OMG	C4-N3	6.17	1.48	1.34
37	BC	75	OMG	C4-N3	6.17	1.48	1.34
10	AA	1844	OMC	C2-N3	6.16	1.48	1.36
10	AA	1603	OMG	C4-N3	6.14	1.48	1.34
36	BB	673	OMG	C4-N3	6.13	1.48	1.34
10	AA	1676	OMG	C4-N3	6.13	1.48	1.34
10	AA	1931	OMG	C4-N3	6.11	1.48	1.34
35	BA	747	OMC	C2-N3	6.11	1.48	1.36
10	AA	66	OMC	C2-N3	6.11	1.48	1.36
10	AA	2123	OMU	C2-N1	6.10	1.48	1.38
35	BA	1028	OMG	C4-N3	6.10	1.48	1.34
35	BA	1605	OMG	C4-N3	6.08	1.48	1.34
36	BB	1062	OMG	C4-N3	6.07	1.48	1.34
10	AA	1932	OMC	C2-N3	6.07	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	72	OMG	C4-N3	6.05	1.48	1.34
10	AA	2123	OMU	C2-N3	6.05	1.48	1.38
36	BB	1245	OMG	C4-N3	6.04	1.48	1.34
10	AA	1895	OMG	C4-N3	6.04	1.48	1.34
36	BB	1269	OMG	C4-N3	6.04	1.48	1.34
36	BB	1247	OMG	C4-N3	6.02	1.48	1.34
35	BA	925	OMG	C4-N3	6.02	1.48	1.34
35	BA	760	OMC	C2-N3	6.02	1.48	1.36
36	BB	542	5MC	C4-N3	6.00	1.44	1.34
10	AA	46	OMC	C2-N3	5.99	1.48	1.36
36	BB	1264	OMC	C2-N3	5.99	1.48	1.36
35	BA	1709	OMG	C4-N3	5.98	1.48	1.34
36	BB	552	OMG	C4-N3	5.97	1.48	1.34
36	BB	1094	OMG	C4-N3	5.96	1.48	1.34
35	BA	1621	OMG	C4-N3	5.95	1.48	1.34
35	BA	1329	OMC	C6-C5	5.95	1.48	1.35
35	BA	1608	OMC	C2-N3	5.95	1.48	1.36
35	BA	1006	OMC	C2-N3	5.93	1.48	1.36
35	BA	1267	OMG	C4-N3	5.91	1.48	1.34
36	BB	71	OMG	C4-N3	5.90	1.48	1.34
36	BB	1413	OMC	C2-N3	5.85	1.48	1.36
10	AA	2070	G7M	C5-N7	5.85	1.46	1.39
36	BB	377	OMC	C6-C5	5.85	1.48	1.35
10	AA	2070	G7M	C8-N9	5.84	1.52	1.35
10	AA	1844	OMC	C6-C5	5.84	1.48	1.35
36	BB	659	OMG	C4-N3	5.81	1.48	1.34
36	BB	1324	5MC	C4-N3	5.80	1.43	1.34
36	BB	1264	OMC	C6-C5	5.80	1.48	1.35
10	AA	1932	OMC	C6-C5	5.79	1.48	1.35
36	BB	542	5MC	C2-N3	5.78	1.48	1.36
10	AA	66	OMC	C6-C5	5.75	1.48	1.35
36	BB	601	OMC	C2-N3	5.74	1.48	1.36
10	AA	46	OMC	C6-C5	5.74	1.48	1.35
10	AA	1700	OMG	C4-N3	5.73	1.47	1.34
35	BA	1608	OMC	C6-C5	5.73	1.48	1.35
36	BB	1413	OMC	C6-C5	5.72	1.48	1.35
10	AA	2227	OMG	C4-N3	5.71	1.47	1.34
35	BA	1006	OMC	C6-C5	5.71	1.48	1.35
35	BA	760	OMC	C6-C5	5.70	1.48	1.35
10	AA	1899	OMU	C6-C5	5.64	1.48	1.35
35	BA	747	OMC	C6-C5	5.64	1.48	1.35
10	AA	1674	OMU	C6-C5	5.62	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AA	2154	OMU	C6-C5	5.61	1.48	1.35
35	BA	1448	OMU	C6-C5	5.58	1.48	1.35
10	AA	2054	OMU	C6-C5	5.57	1.48	1.35
36	BB	1324	5MC	C2-N3	5.57	1.47	1.36
35	BA	916	OMU	C6-C5	5.56	1.48	1.35
10	AA	1596	B8N	C2-N1	5.55	1.55	1.39
10	AA	57	OMU	C6-C5	5.54	1.47	1.35
35	BA	1181	OMU	C6-C5	5.53	1.47	1.35
36	BB	1093	OMU	C6-C5	5.52	1.47	1.35
37	BC	167	OMU	C6-C5	5.52	1.47	1.35
35	BA	1330	OMU	C6-C5	5.52	1.47	1.35
36	BB	601	OMC	C6-C5	5.48	1.47	1.35
36	BB	685	OMU	C6-C5	5.47	1.47	1.35
37	BC	7	OMU	C6-C5	5.47	1.47	1.35
36	BB	73	OMU	C6-C5	5.46	1.47	1.35
35	BA	46	OMU	C6-C5	5.45	1.47	1.35
35	BA	1742	OMU	C6-C5	5.44	1.47	1.35
10	AA	714	OMU	C6-C5	5.44	1.47	1.35
36	BB	1435	OMU	C6-C5	5.41	1.47	1.35
36	BB	578	OMU	C6-C5	5.40	1.47	1.35
10	AA	2070	G7M	C4-N3	5.31	1.46	1.34
10	AA	1676	OMG	C2-N3	5.23	1.45	1.33
10	AA	1596	B8N	C6-C5	5.23	1.42	1.34
10	AA	1517	OMG	C2-N3	5.23	1.45	1.33
36	BB	490	PSU	C6-N1	5.21	1.44	1.36
10	AA	2123	OMU	C6-C5	5.21	1.47	1.35
10	AA	1592	PSU	C6-N1	5.20	1.44	1.36
37	BC	74	PSU	C6-N1	5.19	1.44	1.36
35	BA	1166	PSU	C6-N1	5.18	1.44	1.36
35	BA	1169	PSU	C6-N1	5.18	1.44	1.36
36	BB	629	PSU	C6-N1	5.17	1.44	1.36
10	AA	1619	PSU	C6-N1	5.17	1.44	1.36
10	AA	1603	OMG	C2-N3	5.17	1.45	1.33
10	AA	131	PSU	C6-N1	5.16	1.44	1.36
10	AA	61	PSU	C6-N1	5.16	1.44	1.36
35	BA	1605	OMG	C2-N3	5.14	1.45	1.33
36	BB	528	PSU	C6-N1	5.14	1.44	1.36
35	BA	915	OMG	C2-N3	5.14	1.45	1.33
37	BC	75	OMG	C2-N3	5.14	1.45	1.33
35	BA	452	PSU	C6-N1	5.13	1.44	1.36
10	AA	2278	PSU	C6-N1	5.12	1.44	1.36
10	AA	1276	PSU	C6-N1	5.12	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1329	OMC	C4-N3	5.12	1.44	1.34
36	BB	1160	PSU	C6-N1	5.11	1.44	1.36
36	BB	1062	OMG	C2-N3	5.10	1.45	1.33
10	AA	1710	PSU	C6-N1	5.09	1.44	1.36
35	BA	1258	PSU	C6-N1	5.09	1.44	1.36
10	AA	1931	OMG	C2-N3	5.09	1.45	1.33
35	BA	1080	PSU	C6-N1	5.09	1.44	1.36
36	BB	1247	OMG	C2-N3	5.09	1.45	1.33
36	BB	377	OMC	C4-N3	5.09	1.44	1.34
36	BB	1434	PSU	C6-N1	5.09	1.44	1.36
36	BB	1409	PSU	C6-N1	5.08	1.44	1.36
35	BA	1609	PSU	C6-N1	5.07	1.44	1.36
36	BB	611	PSU	C6-N1	5.07	1.44	1.36
10	AA	1895	OMG	C2-N3	5.06	1.45	1.33
36	BB	518	PSU	C6-N1	5.06	1.44	1.36
35	BA	1009	PSU	C6-N1	5.06	1.44	1.36
10	AA	2045	PSU	C6-N1	5.05	1.44	1.36
36	BB	1245	OMG	C2-N3	5.05	1.45	1.33
36	BB	1210	PSU	C6-N1	5.04	1.44	1.36
36	BB	1419	PSU	C6-N1	5.03	1.44	1.36
36	BB	1319	PSU	C6-N1	5.02	1.44	1.36
36	BB	1229	PSU	C6-N1	5.01	1.44	1.36
35	BA	1129	PSU	C6-N1	5.00	1.44	1.36
35	BA	737	PSU	C6-N1	5.00	1.44	1.36
35	BA	1248	PSU	C6-N1	4.99	1.44	1.36
35	BA	1028	OMG	C2-N3	4.99	1.45	1.33
10	AA	1844	OMC	C4-N3	4.99	1.44	1.34
36	BB	615	PSU	C6-N1	4.99	1.44	1.36
36	BB	673	OMG	C2-N3	4.99	1.45	1.33
36	BB	1280	PSU	C6-N1	4.98	1.44	1.36
10	AA	505	PSU	C6-N1	4.97	1.44	1.36
35	BA	1709	OMG	C2-N3	4.97	1.45	1.33
10	AA	1907	PSU	C6-N1	4.97	1.44	1.36
36	BB	72	OMG	C2-N3	4.96	1.45	1.33
36	BB	644	PSU	C6-N1	4.96	1.44	1.36
35	BA	1614	PSU	C6-N1	4.93	1.44	1.36
36	BB	1334	PSU	C6-N1	4.93	1.44	1.36
36	BB	1269	OMG	C2-N3	4.93	1.45	1.33
10	AA	66	OMC	C4-N3	4.93	1.44	1.34
10	AA	2146	PSU	C6-N1	4.92	1.44	1.36
36	BB	1403	PSU	C6-N1	4.91	1.44	1.36
36	BB	552	OMG	C2-N3	4.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	1076	PSU	C6-N1	4.91	1.44	1.36
35	BA	925	OMG	C2-N3	4.90	1.45	1.33
35	BA	1621	OMG	C2-N3	4.88	1.44	1.33
35	BA	1086	PSU	C6-N1	4.88	1.44	1.36
10	AA	1932	OMC	C4-N3	4.86	1.44	1.34
36	BB	1094	OMG	C2-N3	4.85	1.44	1.33
36	BB	71	OMG	C2-N3	4.85	1.44	1.33
35	BA	1267	OMG	C2-N3	4.81	1.44	1.33
10	AA	46	OMC	C4-N3	4.81	1.44	1.34
36	BB	1429	PSU	C6-N1	4.81	1.44	1.36
35	BA	1329	OMC	C4-N4	4.79	1.45	1.33
36	BB	1264	OMC	C4-N3	4.78	1.44	1.34
35	BA	1006	OMC	C4-N3	4.78	1.44	1.34
35	BA	760	OMC	C4-N3	4.78	1.44	1.34
36	BB	377	OMC	C4-N4	4.76	1.45	1.33
10	AA	1700	OMG	C2-N3	4.72	1.44	1.33
36	BB	659	OMG	C2-N3	4.71	1.44	1.33
10	AA	1844	OMC	C4-N4	4.71	1.45	1.33
10	AA	1932	OMC	C4-N4	4.69	1.45	1.33
35	BA	747	OMC	C4-N3	4.67	1.43	1.34
36	BB	601	OMC	C4-N3	4.67	1.43	1.34
35	BA	1608	OMC	C4-N3	4.65	1.43	1.34
36	BB	1076	PSU	C1'-C5	-4.65	1.39	1.50
10	AA	66	OMC	C4-N4	4.64	1.44	1.33
10	AA	46	OMC	C4-N4	4.64	1.44	1.33
10	AA	1603	OMG	C2-N2	4.63	1.45	1.34
36	BB	1264	OMC	C4-N4	4.63	1.44	1.33
10	AA	505	PSU	C1'-C5	-4.60	1.39	1.50
35	BA	760	OMC	C4-N4	4.60	1.44	1.33
10	AA	1676	OMG	C2-N2	4.59	1.45	1.34
36	BB	1413	OMC	C4-N3	4.58	1.43	1.34
35	BA	1248	PSU	C1'-C5	-4.58	1.39	1.50
36	BB	1403	PSU	C1'-C5	-4.57	1.39	1.50
35	BA	1006	OMC	C4-N4	4.55	1.44	1.33
10	AA	2227	OMG	C2-N3	4.55	1.44	1.33
36	BB	1247	OMG	C2-N2	4.54	1.45	1.34
36	BB	1229	PSU	C1'-C5	-4.53	1.39	1.50
36	BB	1245	OMG	C2-N2	4.53	1.45	1.34
36	BB	72	OMG	C2-N2	4.53	1.45	1.34
35	BA	1608	OMC	C4-N4	4.52	1.44	1.33
10	AA	61	PSU	C1'-C5	-4.52	1.39	1.50
10	AA	1931	OMG	C2-N2	4.51	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AA	1700	OMG	C2-N2	4.51	1.44	1.34
35	BA	915	OMG	C2-N2	4.51	1.44	1.34
36	BB	1319	PSU	C1'-C5	-4.51	1.39	1.50
36	BB	601	OMC	C4-N4	4.50	1.44	1.33
35	BA	1709	OMG	C2-N2	4.50	1.44	1.34
35	BA	1258	PSU	C1'-C5	-4.50	1.39	1.50
10	AA	1907	PSU	C1'-C5	-4.49	1.39	1.50
36	BB	1210	PSU	C1'-C5	-4.49	1.39	1.50
10	AA	1517	OMG	C2-N2	4.48	1.44	1.34
35	BA	1086	PSU	C1'-C5	-4.48	1.39	1.50
36	BB	490	PSU	C1'-C5	-4.48	1.39	1.50
10	AA	131	PSU	C1'-C5	-4.48	1.39	1.50
10	AA	2146	PSU	C1'-C5	-4.48	1.39	1.50
36	BB	1280	PSU	C1'-C5	-4.48	1.40	1.50
35	BA	1614	PSU	C1'-C5	-4.48	1.40	1.50
36	BB	644	PSU	C1'-C5	-4.47	1.40	1.50
36	BB	1419	PSU	C1'-C5	-4.47	1.40	1.50
36	BB	1434	PSU	C1'-C5	-4.47	1.40	1.50
36	BB	659	OMG	C2-N2	4.47	1.44	1.34
36	BB	1413	OMC	C4-N4	4.47	1.44	1.33
37	BC	75	OMG	C2-N2	4.47	1.44	1.34
36	BB	673	OMG	C2-N2	4.47	1.44	1.34
36	BB	1062	OMG	C2-N2	4.46	1.44	1.34
37	BC	74	PSU	C1'-C5	-4.46	1.40	1.50
35	BA	452	PSU	C1'-C5	-4.46	1.40	1.50
35	BA	1009	PSU	C1'-C5	-4.46	1.40	1.50
35	BA	1169	PSU	C1'-C5	-4.46	1.40	1.50
35	BA	747	OMC	C4-N4	4.45	1.44	1.33
36	BB	615	PSU	C1'-C5	-4.44	1.40	1.50
10	AA	1592	PSU	C1'-C5	-4.44	1.40	1.50
36	BB	1094	OMG	C2-N2	4.44	1.44	1.34
36	BB	71	OMG	C2-N2	4.43	1.44	1.34
36	BB	528	PSU	C1'-C5	-4.43	1.40	1.50
10	AA	1895	OMG	C2-N2	4.43	1.44	1.34
36	BB	1160	PSU	C1'-C5	-4.43	1.40	1.50
35	BA	1267	OMG	C2-N2	4.42	1.44	1.34
35	BA	1028	OMG	C2-N2	4.42	1.44	1.34
36	BB	1334	PSU	C1'-C5	-4.42	1.40	1.50
35	BA	1605	OMG	C2-N2	4.42	1.44	1.34
35	BA	1621	OMG	C2-N2	4.42	1.44	1.34
36	BB	1429	PSU	C1'-C5	-4.41	1.40	1.50
35	BA	1129	PSU	C1'-C5	-4.41	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1166	PSU	C1'-C5	-4.41	1.40	1.50
10	AA	1276	PSU	C1'-C5	-4.40	1.40	1.50
36	BB	552	OMG	C2-N2	4.39	1.44	1.34
10	AA	2153	A2M	C6-N6	4.39	1.45	1.34
10	AA	2096	A2M	C6-N6	4.39	1.45	1.34
35	BA	925	OMG	C2-N2	4.39	1.44	1.34
35	BA	1080	PSU	C1'-C5	-4.38	1.40	1.50
36	BB	1269	OMG	C2-N2	4.36	1.44	1.34
10	AA	2278	PSU	C1'-C5	-4.36	1.40	1.50
35	BA	737	PSU	C1'-C5	-4.36	1.40	1.50
36	BB	1388	A2M	C6-N6	4.35	1.45	1.34
36	BB	1409	PSU	C1'-C5	-4.34	1.40	1.50
36	BB	646	A2M	C6-N6	4.34	1.45	1.34
35	BA	743	A2M	C6-N6	4.33	1.45	1.34
35	BA	254	A2M	C6-N6	4.33	1.45	1.34
36	BB	629	PSU	C1'-C5	-4.32	1.40	1.50
35	BA	927	A2M	C6-N6	4.32	1.45	1.34
36	BB	609	A2M	C6-N6	4.32	1.45	1.34
35	BA	1609	PSU	C1'-C5	-4.32	1.40	1.50
10	AA	56	A2M	C6-N6	4.32	1.45	1.34
36	BB	622	A2M	C6-N6	4.31	1.45	1.34
36	BB	1324	5MC	C6-N1	4.31	1.45	1.38
35	BA	1024	A2M	C6-N6	4.31	1.44	1.34
36	BB	1264	OMC	C2-N1	4.31	1.49	1.40
35	BA	1329	OMC	C2-N1	4.30	1.49	1.40
36	BB	590	A2M	C6-N6	4.29	1.44	1.34
36	BB	1201	A2M	C6-N6	4.29	1.44	1.34
10	AA	2227	OMG	C2-N2	4.29	1.44	1.34
10	AA	721	A2M	C6-N6	4.29	1.44	1.34
35	BA	762	A2M	C6-N6	4.27	1.44	1.34
36	BB	95	A2M	C6-N6	4.27	1.44	1.34
37	BC	163	A2M	C6-N6	4.27	1.44	1.34
35	BA	1665	A2M	C6-N6	4.26	1.44	1.34
10	AA	125	A2M	C6-N6	4.26	1.44	1.34
36	BB	400	A2M	C6-N6	4.25	1.44	1.34
10	AA	2045	PSU	C1'-C5	-4.24	1.40	1.50
37	BC	41	A2M	C6-N6	4.24	1.44	1.34
35	BA	1620	A2M	C6-N6	4.22	1.44	1.34
37	BC	43	A2M	C6-N6	4.21	1.44	1.34
35	BA	996	A2M	C6-N6	4.21	1.44	1.34
36	BB	545	A2M	C6-N6	4.21	1.44	1.34
35	BA	1608	OMC	C2-N1	4.21	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	518	PSU	C1'-C5	-4.20	1.40	1.50
36	BB	377	OMC	C2-N1	4.20	1.49	1.40
10	AA	1596	B8N	C1'-C5	-4.19	1.40	1.50
10	AA	66	OMC	C2-N1	4.16	1.49	1.40
35	BA	760	OMC	C2-N1	4.15	1.49	1.40
36	BB	611	PSU	C1'-C5	-4.14	1.40	1.50
35	BA	747	OMC	C2-N1	4.13	1.49	1.40
10	AA	1710	PSU	C1'-C5	-4.13	1.40	1.50
10	AA	1932	OMC	C2-N1	4.13	1.48	1.40
36	BB	542	5MC	C4-N4	4.12	1.44	1.34
36	BB	542	5MC	C6-N1	4.10	1.45	1.38
36	BB	1324	5MC	C4-N4	4.09	1.44	1.34
10	AA	1844	OMC	C2-N1	4.09	1.48	1.40
35	BA	746	A2M	C6-N6	4.08	1.44	1.34
10	AA	46	OMC	C2-N1	4.07	1.48	1.40
10	AA	1619	PSU	C1'-C5	-4.05	1.40	1.50
36	BB	1413	OMC	C2-N1	4.05	1.48	1.40
35	BA	1006	OMC	C2-N1	3.99	1.48	1.40
35	BA	1330	OMU	C4-N3	3.99	1.45	1.38
10	AA	1674	OMU	C4-N3	3.93	1.45	1.38
10	AA	1899	OMU	C4-N3	3.92	1.45	1.38
10	AA	2054	OMU	C4-N3	3.87	1.45	1.38
36	BB	542	5MC	C2-N1	3.86	1.48	1.40
37	BC	167	OMU	C4-N3	3.85	1.45	1.38
10	AA	1619	PSU	C4-N3	3.85	1.46	1.38
10	AA	2154	OMU	C4-N3	3.84	1.45	1.38
36	BB	1324	5MC	C2-N1	3.82	1.48	1.40
36	BB	528	PSU	C4-N3	3.82	1.45	1.38
36	BB	1093	OMU	C4-N3	3.81	1.45	1.38
10	AA	2045	PSU	C4-N3	3.81	1.45	1.38
10	AA	57	OMU	C4-N3	3.81	1.45	1.38
35	BA	1181	OMU	C4-N3	3.80	1.45	1.38
37	BC	7	OMU	C4-N3	3.80	1.45	1.38
36	BB	601	OMC	C2-N1	3.79	1.48	1.40
35	BA	742	1MA	C5-C6	3.79	1.53	1.43
36	BB	490	PSU	C4-N3	3.78	1.45	1.38
35	BA	46	OMU	C4-N3	3.76	1.45	1.38
36	BB	73	OMU	C4-N3	3.76	1.45	1.38
36	BB	1409	PSU	C4-N3	3.76	1.45	1.38
10	AA	1592	PSU	C4-N3	3.75	1.45	1.38
35	BA	1166	PSU	C4-N3	3.75	1.45	1.38
36	BB	578	OMU	C4-N3	3.74	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AA	714	OMU	C4-N3	3.74	1.45	1.38
36	BB	1435	OMU	C4-N3	3.71	1.45	1.38
35	BA	916	OMU	C4-N3	3.71	1.45	1.38
35	BA	1742	OMU	C4-N3	3.70	1.45	1.38
10	AA	61	PSU	C4-N3	3.70	1.45	1.38
35	BA	737	PSU	C4-N3	3.70	1.45	1.38
36	BB	518	PSU	C4-N3	3.70	1.45	1.38
37	BC	74	PSU	C4-N3	3.68	1.45	1.38
35	BA	1080	PSU	C4-N3	3.68	1.45	1.38
35	BA	1448	OMU	C4-N3	3.67	1.45	1.38
35	BA	452	PSU	C4-N3	3.65	1.45	1.38
10	AA	1907	PSU	C4-N3	3.64	1.45	1.38
10	AA	2278	PSU	C4-N3	3.64	1.45	1.38
36	BB	629	PSU	C4-N3	3.63	1.45	1.38
10	AA	2261	MA6	C5-C4	-3.61	1.32	1.39
35	BA	1614	PSU	C4-N3	3.61	1.45	1.38
36	BB	685	OMU	C4-N3	3.60	1.45	1.38
36	BB	1319	PSU	C4-N3	3.60	1.45	1.38
10	AA	131	PSU	C4-N3	3.60	1.45	1.38
35	BA	1129	PSU	C4-N3	3.60	1.45	1.38
35	BA	1609	PSU	C4-N3	3.58	1.45	1.38
36	BB	1210	PSU	C4-N3	3.58	1.45	1.38
36	BB	1229	PSU	C4-N3	3.58	1.45	1.38
36	BB	1419	PSU	C4-N3	3.58	1.45	1.38
35	BA	742	1MA	C2-N1	3.57	1.42	1.35
36	BB	615	PSU	C4-N3	3.56	1.45	1.38
36	BB	611	PSU	C4-N3	3.55	1.45	1.38
35	BA	1169	PSU	C4-N3	3.55	1.45	1.38
36	BB	1160	PSU	C4-N3	3.54	1.45	1.38
10	AA	1276	PSU	C4-N3	3.53	1.45	1.38
36	BB	1434	PSU	C4-N3	3.53	1.45	1.38
36	BB	1076	PSU	C4-N3	3.52	1.45	1.38
35	BA	1248	PSU	C4-N3	3.51	1.45	1.38
36	BB	644	PSU	C4-N3	3.51	1.45	1.38
36	BB	1429	PSU	C4-N3	3.50	1.45	1.38
36	BB	1280	PSU	C4-N3	3.49	1.45	1.38
35	BA	1086	PSU	C4-N3	3.49	1.45	1.38
10	AA	2123	OMU	O4-C4	-3.46	1.17	1.24
36	BB	1334	PSU	C4-N3	3.45	1.45	1.38
35	BA	1258	PSU	C4-N3	3.45	1.45	1.38
36	BB	1403	PSU	C4-N3	3.43	1.45	1.38
10	AA	1710	PSU	C4-N3	3.42	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1009	PSU	C4-N3	3.42	1.45	1.38
10	AA	2260	MA6	C6-N6	3.40	1.46	1.36
10	AA	2070	G7M	C6-N1	3.40	1.45	1.38
36	BB	680	PSU	C6-C5	3.39	1.39	1.35
36	BB	455	PSU	C6-C5	3.38	1.39	1.35
10	AA	505	PSU	C4-N3	3.37	1.45	1.38
10	AA	2070	G7M	C2-N1	3.37	1.46	1.37
36	BB	601	OMC	O2-C2	-3.33	1.17	1.23
36	BB	71	OMG	C5-N7	-3.33	1.32	1.39
10	AA	2146	PSU	C4-N3	3.33	1.45	1.38
10	AA	2227	OMG	C5-N7	-3.32	1.32	1.39
35	BA	46	OMU	O4-C4	-3.31	1.18	1.24
35	BA	762	A2M	C5-C4	-3.30	1.32	1.39
10	AA	714	OMU	O4-C4	-3.30	1.18	1.24
35	BA	996	A2M	C5-C4	-3.30	1.32	1.39
36	BB	685	OMU	O4-C4	-3.29	1.18	1.24
10	AA	1612	PSU	C6-C5	3.28	1.39	1.35
10	AA	1517	OMG	C5-N7	-3.26	1.32	1.39
36	BB	73	OMU	O4-C4	-3.25	1.18	1.24
35	BA	1620	A2M	C5-C4	-3.25	1.32	1.39
10	AA	2070	G7M	C2-N2	3.25	1.41	1.34
35	BA	742	1MA	C5-N7	-3.24	1.32	1.39
37	BC	41	A2M	C5-C4	-3.24	1.33	1.39
36	BB	1435	OMU	O4-C4	-3.24	1.18	1.24
36	BB	1201	A2M	C5-C4	-3.24	1.33	1.39
10	AA	2070	G7M	O6-C6	-3.23	1.17	1.23
35	BA	1181	OMU	O4-C4	-3.23	1.18	1.24
35	BA	1024	A2M	C5-C4	-3.23	1.33	1.39
35	BA	916	OMU	O4-C4	-3.23	1.18	1.24
36	BB	545	A2M	C5-C4	-3.22	1.33	1.39
10	AA	2153	A2M	C5-C4	-3.22	1.33	1.39
10	AA	721	A2M	C5-C4	-3.21	1.33	1.39
35	BA	1329	OMC	C6-N1	3.21	1.45	1.38
36	BB	646	A2M	C5-C4	-3.21	1.33	1.39
35	BA	1448	OMU	O4-C4	-3.20	1.18	1.24
36	BB	1388	A2M	C5-C4	-3.20	1.33	1.39
37	BC	43	A2M	C5-C4	-3.20	1.33	1.39
36	BB	72	OMG	C5-N7	-3.19	1.32	1.39
10	AA	56	A2M	C5-C4	-3.19	1.33	1.39
10	AA	2153	A2M	O3'-C3'	-3.18	1.35	1.43
36	BB	71	OMG	O6-C6	-3.18	1.17	1.23
36	BB	95	A2M	C5-C4	-3.18	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1028	OMG	C5-N7	-3.18	1.32	1.39
10	AA	2123	OMU	C4-N3	3.17	1.44	1.38
35	BA	1742	OMU	O4-C4	-3.17	1.18	1.24
37	BC	43	A2M	O3'-C3'	-3.17	1.35	1.43
35	BA	762	A2M	O3'-C3'	-3.17	1.35	1.43
10	AA	2261	MA6	C6-N6	3.17	1.46	1.36
10	AA	1895	OMG	C5-N7	-3.17	1.32	1.39
35	BA	927	A2M	C5-C4	-3.16	1.33	1.39
35	BA	743	A2M	O3'-C3'	-3.16	1.35	1.43
36	BB	1269	OMG	C5-N7	-3.16	1.33	1.39
10	AA	1676	OMG	C5-N7	-3.16	1.33	1.39
10	AA	1710	PSU	O4-C4	-3.16	1.17	1.23
36	BB	578	OMU	O4-C4	-3.15	1.18	1.24
10	AA	2260	MA6	C5-C4	-3.15	1.33	1.39
37	BC	163	A2M	O3'-C3'	-3.15	1.35	1.43
10	AA	2154	OMU	O4-C4	-3.14	1.18	1.24
35	BA	254	A2M	C5-C4	-3.14	1.33	1.39
10	AA	57	OMU	O4-C4	-3.14	1.18	1.24
35	BA	1620	A2M	O3'-C3'	-3.14	1.35	1.43
35	BA	746	A2M	C5-C4	-3.14	1.33	1.39
36	BB	590	A2M	C5-C4	-3.13	1.33	1.39
35	BA	1024	A2M	O3'-C3'	-3.13	1.35	1.43
35	BA	743	A2M	C5-C4	-3.13	1.33	1.39
36	BB	95	A2M	O3'-C3'	-3.13	1.35	1.43
36	BB	377	OMC	C6-N1	3.12	1.45	1.38
10	AA	2261	MA6	C5-N7	-3.12	1.33	1.39
10	AA	125	A2M	C5-C4	-3.12	1.33	1.39
37	BC	167	OMU	O4-C4	-3.12	1.18	1.24
10	AA	1674	OMU	O4-C4	-3.12	1.18	1.24
35	BA	747	OMC	O2-C2	-3.12	1.17	1.23
36	BB	609	A2M	C5-C4	-3.12	1.33	1.39
37	BC	41	A2M	O3'-C3'	-3.12	1.35	1.43
36	BB	1062	OMG	C5-N7	-3.11	1.33	1.39
37	BC	7	OMU	O4-C4	-3.11	1.18	1.24
36	BB	1093	OMU	O4-C4	-3.10	1.18	1.24
35	BA	1665	A2M	O3'-C3'	-3.10	1.35	1.43
36	BB	622	A2M	C5-C4	-3.10	1.33	1.39
10	AA	56	A2M	O3'-C3'	-3.10	1.35	1.43
36	BB	552	OMG	C5-N7	-3.10	1.33	1.39
36	BB	400	A2M	C5-C4	-3.10	1.33	1.39
36	BB	95	A2M	C5-N7	-3.09	1.33	1.39
10	AA	2227	OMG	O6-C6	-3.09	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AA	2054	OMU	O4-C4	-3.09	1.18	1.24
10	AA	1931	OMG	C5-N7	-3.08	1.33	1.39
35	BA	760	OMC	C6-N1	3.08	1.45	1.38
10	AA	2070	G7M	C4-N9	3.08	1.46	1.38
35	BA	996	A2M	O3'-C3'	-3.08	1.35	1.43
36	BB	1324	5MC	O2-C2	-3.08	1.18	1.23
35	BA	1621	OMG	C5-N7	-3.08	1.33	1.39
10	AA	1899	OMU	O4-C4	-3.07	1.18	1.24
35	BA	915	OMG	C5-N7	-3.07	1.33	1.39
10	AA	125	A2M	O3'-C3'	-3.07	1.35	1.43
36	BB	673	OMG	C5-N7	-3.07	1.33	1.39
10	AA	2070	G7M	C5-C6	3.07	1.51	1.43
10	AA	66	OMC	C6-N1	3.06	1.45	1.38
36	BB	1247	OMG	C5-N7	-3.06	1.33	1.39
37	BC	163	A2M	C5-C4	-3.06	1.33	1.39
10	AA	1700	OMG	C5-N7	-3.06	1.33	1.39
36	BB	1413	OMC	O2-C2	-3.05	1.18	1.23
37	BC	75	OMG	C5-N7	-3.05	1.33	1.39
35	BA	1608	OMC	O2-C2	-3.05	1.18	1.23
36	BB	400	A2M	C5-N7	-3.05	1.33	1.39
35	BA	1006	OMC	O2-C2	-3.05	1.18	1.23
36	BB	400	A2M	O3'-C3'	-3.05	1.35	1.43
35	BA	1267	OMG	C5-N7	-3.04	1.33	1.39
10	AA	2096	A2M	C5-C4	-3.04	1.33	1.39
36	BB	609	A2M	O3'-C3'	-3.04	1.35	1.43
35	BA	1665	A2M	C5-C4	-3.04	1.33	1.39
10	AA	1844	OMC	C6-N1	3.04	1.45	1.38
35	BA	1605	OMG	C5-N7	-3.04	1.33	1.39
35	BA	1608	OMC	C6-N1	3.04	1.45	1.38
36	BB	1201	A2M	O3'-C3'	-3.04	1.35	1.43
35	BA	254	A2M	O3'-C3'	-3.02	1.35	1.43
10	AA	2096	A2M	O2'-C2'	3.02	1.50	1.42
36	BB	646	A2M	O3'-C3'	-3.02	1.35	1.43
35	BA	762	A2M	C5-N7	-3.02	1.33	1.39
10	AA	2146	PSU	O4-C4	-3.02	1.17	1.23
35	BA	1009	PSU	O4-C4	-3.02	1.17	1.23
36	BB	622	A2M	O3'-C3'	-3.01	1.35	1.43
36	BB	590	A2M	O3'-C3'	-3.01	1.35	1.43
35	BA	925	OMG	C5-N7	-3.01	1.33	1.39
10	AA	1603	OMG	C5-N7	-3.01	1.33	1.39
36	BB	1264	OMC	O2-C2	-3.00	1.18	1.23
35	BA	1620	A2M	C5-N7	-3.00	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1709	OMG	C5-N7	-3.00	1.33	1.39
35	BA	927	A2M	O3'-C3'	-3.00	1.35	1.43
35	BA	760	OMC	O2-C2	-3.00	1.18	1.23
10	AA	66	OMC	O2-C2	-2.99	1.18	1.23
35	BA	1086	PSU	O4-C4	-2.99	1.17	1.23
10	AA	1932	OMC	C6-N1	2.99	1.45	1.38
35	BA	1330	OMU	O4-C4	-2.99	1.18	1.24
10	AA	46	OMC	O2-C2	-2.99	1.18	1.23
36	BB	1264	OMC	C6-N1	2.98	1.45	1.38
35	BA	927	A2M	C5-N7	-2.98	1.33	1.39
10	AA	1932	OMC	O2-C2	-2.98	1.18	1.23
35	BA	1248	PSU	O4-C4	-2.98	1.17	1.23
36	BB	1269	OMG	O6-C6	-2.98	1.17	1.23
36	BB	1160	PSU	O4-C4	-2.97	1.17	1.23
36	BB	1334	PSU	O4-C4	-2.97	1.17	1.23
36	BB	1388	A2M	O3'-C3'	-2.97	1.36	1.43
10	AA	125	A2M	C5-N7	-2.96	1.33	1.39
37	BC	41	A2M	C5-N7	-2.96	1.33	1.39
35	BA	1006	OMC	C6-N1	2.95	1.45	1.38
35	BA	915	OMG	O6-C6	-2.95	1.18	1.23
10	AA	2096	A2M	O3'-C3'	-2.95	1.36	1.43
36	BB	545	A2M	C5-N7	-2.95	1.33	1.39
36	BB	1210	PSU	O4-C4	-2.95	1.18	1.23
36	BB	1245	OMG	C5-N7	-2.94	1.33	1.39
36	BB	1201	A2M	C5-N7	-2.94	1.33	1.39
10	AA	46	OMC	C6-N1	2.94	1.45	1.38
35	BA	746	A2M	C5-N7	-2.94	1.33	1.39
10	AA	721	A2M	C5-N7	-2.93	1.33	1.39
10	AA	2261	MA6	C4-N9	-2.93	1.31	1.37
36	BB	659	OMG	C5-N7	-2.93	1.33	1.39
36	BB	1429	PSU	O4-C4	-2.93	1.18	1.23
36	BB	1280	PSU	O4-C4	-2.92	1.18	1.23
36	BB	1388	A2M	C5-N7	-2.92	1.33	1.39
36	BB	1413	OMC	C6-N1	2.91	1.45	1.38
35	BA	737	PSU	O4-C4	-2.91	1.18	1.23
35	BA	254	A2M	C5-N7	-2.91	1.33	1.39
36	BB	609	A2M	C5-N7	-2.90	1.33	1.39
36	BB	1403	PSU	O4-C4	-2.90	1.18	1.23
10	AA	2227	OMG	C4-N9	-2.90	1.30	1.38
35	BA	1267	OMG	O6-C6	-2.90	1.18	1.23
36	BB	615	PSU	O4-C4	-2.90	1.18	1.23
35	BA	925	OMG	O6-C6	-2.90	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1621	OMG	O6-C6	-2.89	1.18	1.23
35	BA	1258	PSU	O4-C4	-2.89	1.18	1.23
10	AA	1700	OMG	O6-C6	-2.89	1.18	1.23
36	BB	673	OMG	O6-C6	-2.89	1.18	1.23
35	BA	996	A2M	C5-N7	-2.89	1.33	1.39
36	BB	1094	OMG	C5-N7	-2.88	1.33	1.39
10	AA	1907	PSU	O4-C4	-2.88	1.18	1.23
10	AA	2123	OMU	O2-C2	-2.87	1.17	1.23
36	BB	622	A2M	C5-N7	-2.87	1.33	1.39
10	AA	2260	MA6	C5-N7	-2.86	1.33	1.39
36	BB	377	OMC	O2-C2	-2.86	1.18	1.23
36	BB	1247	OMG	O6-C6	-2.86	1.18	1.23
10	AA	505	PSU	O4-C4	-2.86	1.18	1.23
35	BA	746	A2M	O3'-C3'	-2.85	1.36	1.43
36	BB	611	PSU	O4-C4	-2.85	1.18	1.23
36	BB	1434	PSU	O4-C4	-2.85	1.18	1.23
35	BA	743	A2M	C5-N7	-2.85	1.33	1.39
35	BA	1609	PSU	O4-C4	-2.85	1.18	1.23
36	BB	590	A2M	C5-N7	-2.85	1.33	1.39
10	AA	1844	OMC	O2-C2	-2.85	1.18	1.23
37	BC	74	PSU	O4-C4	-2.85	1.18	1.23
35	BA	1024	A2M	C5-N7	-2.84	1.33	1.39
37	BC	163	A2M	C5-N7	-2.84	1.33	1.39
10	AA	1895	OMG	O6-C6	-2.83	1.18	1.23
36	BB	646	A2M	C5-N7	-2.83	1.33	1.39
10	AA	1276	PSU	O4-C4	-2.83	1.18	1.23
36	BB	644	PSU	O4-C4	-2.82	1.18	1.23
36	BB	552	OMG	O6-C6	-2.82	1.18	1.23
36	BB	659	OMG	O6-C6	-2.82	1.18	1.23
35	BA	1665	A2M	C5-N7	-2.81	1.33	1.39
36	BB	71	OMG	C4-N9	-2.81	1.30	1.38
35	BA	1169	PSU	O4-C4	-2.81	1.18	1.23
10	AA	1700	OMG	C4-N9	-2.80	1.30	1.38
37	BC	43	A2M	C5-N7	-2.80	1.33	1.39
10	AA	721	A2M	O3'-C3'	-2.80	1.36	1.43
36	BB	72	OMG	O6-C6	-2.80	1.18	1.23
36	BB	95	A2M	O2'-C2'	2.80	1.49	1.42
35	BA	1080	PSU	O4-C4	-2.79	1.18	1.23
10	AA	1931	OMG	O6-C6	-2.79	1.18	1.23
36	BB	1419	PSU	O4-C4	-2.79	1.18	1.23
36	BB	629	PSU	O4-C4	-2.79	1.18	1.23
35	BA	1129	PSU	O4-C4	-2.79	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	1245	OMG	O6-C6	-2.79	1.18	1.23
36	BB	1062	OMG	O6-C6	-2.79	1.18	1.23
35	BA	1028	OMG	O6-C6	-2.79	1.18	1.23
36	BB	545	A2M	O3'-C3'	-2.79	1.36	1.43
36	BB	1076	PSU	O4-C4	-2.78	1.18	1.23
10	AA	1517	OMG	O6-C6	-2.78	1.18	1.23
36	BB	601	OMC	C6-N1	2.78	1.44	1.38
36	BB	659	OMG	C4-N9	-2.78	1.30	1.38
10	AA	56	A2M	C5-N7	-2.78	1.33	1.39
35	BA	1709	OMG	O6-C6	-2.78	1.18	1.23
10	AA	2096	A2M	C5-N7	-2.78	1.33	1.39
36	BB	518	PSU	O4-C4	-2.77	1.18	1.23
10	AA	2278	PSU	O4-C4	-2.77	1.18	1.23
36	BB	1229	PSU	O4-C4	-2.77	1.18	1.23
10	AA	1676	OMG	O6-C6	-2.77	1.18	1.23
35	BA	747	OMC	C6-N1	2.77	1.44	1.38
35	BA	1330	OMU	C6-N1	2.77	1.44	1.38
36	BB	1319	PSU	O4-C4	-2.77	1.18	1.23
10	AA	721	A2M	O2'-C2'	2.77	1.49	1.42
10	AA	1592	PSU	O4-C4	-2.76	1.18	1.23
35	BA	1166	PSU	O4-C4	-2.76	1.18	1.23
10	AA	1899	OMU	C6-N1	2.76	1.44	1.38
35	BA	452	PSU	O4-C4	-2.76	1.18	1.23
36	BB	542	5MC	O2-C2	-2.76	1.18	1.23
36	BB	1094	OMG	O6-C6	-2.75	1.18	1.23
35	BA	1267	OMG	C4-N9	-2.75	1.30	1.38
35	BA	1329	OMC	O2-C2	-2.75	1.18	1.23
10	AA	1674	OMU	C6-N1	2.75	1.44	1.38
35	BA	1614	PSU	O4-C4	-2.74	1.18	1.23
10	AA	131	PSU	O4-C4	-2.74	1.18	1.23
10	AA	1603	OMG	O6-C6	-2.74	1.18	1.23
10	AA	2153	A2M	C5-N7	-2.73	1.33	1.39
10	AA	2045	PSU	O4-C4	-2.73	1.18	1.23
36	BB	490	PSU	O4-C4	-2.73	1.18	1.23
36	BB	1409	PSU	O4-C4	-2.73	1.18	1.23
35	BA	1181	OMU	C6-N1	2.72	1.44	1.38
10	AA	2054	OMU	C6-N1	2.72	1.44	1.38
37	BC	167	OMU	C6-N1	2.71	1.44	1.38
37	BC	75	OMG	O6-C6	-2.71	1.18	1.23
35	BA	762	A2M	O2'-C2'	2.70	1.49	1.42
36	BB	1388	A2M	O2'-C2'	2.70	1.49	1.42
37	BC	7	OMU	C6-N1	2.70	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	646	A2M	O2'-C2'	2.70	1.49	1.42
36	BB	528	PSU	O4-C4	-2.70	1.18	1.23
36	BB	622	A2M	O2'-C2'	2.69	1.49	1.42
10	AA	56	A2M	O2'-C2'	2.69	1.49	1.42
36	BB	609	A2M	O2'-C2'	2.69	1.49	1.42
37	BC	43	A2M	O2'-C2'	2.69	1.49	1.42
37	BC	163	A2M	O2'-C2'	2.69	1.49	1.42
35	BA	1742	OMU	O2-C2	-2.68	1.18	1.23
10	AA	61	PSU	O4-C4	-2.68	1.18	1.23
35	BA	762	A2M	C8-N9	-2.68	1.32	1.37
35	BA	1024	A2M	O2'-C2'	2.68	1.49	1.42
10	AA	57	OMU	C6-N1	2.68	1.44	1.38
36	BB	73	OMU	C6-N1	2.68	1.44	1.38
36	BB	400	A2M	O2'-C2'	2.67	1.49	1.42
35	BA	1665	A2M	O2'-C2'	2.67	1.49	1.42
35	BA	46	OMU	C6-N1	2.67	1.44	1.38
36	BB	590	A2M	O2'-C2'	2.67	1.49	1.42
35	BA	1448	OMU	C6-N1	2.66	1.44	1.38
35	BA	746	A2M	O2'-C2'	2.66	1.49	1.42
36	BB	552	OMG	C4-N9	-2.66	1.31	1.38
37	BC	41	A2M	O2'-C2'	2.66	1.49	1.42
36	BB	1201	A2M	O2'-C2'	2.65	1.49	1.42
10	AA	1603	OMG	C2-N1	2.65	1.44	1.37
36	BB	1093	OMU	C6-N1	2.64	1.44	1.38
35	BA	927	A2M	O2'-C2'	2.64	1.49	1.42
36	BB	545	A2M	O2'-C2'	2.64	1.49	1.42
10	AA	1619	PSU	O4-C4	-2.63	1.18	1.23
10	AA	57	OMU	O2-C2	-2.63	1.18	1.23
10	AA	2154	OMU	C6-N1	2.63	1.44	1.38
36	BB	685	OMU	C6-N1	2.63	1.44	1.38
10	AA	714	OMU	O2-C2	-2.63	1.18	1.23
10	AA	125	A2M	O2'-C2'	2.63	1.49	1.42
35	BA	1605	OMG	C2-N1	2.63	1.44	1.37
35	BA	1620	A2M	O2'-C2'	2.63	1.49	1.42
10	AA	714	OMU	C6-N1	2.62	1.44	1.38
35	BA	1605	OMG	O6-C6	-2.62	1.18	1.23
35	BA	1448	OMU	O2-C2	-2.62	1.18	1.23
35	BA	1621	OMG	C4-N9	-2.62	1.31	1.38
35	BA	996	A2M	O2'-C2'	2.62	1.49	1.42
35	BA	254	A2M	O2'-C2'	2.62	1.49	1.42
36	BB	95	A2M	C8-N9	-2.62	1.32	1.37
36	BB	73	OMU	O2-C2	-2.61	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	1094	OMG	C2-N1	2.61	1.44	1.37
36	BB	1435	OMU	C6-N1	2.61	1.44	1.38
36	BB	1062	OMG	C2-N1	2.61	1.44	1.37
35	BA	916	OMU	C6-N1	2.60	1.44	1.38
35	BA	742	1MA	C4-N9	-2.60	1.31	1.38
35	BA	1709	OMG	C4-N9	-2.60	1.31	1.38
35	BA	925	OMG	C4-N9	-2.60	1.31	1.38
36	BB	1094	OMG	C4-N9	-2.59	1.31	1.38
37	BC	75	OMG	C2-N1	2.59	1.44	1.37
35	BA	1267	OMG	C2-N1	2.59	1.44	1.37
35	BA	916	OMU	O2-C2	-2.59	1.18	1.23
36	BB	1201	A2M	C8-N9	-2.59	1.32	1.37
35	BA	46	OMU	O2-C2	-2.59	1.18	1.23
36	BB	1435	OMU	O2-C2	-2.58	1.18	1.23
36	BB	673	OMG	C2-N1	2.58	1.44	1.37
37	BC	167	OMU	O2-C2	-2.58	1.18	1.23
35	BA	1742	OMU	C6-N1	2.58	1.44	1.38
36	BB	1247	OMG	C2-N1	2.57	1.44	1.37
36	BB	1093	OMU	O2-C2	-2.57	1.18	1.23
10	AA	1931	OMG	C2-N1	2.57	1.44	1.37
35	BA	1709	OMG	C2-N1	2.56	1.44	1.37
36	BB	685	OMU	O2-C2	-2.56	1.18	1.23
10	AA	1895	OMG	C4-N9	-2.56	1.31	1.38
35	BA	1024	A2M	C8-N9	-2.55	1.32	1.37
10	AA	1895	OMG	C2-N1	2.54	1.44	1.37
36	BB	578	OMU	C6-N1	2.54	1.44	1.38
35	BA	743	A2M	O2'-C2'	2.54	1.49	1.42
10	AA	2054	OMU	O2-C2	-2.54	1.18	1.23
35	BA	1028	OMG	C2-N1	2.53	1.43	1.37
35	BA	1621	OMG	C2-N1	2.52	1.43	1.37
10	AA	2154	OMU	O2-C2	-2.52	1.18	1.23
36	BB	1245	OMG	C2-N1	2.52	1.43	1.37
10	AA	2153	A2M	O2'-C2'	2.51	1.49	1.42
35	BA	1181	OMU	O2-C2	-2.51	1.18	1.23
10	AA	1676	OMG	C2-N1	2.51	1.43	1.37
37	BC	7	OMU	O2-C2	-2.50	1.18	1.23
35	BA	925	OMG	C2-N1	2.48	1.43	1.37
10	AA	1517	OMG	C2-N1	2.48	1.43	1.37
35	BA	1329	OMC	C5-C4	2.47	1.48	1.42
35	BA	996	A2M	C8-N9	-2.47	1.33	1.37
36	BB	1247	OMG	C4-N9	-2.47	1.31	1.38
35	BA	1330	OMU	O2-C2	-2.47	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	552	OMG	C2-N1	2.46	1.43	1.37
36	BB	1388	A2M	C8-N9	-2.46	1.33	1.37
36	BB	71	OMG	C2-N1	2.46	1.43	1.37
36	BB	609	A2M	C8-N9	-2.45	1.33	1.37
35	BA	915	OMG	C4-N9	-2.45	1.31	1.38
35	BA	915	OMG	C2-N1	2.45	1.43	1.37
36	BB	578	OMU	O2-C2	-2.45	1.18	1.23
37	BC	41	A2M	C8-N9	-2.45	1.33	1.37
36	BB	72	OMG	C2-N1	2.44	1.43	1.37
36	BB	72	OMG	C4-N9	-2.44	1.31	1.38
10	AA	1931	OMG	C4-N9	-2.44	1.31	1.38
10	AA	1700	OMG	C2-N1	2.44	1.43	1.37
10	AA	1603	OMG	C4-N9	-2.44	1.31	1.38
10	AA	1899	OMU	O2-C2	-2.43	1.18	1.23
36	BB	622	A2M	C8-N9	-2.43	1.33	1.37
10	AA	1674	OMU	O2-C2	-2.43	1.18	1.23
10	AA	2260	MA6	C4-N9	-2.43	1.32	1.37
36	BB	1094	OMG	C5-C6	2.42	1.53	1.44
36	BB	1245	OMG	C4-N9	-2.42	1.31	1.38
35	BA	1605	OMG	C5-C6	2.42	1.53	1.44
35	BA	927	A2M	C8-N9	-2.41	1.33	1.37
36	BB	1269	OMG	C4-N9	-2.41	1.31	1.38
10	AA	125	A2M	C8-N9	-2.41	1.33	1.37
35	BA	1620	A2M	C8-N9	-2.40	1.33	1.37
10	AA	721	A2M	O5'-C5'	-2.40	1.38	1.44
36	BB	1269	OMG	C2-N1	2.40	1.43	1.37
36	BB	673	OMG	C5-C6	2.39	1.53	1.44
35	BA	1709	OMG	C5-C6	2.39	1.53	1.44
36	BB	659	OMG	C2-N1	2.39	1.43	1.37
10	AA	56	A2M	C8-N9	-2.39	1.33	1.37
10	AA	721	A2M	C8-N9	-2.38	1.33	1.37
36	BB	400	A2M	C8-N9	-2.38	1.33	1.37
37	BC	75	OMG	C4-N9	-2.38	1.31	1.38
35	BA	746	A2M	C8-N9	-2.38	1.33	1.37
36	BB	1245	OMG	C5-C6	2.37	1.53	1.44
10	AA	1899	OMU	C5-C4	2.37	1.48	1.43
35	BA	743	A2M	C8-N9	-2.37	1.33	1.37
35	BA	915	OMG	C5-C6	2.36	1.53	1.44
10	AA	2153	A2M	C8-N9	-2.35	1.33	1.37
36	BB	1062	OMG	C4-N9	-2.35	1.32	1.38
37	BC	75	OMG	C6-N1	2.35	1.43	1.38
10	AA	1844	OMC	C5-C4	2.34	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1028	OMG	C4-N9	-2.34	1.32	1.38
36	BB	545	A2M	C8-N9	-2.33	1.33	1.37
37	BC	75	OMG	C5-C6	2.33	1.53	1.44
35	BA	1605	OMG	C6-N1	2.33	1.43	1.38
35	BA	925	OMG	C5-C6	2.33	1.53	1.44
10	AA	1603	OMG	C6-N1	2.33	1.43	1.38
10	AA	1603	OMG	C5-C6	2.32	1.53	1.44
10	AA	1931	OMG	C5-C6	2.32	1.53	1.44
35	BA	254	A2M	C8-N9	-2.32	1.33	1.37
35	BA	743	A2M	O5'-C5'	-2.32	1.39	1.44
10	AA	1517	OMG	C5-C6	2.32	1.53	1.44
37	BC	43	A2M	C8-N9	-2.32	1.33	1.37
36	BB	377	OMC	C5-C4	2.32	1.48	1.42
35	BA	1621	OMG	C5-C6	2.32	1.53	1.44
10	AA	2096	A2M	C8-N9	-2.31	1.33	1.37
36	BB	1247	OMG	C5-C6	2.31	1.53	1.44
35	BA	1267	OMG	C6-N1	2.30	1.43	1.38
36	BB	1093	OMU	C5-C4	2.30	1.48	1.43
36	BB	673	OMG	C4-N9	-2.30	1.32	1.38
36	BB	646	A2M	C8-N9	-2.30	1.33	1.37
35	BA	1028	OMG	C5-C6	2.29	1.52	1.44
10	AA	1895	OMG	C5-C6	2.29	1.52	1.44
36	BB	72	OMG	C5-C6	2.29	1.52	1.44
36	BB	590	A2M	C8-N9	-2.29	1.33	1.37
36	BB	659	OMG	C5-C6	2.29	1.52	1.44
36	BB	1269	OMG	C5-C6	2.28	1.52	1.44
10	AA	66	OMC	C5-C4	2.28	1.48	1.42
37	BC	163	A2M	C8-N9	-2.28	1.33	1.37
36	BB	1062	OMG	C5-C6	2.28	1.52	1.44
35	BA	1665	A2M	C8-N9	-2.28	1.33	1.37
36	BB	552	OMG	C5-C6	2.27	1.52	1.44
10	AA	1674	OMU	C5-C4	2.27	1.48	1.43
35	BA	1709	OMG	C6-N1	2.27	1.43	1.38
35	BA	1267	OMG	C5-C6	2.26	1.52	1.44
35	BA	1605	OMG	C4-N9	-2.25	1.32	1.38
10	AA	2153	A2M	O5'-C5'	-2.25	1.39	1.44
36	BB	1094	OMG	C6-N1	2.25	1.43	1.38
10	AA	2123	OMU	C6-N1	2.25	1.43	1.38
10	AA	1932	OMC	C5-C4	2.24	1.48	1.42
10	AA	1676	OMG	C5-C6	2.23	1.52	1.44
10	AA	2261	MA6	C8-N9	-2.23	1.33	1.37
10	AA	1517	OMG	C4-N9	-2.23	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	1245	OMG	C6-N1	2.23	1.43	1.38
35	BA	1006	OMC	C5-C4	2.23	1.48	1.42
10	AA	1700	OMG	C5-C6	2.23	1.52	1.44
36	BB	1264	OMC	C5-C4	2.23	1.48	1.42
36	BB	1403	PSU	O4'-C1'	-2.22	1.40	1.43
10	AA	2154	OMU	C5-C4	2.21	1.48	1.43
35	BA	1448	OMU	C5-C4	2.19	1.48	1.43
10	AA	2260	MA6	C8-N9	-2.19	1.33	1.37
36	BB	545	A2M	O5'-C5'	-2.19	1.39	1.44
10	AA	2054	OMU	C5-C4	2.19	1.48	1.43
35	BA	1248	PSU	O4'-C1'	-2.18	1.40	1.43
35	BA	1181	OMU	C5-C4	2.18	1.48	1.43
36	BB	1319	PSU	O4'-C1'	-2.18	1.40	1.43
37	BC	167	OMU	C5-C4	2.18	1.48	1.43
37	BC	7	OMU	C5-C4	2.18	1.48	1.43
35	BA	1330	OMU	C5-C4	2.17	1.48	1.43
36	BB	1280	PSU	O4'-C1'	-2.17	1.40	1.43
10	AA	1931	OMG	C6-N1	2.17	1.42	1.38
10	AA	57	OMU	C5-C4	2.17	1.48	1.43
35	BA	1665	A2M	O5'-C5'	-2.16	1.39	1.44
35	BA	1620	A2M	O5'-C5'	-2.16	1.39	1.44
36	BB	1247	OMG	C6-N1	2.16	1.42	1.38
10	AA	1676	OMG	C4-N9	-2.15	1.32	1.38
36	BB	71	OMG	C5-C6	2.15	1.52	1.44
10	AA	1596	B8N	O2-C2	-2.15	1.18	1.22
35	BA	46	OMU	C5-C4	2.15	1.48	1.43
35	BA	1621	OMG	C6-N1	2.15	1.42	1.38
36	BB	685	OMU	C5-C4	2.15	1.48	1.43
10	AA	46	OMC	C5-C4	2.15	1.47	1.42
36	BB	518	PSU	O4'-C1'	-2.15	1.40	1.43
35	BA	916	OMU	C5-C4	2.14	1.48	1.43
36	BB	552	OMG	C6-N1	2.13	1.42	1.38
35	BA	1028	OMG	C6-N1	2.12	1.42	1.38
10	AA	1517	OMG	C6-N1	2.12	1.42	1.38
10	AA	2227	OMG	C2-N1	2.12	1.42	1.37
36	BB	1201	A2M	O5'-C5'	-2.11	1.39	1.44
35	BA	996	A2M	O5'-C5'	-2.11	1.39	1.44
35	BA	927	A2M	O5'-C5'	-2.11	1.39	1.44
35	BA	762	A2M	O5'-C5'	-2.11	1.39	1.44
36	BB	1413	OMC	C5-C4	2.11	1.47	1.42
37	BC	41	A2M	O5'-C5'	-2.10	1.39	1.44
37	BC	163	A2M	O5'-C5'	-2.10	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	1062	OMG	C6-N1	2.10	1.42	1.38
10	AA	1895	OMG	C6-N1	2.10	1.42	1.38
35	BA	760	OMC	C5-C4	2.10	1.47	1.42
36	BB	646	A2M	O5'-C5'	-2.10	1.39	1.44
36	BB	673	OMG	C6-N1	2.09	1.42	1.38
36	BB	73	OMU	C5-C4	2.08	1.48	1.43
36	BB	659	OMG	C6-N1	2.08	1.42	1.38
35	BA	1024	A2M	O5'-C5'	-2.08	1.39	1.44
36	BB	590	A2M	O5'-C5'	-2.07	1.39	1.44
36	BB	1435	OMU	C5-C4	2.07	1.48	1.43
37	BC	43	A2M	O5'-C5'	-2.07	1.39	1.44
10	AA	714	OMU	C5-C4	2.07	1.48	1.43
10	AA	56	A2M	O5'-C5'	-2.05	1.39	1.44
10	AA	2227	OMG	C5-C6	2.05	1.52	1.44
35	BA	1742	OMU	C5-C4	2.05	1.48	1.43
10	AA	1700	OMG	C6-N1	2.05	1.42	1.38
36	BB	1419	PSU	O4'-C1'	-2.04	1.41	1.43
36	BB	578	OMU	C5-C4	2.04	1.48	1.43
10	AA	2153	A2M	C4-N9	-2.04	1.33	1.37
10	AA	125	A2M	O5'-C5'	-2.04	1.39	1.44
10	AA	1619	PSU	C4-C5	2.04	1.50	1.44
35	BA	925	OMG	C6-N1	2.03	1.42	1.38
36	BB	609	A2M	O5'-C5'	-2.03	1.39	1.44
36	BB	400	A2M	O5'-C5'	-2.03	1.39	1.44
35	BA	915	OMG	C6-N1	2.03	1.42	1.38
10	AA	1676	OMG	C6-N1	2.03	1.42	1.38
36	BB	95	A2M	O5'-C5'	-2.02	1.39	1.44
35	BA	1608	OMC	C5-C4	2.01	1.47	1.42
10	AA	1907	PSU	O4'-C1'	-2.01	1.41	1.43
35	BA	762	A2M	C4-N9	-2.00	1.33	1.37

All (889) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	2261	MA6	N1-C6-N6	-11.57	104.44	117.08
10	AA	2260	MA6	N1-C6-N6	-11.11	104.94	117.08
35	BA	742	1MA	C1'-N9-C8	-9.31	100.20	126.70
35	BA	742	1MA	C1'-N9-C4	8.91	152.98	126.50
10	AA	1676	OMG	C1'-N9-C8	-8.24	103.25	126.70
36	BB	72	OMG	C1'-N9-C8	-7.87	104.31	126.70
10	AA	1517	OMG	C1'-N9-C8	-7.86	104.31	126.70
36	BB	552	OMG	C1'-N9-C8	-7.82	104.43	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1605	OMG	C1'-N9-C8	-7.81	104.45	126.70
10	AA	1895	OMG	C1'-N9-C8	-7.78	104.56	126.70
36	BB	1062	OMG	C1'-N9-C8	-7.75	104.63	126.70
36	BB	1247	OMG	C1'-N9-C8	-7.72	104.71	126.70
35	BA	1621	OMG	C1'-N9-C8	-7.72	104.73	126.70
10	AA	1931	OMG	C1'-N9-C8	-7.70	104.77	126.70
36	BB	673	OMG	C1'-N9-C8	-7.66	104.88	126.70
37	BC	75	OMG	C1'-N9-C8	-7.66	104.89	126.70
36	BB	1269	OMG	C1'-N9-C8	-7.64	104.96	126.70
10	AA	1603	OMG	C1'-N9-C8	-7.55	105.21	126.70
36	BB	1245	OMG	C1'-N9-C8	-7.52	105.28	126.70
35	BA	915	OMG	C1'-N9-C8	-7.50	105.36	126.70
35	BA	925	OMG	C1'-N9-C8	-7.36	105.75	126.70
10	AA	2227	OMG	C1'-N9-C8	-7.30	105.92	126.70
35	BA	1709	OMG	C1'-N9-C8	-7.16	106.33	126.70
10	AA	1676	OMG	C1'-N9-C4	7.08	147.54	126.50
10	AA	1700	OMG	C1'-N9-C8	-7.07	106.57	126.70
36	BB	71	OMG	C1'-N9-C8	-6.99	106.79	126.70
36	BB	1094	OMG	C1'-N9-C8	-6.97	106.84	126.70
10	AA	1517	OMG	C1'-N9-C4	6.89	146.96	126.50
35	BA	1267	OMG	C1'-N9-C8	-6.77	107.42	126.70
36	BB	659	OMG	C1'-N9-C8	-6.77	107.42	126.70
36	BB	72	OMG	C1'-N9-C4	6.76	146.58	126.50
35	BA	1605	OMG	C1'-N9-C4	6.72	146.45	126.50
36	BB	1062	OMG	C1'-N9-C4	6.65	146.24	126.50
36	BB	1269	OMG	C1'-N9-C4	6.62	146.17	126.50
10	AA	1895	OMG	C1'-N9-C4	6.60	146.11	126.50
36	BB	552	OMG	C1'-N9-C4	6.56	145.99	126.50
36	BB	673	OMG	C1'-N9-C4	6.56	145.98	126.50
35	BA	1621	OMG	C1'-N9-C4	6.53	145.90	126.50
36	BB	1247	OMG	C1'-N9-C4	6.53	145.89	126.50
37	BC	75	OMG	C1'-N9-C4	6.50	145.81	126.50
10	AA	1931	OMG	C1'-N9-C4	6.49	145.78	126.50
10	AA	1603	OMG	C1'-N9-C4	6.38	145.44	126.50
36	BB	1245	OMG	C1'-N9-C4	6.30	145.23	126.50
35	BA	1028	OMG	C1'-N9-C8	-6.30	108.75	126.70
35	BA	915	OMG	C1'-N9-C4	6.28	145.17	126.50
10	AA	2227	OMG	C1'-N9-C4	6.16	144.81	126.50
35	BA	925	OMG	C1'-N9-C4	6.13	144.70	126.50
35	BA	742	1MA	N1-C2-N3	-5.97	118.90	126.00
35	BA	1709	OMG	C1'-N9-C4	5.94	144.15	126.50
36	BB	71	OMG	C1'-N9-C4	5.89	144.00	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	2261	MA6	C5-C6-N6	5.85	135.50	125.30
10	AA	1700	OMG	C1'-N9-C4	5.80	143.72	126.50
10	AA	125	A2M	C5-C4-N3	-5.80	119.19	126.75
36	BB	1094	OMG	C1'-N9-C4	5.77	143.63	126.50
35	BA	762	A2M	N3-C2-N1	-5.71	119.67	128.60
10	AA	2260	MA6	C5-C6-N6	5.66	135.17	125.30
35	BA	1028	OMG	C1'-N9-C4	5.66	143.31	126.50
35	BA	46	OMU	C4-N3-C2	-5.65	119.13	126.58
36	BB	95	A2M	C5-C4-N3	-5.65	119.38	126.75
35	BA	1024	A2M	N3-C2-N1	-5.63	119.79	128.60
10	AA	56	A2M	N3-C2-N1	-5.63	119.80	128.60
35	BA	743	A2M	C5-C4-N3	-5.63	119.41	126.75
36	BB	400	A2M	C5-C4-N3	-5.62	119.42	126.75
37	BC	43	A2M	N3-C2-N1	-5.62	119.81	128.60
10	AA	2261	MA6	N1-C2-N3	-5.61	119.83	128.60
10	AA	2153	A2M	N3-C2-N1	-5.60	119.84	128.60
10	AA	2054	OMU	C4-N3-C2	-5.59	119.21	126.58
10	AA	2154	OMU	C4-N3-C2	-5.59	119.21	126.58
36	BB	1093	OMU	C4-N3-C2	-5.59	119.21	126.58
35	BA	254	A2M	C5-C4-N3	-5.58	119.47	126.75
36	BB	646	A2M	N3-C2-N1	-5.58	119.88	128.60
35	BA	746	A2M	N3-C2-N1	-5.58	119.88	128.60
37	BC	41	A2M	N3-C2-N1	-5.55	119.92	128.60
35	BA	1181	OMU	C4-N3-C2	-5.55	119.26	126.58
10	AA	1899	OMU	C4-N3-C2	-5.55	119.26	126.58
36	BB	1388	A2M	N3-C2-N1	-5.54	119.94	128.60
10	AA	721	A2M	N3-C2-N1	-5.53	119.94	128.60
10	AA	714	OMU	C4-N3-C2	-5.53	119.28	126.58
35	BA	996	A2M	C5-C4-N3	-5.53	119.54	126.75
36	BB	1201	A2M	C5-C4-N3	-5.53	119.54	126.75
35	BA	916	OMU	C4-N3-C2	-5.53	119.29	126.58
36	BB	659	OMG	C1'-N9-C4	5.52	142.91	126.50
35	BA	1620	A2M	N3-C2-N1	-5.52	119.97	128.60
35	BA	1665	A2M	N3-C2-N1	-5.52	119.97	128.60
36	BB	685	OMU	C4-N3-C2	-5.51	119.31	126.58
35	BA	1448	OMU	C4-N3-C2	-5.49	119.34	126.58
35	BA	1742	OMU	C4-N3-C2	-5.48	119.35	126.58
10	AA	2096	A2M	C5-C4-N3	-5.48	119.60	126.75
10	AA	721	A2M	C5-C4-N3	-5.48	119.61	126.75
36	BB	590	A2M	N3-C2-N1	-5.47	120.04	128.60
35	BA	1267	OMG	C1'-N9-C4	5.47	142.75	126.50
37	BC	163	A2M	N3-C2-N1	-5.47	120.05	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1665	A2M	C5-C4-N3	-5.46	119.62	126.75
37	BC	167	OMU	C4-N3-C2	-5.46	119.38	126.58
35	BA	927	A2M	N3-C2-N1	-5.46	120.06	128.60
36	BB	609	A2M	N3-C2-N1	-5.46	120.06	128.60
36	BB	545	A2M	C5-C4-N3	-5.46	119.63	126.75
36	BB	1201	A2M	N3-C2-N1	-5.45	120.07	128.60
35	BA	996	A2M	N3-C2-N1	-5.45	120.07	128.60
35	BA	743	A2M	N3-C2-N1	-5.45	120.08	128.60
10	AA	2123	OMU	C4-N3-C2	-5.44	119.40	126.58
36	BB	622	A2M	C5-C4-N3	-5.43	119.67	126.75
35	BA	1620	A2M	C5-C4-N3	-5.42	119.68	126.75
35	BA	1024	A2M	C5-C4-N3	-5.42	119.68	126.75
36	BB	73	OMU	C4-N3-C2	-5.42	119.43	126.58
36	BB	578	OMU	C4-N3-C2	-5.42	119.43	126.58
36	BB	590	A2M	C5-C4-N3	-5.41	119.69	126.75
36	BB	400	A2M	N3-C2-N1	-5.41	120.14	128.60
35	BA	254	A2M	N3-C2-N1	-5.41	120.14	128.60
36	BB	609	A2M	C5-C4-N3	-5.40	119.70	126.75
37	BC	7	OMU	C4-N3-C2	-5.40	119.46	126.58
36	BB	1435	OMU	C4-N3-C2	-5.39	119.47	126.58
36	BB	545	A2M	N3-C2-N1	-5.39	120.17	128.60
10	AA	56	A2M	C5-C4-N3	-5.39	119.72	126.75
35	BA	927	A2M	C5-C4-N3	-5.36	119.75	126.75
36	BB	622	A2M	N3-C2-N1	-5.36	120.22	128.60
36	BB	646	A2M	N6-C6-N1	-5.35	106.64	118.35
36	BB	1388	A2M	C5-C4-N3	-5.35	119.77	126.75
36	BB	646	A2M	C5-C4-N3	-5.34	119.78	126.75
37	BC	41	A2M	C5-C4-N3	-5.34	119.78	126.75
10	AA	125	A2M	N3-C2-N1	-5.34	120.25	128.60
10	AA	2096	A2M	N3-C2-N1	-5.32	120.28	128.60
35	BA	746	A2M	C5-C4-N3	-5.32	119.81	126.75
37	BC	163	A2M	C5-C4-N3	-5.31	119.82	126.75
37	BC	41	A2M	N6-C6-N1	-5.31	106.73	118.35
10	AA	1674	OMU	C4-N3-C2	-5.29	119.60	126.58
36	BB	95	A2M	N3-C2-N1	-5.29	120.33	128.60
10	AA	2260	MA6	N1-C2-N3	-5.28	120.35	128.60
37	BC	43	A2M	C5-C4-N3	-5.26	119.89	126.75
10	AA	2260	MA6	C5-C4-N3	-5.26	119.89	126.75
35	BA	762	A2M	N6-C6-N1	-5.25	106.86	118.35
35	BA	746	A2M	N6-C6-N1	-5.23	106.90	118.35
35	BA	743	A2M	N6-C6-N1	-5.21	106.93	118.35
10	AA	57	OMU	C4-N3-C2	-5.21	119.71	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	996	A2M	N6-C6-N1	-5.20	106.97	118.35
35	BA	1665	A2M	N6-C6-N1	-5.19	106.98	118.35
10	AA	721	A2M	N6-C6-N1	-5.18	107.01	118.35
10	AA	56	A2M	N6-C6-N1	-5.17	107.03	118.35
35	BA	1024	A2M	N6-C6-N1	-5.16	107.04	118.35
36	BB	609	A2M	N6-C6-N1	-5.15	107.06	118.35
10	AA	1596	B8N	C5-C4-N3	5.15	125.71	116.17
37	BC	163	A2M	N6-C6-N1	-5.15	107.08	118.35
10	AA	2096	A2M	N6-C6-N1	-5.13	107.11	118.35
10	AA	1710	PSU	C4-N3-C2	-5.11	118.97	126.34
36	BB	95	A2M	N6-C6-N1	-5.09	107.21	118.35
35	BA	762	A2M	C5-C4-N3	-5.09	120.11	126.75
35	BA	1620	A2M	N6-C6-N1	-5.08	107.22	118.35
37	BC	43	A2M	N6-C6-N1	-5.07	107.25	118.35
35	BA	1330	OMU	C4-N3-C2	-5.06	119.90	126.58
36	BB	622	A2M	N6-C6-N1	-5.05	107.28	118.35
36	BB	1388	A2M	N6-C6-N1	-5.01	107.37	118.35
36	BB	590	A2M	N6-C6-N1	-5.01	107.38	118.35
36	BB	1201	A2M	N6-C6-N1	-4.97	107.46	118.35
35	BA	254	A2M	N6-C6-N1	-4.97	107.46	118.35
10	AA	125	A2M	N6-C6-N1	-4.92	107.58	118.35
35	BA	927	A2M	N6-C6-N1	-4.90	107.62	118.35
10	AA	1517	OMG	C5-C4-N3	-4.90	120.52	128.46
36	BB	400	A2M	N6-C6-N1	-4.87	107.69	118.35
10	AA	2153	A2M	N6-C6-N1	-4.85	107.73	118.35
36	BB	545	A2M	N6-C6-N1	-4.81	107.81	118.35
10	AA	505	PSU	C4-N3-C2	-4.80	119.42	126.34
10	AA	2153	A2M	C5-C4-N3	-4.80	120.49	126.75
35	BA	1169	PSU	C4-N3-C2	-4.79	119.43	126.34
36	BB	1334	PSU	C4-N3-C2	-4.78	119.45	126.34
35	BA	1248	PSU	C4-N3-C2	-4.77	119.47	126.34
10	AA	1676	OMG	C5-C4-N3	-4.77	120.73	128.46
36	BB	1076	PSU	C4-N3-C2	-4.75	119.50	126.34
10	AA	131	PSU	C4-N3-C2	-4.74	119.51	126.34
35	BA	1080	PSU	C4-N3-C2	-4.73	119.53	126.34
35	BA	1009	PSU	C4-N3-C2	-4.70	119.56	126.34
37	BC	74	PSU	C4-N3-C2	-4.70	119.56	126.34
35	BA	452	PSU	C4-N3-C2	-4.70	119.57	126.34
10	AA	2146	PSU	C4-N3-C2	-4.70	119.57	126.34
35	BA	1605	OMG	C5-C4-N3	-4.68	120.87	128.46
35	BA	1028	OMG	C5-C4-N3	-4.67	120.88	128.46
36	BB	1269	OMG	C5-C4-N3	-4.67	120.89	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	1160	PSU	C4-N3-C2	-4.66	119.63	126.34
36	BB	1319	PSU	C4-N3-C2	-4.65	119.64	126.34
36	BB	1062	OMG	C5-C4-N3	-4.65	120.92	128.46
36	BB	1419	PSU	C4-N3-C2	-4.65	119.64	126.34
35	BA	1258	PSU	C4-N3-C2	-4.64	119.65	126.34
36	BB	1280	PSU	C4-N3-C2	-4.64	119.65	126.34
36	BB	1403	PSU	C4-N3-C2	-4.64	119.66	126.34
36	BB	673	OMG	C5-C4-N3	-4.64	120.94	128.46
36	BB	1076	PSU	N1-C2-N3	4.63	120.38	115.13
36	BB	490	PSU	C4-N3-C2	-4.63	119.67	126.34
10	AA	1276	PSU	C4-N3-C2	-4.62	119.68	126.34
36	BB	528	PSU	C4-N3-C2	-4.62	119.68	126.34
10	AA	2261	MA6	C5-C4-N3	-4.62	120.72	126.75
36	BB	1429	PSU	C4-N3-C2	-4.60	119.71	126.34
36	BB	1210	PSU	C4-N3-C2	-4.60	119.71	126.34
35	BA	915	OMG	C5-C4-N3	-4.59	121.01	128.46
10	AA	505	PSU	N1-C2-N3	4.59	120.33	115.13
36	BB	1229	PSU	C4-N3-C2	-4.58	119.73	126.34
10	AA	2278	PSU	C4-N3-C2	-4.58	119.74	126.34
10	AA	1592	PSU	C4-N3-C2	-4.58	119.75	126.34
35	BA	1129	PSU	C4-N3-C2	-4.57	119.75	126.34
10	AA	61	PSU	C4-N3-C2	-4.56	119.77	126.34
10	AA	2153	A2M	N9-C8-N7	-4.56	107.68	113.91
35	BA	1086	PSU	C4-N3-C2	-4.54	119.79	126.34
36	BB	615	PSU	C4-N3-C2	-4.54	119.80	126.34
10	AA	1931	OMG	C5-C4-N3	-4.52	121.12	128.46
35	BA	762	A2M	C5-C6-N6	4.52	133.26	123.43
35	BA	1614	PSU	C4-N3-C2	-4.50	119.85	126.34
37	BC	75	OMG	C5-C4-N3	-4.50	121.16	128.46
36	BB	644	PSU	C4-N3-C2	-4.49	119.87	126.34
35	BA	1166	PSU	C4-N3-C2	-4.49	119.88	126.34
36	BB	1245	OMG	C5-C4-N3	-4.47	121.21	128.46
35	BA	737	PSU	C4-N3-C2	-4.46	119.91	126.34
10	AA	2261	MA6	N9-C8-N7	-4.46	107.82	113.91
35	BA	1609	PSU	C4-N3-C2	-4.45	119.92	126.34
36	BB	1247	OMG	C5-C4-N3	-4.45	121.24	128.46
36	BB	629	PSU	C4-N3-C2	-4.44	119.94	126.34
10	AA	1895	OMG	C5-C4-N3	-4.44	121.26	128.46
36	BB	1334	PSU	N1-C2-N3	4.44	120.16	115.13
10	AA	1907	PSU	C4-N3-C2	-4.43	119.95	126.34
35	BA	1258	PSU	N1-C2-N3	4.43	120.15	115.13
10	AA	1603	OMG	C5-C4-N3	-4.43	121.27	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	1409	PSU	C4-N3-C2	-4.43	119.96	126.34
10	AA	2260	MA6	N9-C8-N7	-4.43	107.86	113.91
36	BB	1434	PSU	C4-N3-C2	-4.42	119.97	126.34
36	BB	72	OMG	C5-C4-N3	-4.42	121.29	128.46
35	BA	1614	PSU	N1-C2-N3	4.41	120.13	115.13
36	BB	609	A2M	C5-C6-N6	4.39	132.98	123.43
35	BA	452	PSU	N1-C2-N3	4.38	120.09	115.13
36	BB	673	OMG	C2-N3-C4	4.38	120.10	112.30
36	BB	1280	PSU	N1-C2-N3	4.37	120.08	115.13
36	BB	1160	PSU	N1-C2-N3	4.36	120.07	115.13
36	BB	1403	PSU	N1-C2-N3	4.36	120.07	115.13
36	BB	646	A2M	C5-C6-N6	4.36	132.92	123.43
37	BC	74	PSU	N1-C2-N3	4.36	120.07	115.13
35	BA	746	A2M	C5-C6-N6	4.36	132.92	123.43
35	BA	1080	PSU	N1-C2-N3	4.36	120.07	115.13
10	AA	2146	PSU	N1-C2-N3	4.35	120.06	115.13
35	BA	743	A2M	C5-C6-N6	4.35	132.89	123.43
35	BA	1169	PSU	N1-C2-N3	4.34	120.05	115.13
36	BB	1319	PSU	N1-C2-N3	4.34	120.05	115.13
37	BC	41	A2M	C5-C6-N6	4.33	132.86	123.43
36	BB	518	PSU	C4-N3-C2	-4.33	120.10	126.34
10	AA	2070	G7M	C2-N3-C4	4.33	120.01	112.30
36	BB	1419	PSU	N1-C2-N3	4.33	120.03	115.13
37	BC	163	A2M	C5-C6-N6	4.32	132.83	123.43
10	AA	1517	OMG	C2-N3-C4	4.32	119.99	112.30
36	BB	490	PSU	N1-C2-N3	4.31	120.02	115.13
36	BB	1269	OMG	C2-N3-C4	4.31	119.98	112.30
10	AA	61	PSU	N1-C2-N3	4.30	120.00	115.13
36	BB	611	PSU	C4-N3-C2	-4.29	120.16	126.34
10	AA	131	PSU	N1-C2-N3	4.29	119.98	115.13
35	BA	1024	A2M	C5-C6-N6	4.28	132.75	123.43
10	AA	2123	OMU	N3-C2-N1	4.28	120.57	114.89
35	BA	1086	PSU	N1-C2-N3	4.28	119.98	115.13
36	BB	1245	OMG	C2-N3-C4	4.28	119.92	112.30
35	BA	996	A2M	C5-C6-N6	4.27	132.72	123.43
35	BA	1665	A2M	C5-C6-N6	4.27	132.72	123.43
35	BA	1248	PSU	N1-C2-N3	4.27	119.96	115.13
36	BB	1062	OMG	C2-N3-C4	4.26	119.89	112.30
35	BA	1024	A2M	N9-C8-N7	-4.26	108.09	113.91
10	AA	1931	OMG	C2-N3-C4	4.26	119.89	112.30
35	BA	1129	PSU	N1-C2-N3	4.25	119.95	115.13
35	BA	1028	OMG	C2-N3-C4	4.25	119.87	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	1700	OMG	C2-N3-C4	4.25	119.87	112.30
36	BB	1201	A2M	N9-C8-N7	-4.25	108.10	113.91
36	BB	71	OMG	C5-C4-N3	-4.25	121.57	128.46
35	BA	915	OMG	C2-N3-C4	4.24	119.86	112.30
10	AA	2045	PSU	C4-N3-C2	-4.24	120.23	126.34
10	AA	1603	OMG	C2-N3-C4	4.24	119.85	112.30
10	AA	56	A2M	C5-C6-N6	4.24	132.66	123.43
10	AA	2096	A2M	C5-C6-N6	4.24	132.66	123.43
36	BB	1210	PSU	N1-C2-N3	4.24	119.93	115.13
10	AA	2278	PSU	N1-C2-N3	4.24	119.93	115.13
10	AA	1907	PSU	N1-C2-N3	4.23	119.93	115.13
35	BA	1621	OMG	C5-C4-N3	-4.23	121.59	128.46
35	BA	1665	A2M	N9-C8-N7	-4.23	108.12	113.91
36	BB	95	A2M	C5-C6-N6	4.23	132.64	123.43
36	BB	528	PSU	N1-C2-N3	4.23	119.92	115.13
36	BB	644	PSU	N1-C2-N3	4.23	119.92	115.13
35	BA	1009	PSU	N1-C2-N3	4.23	119.92	115.13
36	BB	615	PSU	N1-C2-N3	4.23	119.92	115.13
10	AA	1592	PSU	N1-C2-N3	4.23	119.92	115.13
37	BC	43	A2M	N9-C8-N7	-4.22	108.14	113.91
36	BB	545	A2M	N9-C8-N7	-4.22	108.14	113.91
10	AA	1276	PSU	N1-C2-N3	4.22	119.91	115.13
36	BB	1434	PSU	N1-C2-N3	4.21	119.90	115.13
36	BB	1229	PSU	N1-C2-N3	4.21	119.90	115.13
10	AA	721	A2M	C5-C6-N6	4.20	132.58	123.43
36	BB	1094	OMG	C2-N3-C4	4.20	119.78	112.30
37	BC	43	A2M	C5-C6-N6	4.19	132.56	123.43
36	BB	1247	OMG	C2-N3-C4	4.19	119.77	112.30
36	BB	552	OMG	C5-C4-N3	-4.19	121.67	128.46
10	AA	1619	PSU	C4-N3-C2	-4.18	120.31	126.34
35	BA	1605	OMG	C2-N3-C4	4.18	119.75	112.30
10	AA	721	A2M	N9-C8-N7	-4.18	108.20	113.91
10	AA	1676	OMG	C2-N3-C4	4.18	119.74	112.30
36	BB	622	A2M	C5-C6-N6	4.17	132.51	123.43
36	BB	622	A2M	N9-C8-N7	-4.16	108.22	113.91
36	BB	646	A2M	N9-C8-N7	-4.16	108.22	113.91
35	BA	1620	A2M	C5-C6-N6	4.16	132.49	123.43
35	BA	1267	OMG	C2-N3-C4	4.16	119.71	112.30
10	AA	2070	G7M	C5-C4-N3	-4.16	120.18	128.15
36	BB	590	A2M	C5-C6-N6	4.16	132.48	123.43
36	BB	71	OMG	C2-N3-C4	4.14	119.68	112.30
10	AA	56	A2M	N9-C8-N7	-4.14	108.25	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	925	OMG	C5-C4-N3	-4.14	121.75	128.46
35	BA	1609	PSU	N1-C2-N3	4.14	119.82	115.13
35	BA	254	A2M	C5-C6-N6	4.14	132.43	123.43
36	BB	1201	A2M	C5-C6-N6	4.13	132.43	123.43
35	BA	1709	OMG	C2-N3-C4	4.13	119.66	112.30
36	BB	659	OMG	C2-N3-C4	4.13	119.65	112.30
35	BA	1166	PSU	N1-C2-N3	4.13	119.81	115.13
35	BA	1709	OMG	C5-C4-N3	-4.13	121.77	128.46
10	AA	2045	PSU	N1-C2-N3	4.13	119.80	115.13
36	BB	1429	PSU	N1-C2-N3	4.12	119.80	115.13
10	AA	125	A2M	N9-C8-N7	-4.12	108.28	113.91
10	AA	1710	PSU	N1-C2-N3	4.12	119.80	115.13
37	BC	75	OMG	C2-N3-C4	4.12	119.64	112.30
10	AA	1700	OMG	C5-C4-N3	-4.12	121.78	128.46
36	BB	590	A2M	N9-C8-N7	-4.12	108.28	113.91
10	AA	2227	OMG	C2-N3-C4	4.11	119.63	112.30
36	BB	629	PSU	N1-C2-N3	4.11	119.79	115.13
36	BB	1388	A2M	C5-C6-N6	4.11	132.38	123.43
36	BB	552	OMG	C2-N3-C4	4.11	119.62	112.30
36	BB	1094	OMG	C5-C4-N3	-4.10	121.80	128.46
35	BA	916	OMU	N3-C2-N1	4.10	120.34	114.89
35	BA	1621	OMG	C2-N3-C4	4.10	119.61	112.30
36	BB	1324	5MC	C5-C6-N1	-4.10	119.12	123.34
36	BB	518	PSU	N1-C2-N3	4.10	119.77	115.13
10	AA	2096	A2M	N9-C8-N7	-4.10	108.31	113.91
10	AA	2227	OMG	C5-C4-N3	-4.10	121.82	128.46
35	BA	925	OMG	C2-N3-C4	4.09	119.59	112.30
36	BB	1409	PSU	N1-C2-N3	4.09	119.76	115.13
35	BA	927	A2M	C5-C6-N6	4.09	132.32	123.43
10	AA	1895	OMG	C2-N3-C4	4.08	119.57	112.30
35	BA	1620	A2M	N9-C8-N7	-4.08	108.33	113.91
10	AA	1596	B8N	C4-N3-C2	-4.08	120.31	125.46
36	BB	1388	A2M	N9-C8-N7	-4.07	108.34	113.91
37	BC	41	A2M	N9-C8-N7	-4.06	108.36	113.91
10	AA	2054	OMU	N3-C2-N1	4.05	120.27	114.89
10	AA	2153	A2M	C5-C6-N6	4.05	132.25	123.43
36	BB	72	OMG	C2-N3-C4	4.05	119.51	112.30
36	BB	400	A2M	C5-C6-N6	4.04	132.23	123.43
36	BB	685	OMU	N3-C2-N1	4.04	120.25	114.89
10	AA	2154	OMU	N3-C2-N1	4.04	120.25	114.89
35	BA	746	A2M	N9-C8-N7	-4.03	108.41	113.91
36	BB	659	OMG	C5-C4-N3	-4.01	121.95	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1448	OMU	N3-C2-N1	4.01	120.22	114.89
37	BC	163	A2M	N9-C8-N7	-4.00	108.44	113.91
10	AA	125	A2M	C5-C6-N6	4.00	132.13	123.43
10	AA	1899	OMU	N3-C2-N1	3.99	120.19	114.89
35	BA	1267	OMG	C5-C4-N3	-3.99	121.98	128.46
35	BA	996	A2M	N9-C8-N7	-3.99	108.46	113.91
35	BA	46	OMU	N3-C2-N1	3.99	120.18	114.89
37	BC	167	OMU	N3-C2-N1	3.97	120.17	114.89
35	BA	742	1MA	C2-N3-C4	3.97	120.21	112.41
35	BA	762	A2M	N9-C8-N7	-3.96	108.49	113.91
10	AA	1619	PSU	N1-C2-N3	3.96	119.62	115.13
35	BA	1181	OMU	N3-C2-N1	3.94	120.12	114.89
36	BB	95	A2M	N9-C8-N7	-3.94	108.53	113.91
10	AA	57	OMU	N3-C2-N1	3.93	120.11	114.89
35	BA	254	A2M	N9-C8-N7	-3.92	108.56	113.91
35	BA	1742	OMU	N3-C2-N1	3.91	120.08	114.89
10	AA	2260	MA6	C4-C5-C6	3.90	120.25	115.88
36	BB	1093	OMU	N3-C2-N1	3.90	120.07	114.89
36	BB	609	A2M	N9-C8-N7	-3.90	108.58	113.91
36	BB	611	PSU	N1-C2-N3	3.89	119.54	115.13
10	AA	1674	OMU	N3-C2-N1	3.88	120.05	114.89
10	AA	2070	G7M	C5-C6-N1	3.88	119.88	111.79
35	BA	742	1MA	C5-C4-N3	-3.87	121.48	127.26
10	AA	714	OMU	N3-C2-N1	3.87	120.03	114.89
35	BA	737	PSU	N1-C2-N3	3.87	119.51	115.13
35	BA	927	A2M	N9-C8-N7	-3.87	108.62	113.91
10	AA	1700	OMG	N9-C8-N7	-3.84	106.16	113.39
36	BB	545	A2M	C5-C6-N6	3.84	131.78	123.43
35	BA	1267	OMG	N9-C8-N7	-3.83	106.18	113.39
36	BB	73	OMU	N3-C2-N1	3.83	119.97	114.89
35	BA	743	A2M	N9-C8-N7	-3.80	108.71	113.91
35	BA	1330	OMU	N3-C2-N1	3.79	119.92	114.89
36	BB	578	OMU	N3-C2-N1	3.78	119.91	114.89
37	BC	7	OMU	N3-C2-N1	3.75	119.87	114.89
36	BB	659	OMG	N9-C8-N7	-3.75	106.34	113.39
36	BB	1435	OMU	N3-C2-N1	3.73	119.84	114.89
36	BB	1094	OMG	N9-C8-N7	-3.71	106.40	113.39
35	BA	1024	A2M	C2-N3-C4	3.70	120.49	111.75
35	BA	743	A2M	C2-N3-C4	3.69	120.47	111.75
10	AA	56	A2M	C2-N3-C4	3.69	120.46	111.75
35	BA	1181	OMU	C5-C4-N3	3.67	120.33	114.84
36	BB	400	A2M	N9-C8-N7	-3.65	108.92	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1665	A2M	C2-N3-C4	3.65	120.38	111.75
36	BB	646	A2M	C2-N3-C4	3.65	120.38	111.75
35	BA	996	A2M	C2-N3-C4	3.65	120.38	111.75
10	AA	721	A2M	C2-N3-C4	3.65	120.37	111.75
35	BA	254	A2M	C2-N3-C4	3.64	120.35	111.75
35	BA	46	OMU	C5-C4-N3	3.62	120.26	114.84
10	AA	125	A2M	C2-N3-C4	3.62	120.31	111.75
10	AA	714	OMU	C5-C4-N3	3.62	120.26	114.84
36	BB	1245	OMG	N9-C8-N7	-3.62	106.57	113.39
37	BC	41	A2M	C2-N3-C4	3.62	120.30	111.75
36	BB	1435	OMU	C5-C4-N3	3.62	120.25	114.84
36	BB	400	A2M	C2-N3-C4	3.61	120.27	111.75
35	BA	925	OMG	N9-C8-N7	-3.60	106.61	113.39
35	BA	1709	OMG	N9-C8-N7	-3.60	106.61	113.39
36	BB	1388	A2M	C2-N3-C4	3.60	120.26	111.75
36	BB	73	OMU	C5-C4-N3	3.60	120.23	114.84
35	BA	915	OMG	N9-C8-N7	-3.60	106.61	113.39
35	BA	1620	A2M	C2-N3-C4	3.60	120.25	111.75
35	BA	746	A2M	C2-N3-C4	3.59	120.23	111.75
36	BB	1201	A2M	C2-N3-C4	3.58	120.22	111.75
35	BA	1330	OMU	C1'-N1-C2	3.58	124.06	117.57
36	BB	590	A2M	C2-N3-C4	3.58	120.21	111.75
35	BA	927	A2M	C2-N3-C4	3.58	120.20	111.75
36	BB	622	A2M	C2-N3-C4	3.57	120.19	111.75
36	BB	1093	OMU	C5-C4-N3	3.57	120.18	114.84
10	AA	2096	A2M	C2-N3-C4	3.57	120.17	111.75
37	BC	43	A2M	C2-N3-C4	3.55	120.15	111.75
36	BB	545	A2M	C2-N3-C4	3.55	120.15	111.75
36	BB	95	A2M	C2-N3-C4	3.55	120.14	111.75
36	BB	609	A2M	C2-N3-C4	3.55	120.13	111.75
35	BA	1742	OMU	C5-C4-N3	3.55	120.15	114.84
37	BC	163	A2M	C2-N3-C4	3.54	120.12	111.75
37	BC	7	OMU	C5-C4-N3	3.54	120.13	114.84
10	AA	1931	OMG	N9-C8-N7	-3.53	106.74	113.39
35	BA	762	A2M	C2-N3-C4	3.53	120.09	111.75
10	AA	2227	OMG	N9-C8-N7	-3.52	106.75	113.39
35	BA	1621	OMG	N9-C8-N7	-3.52	106.76	113.39
35	BA	1448	OMU	C5-C4-N3	3.52	120.10	114.84
10	AA	2154	OMU	C5-C4-N3	3.51	120.09	114.84
10	AA	2054	OMU	C5-C4-N3	3.50	120.07	114.84
36	BB	673	OMG	N9-C8-N7	-3.50	106.80	113.39
36	BB	685	OMU	C5-C4-N3	3.50	120.07	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	2261	MA6	C2-N1-C6	3.49	120.00	111.75
36	BB	552	OMG	N9-C8-N7	-3.49	106.82	113.39
10	AA	1603	OMG	N9-C8-N7	-3.48	106.84	113.39
36	BB	71	OMG	N9-C8-N7	-3.48	106.84	113.39
36	BB	1247	OMG	N9-C8-N7	-3.48	106.84	113.39
10	AA	1899	OMU	C5-C4-N3	3.47	120.03	114.84
37	BC	167	OMU	C5-C4-N3	3.47	120.03	114.84
10	AA	2260	MA6	C2-N3-C4	3.47	119.94	111.75
10	AA	1895	OMG	N9-C8-N7	-3.46	106.87	113.39
36	BB	578	OMU	C5-C4-N3	3.45	120.01	114.84
10	AA	125	A2M	N3-C4-N9	3.45	132.77	127.08
36	BB	1062	OMG	N9-C8-N7	-3.43	106.92	113.39
10	AA	2261	MA6	C2-N3-C4	3.42	119.83	111.75
37	BC	75	OMG	N9-C8-N7	-3.42	106.96	113.39
10	AA	2153	A2M	C2-N3-C4	3.41	119.80	111.75
36	BB	518	PSU	C6-N1-C2	-3.40	119.21	122.68
35	BA	1605	OMG	N9-C8-N7	-3.39	107.02	113.39
36	BB	545	A2M	O4'-C1'-N9	3.38	114.72	108.06
36	BB	545	A2M	N3-C4-N9	3.38	132.65	127.08
35	BA	916	OMU	C5-C4-N3	3.38	119.89	114.84
10	AA	1674	OMU	C5-C4-N3	3.36	119.86	114.84
10	AA	2260	MA6	C2-N1-C6	3.36	119.68	111.75
36	BB	72	OMG	N9-C8-N7	-3.35	107.08	113.39
10	AA	2123	OMU	C5-C4-N3	3.33	119.83	114.84
36	BB	1201	A2M	N3-C4-N9	3.31	132.54	127.08
36	BB	542	5MC	C5-C6-N1	-3.31	119.94	123.34
10	AA	1676	OMG	N9-C8-N7	-3.30	107.17	113.39
10	AA	2070	G7M	O6-C6-C5	-3.30	120.61	128.06
10	AA	2045	PSU	C6-N1-C2	-3.30	119.31	122.68
36	BB	400	A2M	N3-C4-N9	3.29	132.50	127.08
10	AA	57	OMU	C5-C4-N3	3.29	119.76	114.84
10	AA	2261	MA6	C4-C5-C6	3.28	119.55	115.88
36	BB	1269	OMG	N9-C8-N7	-3.28	107.22	113.39
35	BA	1665	A2M	N3-C4-N9	3.27	132.47	127.08
35	BA	996	A2M	N3-C4-N9	3.26	132.45	127.08
35	BA	1330	OMU	C5-C4-N3	3.26	119.72	114.84
10	AA	1907	PSU	C6-N1-C2	-3.26	119.35	122.68
35	BA	1614	PSU	C6-N1-C2	-3.26	119.35	122.68
36	BB	545	A2M	C2'-C1'-N9	-3.25	108.06	113.53
36	BB	1076	PSU	C6-N1-C2	-3.24	119.36	122.68
36	BB	95	A2M	N3-C4-N9	3.24	132.42	127.08
10	AA	505	PSU	C6-C5-C4	3.24	120.46	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	1201	A2M	C5-N7-C8	3.21	108.06	103.51
35	BA	1024	A2M	C5-N7-C8	3.19	108.05	103.51
35	BA	1086	PSU	C6-N1-C2	-3.19	119.42	122.68
35	BA	927	A2M	N3-C4-N9	3.18	132.32	127.08
35	BA	1620	A2M	N3-C4-N9	3.18	132.32	127.08
10	AA	125	A2M	C5-N7-C8	3.18	108.03	103.51
36	BB	644	PSU	C6-N1-C2	-3.18	119.43	122.68
36	BB	1269	OMG	C2-N1-C6	-3.17	119.31	125.10
35	BA	1665	A2M	C5-N7-C8	3.17	108.02	103.51
36	BB	622	A2M	C5-N7-C8	3.17	108.01	103.51
10	AA	2227	OMG	C2-N1-C6	-3.17	119.32	125.10
10	AA	1517	OMG	N9-C8-N7	-3.17	107.43	113.39
36	BB	1076	PSU	C6-C5-C4	3.16	120.41	118.20
10	AA	2260	MA6	N3-C4-N9	3.15	132.28	127.08
36	BB	73	OMU	O4-C4-C5	-3.15	119.62	125.16
36	BB	622	A2M	N3-C4-N9	3.15	132.27	127.08
10	AA	56	A2M	N3-C4-N9	3.14	132.26	127.08
36	BB	1388	A2M	N3-C4-N9	3.14	132.25	127.08
36	BB	590	A2M	N3-C4-N9	3.13	132.24	127.08
36	BB	1434	PSU	C6-N1-C2	-3.12	119.49	122.68
10	AA	1517	OMG	C2-N1-C6	-3.12	119.40	125.10
35	BA	1742	OMU	O4-C4-C5	-3.12	119.68	125.16
10	AA	721	A2M	C5-N7-C8	3.12	107.94	103.51
35	BA	1605	OMG	C2-N1-C6	-3.11	119.42	125.10
10	AA	2096	A2M	N3-C4-N9	3.10	132.19	127.08
35	BA	254	A2M	N3-C4-N9	3.10	132.19	127.08
37	BC	43	A2M	C5-N7-C8	3.10	107.91	103.51
10	AA	721	A2M	N3-C4-N9	3.09	132.18	127.08
36	BB	1280	PSU	C6-N1-C2	-3.09	119.52	122.68
35	BA	1609	PSU	C6-N1-C2	-3.09	119.52	122.68
36	BB	615	PSU	C6-N1-C2	-3.09	119.52	122.68
10	AA	2153	A2M	C5-N7-C8	3.08	107.89	103.51
10	AA	2260	MA6	C5-N7-C8	3.08	107.89	103.51
35	BA	1024	A2M	N3-C4-N9	3.08	132.16	127.08
36	BB	490	PSU	C6-C5-C4	3.08	120.35	118.20
10	AA	2096	A2M	C5-N7-C8	3.08	107.88	103.51
10	AA	1676	OMG	N9-C4-N3	3.08	132.12	125.94
10	AA	1619	PSU	C6-N1-C2	-3.07	119.54	122.68
10	AA	1603	OMG	C2-N1-C6	-3.06	119.51	125.10
36	BB	1062	OMG	C2-N1-C6	-3.06	119.51	125.10
35	BA	743	A2M	C5-N7-C8	3.06	107.86	103.51
36	BB	590	A2M	C5-N7-C8	3.06	107.86	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	61	PSU	C6-N1-C2	-3.06	119.55	122.68
36	BB	1403	PSU	C6-N1-C2	-3.06	119.55	122.68
35	BA	915	OMG	C2-N1-C6	-3.06	119.52	125.10
35	BA	1258	PSU	C6-N1-C2	-3.06	119.56	122.68
36	BB	646	A2M	N3-C4-N9	3.06	132.12	127.08
36	BB	646	A2M	C5-N7-C8	3.05	107.85	103.51
36	BB	95	A2M	C5-N7-C8	3.05	107.84	103.51
36	BB	1210	PSU	C6-N1-C2	-3.05	119.57	122.68
10	AA	1700	OMG	C2-N1-C6	-3.04	119.55	125.10
35	BA	743	A2M	N3-C4-N9	3.04	132.09	127.08
10	AA	1931	OMG	C2-N1-C6	-3.04	119.56	125.10
35	BA	746	A2M	N3-C4-N9	3.04	132.09	127.08
36	BB	71	OMG	C2-N1-C6	-3.04	119.56	125.10
36	BB	545	A2M	C5-N7-C8	3.03	107.82	103.51
35	BA	746	A2M	C5-N7-C8	3.03	107.82	103.51
36	BB	673	OMG	C2-N1-C6	-3.03	119.57	125.10
35	BA	996	A2M	C5-N7-C8	3.03	107.82	103.51
37	BC	167	OMU	O4-C4-C5	-3.03	119.84	125.16
37	BC	43	A2M	N3-C4-N9	3.02	132.05	127.08
10	AA	714	OMU	O4-C4-C5	-3.01	119.86	125.16
36	BB	1245	OMG	C2-N1-C6	-3.01	119.61	125.10
36	BB	609	A2M	N3-C4-N9	3.01	132.04	127.08
10	AA	2070	G7M	C2-N1-C6	-3.01	119.61	125.10
35	BA	1080	PSU	C6-N1-C2	-3.01	119.61	122.68
35	BA	46	OMU	O4-C4-C5	-3.01	119.87	125.16
37	BC	41	A2M	C5-N7-C8	3.00	107.78	103.51
36	BB	1419	PSU	C6-N1-C2	-3.00	119.61	122.68
36	BB	1160	PSU	C6-N1-C2	-3.00	119.61	122.68
37	BC	7	OMU	O4-C4-C5	-3.00	119.89	125.16
35	BA	1620	A2M	C5-N7-C8	3.00	107.77	103.51
10	AA	2278	PSU	C6-N1-C2	-3.00	119.62	122.68
36	BB	609	A2M	C5-N7-C8	3.00	107.77	103.51
10	AA	2227	OMG	C5-C6-N1	3.00	120.80	113.19
10	AA	1676	OMG	C2-N1-C6	-2.99	119.64	125.10
10	AA	2146	PSU	C6-N1-C2	-2.99	119.63	122.68
37	BC	163	A2M	N3-C4-N9	2.99	132.01	127.08
35	BA	1028	OMG	C2-N1-C6	-2.99	119.65	125.10
10	AA	1592	PSU	C6-N1-C2	-2.98	119.63	122.68
37	BC	75	OMG	C2-N1-C6	-2.98	119.66	125.10
36	BB	1388	A2M	C5-N7-C8	2.98	107.74	103.51
35	BA	1267	OMG	C2-N1-C6	-2.97	119.68	125.10
10	AA	2154	OMU	O4-C4-C5	-2.97	119.94	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BC	163	A2M	C5-N7-C8	2.97	107.72	103.51
36	BB	1419	PSU	C6-C5-C4	2.96	120.27	118.20
37	BC	41	A2M	N3-C4-N9	2.96	131.97	127.08
36	BB	1094	OMG	C2-N1-C6	-2.96	119.70	125.10
10	AA	1276	PSU	C6-N1-C2	-2.96	119.66	122.68
36	BB	629	PSU	C6-N1-C2	-2.96	119.66	122.68
10	AA	56	A2M	C5-N7-C8	2.96	107.71	103.51
37	BC	74	PSU	C6-N1-C2	-2.95	119.66	122.68
35	BA	1129	PSU	C6-N1-C2	-2.95	119.66	122.68
35	BA	254	A2M	C5-N7-C8	2.95	107.70	103.51
36	BB	490	PSU	C6-N1-C2	-2.95	119.67	122.68
10	AA	1895	OMG	C2-N1-C6	-2.95	119.72	125.10
36	BB	1247	OMG	C2-N1-C6	-2.95	119.72	125.10
36	BB	1435	OMU	O4-C4-C5	-2.94	119.98	125.16
10	AA	2123	OMU	O4-C4-C5	-2.94	120.00	125.16
36	BB	1403	PSU	C6-C5-C4	2.93	120.25	118.20
36	BB	1269	OMG	C5-C6-N1	2.93	120.63	113.19
35	BA	1621	OMG	C2-N1-C6	-2.92	119.77	125.10
35	BA	1330	OMU	O4-C4-C5	-2.92	120.02	125.16
35	BA	1709	OMG	C2-N1-C6	-2.92	119.77	125.10
36	BB	1229	PSU	C6-N1-C2	-2.92	119.70	122.68
36	BB	1319	PSU	C6-N1-C2	-2.92	119.70	122.68
10	AA	1517	OMG	N9-C4-N3	2.92	131.79	125.94
36	BB	528	PSU	C6-N1-C2	-2.92	119.70	122.68
35	BA	452	PSU	C6-N1-C2	-2.91	119.70	122.68
36	BB	578	OMU	O4-C4-C5	-2.91	120.04	125.16
36	BB	611	PSU	C6-N1-C2	-2.91	119.71	122.68
10	AA	2153	A2M	N3-C4-N9	2.90	131.86	127.08
36	BB	685	OMU	O4-C4-C5	-2.90	120.06	125.16
35	BA	1009	PSU	C6-N1-C2	-2.90	119.72	122.68
35	BA	1166	PSU	C6-N1-C2	-2.90	119.72	122.68
35	BA	915	OMG	C5-C6-N1	2.90	120.54	113.19
36	BB	1093	OMU	O4-C4-C5	-2.89	120.07	125.16
10	AA	505	PSU	C6-N1-C2	-2.89	119.73	122.68
36	BB	71	OMG	C5-C6-N1	2.89	120.52	113.19
36	BB	1429	PSU	C6-N1-C2	-2.88	119.74	122.68
36	BB	659	OMG	C2-N1-C6	-2.88	119.85	125.10
35	BA	762	A2M	C5-N7-C8	2.87	107.59	103.51
35	BA	925	OMG	C2-N1-C6	-2.87	119.86	125.10
10	AA	1674	OMU	O4-C4-C5	-2.87	120.12	125.16
35	BA	1028	OMG	N9-C8-N7	-2.87	107.99	113.39
10	AA	1603	OMG	C5-C6-N1	2.87	120.47	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	2054	OMU	O4-C4-C5	-2.86	120.12	125.16
35	BA	1181	OMU	O4-C4-C5	-2.86	120.13	125.16
36	BB	72	OMG	C2-N1-C6	-2.86	119.89	125.10
36	BB	1319	PSU	C6-C5-C4	2.86	120.19	118.20
36	BB	400	A2M	C5-N7-C8	2.85	107.56	103.51
36	BB	1334	PSU	C6-N1-C2	-2.85	119.77	122.68
36	BB	1409	PSU	C6-N1-C2	-2.85	119.77	122.68
10	AA	1700	OMG	C5-C6-N1	2.85	120.43	113.19
36	BB	673	OMG	C5-C6-N1	2.85	120.42	113.19
10	AA	1899	OMU	O4-C4-C5	-2.84	120.16	125.16
10	AA	1931	OMG	C5-C6-N1	2.83	120.39	113.19
10	AA	1517	OMG	C5-C6-N1	2.83	120.38	113.19
35	BA	1169	PSU	C6-N1-C2	-2.83	119.79	122.68
35	BA	927	A2M	C5-N7-C8	2.82	107.51	103.51
35	BA	1267	OMG	C5-C6-N1	2.81	120.32	113.19
35	BA	925	OMG	C5-C6-N1	2.81	120.31	113.19
36	BB	1062	OMG	C5-C6-N1	2.80	120.30	113.19
36	BB	1245	OMG	C5-C6-N1	2.80	120.30	113.19
35	BA	1248	PSU	C6-N1-C2	-2.80	119.82	122.68
10	AA	1596	B8N	N3-C2-N1	2.79	120.70	116.76
36	BB	552	OMG	C2-N1-C6	-2.79	120.01	125.10
36	BB	1094	OMG	C5-C6-N1	2.79	120.27	113.19
35	BA	916	OMU	O4-C4-C5	-2.79	120.26	125.16
10	AA	2261	MA6	C5-N7-C8	2.78	107.46	103.51
35	BA	762	A2M	N3-C4-N9	2.78	131.66	127.08
35	BA	737	PSU	O2-C2-N1	-2.78	119.73	122.79
35	BA	1709	OMG	C5-C6-N1	2.77	120.22	113.19
10	AA	131	PSU	C6-N1-C2	-2.77	119.85	122.68
10	AA	1676	OMG	C5-C6-N1	2.77	120.22	113.19
36	BB	1229	PSU	C6-C5-C4	2.76	120.13	118.20
36	BB	659	OMG	C5-C6-N1	2.75	120.18	113.19
36	BB	1247	OMG	C5-C6-N1	2.75	120.17	113.19
35	BA	1028	OMG	C5-C6-N1	2.74	120.16	113.19
10	AA	1596	B8N	O4-C4-N3	-2.74	115.32	119.98
35	BA	452	PSU	C6-C5-C4	2.74	120.11	118.20
35	BA	1614	PSU	O2-C2-N1	-2.74	119.78	122.79
10	AA	61	PSU	C6-C5-C4	2.73	120.11	118.20
36	BB	528	PSU	O2-C2-N1	-2.72	119.79	122.79
35	BA	743	A2M	O4'-C1'-N9	2.72	113.42	108.06
37	BC	75	OMG	C5-C6-N1	2.72	120.10	113.19
10	AA	57	OMU	O4-C4-C5	-2.72	120.38	125.16
10	AA	1895	OMG	C5-C6-N1	2.72	120.08	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	72	OMG	C5-C6-N1	2.71	120.08	113.19
36	BB	552	OMG	C5-C6-N1	2.71	120.08	113.19
35	BA	1621	OMG	C5-C6-N1	2.71	120.07	113.19
35	BA	742	1MA	N9-C8-N7	-2.71	108.29	113.39
10	AA	131	PSU	C6-C5-C4	2.71	120.09	118.20
35	BA	1605	OMG	C5-C6-N1	2.69	120.03	113.19
36	BB	1062	OMG	N9-C4-N3	2.69	131.35	125.94
10	AA	1931	OMG	N9-C4-N3	2.69	131.35	125.94
10	AA	1603	OMG	O6-C6-C5	-2.69	119.46	126.60
36	BB	1076	PSU	O2-C2-N1	-2.69	119.83	122.79
35	BA	1605	OMG	N9-C4-N3	2.69	131.33	125.94
36	BB	490	PSU	O2-C2-N1	-2.68	119.84	122.79
37	BC	75	OMG	N9-C4-N3	2.67	131.31	125.94
35	BA	1448	OMU	O4-C4-C5	-2.67	120.46	125.16
36	BB	1269	OMG	N9-C4-N3	2.67	131.30	125.94
36	BB	1419	PSU	O2-C2-N1	-2.66	119.86	122.79
35	BA	915	OMG	N9-C4-N3	2.66	131.27	125.94
35	BA	1267	OMG	O6-C6-C5	-2.65	119.58	126.60
35	BA	1129	PSU	O2-C2-N1	-2.64	119.88	122.79
36	BB	1403	PSU	O2-C2-N1	-2.64	119.89	122.79
36	BB	1280	PSU	O2-C2-N1	-2.63	119.89	122.79
35	BA	737	PSU	C6-N1-C2	-2.63	119.99	122.68
10	AA	2153	A2M	C4-N9-C8	2.63	108.58	105.73
35	BA	1169	PSU	C6-C5-C4	2.62	120.03	118.20
10	AA	2227	OMG	O6-C6-C5	-2.62	119.64	126.60
10	AA	1931	OMG	O6-C6-C5	-2.61	119.67	126.60
35	BA	1080	PSU	O2-C2-N1	-2.61	119.92	122.79
36	BB	1247	OMG	N9-C4-N3	2.61	131.18	125.94
36	BB	1280	PSU	C6-C5-C4	2.61	120.02	118.20
10	AA	1676	OMG	O6-C6-C5	-2.60	119.71	126.60
36	BB	518	PSU	O2-C2-N1	-2.59	119.94	122.79
36	BB	71	OMG	O6-C6-C5	-2.59	119.73	126.60
36	BB	673	OMG	N9-C4-N3	2.59	131.14	125.94
36	BB	1319	PSU	O2-C2-N1	-2.59	119.94	122.79
10	AA	1276	PSU	C6-C5-C4	2.59	120.01	118.20
10	AA	2045	PSU	O2-C2-N1	-2.58	119.95	122.79
36	BB	615	PSU	O2-C2-N1	-2.58	119.95	122.79
36	BB	72	OMG	N9-C4-N3	2.58	131.12	125.94
35	BA	916	OMU	O2-C2-N1	-2.57	119.36	122.79
36	BB	1062	OMG	O6-C6-C5	-2.57	119.77	126.60
10	AA	61	PSU	O2-C2-N1	-2.57	119.96	122.79
36	BB	629	PSU	O2-C2-N1	-2.56	119.97	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	2146	PSU	O2-C2-N1	-2.56	119.97	122.79
10	AA	1603	OMG	N9-C4-N3	2.56	131.09	125.94
10	AA	2261	MA6	N3-C4-N9	2.56	131.30	127.08
37	BC	75	OMG	O6-C6-C5	-2.56	119.81	126.60
36	BB	1334	PSU	O2-C2-N1	-2.56	119.98	122.79
10	AA	1895	OMG	N9-C4-N3	2.55	131.07	125.94
10	AA	721	A2M	C3'-C2'-C1'	2.55	107.69	102.89
10	AA	2154	OMU	O2-C2-N1	-2.55	119.39	122.79
36	BB	1245	OMG	N9-C4-N3	2.54	131.03	125.94
35	BA	1086	PSU	O2-C2-N1	-2.53	120.00	122.79
37	BC	74	PSU	C6-C5-C4	2.53	119.97	118.20
10	AA	1700	OMG	O6-C6-C5	-2.52	119.91	126.60
36	BB	1269	OMG	O6-C6-C5	-2.52	119.91	126.60
36	BB	1210	PSU	O2-C2-N1	-2.51	120.03	122.79
36	BB	1160	PSU	O2-C2-N1	-2.51	120.03	122.79
36	BB	1247	OMG	O6-C6-C5	-2.50	119.97	126.60
35	BA	1709	OMG	O6-C6-C5	-2.50	119.97	126.60
36	BB	552	OMG	N9-C4-N3	2.47	130.90	125.94
35	BA	1614	PSU	C6-C5-C4	2.47	119.92	118.20
36	BB	1245	OMG	O6-C6-C5	-2.47	120.06	126.60
10	AA	2278	PSU	O2-C2-N1	-2.47	120.08	122.79
10	AA	131	PSU	O2-C2-N1	-2.46	120.08	122.79
36	BB	644	PSU	O2-C2-N1	-2.46	120.08	122.79
35	BA	1028	OMG	O6-C6-C5	-2.46	120.08	126.60
35	BA	1605	OMG	O6-C6-C5	-2.46	120.08	126.60
35	BA	915	OMG	O6-C6-C5	-2.45	120.10	126.60
10	AA	1895	OMG	O6-C6-C5	-2.45	120.11	126.60
35	BA	1609	PSU	O2-C2-N1	-2.45	120.10	122.79
35	BA	452	PSU	O2-C2-N1	-2.45	120.10	122.79
10	AA	2054	OMU	O2-C2-N1	-2.45	119.54	122.79
36	BB	1409	PSU	O2-C2-N1	-2.44	120.10	122.79
10	AA	1592	PSU	C6-C5-C4	2.44	119.91	118.20
36	BB	528	PSU	C6-C5-C4	2.44	119.91	118.20
35	BA	1009	PSU	O2-C2-N1	-2.44	120.11	122.79
35	BA	742	1MA	C5-C4-N9	2.43	110.05	105.63
10	AA	1907	PSU	O2-C2-N1	-2.43	120.11	122.79
35	BA	1248	PSU	O2-C2-N1	-2.43	120.11	122.79
10	AA	1517	OMG	O6-C6-C5	-2.43	120.15	126.60
36	BB	552	OMG	O6-C6-C5	-2.42	120.17	126.60
10	AA	2260	MA6	C4-N9-C8	2.42	108.36	105.73
10	AA	1592	PSU	O2-C2-N1	-2.42	120.13	122.79
35	BA	1258	PSU	C6-C5-C4	2.42	119.89	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	659	OMG	O6-C6-C5	-2.42	120.19	126.60
35	BA	1621	OMG	O6-C6-C5	-2.42	120.19	126.60
10	AA	2261	MA6	C4-N9-C8	2.41	108.34	105.73
36	BB	1334	PSU	C6-C5-C4	2.41	119.88	118.20
36	BB	1094	OMG	O6-C6-C5	-2.41	120.21	126.60
10	AA	1619	PSU	O2-C2-N1	-2.41	120.14	122.79
36	BB	542	5MC	CM5-C5-C6	-2.40	119.64	122.85
10	AA	125	A2M	C6-C5-C4	2.39	120.40	117.18
35	BA	1166	PSU	O2-C2-N1	-2.39	120.17	122.79
35	BA	1248	PSU	C6-C5-C4	2.38	119.86	118.20
36	BB	673	OMG	C8-N7-C5	2.37	108.54	104.24
35	BA	1267	OMG	N2-C2-N1	2.37	121.76	116.71
36	BB	1160	PSU	C6-C5-C4	2.37	119.85	118.20
35	BA	1028	OMG	N9-C4-N3	2.37	130.69	125.94
35	BA	1080	PSU	C6-C5-C4	2.36	119.85	118.20
36	BB	1094	OMG	C8-N7-C5	2.36	108.52	104.24
35	BA	925	OMG	O6-C6-C5	-2.36	120.33	126.60
35	BA	1267	OMG	C2'-C1'-N9	-2.36	109.65	114.22
10	AA	1700	OMG	C8-N7-C5	2.35	108.50	104.24
35	BA	737	PSU	C6-C5-C4	2.35	119.84	118.20
10	AA	1710	PSU	C6-N1-C2	-2.35	120.28	122.68
36	BB	545	A2M	C4'-O4'-C1'	-2.34	104.30	109.47
35	BA	1267	OMG	C8-N7-C5	2.34	108.48	104.24
36	BB	673	OMG	O6-C6-C5	-2.34	120.39	126.60
35	BA	1181	OMU	O2-C2-N1	-2.34	119.68	122.79
35	BA	743	A2M	C5-C4-N9	2.33	108.50	105.78
36	BB	644	PSU	C6-C5-C4	2.33	119.83	118.20
36	BB	1245	OMG	C8-N7-C5	2.33	108.46	104.24
36	BB	545	A2M	O4'-C1'-C2'	-2.33	102.48	106.57
35	BA	743	A2M	C4-C5-N7	-2.33	107.78	110.62
36	BB	95	A2M	C6-C5-C4	2.33	120.32	117.18
36	BB	1403	PSU	O4'-C1'-C2'	2.33	108.42	105.14
35	BA	1621	OMG	N9-C4-N3	2.32	130.61	125.94
35	BA	1169	PSU	O2-C2-N1	-2.32	120.23	122.79
35	BA	1258	PSU	O2-C2-N1	-2.32	120.24	122.79
10	AA	2153	A2M	C2'-C1'-N9	-2.31	109.64	113.53
35	BA	1024	A2M	C4-C5-N7	-2.30	107.81	110.62
35	BA	915	OMG	C8-N7-C5	2.30	108.41	104.24
36	BB	72	OMG	O6-C6-C5	-2.30	120.50	126.60
36	BB	1210	PSU	C6-C5-C4	2.30	119.81	118.20
36	BB	400	A2M	C6-C5-C4	2.29	120.27	117.18
35	BA	742	1MA	C4-C5-N7	-2.29	107.09	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	1201	A2M	C6-C5-C4	2.29	120.26	117.18
36	BB	73	OMU	O2-C2-N1	-2.29	119.74	122.79
35	BA	925	OMG	N9-C4-N3	2.28	130.51	125.94
36	BB	1280	PSU	O4'-C1'-C2'	2.28	108.35	105.14
37	BC	74	PSU	O2-C2-N1	-2.28	120.28	122.79
35	BA	254	A2M	C6-C5-C4	2.27	120.23	117.18
36	BB	659	OMG	C8-N7-C5	2.27	108.35	104.24
10	AA	1596	B8N	O4'-C1'-C2'	2.26	108.33	105.14
36	BB	1229	PSU	O2-C2-N1	-2.26	120.30	122.79
36	BB	1419	PSU	O4'-C1'-C2'	2.26	108.33	105.14
35	BA	1605	OMG	C8-N7-C5	2.25	108.32	104.24
36	BB	1062	OMG	C8-N7-C5	2.25	108.30	104.24
10	AA	1700	OMG	N2-C2-N1	2.24	121.48	116.71
35	BA	1709	OMG	C8-N7-C5	2.23	108.28	104.24
36	BB	1434	PSU	O2-C2-N1	-2.23	120.34	122.79
35	BA	925	OMG	C8-N7-C5	2.23	108.28	104.24
10	AA	1899	OMU	O2-C2-N1	-2.22	119.84	122.79
36	BB	1094	OMG	N2-C2-N1	2.22	121.44	116.71
37	BC	167	OMU	O2-C2-N1	-2.22	119.84	122.79
36	BB	1319	PSU	O4'-C1'-C2'	2.22	108.27	105.14
35	BA	46	OMU	O2-C2-N1	-2.22	119.84	122.79
35	BA	1709	OMG	N9-C4-N3	2.22	130.39	125.94
35	BA	1248	PSU	O4'-C1'-C2'	2.21	108.27	105.14
10	AA	1895	OMG	C8-N7-C5	2.21	108.25	104.24
36	BB	71	OMG	N9-C4-N3	2.21	130.38	125.94
35	BA	1166	PSU	C6-C5-C4	2.21	119.74	118.20
10	AA	2096	A2M	C4-C5-N7	-2.21	107.93	110.62
10	AA	1931	OMG	C8-N7-C5	2.21	108.24	104.24
35	BA	1621	OMG	C8-N7-C5	2.21	108.24	104.24
36	BB	622	A2M	C4-C5-N7	-2.21	107.93	110.62
35	BA	254	A2M	C5-C4-N9	2.20	108.35	105.78
10	AA	1710	PSU	C5-C4-N3	2.20	121.55	116.58
10	AA	714	OMU	O2-C2-N1	-2.19	119.87	122.79
10	AA	1603	OMG	C8-N7-C5	2.19	108.20	104.24
36	BB	1247	OMG	C8-N7-C5	2.19	108.20	104.24
36	BB	95	A2M	C4-C5-N7	-2.18	107.97	110.62
35	BA	1742	OMU	O2-C2-N1	-2.18	119.89	122.79
10	AA	2153	A2M	O4'-C1'-N9	2.17	112.34	108.06
36	BB	609	A2M	C4-C5-N7	-2.17	107.97	110.62
36	BB	1429	PSU	O2-C2-N1	-2.17	120.41	122.79
10	AA	2278	PSU	C6-C5-C4	2.17	119.71	118.20
10	AA	721	A2M	C4-C5-N7	-2.17	107.98	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	71	OMG	N2-C2-N1	2.16	121.32	116.71
10	AA	2070	G7M	N9-C8-N7	-2.16	106.86	112.21
36	BB	72	OMG	C8-N7-C5	2.16	108.15	104.24
37	BC	7	OMU	O2-C2-N1	-2.16	119.91	122.79
36	BB	1201	A2M	C4-C5-N7	-2.16	107.99	110.62
36	BB	545	A2M	C6-C5-C4	2.16	120.08	117.18
36	BB	71	OMG	C8-N7-C5	2.16	108.14	104.24
37	BC	75	OMG	C8-N7-C5	2.16	108.14	104.24
36	BB	609	A2M	C6-C5-C4	2.16	120.08	117.18
10	AA	1517	OMG	C8-N7-C5	2.15	108.13	104.24
10	AA	1276	PSU	O2-C2-N1	-2.15	120.43	122.79
10	AA	1676	OMG	C8-N7-C5	2.15	108.13	104.24
36	BB	1093	OMU	O2-C2-N1	-2.15	119.93	122.79
35	BA	743	A2M	C6-C5-C4	2.15	120.07	117.18
10	AA	125	A2M	C4-C5-N7	-2.14	108.01	110.62
35	BA	1129	PSU	C6-C5-C4	2.14	119.69	118.20
10	AA	505	PSU	O2-C2-N1	-2.14	120.44	122.79
37	BC	41	A2M	C4-C5-N7	-2.14	108.02	110.62
36	BB	611	PSU	O2-C2-N1	-2.14	120.44	122.79
10	AA	57	OMU	O2-C2-N1	-2.14	119.95	122.79
36	BB	1269	OMG	C8-N7-C5	2.13	108.10	104.24
36	BB	1434	PSU	C6-C5-C4	2.13	119.69	118.20
36	BB	659	OMG	N2-C2-N1	2.13	121.25	116.71
35	BA	762	A2M	C4-C5-N7	-2.13	108.03	110.62
10	AA	2096	A2M	C6-C5-C4	2.13	120.04	117.18
37	BC	41	A2M	C5-C4-N9	2.12	108.25	105.78
36	BB	609	A2M	C5-C4-N9	2.12	108.25	105.78
35	BA	254	A2M	C4-C5-N7	-2.12	108.04	110.62
37	BC	43	A2M	C4-C5-N7	-2.11	108.05	110.62
36	BB	659	OMG	C2'-C1'-N9	-2.10	110.14	114.22
36	BB	552	OMG	C8-N7-C5	2.10	108.05	104.24
35	BA	762	A2M	C5-C4-N9	2.10	108.23	105.78
10	AA	2260	MA6	C4-C5-N7	-2.10	108.06	110.62
35	BA	746	A2M	C4-C5-N7	-2.10	108.06	110.62
36	BB	622	A2M	C6-C5-C4	2.10	120.00	117.18
10	AA	2123	OMU	O2-C2-N1	-2.10	120.00	122.79
10	AA	2227	OMG	N9-C4-N3	2.09	130.14	125.94
35	BA	1665	A2M	C4-C5-N7	-2.09	108.07	110.62
35	BA	1709	OMG	N2-C2-N1	2.09	121.17	116.71
10	AA	721	A2M	C5-C4-N9	2.09	108.21	105.78
10	AA	1700	OMG	N9-C4-N3	2.09	130.13	125.94
10	AA	1674	OMU	O2-C2-N1	-2.09	120.01	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	646	A2M	C4-C5-N7	-2.09	108.08	110.62
10	AA	2096	A2M	C5-C4-N9	2.09	108.21	105.78
37	BC	163	A2M	C4-C5-N7	-2.09	108.08	110.62
36	BB	1094	OMG	N9-C4-N3	2.09	130.13	125.94
10	AA	2227	OMG	C8-N7-C5	2.08	108.01	104.24
36	BB	71	OMG	C2'-C1'-N9	-2.08	110.18	114.22
36	BB	1388	A2M	C3'-C2'-C1'	2.08	106.80	102.89
36	BB	590	A2M	C6-C5-C4	2.08	119.98	117.18
35	BA	927	A2M	C4'-O4'-C1'	-2.08	104.89	109.47
36	BB	685	OMU	O2-C2-N1	-2.08	120.03	122.79
36	BB	1201	A2M	C2'-C1'-N9	-2.07	110.04	113.53
35	BA	1267	OMG	N9-C4-N3	2.07	130.10	125.94
35	BA	1620	A2M	C6-C5-C4	2.07	119.97	117.18
36	BB	95	A2M	C5-C4-N9	2.07	108.19	105.78
36	BB	590	A2M	C4-C5-N7	-2.07	108.10	110.62
10	AA	1907	PSU	C6-C5-C4	2.07	119.64	118.20
36	BB	615	PSU	C6-C5-C4	2.07	119.64	118.20
36	BB	1429	PSU	C6-C5-C4	2.07	119.64	118.20
35	BA	1080	PSU	O4'-C1'-C2'	2.06	108.06	105.14
35	BA	996	A2M	C6-C5-C4	2.06	119.96	117.18
35	BA	927	A2M	C6-C5-C4	2.06	119.95	117.18
36	BB	1388	A2M	C6-C5-C4	2.06	119.95	117.18
36	BB	545	A2M	C4-N9-C8	2.06	107.96	105.73
35	BA	996	A2M	C4-C5-N7	-2.05	108.12	110.62
35	BA	1086	PSU	C6-C5-C4	2.05	119.63	118.20
36	BB	1094	OMG	C4-C5-N7	-2.05	107.48	110.72
35	BA	1665	A2M	C6-C5-C4	2.05	119.93	117.18
37	BC	163	A2M	C5-C4-N9	2.05	108.16	105.78
36	BB	629	PSU	C6-C5-C4	2.05	119.63	118.20
35	BA	1609	PSU	C6-C5-C4	2.04	119.63	118.20
35	BA	1024	A2M	C5-C4-N9	2.04	108.16	105.78
36	BB	659	OMG	N9-C4-N3	2.04	130.03	125.94
10	AA	56	A2M	C4-C5-N7	-2.03	108.14	110.62
36	BB	1409	PSU	C6-C5-C4	2.03	119.62	118.20
36	BB	1201	A2M	C4-N9-C8	2.03	107.92	105.73
35	BA	1621	OMG	N2-C2-N1	2.02	121.01	116.71
37	BC	163	A2M	C6-C5-C4	2.02	119.89	117.18
36	BB	1388	A2M	C4-C5-N7	-2.01	108.17	110.62
35	BA	737	PSU	O4'-C1'-C2'	2.01	107.98	105.14
10	AA	2070	G7M	C5-C4-N9	2.01	110.30	105.89
35	BA	1608	OMC	O2-C2-N3	-2.00	119.08	122.33

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	AA	56	A2M	C1'-C2'-O2'-CM'
10	AA	57	OMU	C1'-C2'-O2'-CM2
10	AA	721	A2M	C3'-C4'-C5'-O5'
10	AA	1619	PSU	C2'-C1'-C5-C4
10	AA	1676	OMG	C1'-C2'-O2'-CM2
10	AA	1710	PSU	O4'-C1'-C5-C4
10	AA	1710	PSU	O4'-C1'-C5-C6
10	AA	2054	OMU	O4'-C4'-C5'-O5'
10	AA	2096	A2M	C1'-C2'-O2'-CM'
10	AA	2134	OMC	C3'-C4'-C5'-O5'
10	AA	2153	A2M	C1'-C2'-O2'-CM'
10	AA	2154	OMU	C1'-C2'-O2'-CM2
10	AA	2278	PSU	O4'-C1'-C5-C6
35	BA	762	A2M	C1'-C2'-O2'-CM'
35	BA	1024	A2M	C1'-C2'-O2'-CM'
35	BA	1080	PSU	C2'-C1'-C5-C4
35	BA	1080	PSU	O4'-C1'-C5-C4
35	BA	1080	PSU	O4'-C1'-C5-C6
35	BA	1330	OMU	O4'-C1'-N1-C2
35	BA	1330	OMU	O4'-C1'-N1-C6
35	BA	1330	OMU	C1'-C2'-O2'-CM2
36	BB	552	OMG	O4'-C4'-C5'-O5'
36	BB	552	OMG	C3'-C4'-C5'-O5'
36	BB	578	OMU	C1'-C2'-O2'-CM2
36	BB	629	PSU	C3'-C4'-C5'-O5'
36	BB	629	PSU	O4'-C4'-C5'-O5'
36	BB	646	A2M	C1'-C2'-O2'-CM'
36	BB	685	OMU	C1'-C2'-O2'-CM2
36	BB	1062	OMG	O4'-C4'-C5'-O5'
36	BB	1062	OMG	C3'-C4'-C5'-O5'
36	BB	1400	A2M	C1'-C2'-O2'-CM'
37	BC	7	OMU	C1'-C2'-O2'-CM2
37	BC	163	A2M	C1'-C2'-O2'-CM'
10	AA	721	A2M	O4'-C4'-C5'-O5'
10	AA	1603	OMG	C3'-C4'-C5'-O5'
10	AA	1619	PSU	C3'-C4'-C5'-O5'
10	AA	2045	PSU	C3'-C4'-C5'-O5'
10	AA	2045	PSU	O4'-C4'-C5'-O5'
10	AA	2054	OMU	C3'-C4'-C5'-O5'
10	AA	2134	OMC	O4'-C4'-C5'-O5'
35	BA	1258	PSU	C3'-C4'-C5'-O5'
36	BB	518	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
36	BB	578	OMU	C3'-C4'-C5'-O5'
36	BB	578	OMU	O4'-C4'-C5'-O5'
36	BB	1434	PSU	O4'-C4'-C5'-O5'
10	AA	125	A2M	O4'-C4'-C5'-O5'
10	AA	1603	OMG	O4'-C4'-C5'-O5'
10	AA	1619	PSU	O4'-C4'-C5'-O5'
10	AA	1931	OMG	C3'-C4'-C5'-O5'
35	BA	1614	PSU	C3'-C4'-C5'-O5'
36	BB	1434	PSU	C3'-C4'-C5'-O5'
36	BB	1324	5MC	C2'-C1'-N1-C6
35	BA	1448	OMU	C3'-C4'-C5'-O5'
10	AA	1931	OMG	O4'-C4'-C5'-O5'
35	BA	1258	PSU	O4'-C4'-C5'-O5'
35	BA	1448	OMU	O4'-C4'-C5'-O5'
35	BA	1614	PSU	O4'-C4'-C5'-O5'
36	BB	518	PSU	O4'-C4'-C5'-O5'
36	BB	1201	A2M	C3'-C4'-C5'-O5'
10	AA	1531	OMG	C3'-C4'-C5'-O5'
10	AA	36	OMU	C2'-C1'-N1-C6
36	BB	545	A2M	O4'-C4'-C5'-O5'
35	BA	1006	OMC	C1'-C2'-O2'-CM2
36	BB	588	A2M	C2'-C1'-N9-C8
35	BA	1608	OMC	C3'-C2'-O2'-CM2
36	BB	1324	5MC	O4'-C1'-N1-C6
35	BA	1605	OMG	C3'-C4'-C5'-O5'
36	BB	1324	5MC	C2'-C1'-N1-C2
35	BA	746	A2M	C4'-C5'-O5'-P
36	BB	1324	5MC	O4'-C1'-N1-C2
36	BB	578	OMU	C4'-C5'-O5'-P
36	BB	1264	OMC	C4'-C5'-O5'-P
10	AA	36	OMU	O4'-C1'-N1-C6
35	BA	1329	OMC	C3'-C2'-O2'-CM2
35	BA	1605	OMG	C3'-C2'-O2'-CM2
10	AA	1619	PSU	C4'-C5'-O5'-P
35	BA	1621	OMG	C4'-C5'-O5'-P
35	BA	1608	OMC	O4'-C4'-C5'-O5'
36	BB	545	A2M	C3'-C4'-C5'-O5'
10	AA	721	A2M	C2'-C1'-N9-C8
10	AA	1596	B8N	O4'-C1'-C5-C4
10	AA	1612	PSU	O4'-C1'-C5-C4
10	AA	1907	PSU	C3'-C4'-C5'-O5'
36	BB	588	A2M	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
10	AA	1592	PSU	O4'-C4'-C5'-O5'
35	BA	1329	OMC	C3'-C4'-C5'-O5'
10	AA	36	OMU	O4'-C1'-N1-C2
35	BA	1608	OMC	C2'-C1'-N1-C2
10	AA	125	A2M	C3'-C4'-C5'-O5'
36	BB	542	5MC	O4'-C4'-C5'-O5'
36	BB	659	OMG	O4'-C4'-C5'-O5'
36	BB	73	OMU	C1'-C2'-O2'-CM2
36	BB	95	A2M	C1'-C2'-O2'-CM'
10	AA	1531	OMG	O4'-C4'-C5'-O5'
35	BA	743	A2M	O4'-C4'-C5'-O5'
35	BA	1329	OMC	O4'-C4'-C5'-O5'
10	AA	36	OMU	C2'-C1'-N1-C2
10	AA	36	OMU	O4'-C4'-C5'-O5'
10	AA	1899	OMU	O4'-C4'-C5'-O5'
35	BA	1608	OMC	C3'-C4'-C5'-O5'
10	AA	1895	OMG	C4'-C5'-O5'-P
36	BB	588	A2M	C2'-C1'-N9-C4

There are no ring outliers.

39 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	AA	2261	MA6	1	0
10	AA	1676	OMG	1	0
10	AA	2153	A2M	1	0
10	AA	2045	PSU	2	0
36	BB	1245	OMG	1	0
36	BB	646	A2M	1	0
35	BA	1620	A2M	1	0
36	BB	545	A2M	1	0
36	BB	1375	OMU	1	0
36	BB	644	PSU	1	0
35	BA	1665	A2M	1	0
35	BA	916	OMU	1	0
35	BA	254	A2M	2	0
36	BB	685	OMU	1	0
35	BA	915	OMG	1	0
37	BC	7	OMU	2	0
36	BB	1429	PSU	1	0
10	AA	2123	OMU	1	0
36	BB	578	OMU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	BA	762	A2M	3	0
36	BB	95	A2M	1	0
10	AA	2096	A2M	2	0
10	AA	2260	MA6	1	0
10	AA	57	OMU	1	0
36	BB	609	A2M	2	0
10	AA	2154	OMU	1	0
10	AA	2070	G7M	1	0
35	BA	1181	OMU	1	0
36	BB	400	A2M	1	0
37	BC	163	A2M	1	0
35	BA	743	A2M	3	0
35	BA	747	OMC	2	0
10	AA	1674	OMU	1	0
35	BA	746	A2M	1	0
36	BB	1400	A2M	1	0
10	AA	56	A2M	1	0
35	BA	1024	A2M	1	0
10	AA	46	OMC	1	0
35	BA	1330	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 307 ligands modelled in this entry, 307 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 ⓘ

There are no chain breaks in this entry.

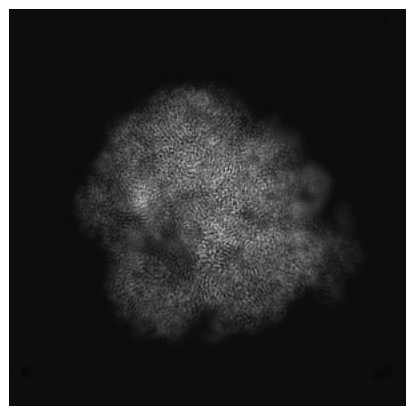
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55348. These allow visual inspection of the internal detail of the map and identification of artifacts.

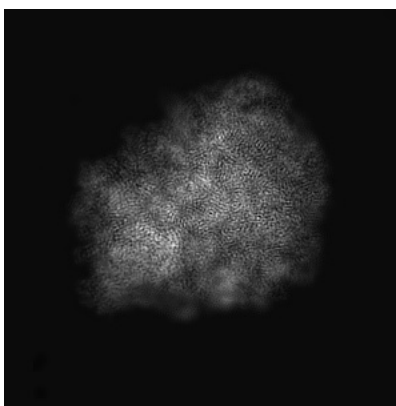
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

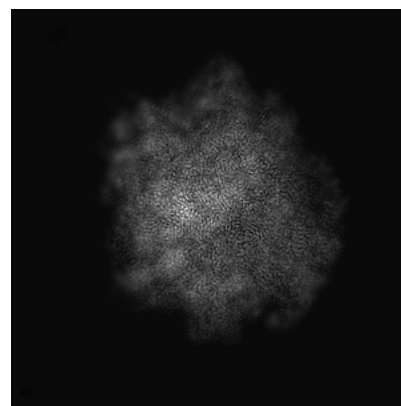
6.1.1 Primary map



X

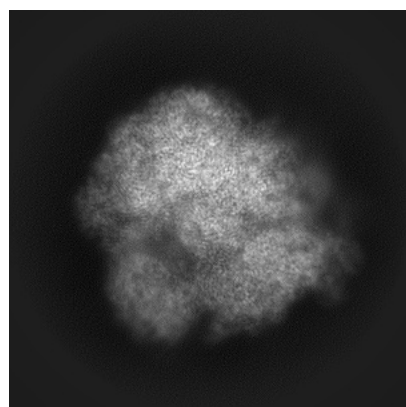


Y

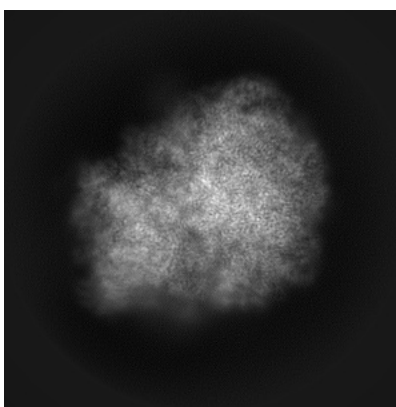


Z

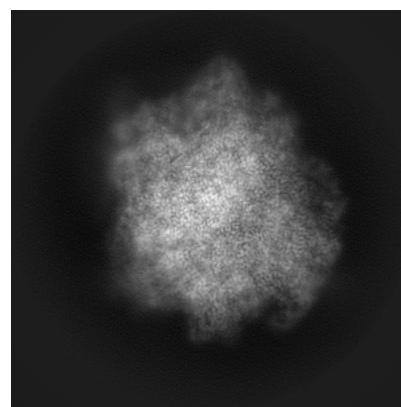
6.1.2 Raw map



X



Y

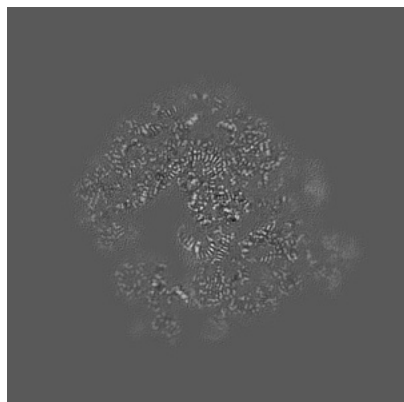


Z

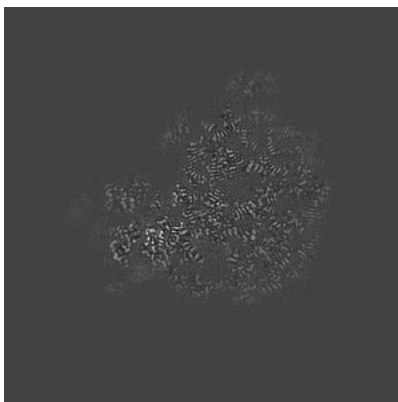
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

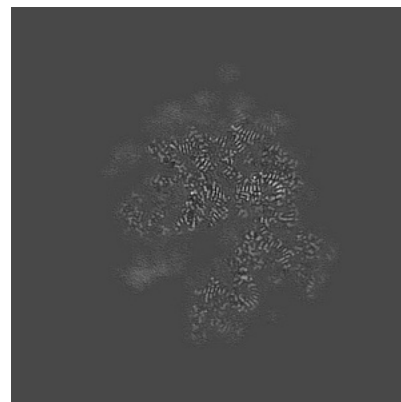
6.2.1 Primary map



X Index: 240

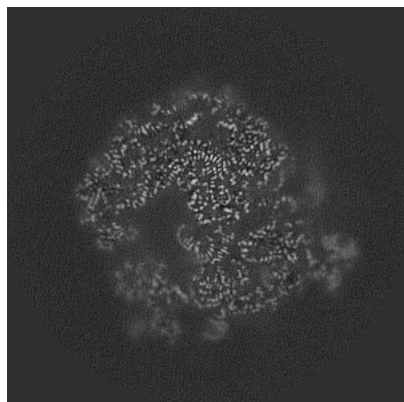


Y Index: 240

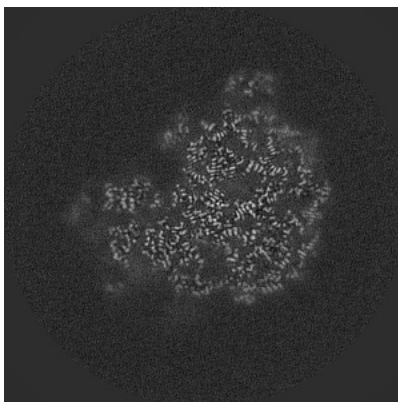


Z Index: 240

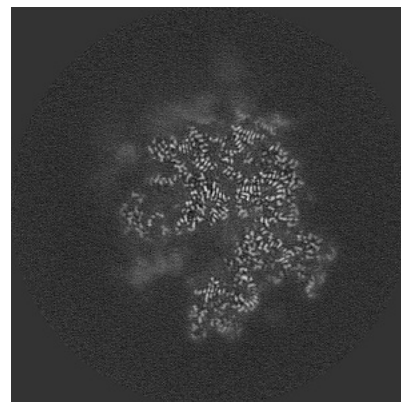
6.2.2 Raw map



X Index: 240



Y Index: 240

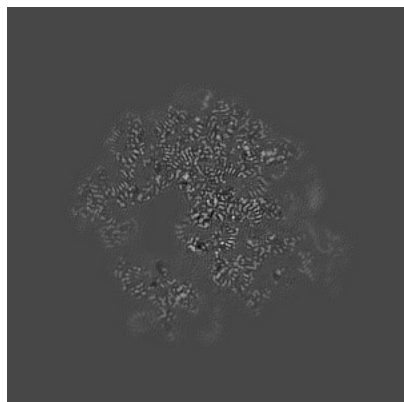


Z Index: 240

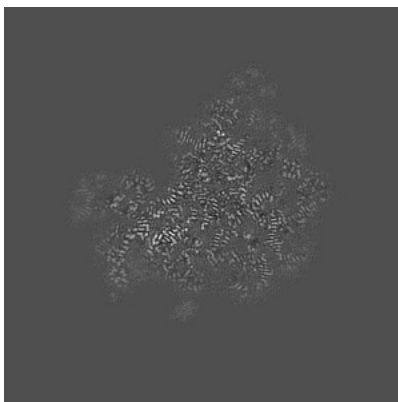
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

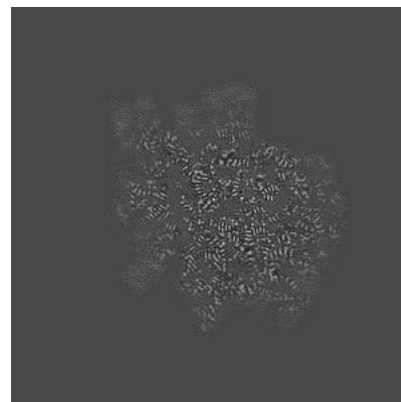
6.3.1 Primary map



X Index: 228

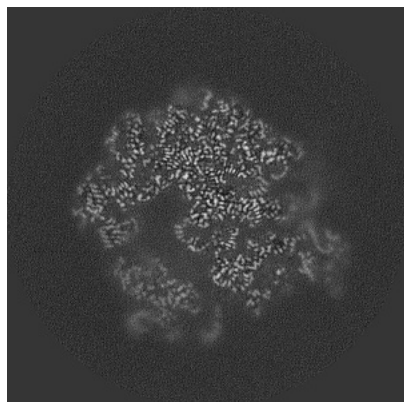


Y Index: 251

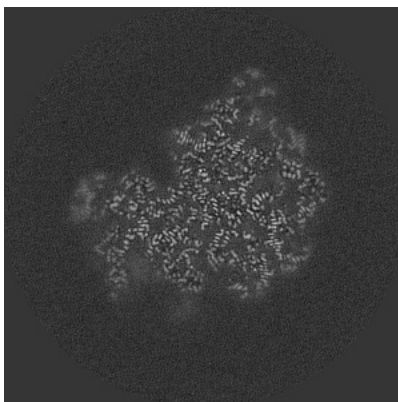


Z Index: 279

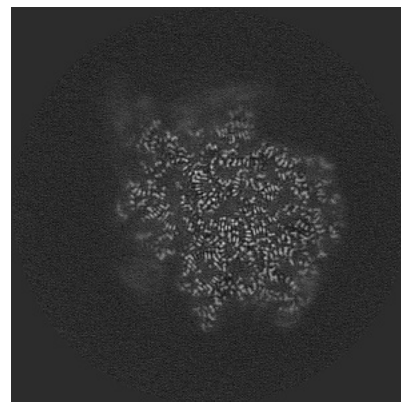
6.3.2 Raw map



X Index: 228



Y Index: 251

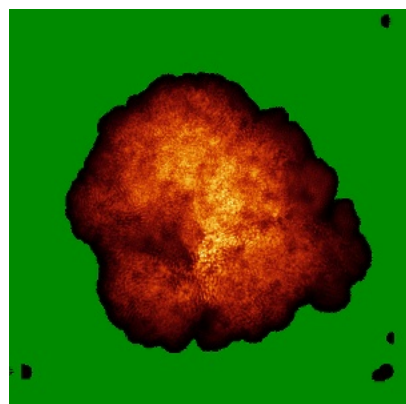


Z Index: 279

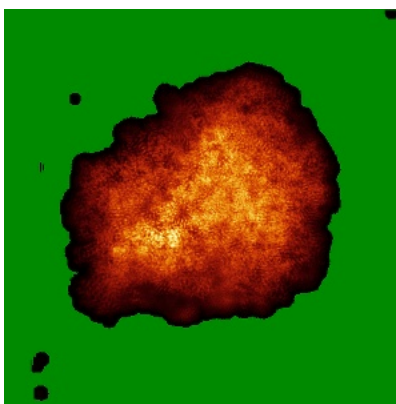
The images above show the largest variance slices of the map in three orthogonal directions.

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

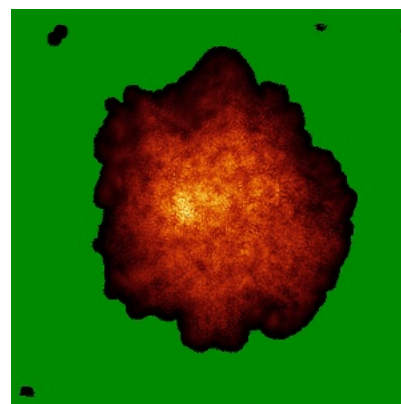
6.4.1 Primary map



X

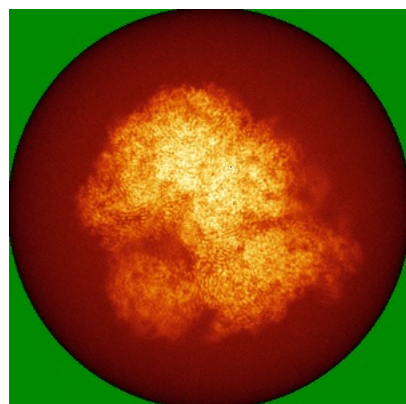


Y

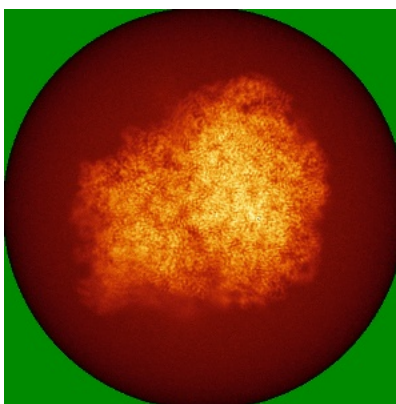


Z

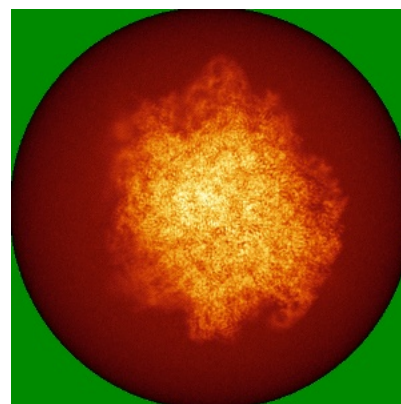
6.4.2 Raw map



X



Y

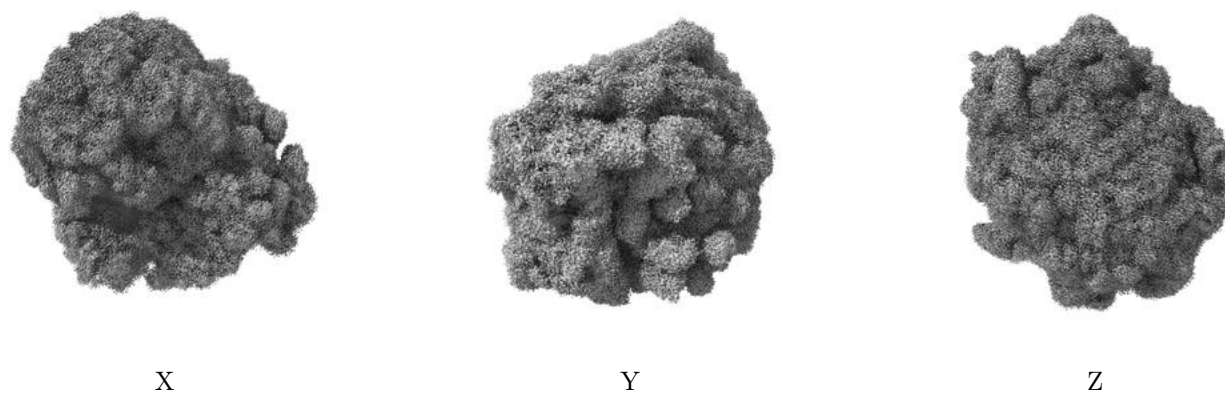


Z

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.

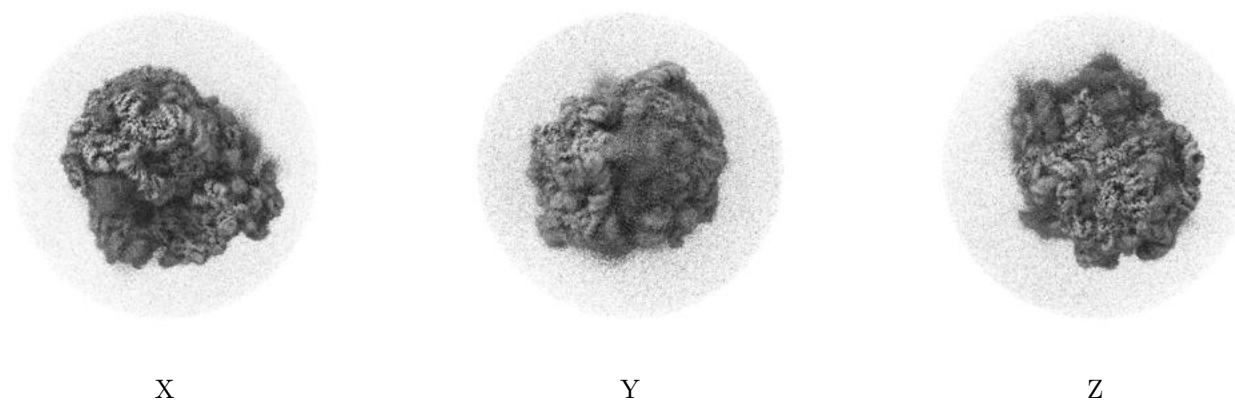
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

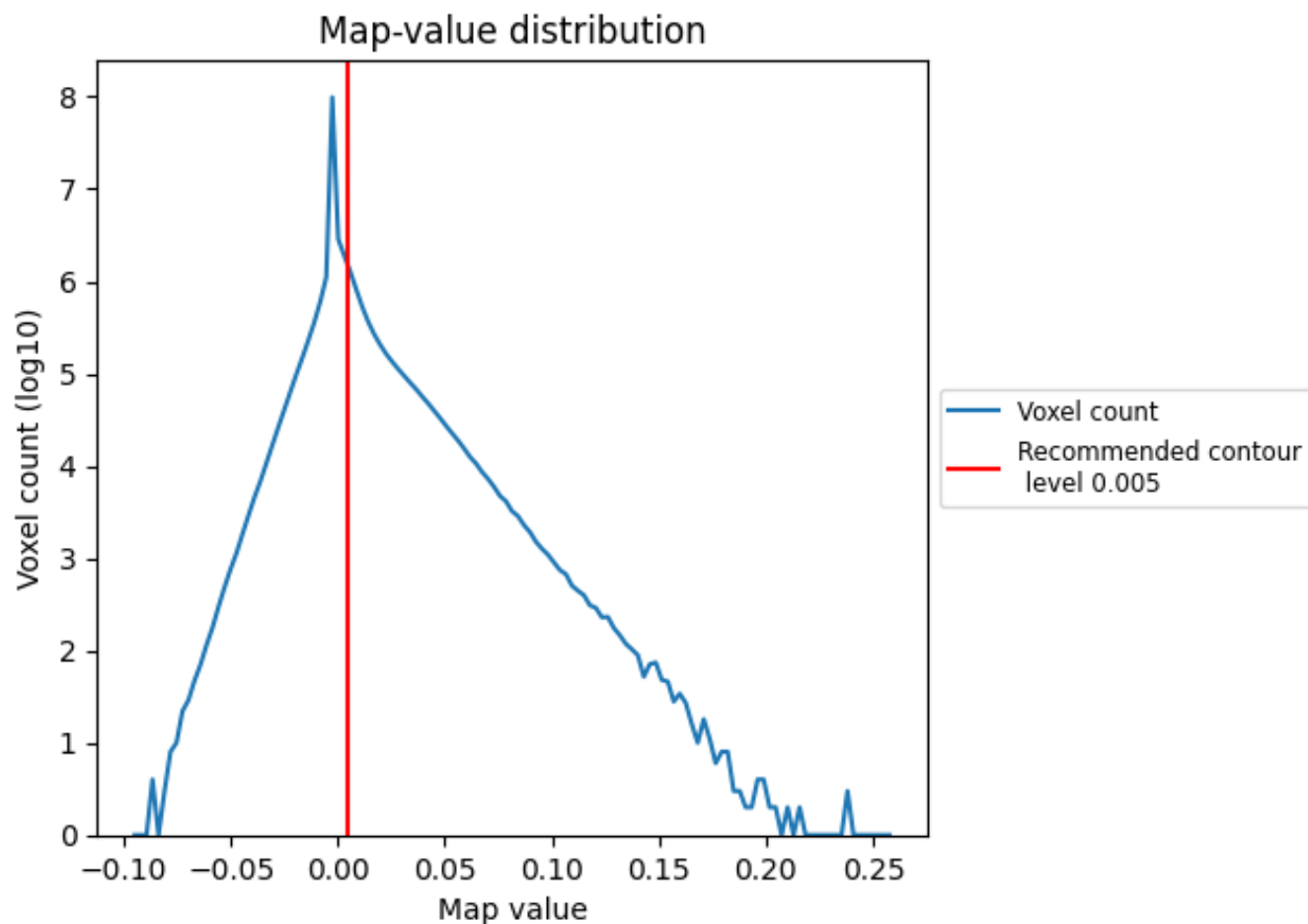
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

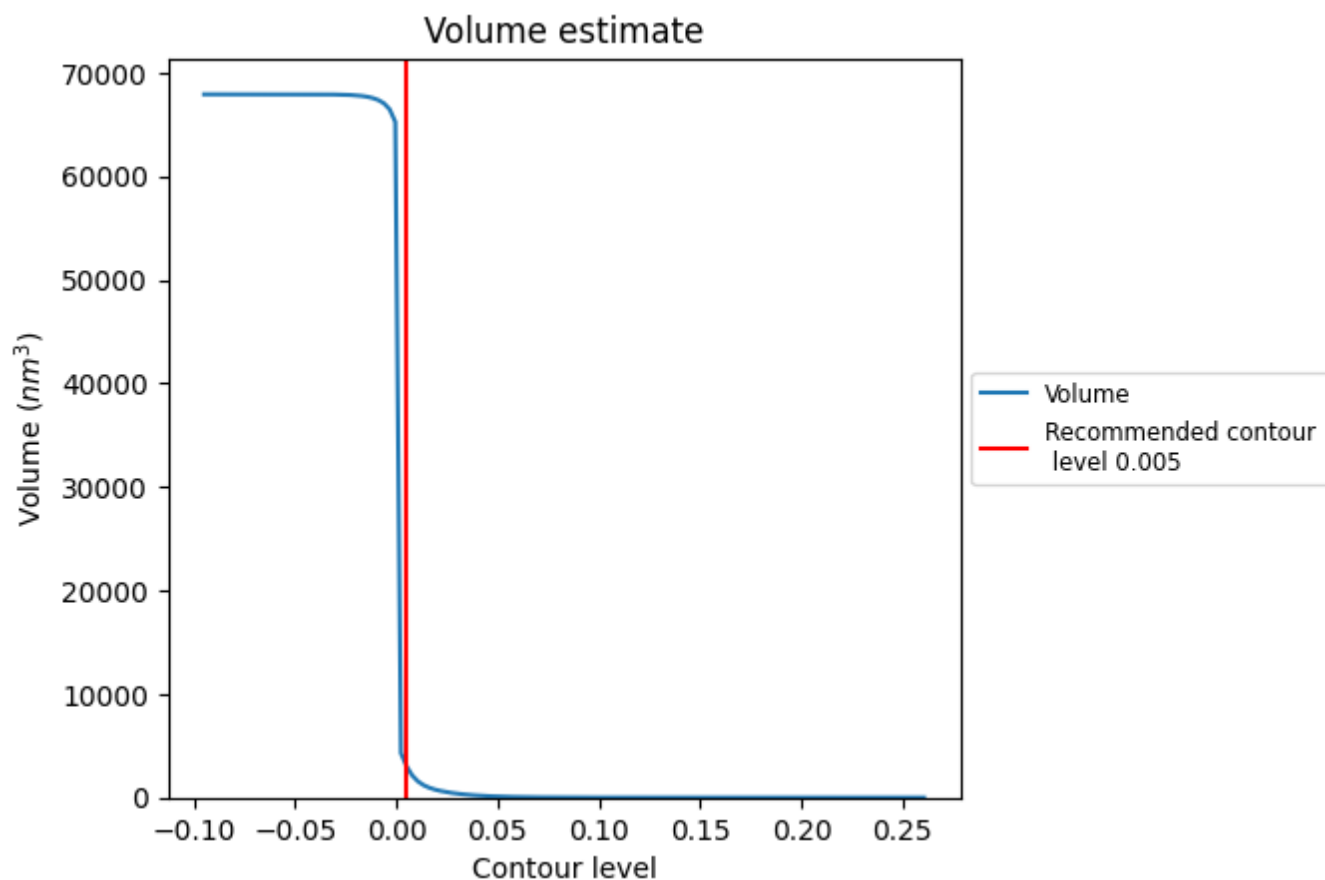
This section contains the results of statistical analysis of the map.

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.

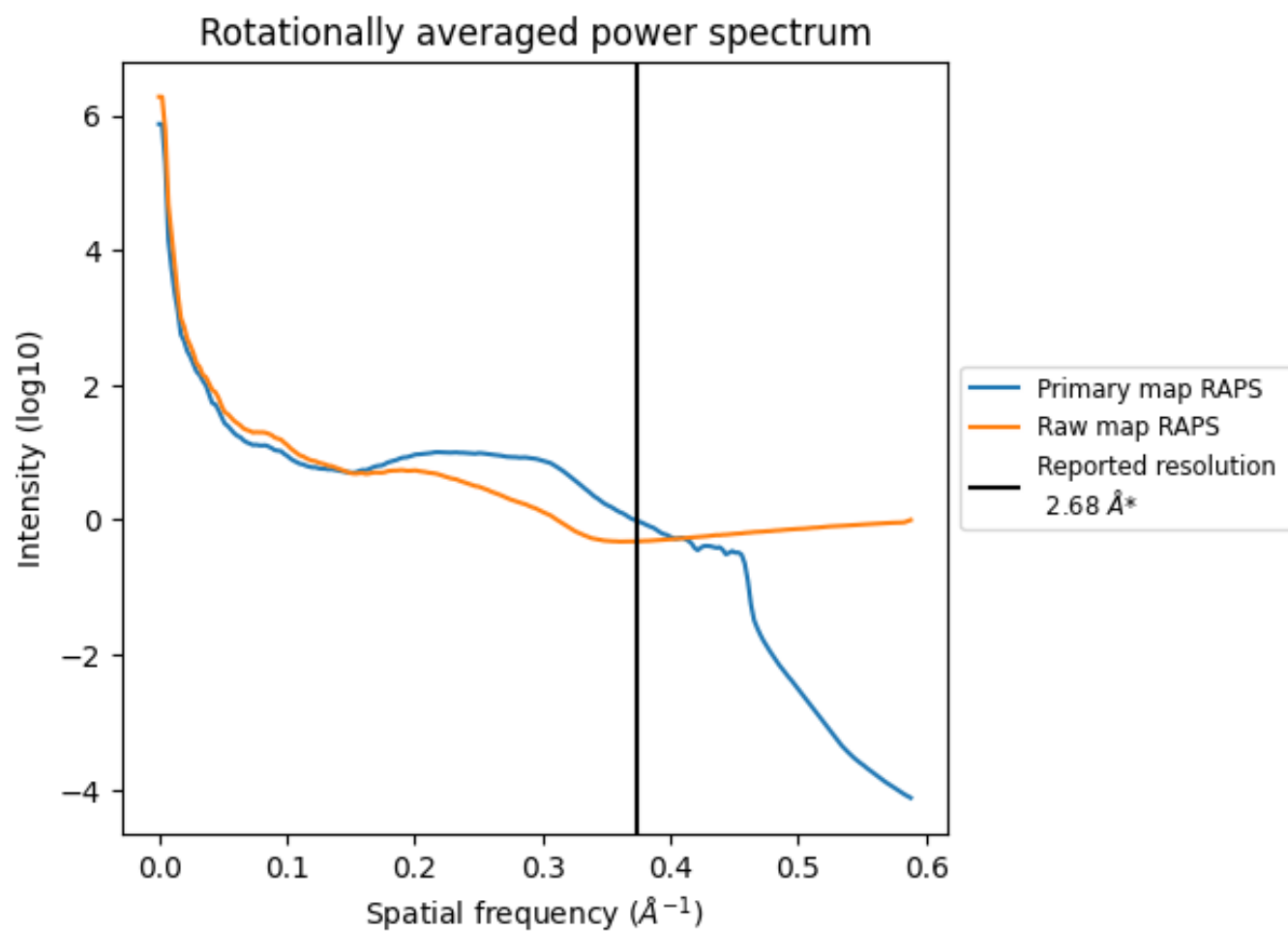
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3041 nm^3 ; this corresponds to an approximate mass of 2747 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 ⓘ

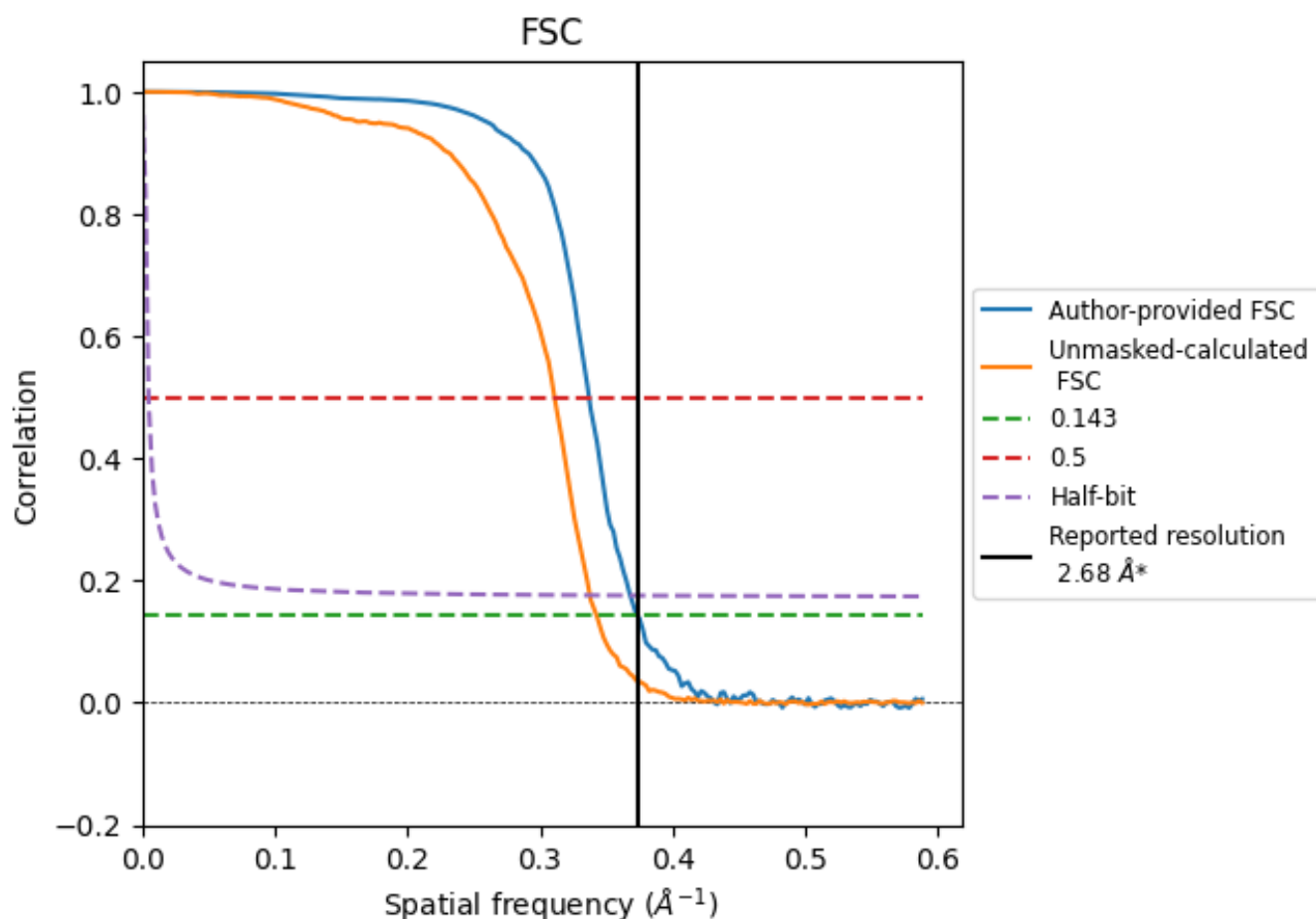


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

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 0.373 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

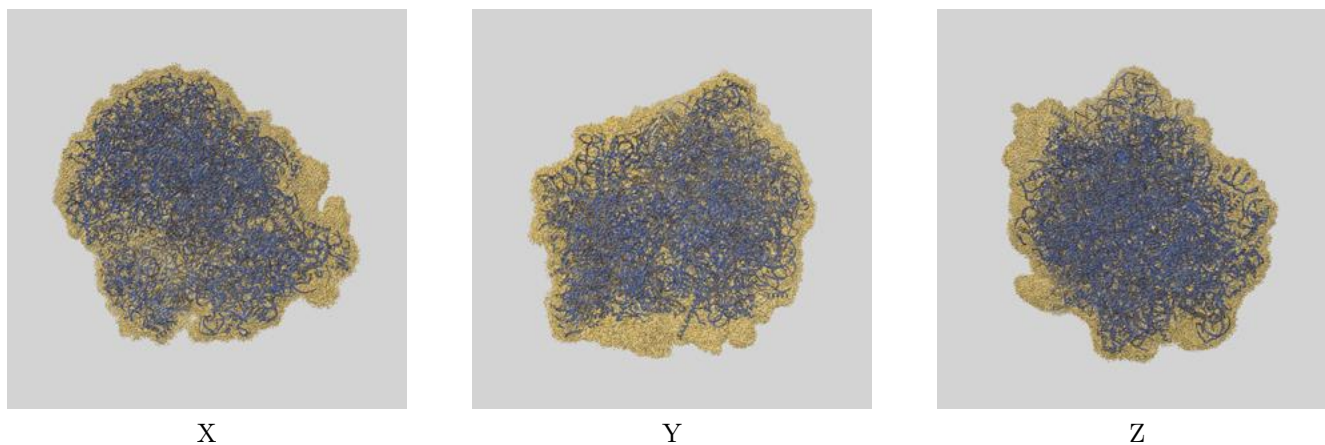
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	2.97	2.72
Unmasked-calculated*	2.92	3.22	2.96

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

9 Map-model fit [i](#)

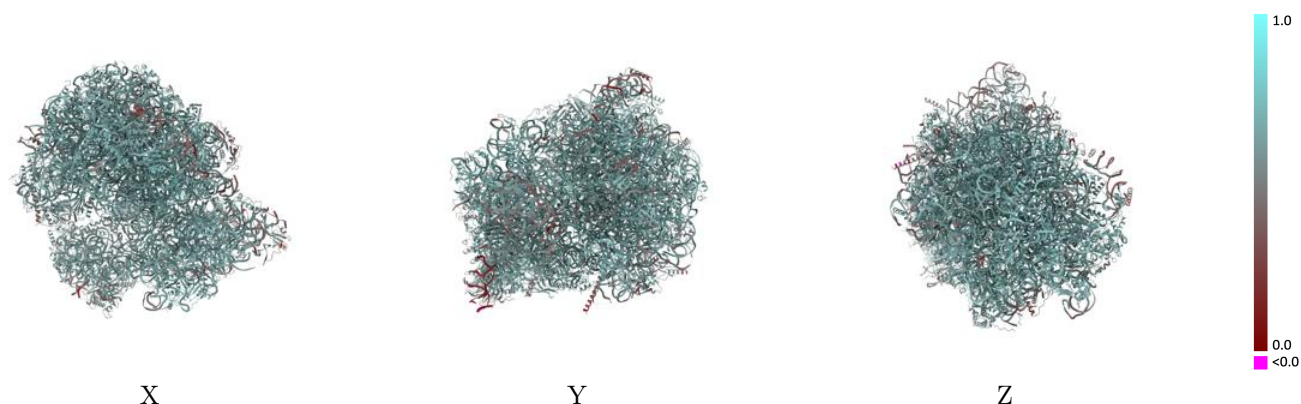
This section contains information regarding the fit between EMDB map EMD-55348 and PDB model 9SYG. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



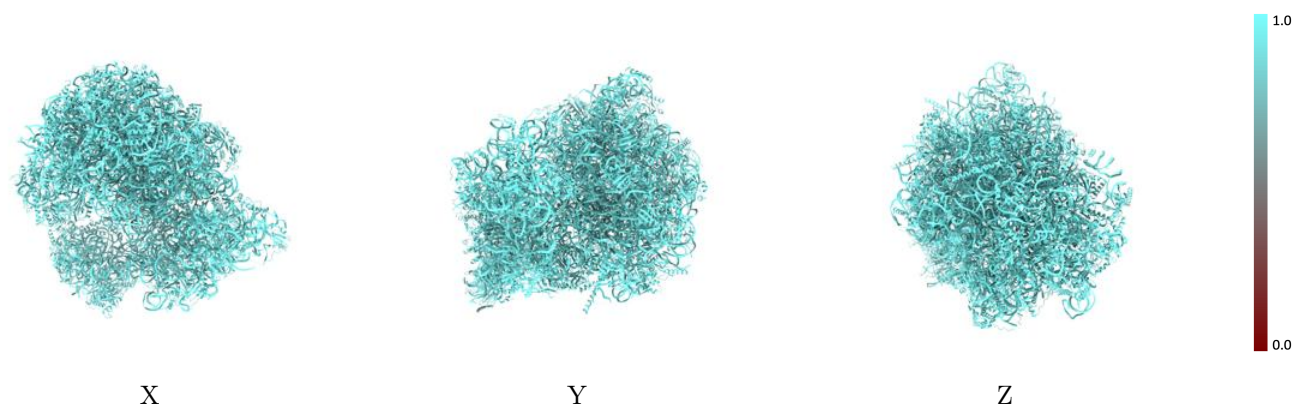
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



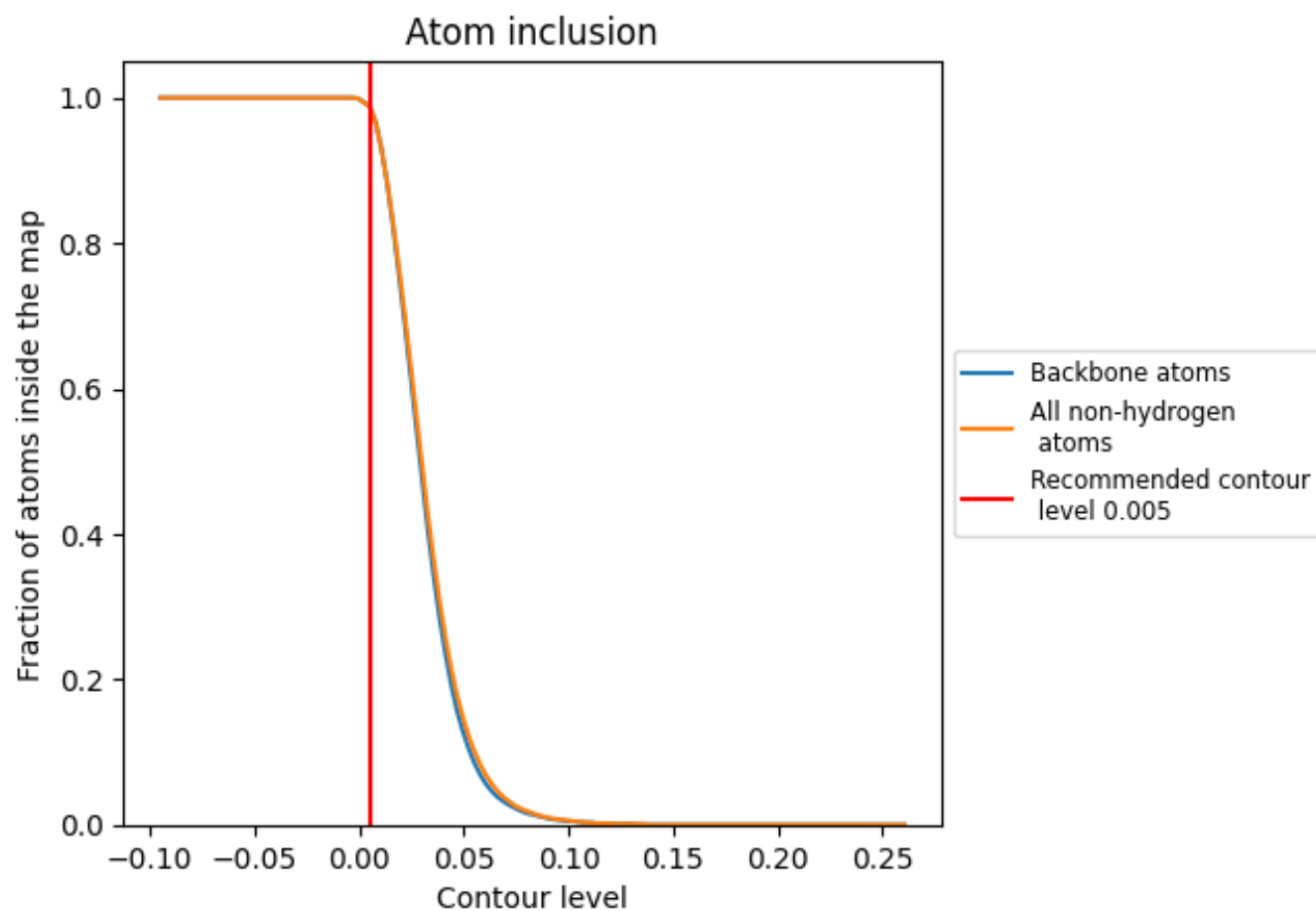
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.6270
A0	 0.9910	 0.6360
A1	 0.9840	 0.6430
A2	 0.9900	 0.6300
A3	 0.9820	 0.6010
A4	 0.9860	 0.6190
A5	 0.9950	 0.6570
A6	 0.9890	 0.6480
A7	 0.9230	 0.5310
A8	 0.9780	 0.6360
AA	 0.9860	 0.6100
AB	 0.9910	 0.5860
AC	 0.9930	 0.6130
AD	 0.9620	 0.5630
AE	 0.9840	 0.6470
AG	 0.9950	 0.6460
AH	 0.9810	 0.6230
AI	 0.9690	 0.5800
AJ	 0.9960	 0.6650
AK	 0.9870	 0.6370
AL	 0.9890	 0.5710
AM	 0.9840	 0.6060
AO	 0.9890	 0.6270
AP	 0.9810	 0.6410
AQ	 0.9500	 0.5890
AR	 0.9790	 0.6070
AS	 0.9850	 0.6440
AT	 0.9790	 0.6310
AU	 0.9720	 0.5950
AV	 0.9940	 0.6430
AW	 0.9810	 0.6180
AX	 0.9740	 0.5990
AY	 0.9780	 0.6160
AZ	 0.9770	 0.5810
Az	 0.9170	 0.4520



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Chain	Atom inclusion	Q-score
BA	 0.9940	 0.6410
BB	 0.9930	 0.6340
BC	 0.9970	 0.6470
BD	 1.0000	 0.6380
BE	 0.9880	 0.6100
BF	 0.9880	 0.6020
BG	 0.9960	 0.6400
BH	 0.9840	 0.6080
BI	 0.9900	 0.6500
BK	 0.9880	 0.6330
BL	 0.9800	 0.5550
BN	 0.9800	 0.6280
BO	 0.9930	 0.6640
BP	 0.9750	 0.5990
BQ	 0.9990	 0.6840
BR	 0.9970	 0.6820
BS	 0.9910	 0.6550
BT	 0.9920	 0.6240
BU	 0.9800	 0.6040
BV	 0.9500	 0.4940
BW	 0.9930	 0.6740
BX	 0.9940	 0.6590
BY	 0.9960	 0.6640
BZ	 0.9900	 0.6440
Ba	 0.9920	 0.6250
Bb	 0.9910	 0.6610
Bc	 0.9920	 0.6400
Bd	 0.9820	 0.6400
Be	 0.9970	 0.6810
Bf	 0.9930	 0.6710
Bg	 0.9930	 0.6530
Bh	 0.9830	 0.6240
Bi	 0.9950	 0.6590
Bj	 0.9770	 0.6090
Bk	 0.9920	 0.6160
Bl	 0.9990	 0.6710
Bm	 0.9930	 0.6240
Bn	 0.9970	 0.6830
Bo	 0.9970	 0.6720
Bp	 0.9760	 0.5900
Bq	 0.9910	 0.6630
Br	 0.9940	 0.6550

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Chain	Atom inclusion	Q-score
Bs	 0.9790	 0.5740
Bt	 0.9900	 0.6530
Bu	 0.9780	 0.5830
Bv	 0.9810	 0.6020
Bw	 0.9950	 0.6570
Bx	 0.9820	 0.6170
By	 0.9870	 0.5990
Bz	 0.9960	 0.6650