



Full wwPDB EM Validation Report ⓘ

Sep 13, 2026 – 09:37 am BST

PDB ID : 31FY / pdb_000031fy
EMDB ID : EMD-58362
Title : Mouse 80S ribosome, Gm10076 KO
Authors : Rabl, J.; Valdivia Francia, F.; Sendoel, A.
Deposited on : 2026-06-02
Resolution : 2.57 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:

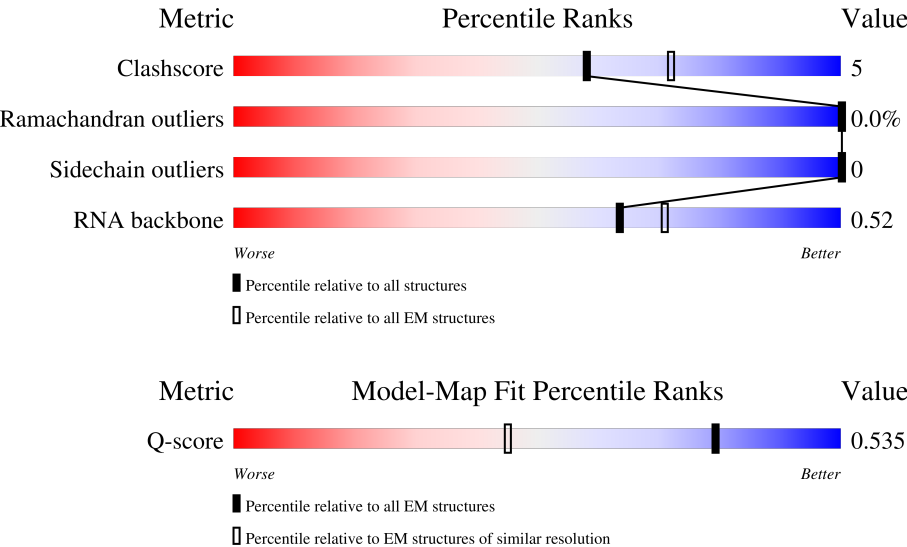
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.57 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	7615 (2.07 - 3.07)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	69	35% 65% 28% 7%
2	AB	56	7% 84% 12% •
3	AC	1871	14% 59% 27% • 9%

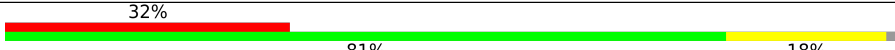
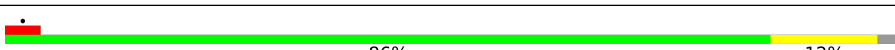
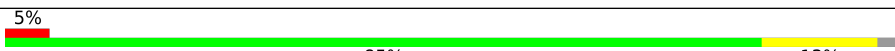
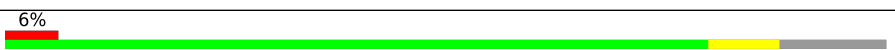
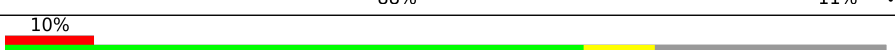
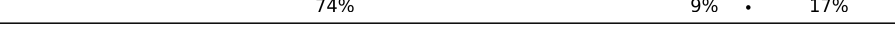
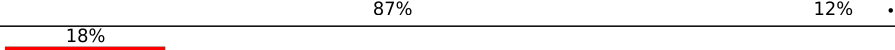
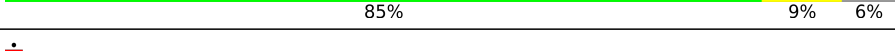
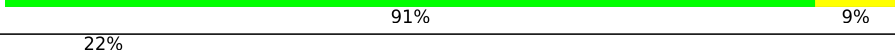
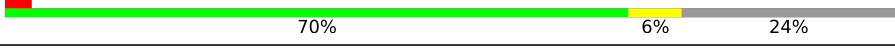
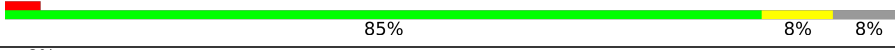
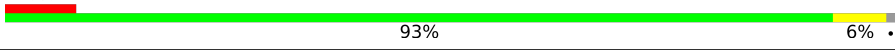
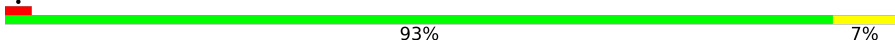
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Mol	Chain	Length	Quality of chain
4	AE	243	
5	AH	135	
6	AJ	204	
7	AK	165	
8	AL	145	
9	AM	146	
10	AN	152	
11	AO	145	
12	AP	119	
13	AT	317	
14	AX	132	
15	Ac	125	
16	Af	156	
17	AD	264	
18	AF	263	
19	AG	158	
20	AI	295	
21	AQ	83	
22	AR	143	
23	AS	115	
24	AU	293	
25	AV	249	
26	AW	194	
27	AY	151	
28	AZ	151	

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Mol	Chain	Length	Quality of chain
29	Aa	130	
30	Ab	133	
31	Ad	84	
32	Ae	133	
33	Ag	194	
34	Ah	208	
35	BA	257	
36	BB	403	
37	BC	419	
38	BD	297	
39	BE	296	
40	BF	203	
41	BG	184	
42	BH	188	
43	BI	196	
44	BJ	176	
45	BK	160	
46	BL	128	
47	BM	140	
48	BN	157	
49	BO	156	
50	BP	145	
51	BQ	136	
52	BR	148	
53	BS	160	

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Mol	Chain	Length	Quality of chain
54	BT	115	
55	BU	125	
56	BV	135	
57	BW	110	
58	BX	117	
59	BY	123	
60	BZ	105	
61	Ba	97	
62	Bb	70	
63	Bc	51	
64	Bd	128	
65	Be	25	
66	Bf	106	
67	Bg	92	
68	Bh	137	
69	CA	270	
70	CB	266	
71	CC	192	
72	CD	214	
73	CE	178	
74	CF	211	
75	CG	217	
76	CH	204	
77	CI	4731	
78	CJ	121	

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Mol	Chain	Length	Quality of chain
79	CK	156	9% 71% 23% 5%

2 Entry composition [i](#)

There are 81 unique types of molecules in this entry. The entry contains 363044 atoms, of which 154659 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 Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	AA	64	Total	C	H	N	O	S	0	0
			1042	308	536	102	94	2		

- Molecule 2 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AB	54	Total	C	H	N	O	S	0	0
			902	284	447	93	73	5		

- Molecule 3 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	AC	1694	Total	C	H	N	O	P	0	0
			54441	16156	18258	6497	11837	1693		

- Molecule 4 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	AE	226	Total	C	H	N	O	S	0	0
			3607	1119	1851	316	314	7		

- Molecule 5 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	AH	134	Total	C	H	N	O	S	0	0
			2215	678	1135	201	197	4		

- Molecule 6 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	AJ	189	Total	C	H	N	O	S	0	0
			3044	934	1549	284	270	7		

- Molecule 7 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	AK	97	Total	C	H	N	O	S	0	0
			1661	534	842	147	133	5		

- Molecule 8 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	AL	123	Total	C	H	N	O	S	0	0
			2053	638	1047	189	172	7		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AM	144	Total	C	H	N	O	S	0	0
			2356	726	1213	216	198	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AN	144	Total	C	H	N	O	S	0	0
			2439	746	1249	241	202	1		

- Molecule 11 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AO	141	Total	C	H	N	O	S	0	0
			2243	691	1139	215	196	2		

- Molecule 12 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AP	102	Total	C	H	N	O	S	0	0
			1681	507	874	153	143	4		

- Molecule 13 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AT	313	Total	C	H	N	O	S	0	0
			4829	1535	2393	424	465	12		

- Molecule 14 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AX	87	Total	C	H	N	O	S	0	0
			1358	418	690	118	125	7		

- Molecule 15 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Ac	75	Total	C	H	N	O	S	0	0
			1254	382	656	111	104	1		

- Molecule 16 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Af	62	Total	C	H	N	O	S	0	0
			1011	317	506	96	85	7		

- Molecule 17 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AD	214	Total	C	H	N	O	S	0	0
			3544	1103	1806	310	311	14		

- Molecule 18 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AF	262	Total	C	H	N	O	S	0	0
			4253	1324	2177	386	358	8		

- Molecule 19 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AG	146	Total	C	H	N	O	S	0	0
			2468	764	1269	224	205	6		

- Molecule 20 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AI	214	Total	C	H	N	O	S	0	0
			3390	1077	1696	297	312	8		

- Molecule 21 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AQ	83	Total	C	H	N	O	S	0	0
			1273	392	635	119	122	5		

- Molecule 22 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AR	141	Total	C	H	N	O	S	0	0
			2266	693	1168	219	183	3		

- Molecule 23 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AS	100	Total	C	H	N	O	S	1	0
			1675	506	864	169	131	5		

- Molecule 24 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AU	222	Total	C	H	N	O	S	0	0
			3540	1116	1815	298	302	9		

- Molecule 25 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AV	227	Total	C	H	N	O	S	0	0
			3829	1149	1989	367	317	7		

- Molecule 26 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AW	147	Total	C	H	N	O	S	0	0
			2577	794	1339	243	199	2		

- Molecule 27 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	AY	150	Total	C	H	N	O	S	0	0
			2502	773	1294	229	205	1		

- Molecule 28 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	AZ	134	Total	C	H	N	O	S	0	0
			2023	612	1021	197	187	6		

- Molecule 29 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Aa	129	Total	C	H	N	O	S	0	0
			2114	659	1080	193	176	6		

- Molecule 30 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	Ab	121	Total	C	H	N	O	S	0	0
			2058	631	1060	195	167	5		

- Molecule 31 is a protein called Small ribosomal subunit protein eS27-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Ad	83	Total	C	H	N	O	S	0	0
			1328	409	676	121	115	7		

- Molecule 32 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	Ae	13	Total	C	H	N	O		0	0
			194	56	101	21	16			

- Molecule 33 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Ag	183	Total	C	H	N	O	S	0	0
			3044	944	1567	270	262	1		

- Molecule 34 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	Ah	206	Total	C	H	N	O	S	0	0
			3458	1058	1772	332	291	5		

- Molecule 35 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	BA	251	Total	C	H	N	O	S	0	0
			3943	1204	2022	393	318	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	BB	396	Total	C	H	N	O	S	0	0
			6540	2036	3343	602	545	14		

- Molecule 37 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	BC	367	Total	C	H	N	O	S	0	0
			6038	1842	3110	583	488	15		

- Molecule 38 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	BD	293	Total	C	H	N	O	S	0	0
			4794	1506	2409	440	425	14		

- Molecule 39 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	BE	218	Total	C	H	N	O	S	0	0
			3668	1130	1902	337	295	4		

- Molecule 40 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	BF	201	Total	C	H	N	O	S	0	0
			3430	1055	1790	320	259	6		

- Molecule 41 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	BG	153	Total	C	H	N	O	S	0	0
			2516	777	1274	241	215	9		

- Molecule 42 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	BH	186	Total	C	H	N	O	S	0	0
			3148	946	1637	313	248	4		

- Molecule 43 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	BI	184	Total	C	H	N	O	S	0	0
			3240	955	1698	332	246	9		

- Molecule 44 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	BJ	175	Total	C	H	N	O	S	0	0
			2938	924	1488	283	233	10		

- Molecule 45 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	BK	159	Total	C	H	N	O	S	0	0
			2669	824	1370	252	217	6		

- Molecule 46 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	BL	101	Total	C	H	N	O	S	0	0
			1675	529	850	144	150	2		

- Molecule 47 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	BM	129	Total	C	H	N	O	S	0	0
			2000	613	1031	182	169	5		

- Molecule 48 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	BN	61	Total	C	H	N	O	S	0	0
			1045	330	530	100	82	3		

- Molecule 49 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	BO	118	Total	C	H	N	O	S	0	0
			2007	618	1040	181	167	1		

- Molecule 50 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	BP	134	Total	C	H	N	O	S	0	0
			2320	700	1205	226	186	3		

- Molecule 51 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	BQ	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 52 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	BR	147	Total	C	H	N	O	S	0	0
			2377	736	1213	239	185	4		

- Molecule 53 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	BS	99	Total	C	H	N	O	S	0	0
			1697	511	884	173	124	5		

- Molecule 54 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	BT	94	Total	C	H	N	O	S	0	0
			1501	465	769	130	131	6		

- Molecule 55 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	BU	107	Total	C	H	N	O	S	0	0
			1817	560	929	171	155	2		

- Molecule 56 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	BV	110	Total	C	H	N	O	S	0	0
			1866	571	971	176	143	5		

- Molecule 57 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	BW	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	143	4		

- Molecule 58 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	BX	114	Total	C	H	N	O	S	0	0
			1903	565	997	187	148	6		

- Molecule 59 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	BY	120	Total	C	H	N	O	S	0	0
			2139	634	1138	201	165	1		

- Molecule 60 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	BZ	102	Total	C	H	N	O	S	0	0
			1749	521	917	177	129	5		

- Molecule 61 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	Ba	86	Total	C	H	N	O	S	0	0
			1442	434	737	155	111	5		

- Molecule 62 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	Bb	69	Total	C	H	N	O	S	0	0
			1203	365	635	103	99	1		

- Molecule 63 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	Bc	50	Total	C	H	N	O	S	0	0
			927	281	483	98	64	1		

- Molecule 64 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	Bd	52	Total	C	H	N	O	S	0	0
			895	267	465	90	67	6		

- Molecule 65 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	Be	25	Total	C	H	N	O	S	0	0
			528	145	289	64	27	3		

- Molecule 66 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	Bf	103	Total	C	H	N	O	S	0	0
			1753	528	911	172	136	6		

- Molecule 67 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	Bg	89	Total	C	H	N	O	S	0	0
			1432	436	738	133	118	7		

- Molecule 68 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	Bh	125	Total	C	H	N	O	S	0	0
			2068	621	1067	207	168	5		

- Molecule 69 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	CA	222	Total	C	H	N	O	S	1	0
			3839	1190	1988	356	297	8		

- Molecule 70 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	CB	230	Total	C	H	N	O	S	1	0
			3866	1188	2003	359	312	4		

- Molecule 71 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	CC	190	Total	C	H	N	O	S	0	0
			3122	956	1603	284	273	6		

- Molecule 72 is a protein called Large ribosomal subunit protein uL16-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	CD	208	Total	C	H	N	O	S	0	0
			3435	1073	1745	327	278	12		

- Molecule 73 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	CE	168	Total	C	H	N	O	S	0	0
			2732	853	1383	251	239	6		

- Molecule 74 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	CF	207	Total	C	H	N	O	S	0	0
			3453	1048	1777	344	280	4		

- Molecule 75 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	CG	139	Total	C	H	N	O	S	0	0
			2360	732	1217	221	183	7		

- Molecule 76 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	CH	203	Total	C	H	N	O	S	0	0
			3450	1072	1749	359	266	4		

- Molecule 77 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	CI	3558	Total	C	H	N	O	P	0	0
			114909	34045	38567	13907	24833	3557		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	248	C	-	insertion	GB 120444900
CI	?	-	C	deletion	GB 120444900
CI	?	-	C	deletion	GB 120444900
CI	831	U	-	insertion	GB 120444900
CI	1887	G	-	insertion	GB 120444900
CI	2324	C	-	insertion	GB 120444900
CI	2325	G	-	insertion	GB 120444900
CI	2326	U	-	insertion	GB 120444900
CI	?	-	G	deletion	GB 120444900
CI	?	-	A	deletion	GB 120444900
CI	?	-	A	deletion	GB 120444900

- Molecule 78 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	CJ	120	Total	C	H	N	O	P	0	0
			3853	1141	1295	456	842	119		

- Molecule 79 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	CK	156	Total	C	H	N	O	P	0	0
			4997	1481	1682	585	1094	155		

- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
80	AB	1	Total	Zn	0
			1	1	
80	Af	1	Total	Zn	0
			1	1	
80	AS	1	Total	Zn	0
			1	1	
80	Ba	1	Total	Zn	0
			1	1	
80	Bd	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
80	Bf	1	Total 1	Zn 1	0
80	Bg	1	Total 1	Zn 1	0

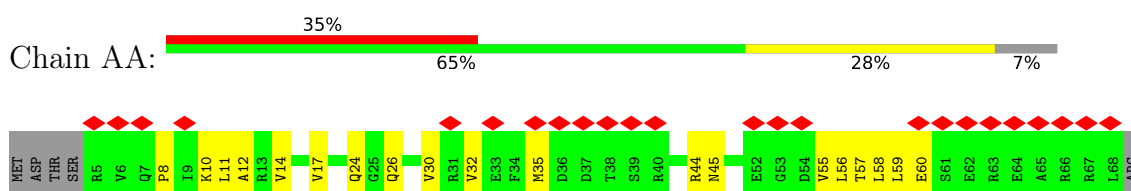
- Molecule 81 is water.

Mol	Chain	Residues	Atoms		AltConf
81	AC	2	Total 2	O 2	0
81	CB	1	Total 1	O 1	0
81	CI	1	Total 1	O 1	0

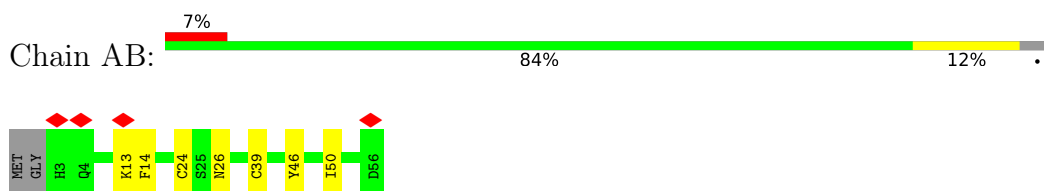
3 Residue-property plots [i](#)

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.

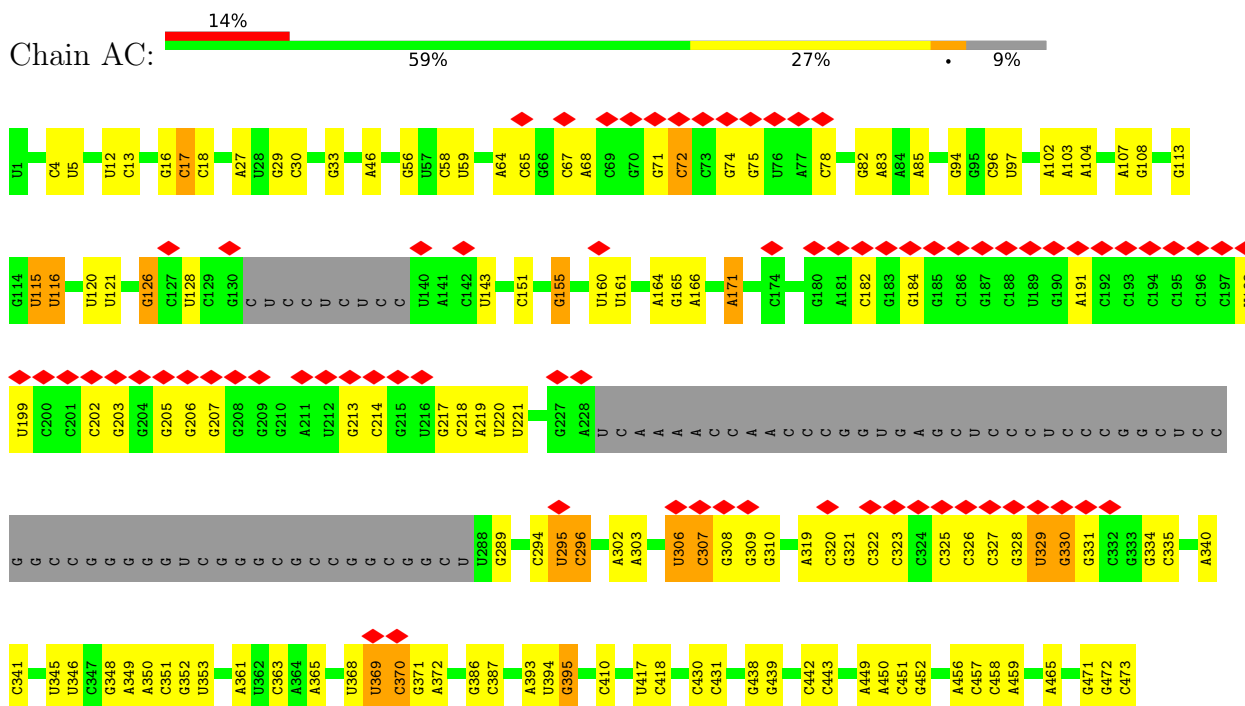
- Molecule 1: Small ribosomal subunit protein eS28

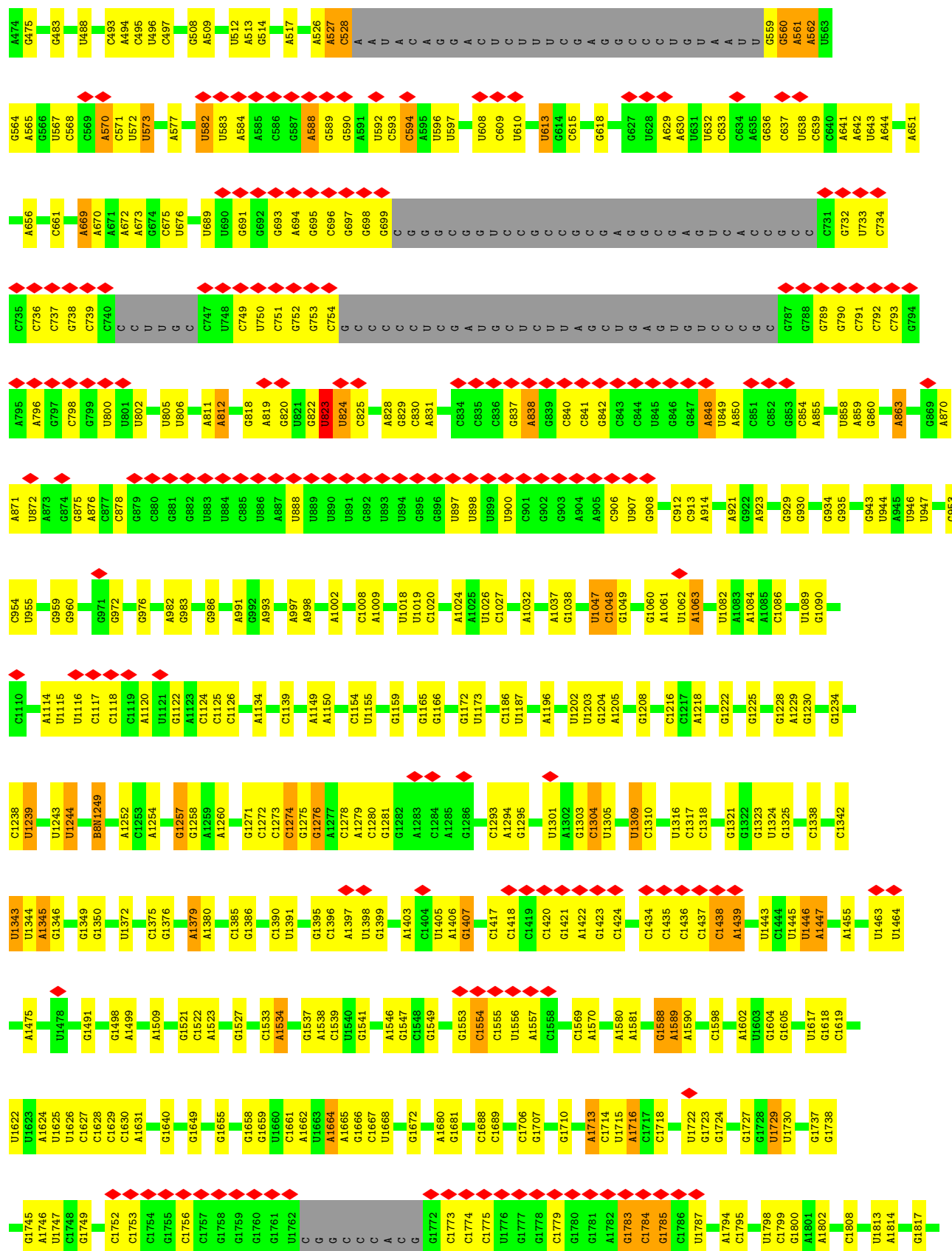


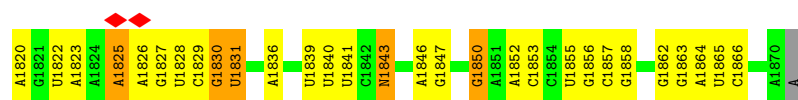
- Molecule 2: Small ribosomal subunit protein uS14



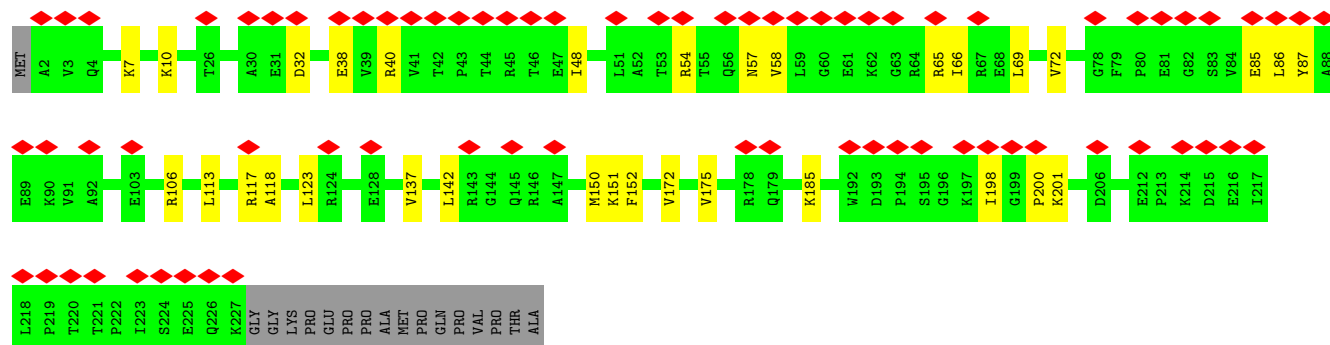
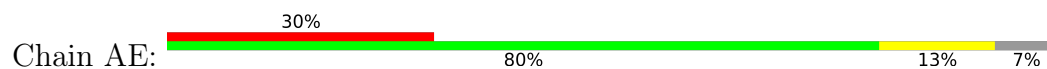
- Molecule 3: 18S rRNA



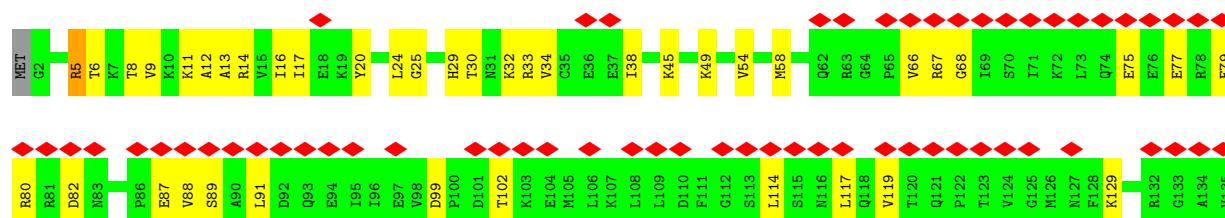




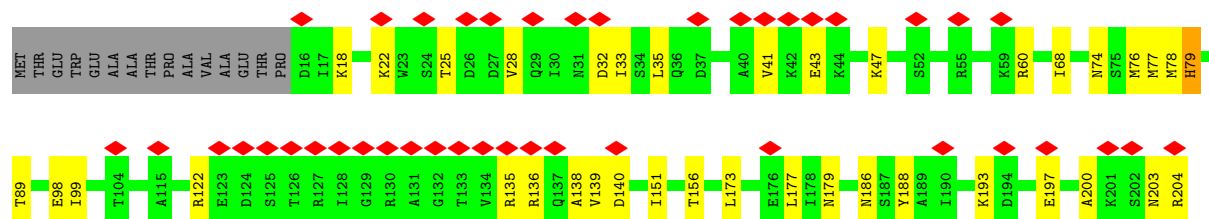
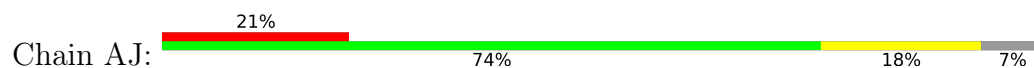
• Molecule 4: Small ribosomal subunit protein uS3



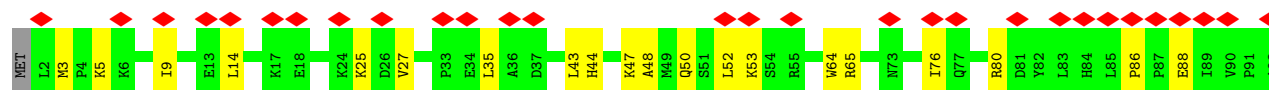
• Molecule 5: Small ribosomal subunit protein eS17

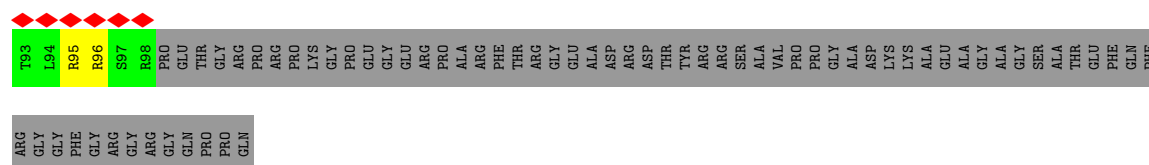


• Molecule 6: Small ribosomal subunit protein uS7

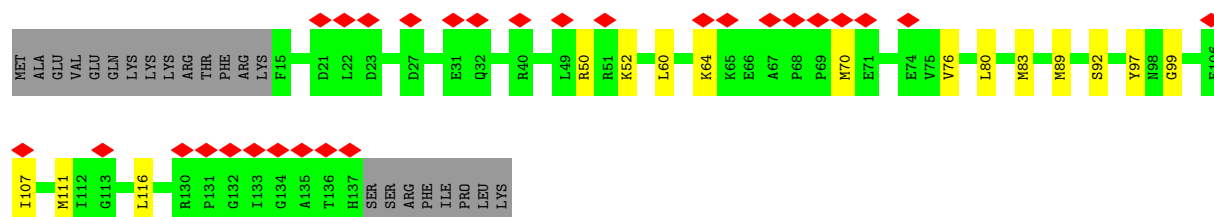
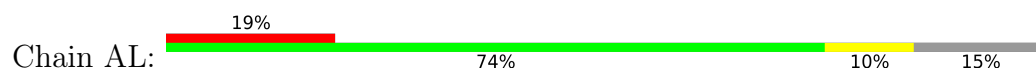


• Molecule 7: Small ribosomal subunit protein eS10

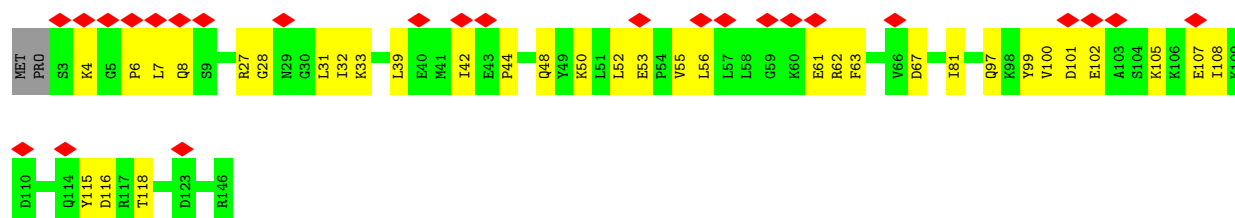
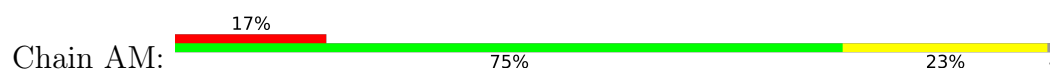




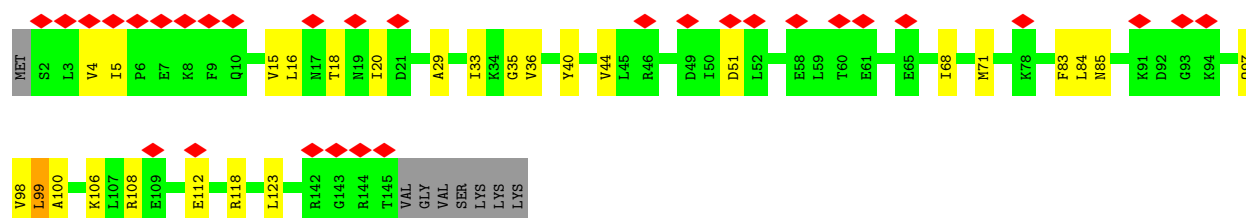
- Molecule 8: Small ribosomal subunit protein uS19



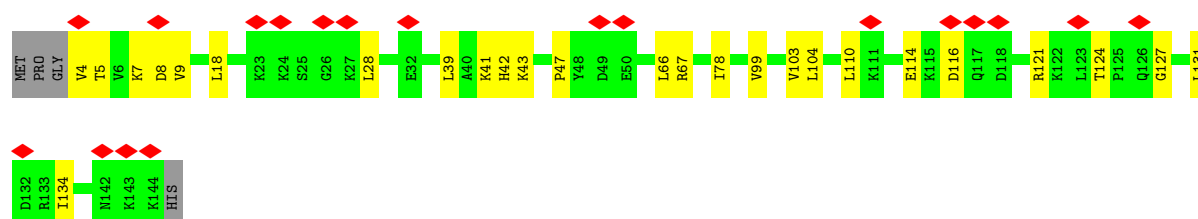
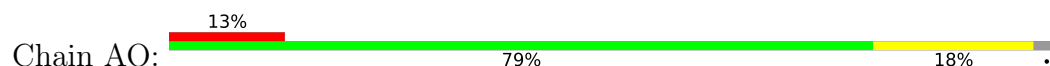
- Molecule 9: Small ribosomal subunit protein uS9

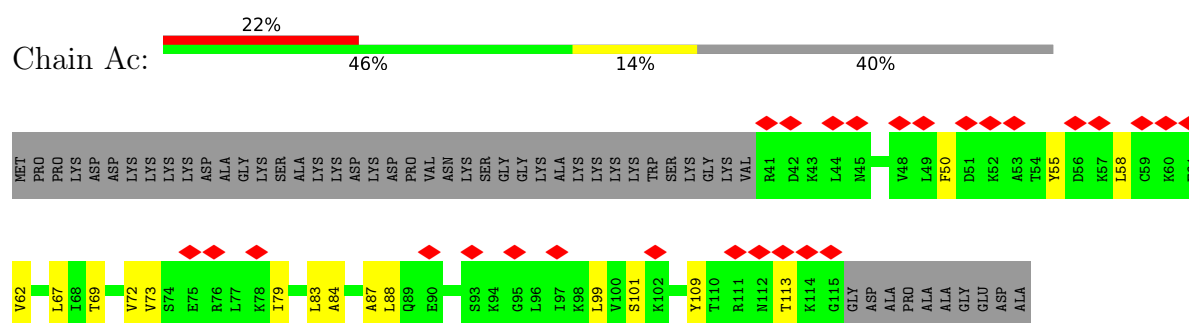


- Molecule 10: Small ribosomal subunit protein uS13

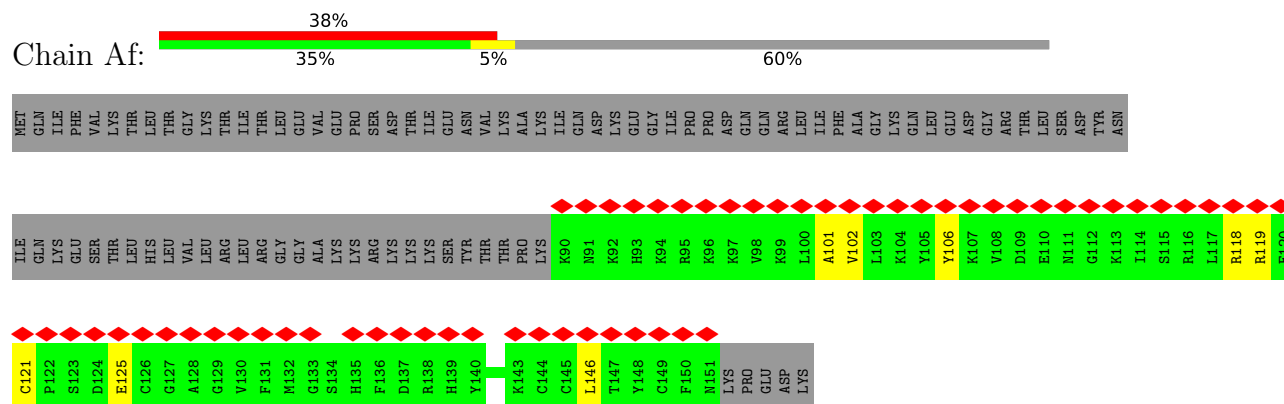


- Molecule 11: Small ribosomal subunit protein eS19

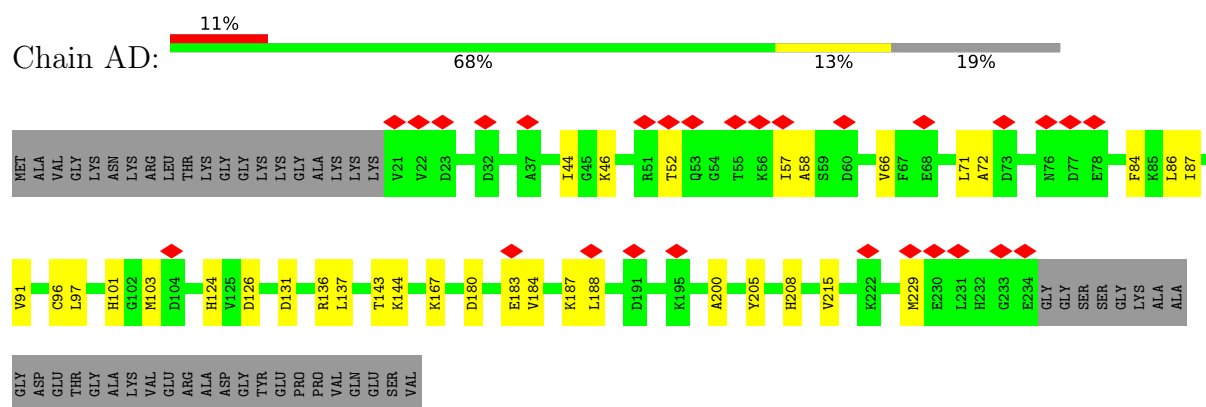




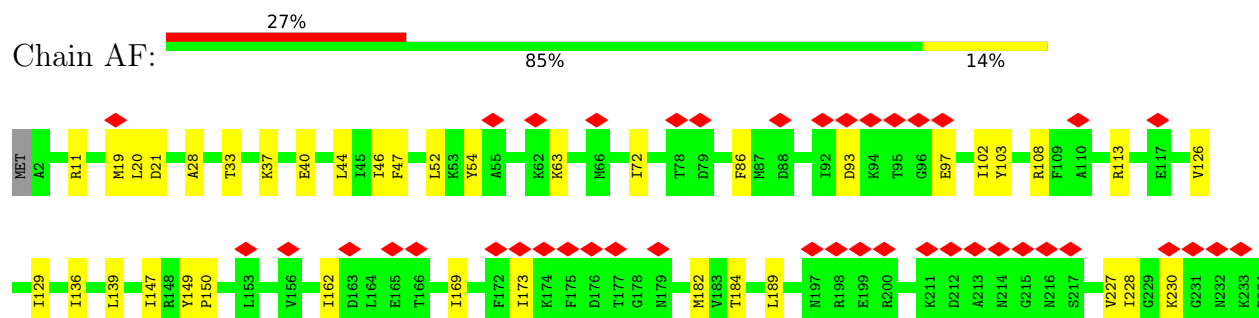
- Molecule 16: Ubiquitin-ribosomal protein eS31 fusion protein.

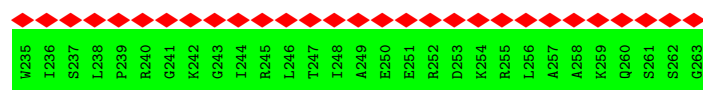


- Molecule 17: 40S ribosomal protein S3a

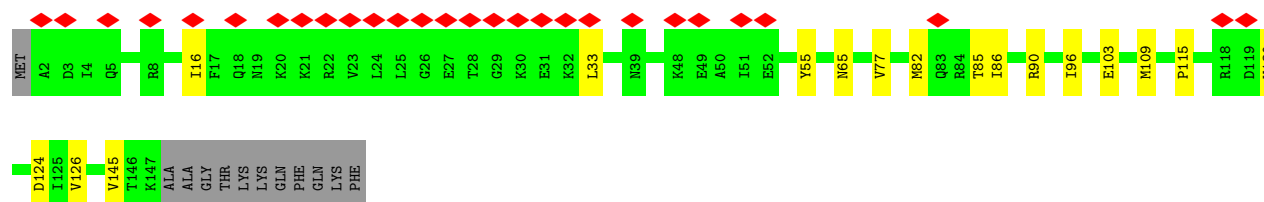
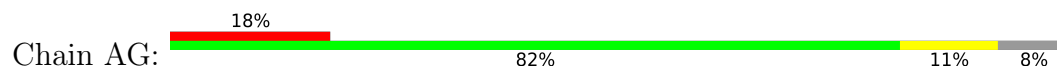


- Molecule 18: Small ribosomal subunit protein eS4

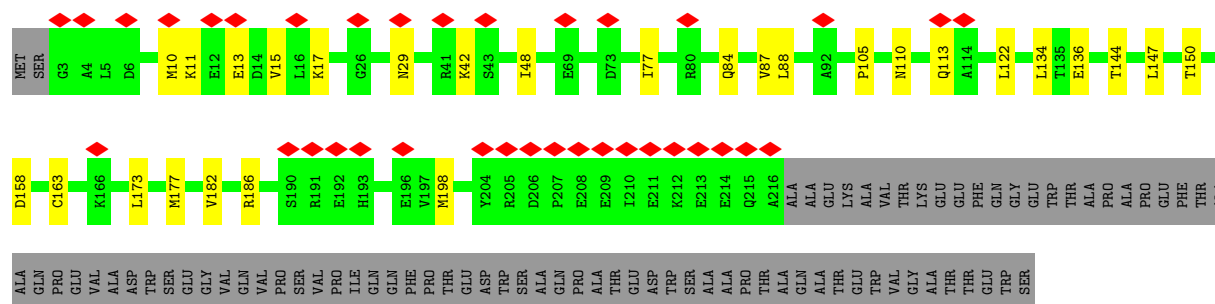




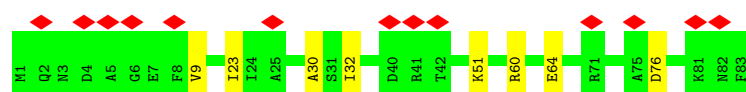
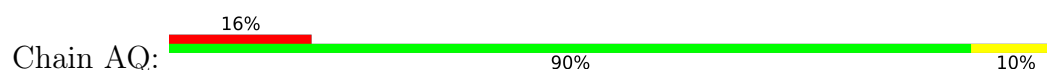
- Molecule 19: Small ribosomal subunit protein uS17



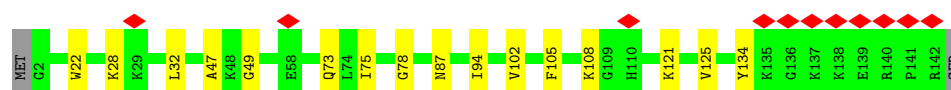
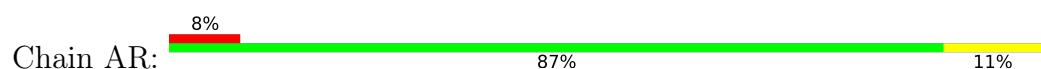
- Molecule 20: Small ribosomal subunit protein uS2



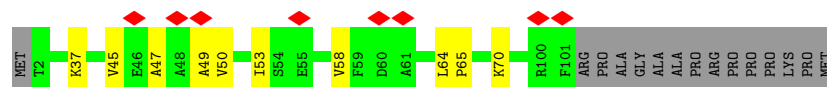
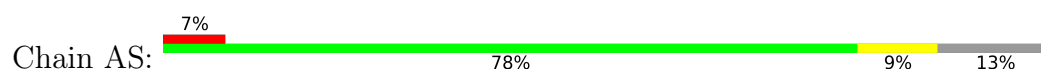
- Molecule 21: Small ribosomal subunit protein eS21



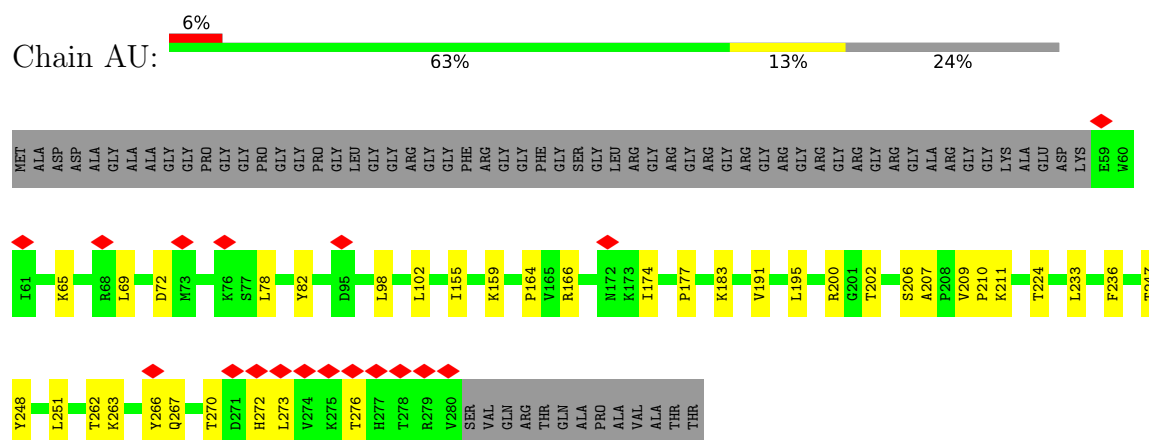
- Molecule 22: Small ribosomal subunit protein uS12



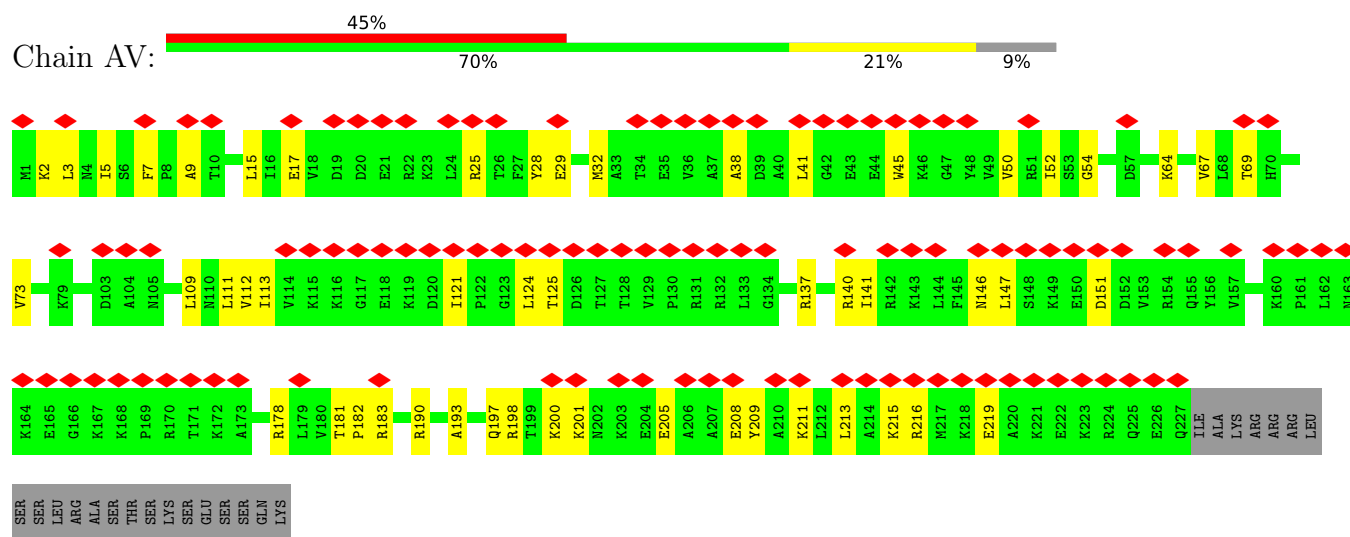
- Molecule 23: Small ribosomal subunit protein eS26



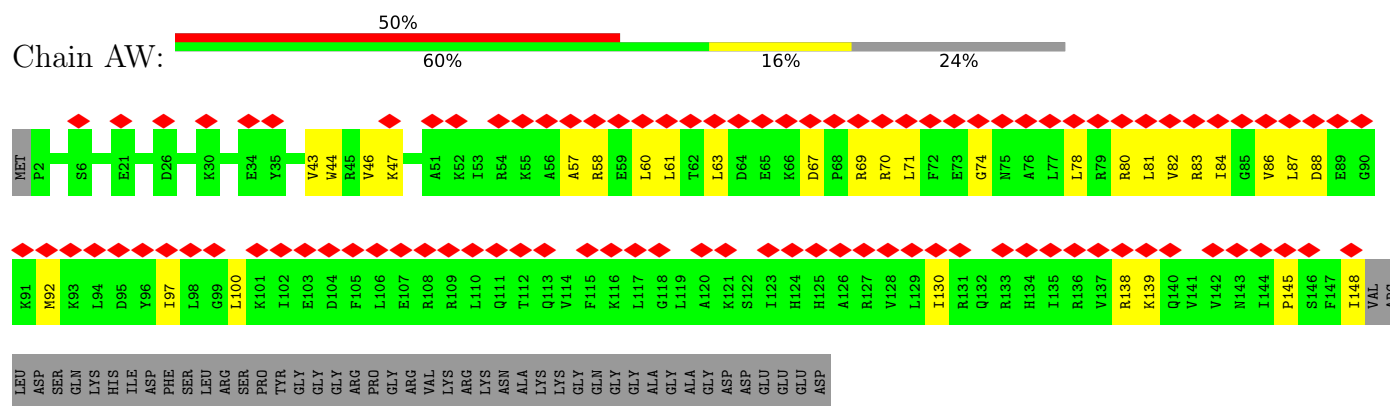
- Molecule 24: Small ribosomal subunit protein uS5



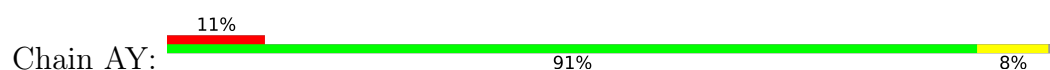
- Molecule 25: Small ribosomal subunit protein eS6

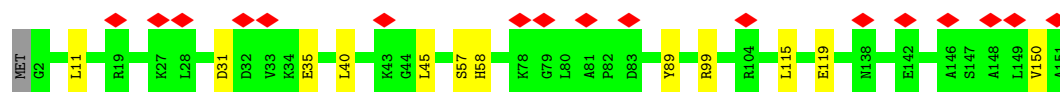


- Molecule 26: Small ribosomal subunit protein uS4

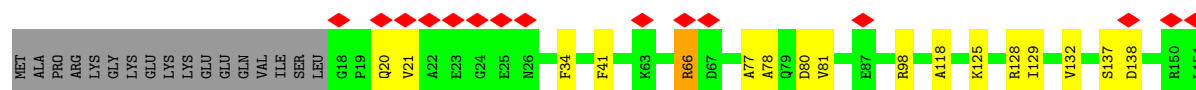
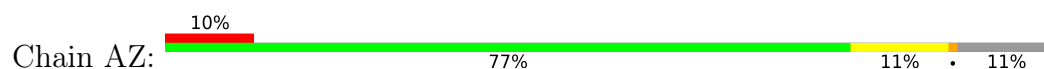


- Molecule 27: Small ribosomal subunit protein uS15

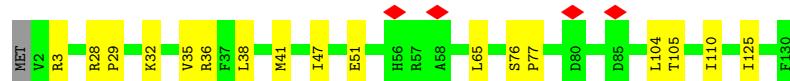




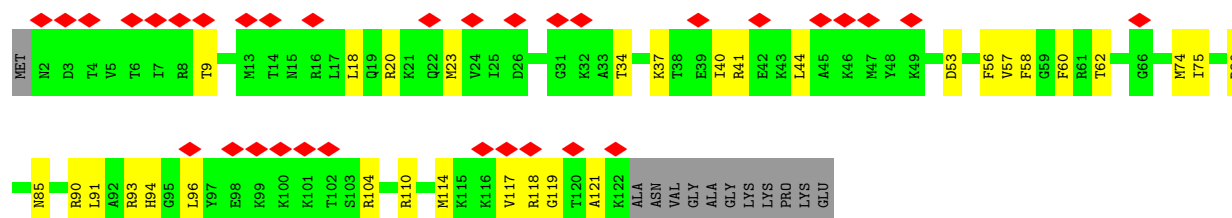
- Molecule 28: Small ribosomal subunit protein uS11



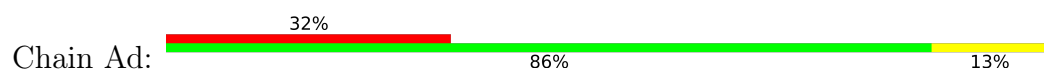
- Molecule 29: Small ribosomal subunit protein uS8



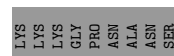
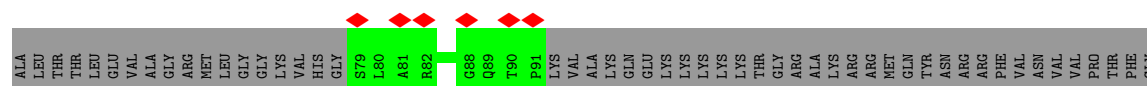
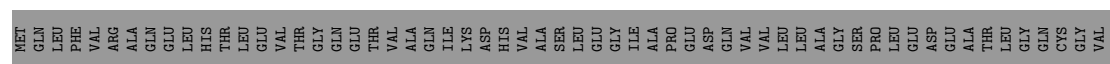
- Molecule 30: Small ribosomal subunit protein eS24



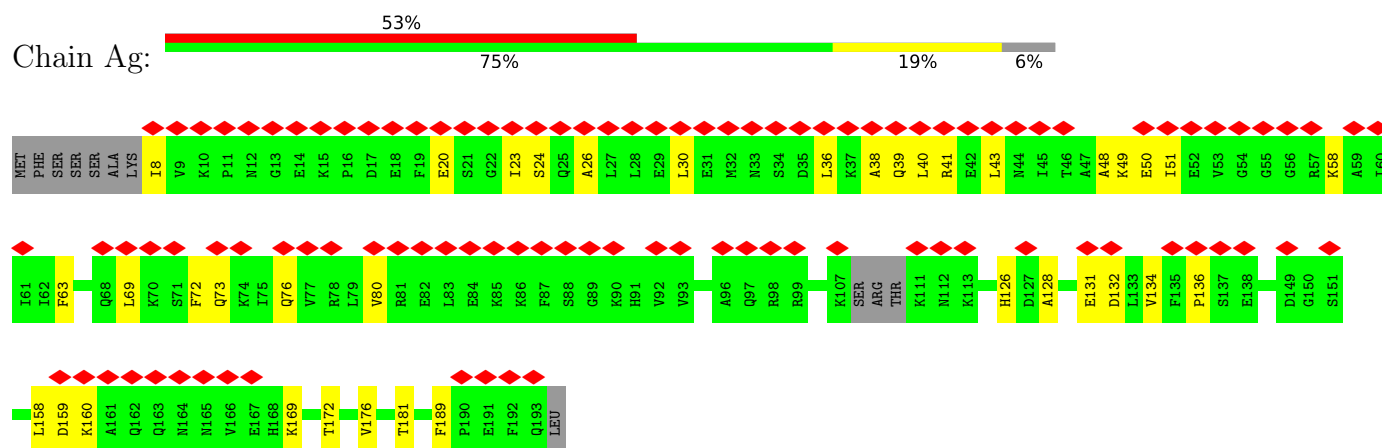
- Molecule 31: Small ribosomal subunit protein eS27-like



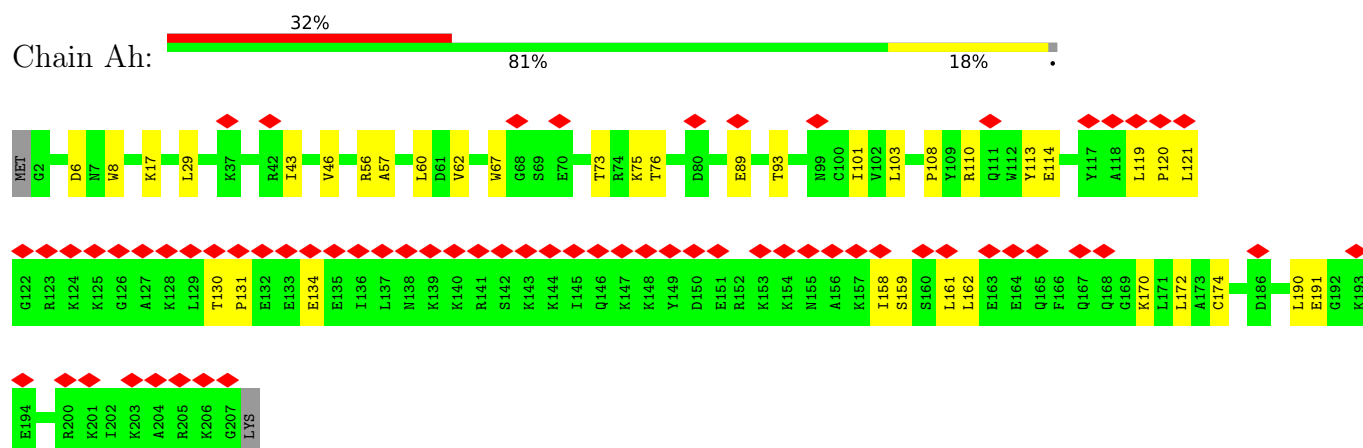
- Molecule 32: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



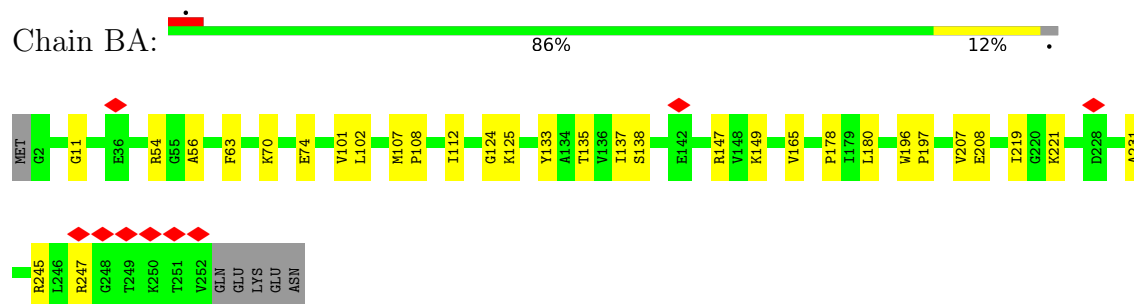
- Molecule 33: Small ribosomal subunit protein eS7



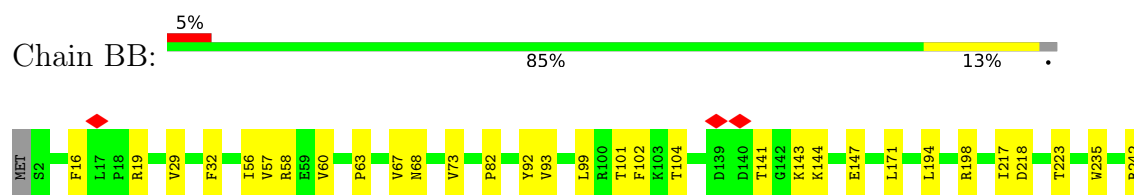
- Molecule 34: Small ribosomal subunit protein eS8

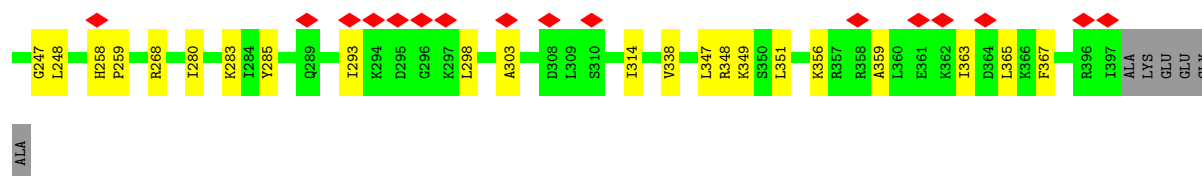


- Molecule 35: Large ribosomal subunit protein uL2

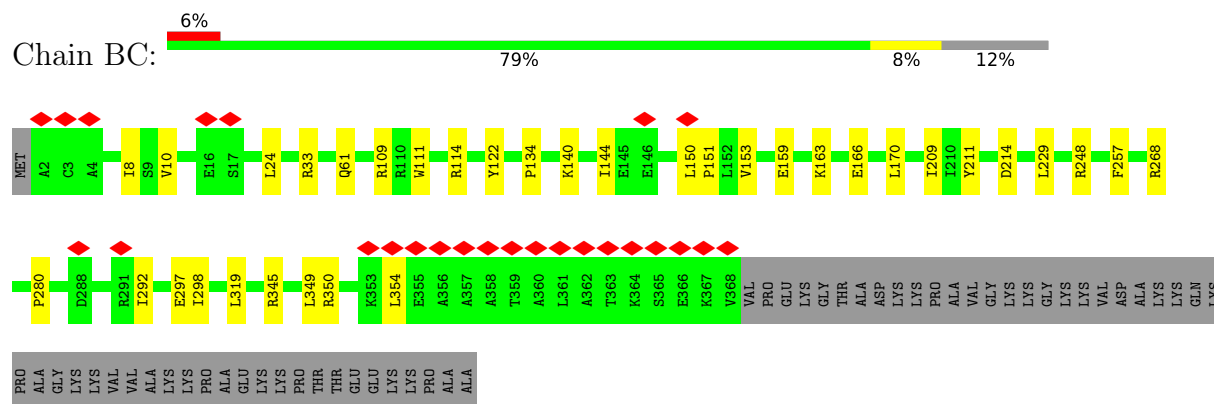


- Molecule 36: Large ribosomal subunit protein uL3

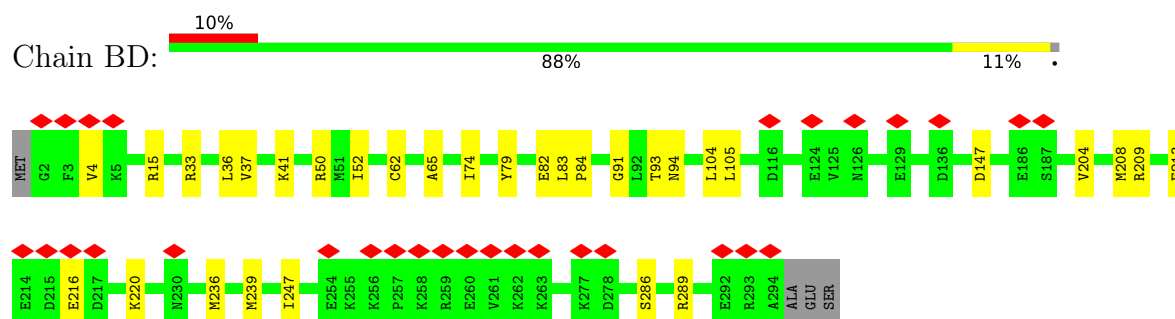




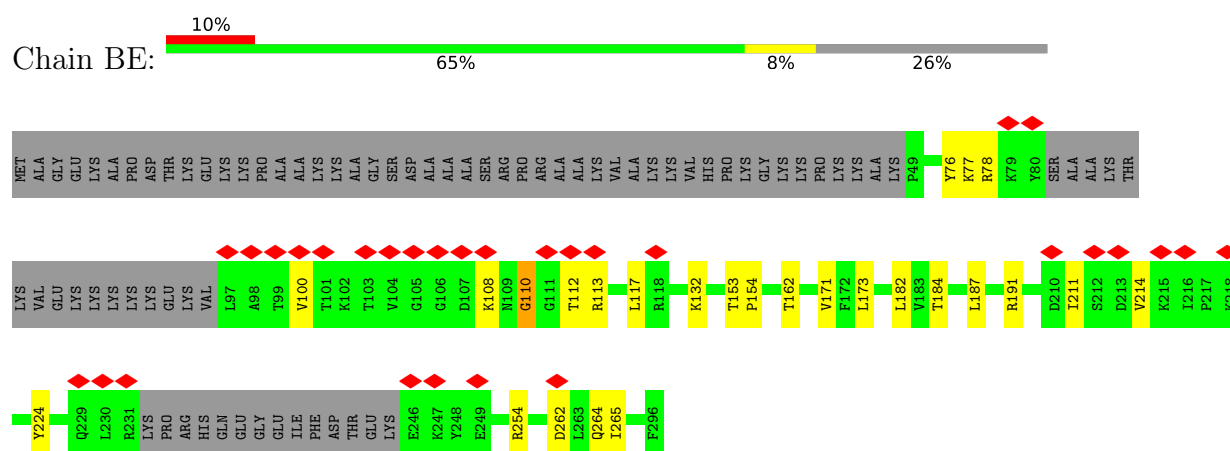
- Molecule 37: Large ribosomal subunit protein uL4



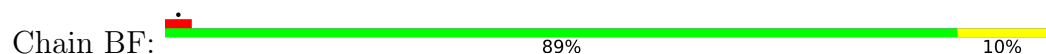
- Molecule 38: Large ribosomal subunit protein uL18

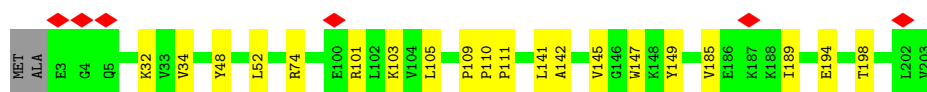


- Molecule 39: Large ribosomal subunit protein eL6

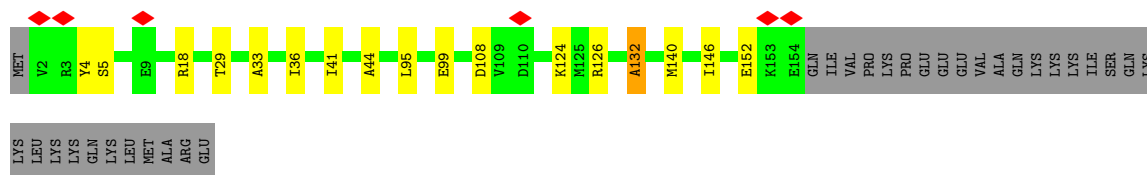
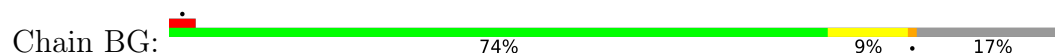


- Molecule 40: Large ribosomal subunit protein uL13

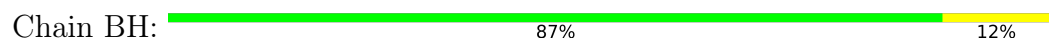




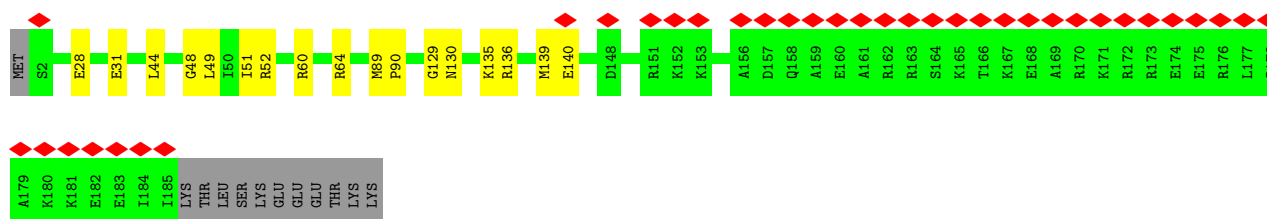
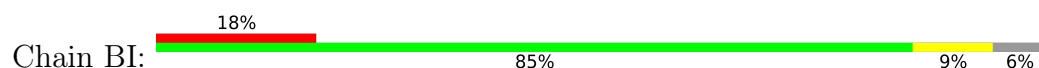
- Molecule 41: Large ribosomal subunit protein uL22



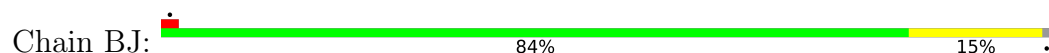
- Molecule 42: Large ribosomal subunit protein eL18



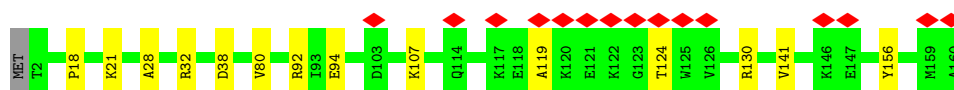
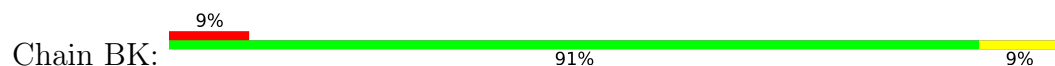
- Molecule 43: Large ribosomal subunit protein eL19



- Molecule 44: Large ribosomal subunit protein eL20



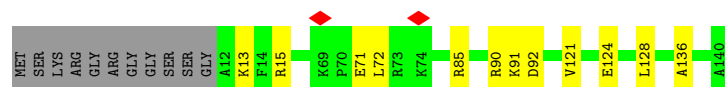
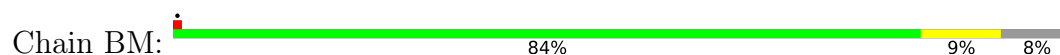
- Molecule 45: Large ribosomal subunit protein eL21



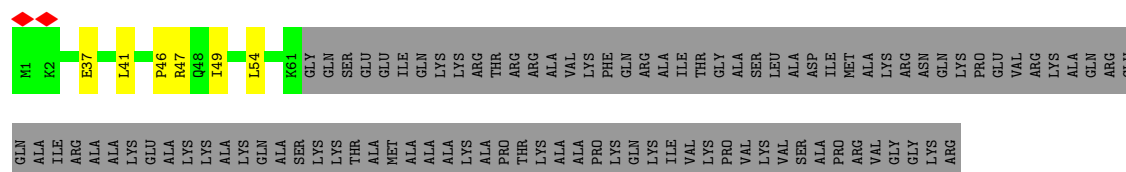
- Molecule 46: Large ribosomal subunit protein eL22



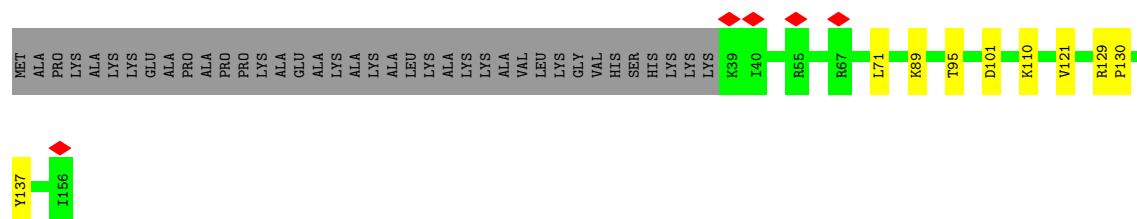
- Molecule 47: Large ribosomal subunit protein uL14



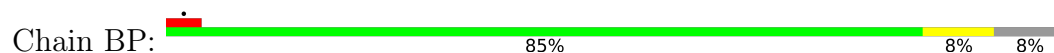
- Molecule 48: Large ribosomal subunit protein eL24



- Molecule 49: Large ribosomal subunit protein uL23



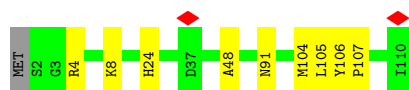
- Molecule 50: Large ribosomal subunit protein uL24



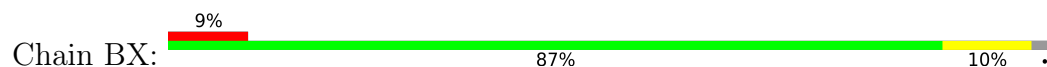
- Molecule 51: Large ribosomal subunit protein eL27



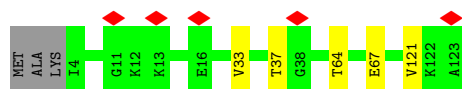




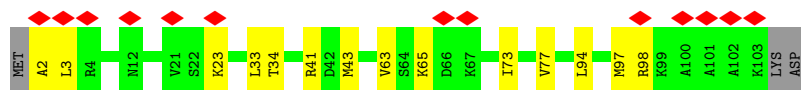
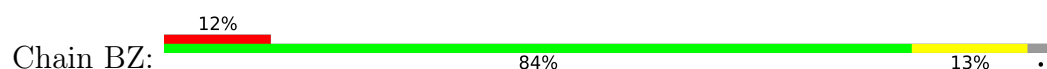
- Molecule 58: Large ribosomal subunit protein eL34



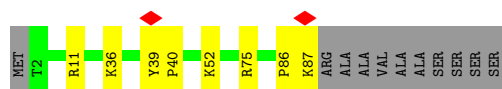
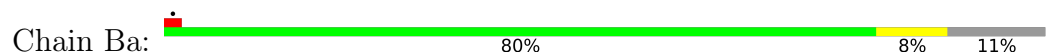
- Molecule 59: Large ribosomal subunit protein uL29



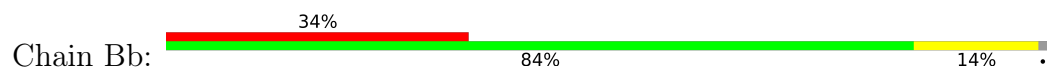
- Molecule 60: Large ribosomal subunit protein eL36



- Molecule 61: Large ribosomal subunit protein eL37



- Molecule 62: Large ribosomal subunit protein eL38



- Molecule 63: Large ribosomal subunit protein eL39



- Molecule 64: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Bd:  38% 59%

MET GLN ILE PHE VAL SER THR LEU THR LEU THR LEU VAL GLU VAL PRO SER ASP THR ILE GLU ASN VAL LYS ALA LYS ILE GLN ASP LYS GLU GLY ILE PRO PRO ASP GLN GLN ARG ARG LEU ILE PHE ALA GLY LYS LYS LEU LEU GLU ASP GLY ARG THR LEU SER ASP TYR ASN

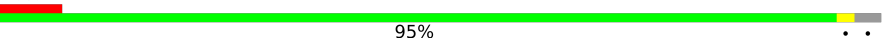
ILE GLN LYS SER THR LEU HIS LEU VAL LEU ARG LEU ARG GLY I77 P80 Q84 N109 N119 K126 V127 K128

- Molecule 65: 60S ribosomal protein L41

Chain Be:  8% 88% 12%

M1 M10 R17 R23 S24 K25

- Molecule 66: Large ribosomal subunit protein eL42

Chain Bf:  8% 95%

MET Y2 P5 R9 S32 R76 C77 R78 D96 R99 K100 G101 Q102 V103 I104 GLN PHE

- Molecule 67: Large ribosomal subunit protein eL43

Chain Bg:  83% 14%

MET ALA R4 T16 R17 Y18 V26 C42 M47 V52 C57 C60 M61 L89 K90 D91 Q92

- Molecule 68: Large ribosomal subunit protein eL28

Chain Bh:  5% 88% 9%

MET S2 A55 D56 G57 K58 N85 A88 S92 M96 V124 V125 V126 LYS ARG LYS ARG THR ARG PRO THR LYS SER SER

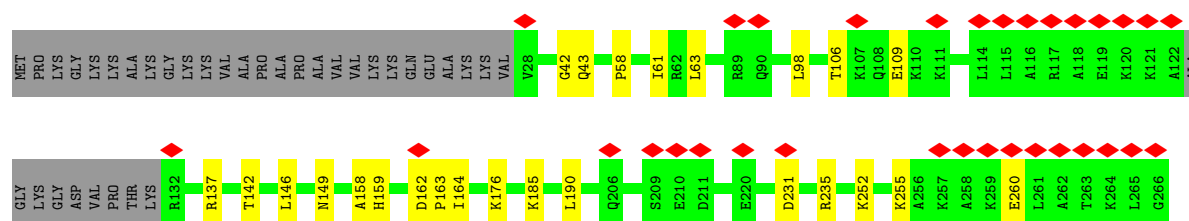
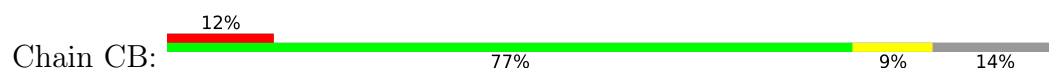
- Molecule 69: Large ribosomal subunit protein uL30

Chain CA:  5% 71% 11% 18%

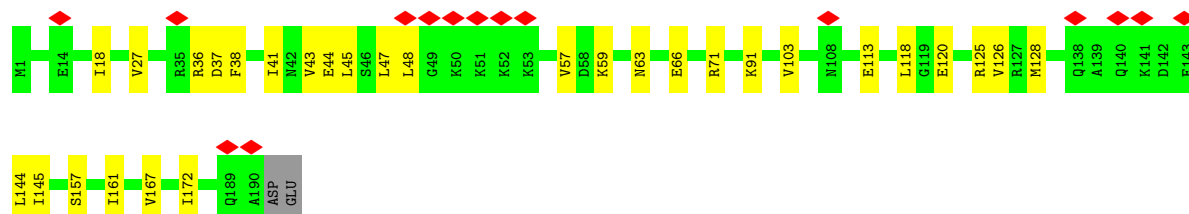
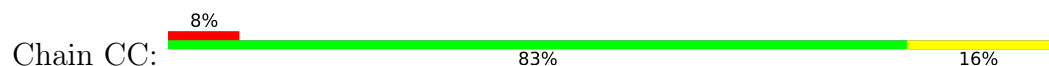
MET GLU ALA VAL PRO GLU LYS LYS VAL ALA THR VAL PRO GLY THR LEU LYS LYS VAL PRO ALA GLY PRO LYS THR LEU LYS LYS VAL VAL PRO GLU THR LYS LYS ARG ARG ASN PHE ALA E49 L50 K51 V52 K53 R54 L55 R56 K57 K58 F59 A60

L61 K81 Q85 P109 A112 I120 S124 R128 L147 I152 H153 M154 I157 Y166 K170 E174 S195 R199 F204 E215 K221 R222 R239 M242 T247 H248 D254 R258 Q261 R264 N270

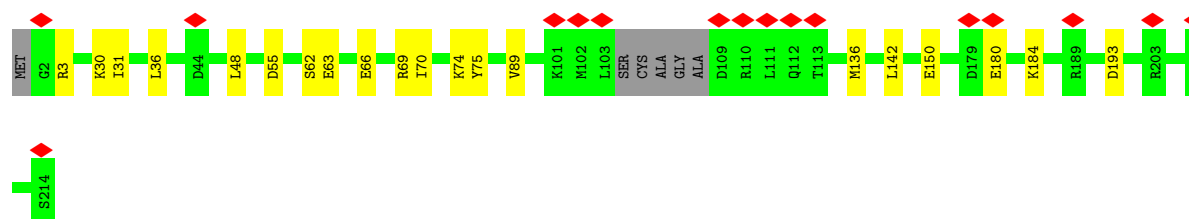
- Molecule 70: Large ribosomal subunit protein eL8



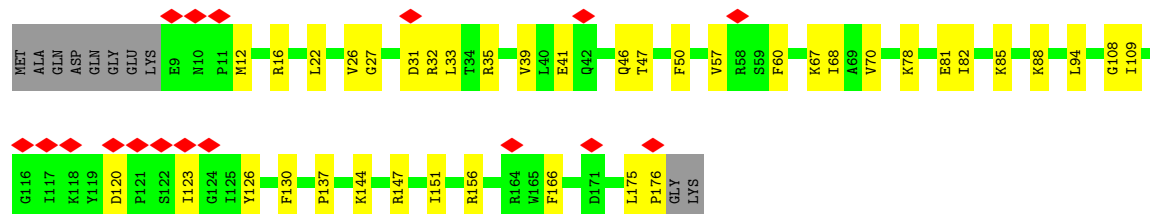
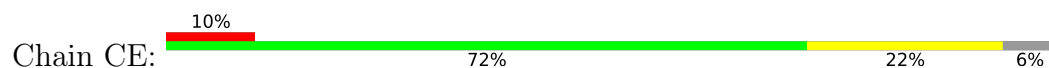
- Molecule 71: Large ribosomal subunit protein uL6



- Molecule 72: Large ribosomal subunit protein uL16-like



- Molecule 73: Large ribosomal subunit protein uL5

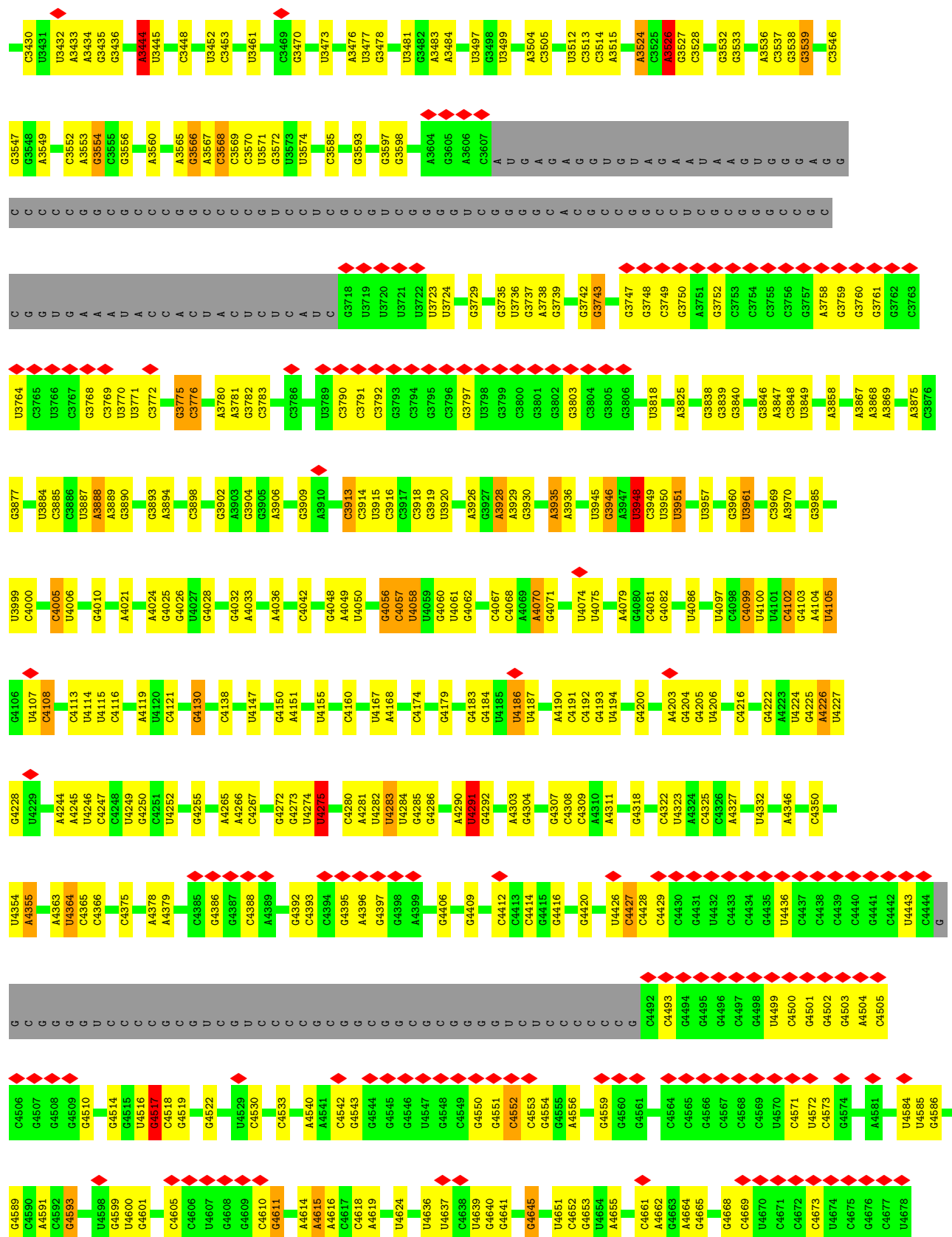


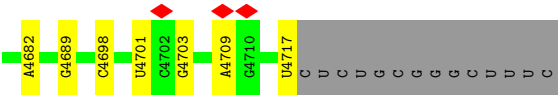
- Molecule 74: Large ribosomal subunit protein eL13



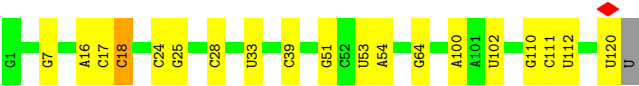
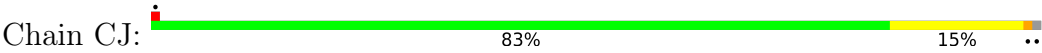




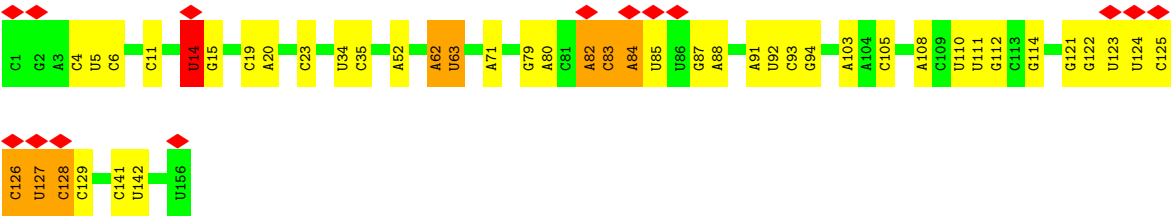




• Molecule 78: 5S rRNA



• Molecule 79: 5.8S rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58407	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 ($e^-/\text{\AA}^2$)	60.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.310	Depositor
Minimum map value	-2.130	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	589.824, 589.824, 589.824	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.152, 1.152, 1.152	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8W, P7G, 5MC, I4U, 1MA, E6G, A2M, B8Q, B8N, OMG, UR3, OMC, ZN, MHG, B8T, MLZ, 2MG, 4AC, B9H, B9B, E7G, 6MZ, OMU, G7M, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.19	0/508	0.45	0/680
2	AB	0.20	0/466	0.46	0/618
3	AC	0.15	1/40063 (0.0%)	0.29	0/62440
4	AE	0.16	0/1784	0.40	0/2402
5	AH	0.22	0/1094	0.56	0/1469
6	AJ	0.22	0/1516	0.43	0/2037
7	AK	0.19	0/843	0.48	0/1137
8	AL	0.22	0/1026	0.49	0/1373
9	AM	0.24	0/1161	0.54	0/1553
10	AN	0.17	0/1208	0.43	0/1618
11	AO	0.17	0/1122	0.37	0/1503
12	AP	0.17	0/817	0.45	0/1097
13	AT	0.17	0/2493	0.45	0/3394
14	AX	0.18	0/673	0.35	0/907
15	Ac	0.18	0/604	0.46	0/810
16	Af	0.13	0/515	0.39	0/682
17	AD	0.17	0/1765	0.39	0/2362
18	AF	0.15	0/2118	0.37	0/2849
19	AG	0.13	0/1220	0.34	0/1633
20	AI	0.16	0/1731	0.38	0/2352
21	AQ	0.15	0/645	0.32	0/863
22	AR	0.16	0/1116	0.44	0/1490
23	AS	0.23	0/828	0.43	0/1109
24	AU	0.20	0/1762	0.41	0/2382
25	AV	0.20	0/1863	0.45	0/2481
26	AW	0.17	0/1258	0.41	0/1683
27	AY	0.21	0/1232	0.40	0/1656
28	AZ	0.24	0/1015	0.46	0/1361
29	Aa	0.18	0/1051	0.41	0/1406
30	Ab	0.26	0/1015	0.51	0/1348
31	Ad	0.16	0/665	0.46	0/890

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ae	0.18	0/93	0.41	0/123
33	Ag	0.19	0/1499	0.42	0/2007
34	Ah	0.16	0/1715	0.42	0/2287
35	BA	0.17	0/1959	0.40	0/2627
36	BB	0.17	0/3264	0.41	0/4368
37	BC	0.18	0/2971	0.40	0/3987
38	BD	0.16	0/2431	0.38	0/3256
39	BE	0.19	0/1799	0.43	2/2413 (0.1%)
40	BF	0.19	0/1670	0.40	0/2232
41	BG	0.17	0/1268	0.41	0/1700
42	BH	0.17	0/1535	0.40	0/2048
43	BI	0.19	0/1558	0.39	0/2059
44	BJ	0.19	0/1490	0.46	0/2000
45	BK	0.15	0/1327	0.34	0/1771
46	BL	0.17	0/839	0.41	0/1126
47	BM	0.15	0/983	0.35	0/1319
48	BN	0.14	0/528	0.32	0/703
49	BO	0.18	0/984	0.39	0/1323
50	BP	0.17	0/1132	0.36	0/1504
51	BQ	0.15	0/1130	0.38	0/1507
52	BR	0.17	0/1193	0.35	0/1593
53	BS	0.20	0/828	0.42	0/1091
54	BT	0.16	0/742	0.39	0/996
55	BU	0.18	0/903	0.41	0/1216
56	BV	0.15	0/910	0.30	0/1216
57	BW	0.16	0/895	0.38	0/1198
58	BX	0.18	0/916	0.39	0/1221
59	BY	0.18	0/1009	0.41	0/1332
60	BZ	0.17	0/843	0.41	0/1115
61	Ba	0.19	0/720	0.40	0/952
62	Bb	0.21	0/574	0.39	0/760
63	Bc	0.19	0/454	0.39	0/599
64	Bd	0.15	0/425	0.34	0/561
65	Be	0.20	0/240	0.44	0/305
66	Bf	0.15	0/855	0.37	0/1128
67	Bg	0.18	0/704	0.35	0/935
68	Bh	0.17	0/1016	0.39	0/1363
69	CA	0.17	0/1888	0.39	0/2516
70	CB	0.20	0/1898	0.44	0/2553
71	CC	0.16	0/1537	0.41	0/2065
72	CD	0.15	0/1728	0.36	0/2306
73	CE	0.19	0/1372	0.46	0/1836
74	CF	0.17	0/1707	0.40	0/2286

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	CG	0.31	1/1165 (0.1%)	0.61	6/1558 (0.4%)
76	CH	0.16	0/1746	0.36	0/2338
77	CI	0.15	3/83322 (0.0%)	0.27	0/129924
78	CJ	0.13	0/2858	0.26	0/4455
79	CK	0.16	0/3679	0.29	0/5732
All	All	0.16	5/221479 (0.0%)	0.34	8/325095 (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
5	AH	0	1
10	AN	0	1
28	AZ	0	1
65	Be	0	1
75	CG	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	1140	A2M	O3'-P	5.34	1.61	1.56
75	CG	56	GLN	CD-OE1	5.26	1.33	1.23
77	CI	3444	A2M	O3'-P	5.13	1.61	1.56
3	AC	669	A2M	O3'-P	5.12	1.61	1.56
77	CI	4226	A2M	O3'-P	5.05	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	CG	56	GLN	N-CA-CB	8.76	123.28	110.06
75	CG	56	GLN	CB-CA-C	-5.40	100.40	109.53
75	CG	56	GLN	N-CA-C	5.36	118.66	110.20
75	CG	56	GLN	CA-C-N	5.29	128.74	120.75
75	CG	56	GLN	C-N-CA	5.29	128.74	120.75
39	BE	108	LYS	CA-C-N	-5.27	115.26	121.90
39	BE	108	LYS	C-N-CA	-5.27	115.26	121.90
75	CG	56	GLN	CG-CD-NE2	-5.03	108.86	116.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AH	5	ARG	Sidechain
10	AN	99	LEU	Peptide
28	AZ	66	ARG	Sidechain
65	Be	23	ARG	Sidechain
75	CG	55	MET	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	506	536	536	14	0
2	AB	455	447	446	9	0
3	AC	36183	18258	18277	239	0
4	AE	1756	1851	1851	23	0
5	AH	1080	1135	1135	30	0
6	AJ	1495	1549	1549	34	0
7	AK	819	842	842	13	0
8	AL	1006	1047	1047	10	0
9	AM	1143	1213	1213	29	0
10	AN	1190	1249	1249	24	0
11	AO	1104	1139	1139	23	0
12	AP	807	874	874	21	0
13	AT	2436	2393	2393	58	0
14	AX	668	690	690	6	0
15	Ac	598	656	656	16	0
16	Af	505	506	505	6	0
17	AD	1738	1806	1809	28	0
18	AF	2076	2177	2177	31	0
19	AG	1199	1269	1269	10	0
20	AI	1694	1696	1696	19	0
21	AQ	638	635	635	7	0
22	AR	1098	1168	1167	9	0
23	AS	811	864	863	8	0
24	AU	1725	1815	1815	32	0
25	AV	1840	1989	1989	41	0
26	AW	1238	1339	1339	22	0
27	AY	1208	1294	1294	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	AZ	1002	1021	1021	18	0
29	Aa	1034	1080	1080	13	0
30	Ab	998	1060	1065	28	0
31	Ad	652	676	676	8	0
32	Ae	93	101	101	0	0
33	Ag	1477	1567	1567	27	0
34	Ah	1686	1772	1772	31	0
35	BA	1921	2022	2022	22	0
36	BB	3197	3343	3342	39	0
37	BC	2928	3110	3110	30	0
38	BD	2385	2409	2409	21	0
39	BE	1766	1902	1902	21	0
40	BF	1640	1790	1790	13	0
41	BG	1242	1274	1274	13	0
42	BH	1511	1637	1636	17	0
43	BI	1542	1698	1698	9	0
44	BJ	1450	1488	1488	17	0
45	BK	1299	1370	1368	10	0
46	BL	825	850	850	18	0
47	BM	969	1031	1031	8	0
48	BN	515	530	530	5	0
49	BO	967	1040	1040	6	0
50	BP	1115	1205	1205	9	0
51	BQ	1107	1182	1182	6	0
52	BR	1164	1213	1213	7	0
53	BS	813	884	884	7	0
54	BT	732	769	769	5	0
55	BU	888	929	929	8	0
56	BV	895	971	971	5	0
57	BW	876	912	912	9	0
58	BX	906	997	997	8	0
59	BY	1001	1138	1138	3	0
60	BZ	832	917	917	10	0
61	Ba	705	737	737	6	0
62	Bb	568	635	635	7	0
63	Bc	444	483	483	1	0
64	Bd	430	465	465	4	0
65	Be	239	289	289	2	0
66	Bf	842	911	912	2	0
67	Bg	694	738	738	13	0
68	Bh	1001	1067	1066	3	0
69	CA	1851	1988	1988	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	CB	1863	2003	2003	20	0
71	CC	1519	1603	1603	19	0
72	CD	1690	1745	1745	13	0
73	CE	1349	1383	1383	29	0
74	CF	1676	1777	1777	19	0
75	CG	1143	1217	1217	16	0
76	CH	1701	1749	1749	11	0
77	CI	76342	38567	38467	433	0
78	CJ	2558	1295	1296	8	0
79	CK	3315	1682	1685	21	0
80	AB	1	0	0	0	0
80	AS	1	0	0	0	0
80	Af	1	0	0	0	0
80	Ba	1	0	0	0	0
80	Bd	1	0	0	0	0
80	Bf	1	0	0	0	0
80	Bg	1	0	0	0	0
81	AC	2	0	0	0	0
81	CB	1	0	0	0	0
81	CI	1	0	0	0	0
All	All	208385	154659	154582	1702	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1702) 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)
77:CI:2542:B9H:N3	77:CI:2542:B9H:C4	1.70	1.50
10:AN:118:ARG:HE	10:AN:123:LEU:HD21	1.30	0.95
77:CI:4274:U:O2'	77:CI:4275:OMU:H6	1.69	0.92
10:AN:15:VAL:HG23	10:AN:68:ILE:HD11	1.52	0.88
77:CI:2542:B9H:C4	77:CI:2542:B9H:C2	2.53	0.86
49:BO:71:LEU:HD11	49:BO:101:ASP:OD2	1.75	0.85
9:AM:102:GLU:OE2	13:AT:58:ALA:HB2	1.77	0.85
4:AE:106:ARG:HG3	4:AE:175:VAL:HG22	1.58	0.84
10:AN:15:VAL:HG12	10:AN:20:ILE:HD13	1.62	0.81
34:Ah:158:ILE:HG21	34:Ah:162:LEU:HD23	1.63	0.80
3:AC:1173:U:H4'	65:Be:10:MET:HE2	1.64	0.79
37:BC:134:PRO:HA	37:BC:150:LEU:HD11	1.65	0.78
46:BL:56:LEU:HD12	46:BL:61:VAL:HG23	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AO:8:ASP:OD1	11:AO:9:VAL:HG13	1.84	0.78
77:CI:1129:C:H2'	77:CI:1130:G:C8	2.20	0.76
36:BB:56:ILE:HD12	36:BB:365:LEU:HD21	1.69	0.74
13:AT:39:THR:HG22	13:AT:60:ARG:HD2	1.70	0.74
75:CG:104:MET:HE3	75:CG:109:ARG:HG2	1.70	0.74
4:AE:123:LEU:HD11	4:AE:152:PHE:HB3	1.71	0.73
23:AS:47:ALA:O	23:AS:50:VAL:HG12	1.89	0.73
13:AT:241:PHE:HE1	13:AT:248:LEU:HD13	1.55	0.72
10:AN:15:VAL:CG2	10:AN:68:ILE:HD11	2.19	0.71
33:Ag:134:VAL:HG12	33:Ag:136:PRO:O	1.91	0.71
36:BB:57:VAL:HG22	36:BB:367:PHE:HB3	1.72	0.71
77:CI:4225:G:H2'	77:CI:4226:A2M:H8	1.71	0.71
77:CI:3312:A:C2	77:CI:3351:A:H4'	2.26	0.71
74:CF:58:ILE:HG23	74:CF:70:VAL:HG11	1.72	0.71
12:AP:24:LEU:CD2	12:AP:112:VAL:HG12	2.20	0.70
13:AT:195:LEU:HD22	13:AT:209:SER:OG	1.90	0.70
57:BW:106:TYR:HB2	57:BW:107:PRO:HD3	1.74	0.70
73:CE:78:LYS:O	73:CE:82:ILE:HD12	1.92	0.70
13:AT:241:PHE:CE1	13:AT:248:LEU:HD13	2.26	0.70
25:AV:209:TYR:CE2	25:AV:213:LEU:HD11	2.26	0.70
59:BY:121:VAL:O	74:CF:150:LEU:HD11	1.90	0.70
62:Bb:8:ILE:HD13	62:Bb:56:LEU:HD11	1.75	0.69
8:AL:64:LYS:HZ1	8:AL:89:MET:HA	1.56	0.69
10:AN:118:ARG:NE	10:AN:123:LEU:HD21	2.05	0.69
1:AA:56:LEU:HD21	6:AJ:140:ASP:OD2	1.93	0.69
37:BC:297:GLU:OE2	42:BH:128:LEU:HD22	1.92	0.69
3:AC:1126:C:OP1	5:AH:129:LYS:HD3	1.93	0.68
26:AW:63:LEU:HD11	26:AW:69:ARG:NH1	2.07	0.68
33:Ag:76:GLN:O	33:Ag:80:VAL:HG23	1.93	0.68
36:BB:223:THR:HG22	36:BB:338:VAL:HG23	1.75	0.68
26:AW:87:LEU:HD13	26:AW:100:LEU:HD21	1.74	0.68
37:BC:8:ILE:HD11	37:BC:24:LEU:HB2	1.75	0.68
8:AL:60:LEU:HD23	8:AL:76:VAL:HG21	1.75	0.67
2:AB:46:TYR:O	2:AB:50:ILE:HD12	1.94	0.67
30:Ab:37:LYS:HD2	30:Ab:57:VAL:HG23	1.75	0.67
75:CG:136:LEU:O	75:CG:136:LEU:HD23	1.94	0.67
70:CB:137[A]:ARG:HD2	70:CB:146:LEU:HD11	1.77	0.67
3:AC:439:G:N2	3:AC:456:A:N1	2.42	0.67
17:AD:103:MET:SD	17:AD:188:LEU:HD21	2.35	0.67
71:CC:103:VAL:HG11	71:CC:144:LEU:HD21	1.75	0.67
18:AF:147:ILE:HG21	18:AF:169:ILE:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:3381:G:H2'	77:CI:3382:A2M:H8	1.75	0.67
15:Ac:69:THR:OG1	15:Ac:72:VAL:HG23	1.95	0.66
24:AU:164:PRO:HB2	24:AU:248:TYR:HE2	1.59	0.66
33:Ag:43:LEU:HD22	33:Ag:72:PHE:CE1	2.30	0.66
34:Ah:119:LEU:HD12	34:Ah:120:PRO:HD2	1.76	0.66
45:BK:119:ALA:HB1	45:BK:124:THR:O	1.95	0.66
34:Ah:62:VAL:HG11	34:Ah:75:LYS:HE2	1.77	0.66
77:CI:4070:1MA:N6	77:CI:4082:G:HO2'	1.94	0.66
56:BV:24:GLN:OE1	77:CI:1129:C:H5'	1.96	0.66
10:AN:15:VAL:CG1	10:AN:20:ILE:HD13	2.26	0.65
25:AV:7:PHE:CE2	25:AV:9:ALA:HB3	2.30	0.65
42:BH:39:THR:HG22	42:BH:41:SER:H	1.61	0.65
36:BB:143:LYS:O	36:BB:147:GLU:OE1	2.14	0.65
5:AH:12:ALA:O	5:AH:16:ILE:HD12	1.95	0.65
75:CG:56:GLN:HB3	77:CI:4517:OMG:C8	2.32	0.65
77:CI:4274:U:HO2'	77:CI:4275:OMU:H6	1.61	0.65
6:AJ:135:ARG:HH22	28:AZ:66:ARG:HD3	1.62	0.65
34:Ah:110:ARG:HG2	34:Ah:121:LEU:HD21	1.79	0.65
54:BT:34:THR:HG23	54:BT:95:ALA:HB2	1.78	0.65
17:AD:71:LEU:HD13	17:AD:84:PHE:CE2	2.32	0.65
48:BN:47:ARG:NH1	48:BN:54:LEU:HD21	2.12	0.64
24:AU:155:ILE:HG22	24:AU:159:LYS:NZ	2.12	0.64
39:BE:187:LEU:HD12	39:BE:191:ARG:HA	1.79	0.64
77:CI:454:U:H2'	77:CI:455:C:C6	2.33	0.64
10:AN:20:ILE:CG2	10:AN:29:ALA:HB1	2.28	0.64
18:AF:147:ILE:HG21	18:AF:169:ILE:CD1	2.27	0.64
60:BZ:43:MET:HE1	70:CB:176:LYS:HG3	1.78	0.64
77:CI:3377:A2M:H2	77:CI:3593:G:O4'	1.98	0.64
70:CB:162:ASP:HB2	70:CB:163:PRO:HD3	1.80	0.64
77:CI:4551:G:H2'	77:CI:4552:C:C6	2.33	0.64
10:AN:20:ILE:HG23	10:AN:29:ALA:HB1	1.81	0.63
30:Ab:117:VAL:HG23	30:Ab:121:ALA:HB2	1.80	0.63
76:CH:200:LEU:HD22	76:CH:204:ARG:HH12	1.62	0.63
33:Ag:69:LEU:HD21	33:Ag:132:ASP:OD1	1.98	0.63
37:BC:134:PRO:CA	37:BC:150:LEU:HD11	2.28	0.63
35:BA:70:LYS:HG2	77:CI:2350:C:H5''	1.81	0.63
49:BO:89:LYS:HG2	49:BO:95:THR:HG23	1.79	0.62
33:Ag:20:GLU:HA	33:Ag:23:ILE:HG22	1.79	0.62
3:AC:1553:G:H3'	3:AC:1554:C:H5''	1.82	0.62
5:AH:17:ILE:HD11	5:AH:54:VAL:HG13	1.81	0.62
10:AN:33:ILE:HG22	10:AN:35:GLY:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Aa:38:LEU:HD23	29:Aa:41:MET:CE	2.29	0.62
39:BE:211:ILE:O	39:BE:211:ILE:HG22	1.99	0.62
68:Bh:85:ASN:OD1	68:Bh:88:ALA:HB3	2.00	0.62
4:AE:113:LEU:HD23	4:AE:118:ALA:HB2	1.81	0.61
25:AV:124:LEU:HD12	25:AV:125:THR:OG1	2.00	0.61
25:AV:137:ARG:O	25:AV:141:ILE:HD12	1.99	0.61
33:Ag:36:LEU:HB3	33:Ag:40:LEU:HD23	1.82	0.61
60:BZ:73:ILE:O	60:BZ:77:VAL:HG22	1.99	0.61
40:BF:32:LYS:HD3	40:BF:101:ARG:HG3	1.80	0.61
77:CI:661:C:H2'	77:CI:662:C:C6	2.35	0.61
77:CI:1129:C:H42	77:CI:1138:A:P	2.23	0.61
21:AQ:9:VAL:HG11	24:AU:177:PRO:HD3	1.81	0.61
30:Ab:94:HIS:HE1	30:Ab:96:LEU:HD12	1.65	0.61
4:AE:48:ILE:HD11	4:AE:86:LEU:HD11	1.83	0.61
15:Ac:84:ALA:O	15:Ac:88:LEU:HD13	2.01	0.61
37:BC:10:VAL:HG22	37:BC:153:VAL:HG11	1.83	0.61
39:BE:112:THR:O	39:BE:113:ARG:HD2	2.00	0.61
77:CI:2542:B9H:C4	77:CI:2542:B9H:C31	2.76	0.61
77:CI:2112:U:C5'	79:CK:14:OMU:HM21	2.31	0.61
9:AM:31:LEU:HD21	9:AM:33:LYS:HG3	1.83	0.61
36:BB:248:LEU:HD23	77:CI:2594:G:OP1	2.00	0.61
74:CF:125:ILE:HG22	74:CF:143:GLU:OE2	2.00	0.61
4:AE:54:ARG:HG3	4:AE:57:ASN:HB2	1.81	0.61
20:AI:84:GLN:O	20:AI:88:LEU:HD23	2.00	0.61
27:AY:40:LEU:HB3	27:AY:45:LEU:HD12	1.83	0.61
3:AC:1588:G:C6	11:AO:78:ILE:HD11	2.35	0.61
68:Bh:92:SER:O	68:Bh:96:MET:HG3	2.01	0.61
13:AT:39:THR:HG22	13:AT:60:ARG:CD	2.31	0.60
13:AT:275:ILE:O	13:AT:277:THR:HG23	2.01	0.60
47:BM:13:LYS:HD2	47:BM:128:LEU:HD11	1.84	0.60
29:Aa:36:ARG:HD2	29:Aa:110:ILE:HD12	1.82	0.60
43:BI:129:GLY:O	43:BI:130:ASN:OD1	2.19	0.60
43:BI:136:ARG:O	43:BI:140:GLU:OE1	2.19	0.60
12:AP:20:ILE:HD11	12:AP:114:VAL:CG1	2.31	0.60
30:Ab:58:PHE:HE1	30:Ab:74:MET:HE1	1.66	0.60
74:CF:46:ILE:HD11	74:CF:51:ALA:HA	1.83	0.60
77:CI:3312:A:N1	77:CI:3351:A:H4'	2.17	0.60
78:CJ:28:C:H1'	78:CJ:54:A:H61	1.67	0.60
75:CG:56:GLN:HB3	77:CI:4517:OMG:N7	2.17	0.60
74:CF:23:ASP:OD2	76:CH:197:THR:HG21	2.01	0.60
3:AC:1417:C:HO2'	11:AO:4:VAL:N	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AU:272:HIS:O	24:AU:276:THR:HG23	2.02	0.59
35:BA:231:ALA:HB1	77:CI:3326:C:H5'	1.83	0.59
48:BN:47:ARG:CZ	48:BN:54:LEU:HD21	2.32	0.59
1:AA:11:LEU:HD23	1:AA:57:THR:HA	1.84	0.59
2:AB:14:PHE:HA	3:AC:1557:A:C2	2.36	0.59
7:AK:47:LYS:O	7:AK:50:GLN:HG2	2.02	0.59
20:AI:77:ILE:HD12	20:AI:122:LEU:HD11	1.85	0.59
35:BA:180:LEU:HD11	67:Bg:26:VAL:HG21	1.84	0.59
38:BD:209:ARG:O	38:BD:213:GLU:OE1	2.19	0.59
60:BZ:63:VAL:HG21	60:BZ:65:LYS:HE2	1.84	0.59
50:BP:51:LYS:O	50:BP:52:ASP:OD2	2.20	0.59
51:BQ:87:VAL:HG11	51:BQ:89:ILE:HD12	1.84	0.59
71:CC:118:LEU:HD11	71:CC:167:VAL:HG12	1.84	0.59
72:CD:36:LEU:HD11	72:CD:69:ARG:HD2	1.85	0.59
12:AP:24:LEU:HD23	12:AP:112:VAL:HG12	1.84	0.59
20:AI:42:LYS:HE2	20:AI:48:ILE:HD11	1.84	0.59
24:AU:166:ARG:HB2	24:AU:248:TYR:CD1	2.38	0.59
62:Bb:13:LEU:HD23	62:Bb:16:ARG:NH2	2.18	0.59
15:Ac:113:THR:O	15:Ac:113:THR:HG22	2.02	0.59
74:CF:58:ILE:HG23	74:CF:70:VAL:CG1	2.32	0.59
72:CD:69:ARG:HA	72:CD:136:MET:HE1	1.84	0.58
3:AC:64:A:H2	3:AC:83:A:H62	1.50	0.58
46:BL:63:ILE:HG23	46:BL:70:ILE:HG23	1.85	0.58
9:AM:42:ILE:HG22	9:AM:48:GLN:OE1	2.03	0.58
6:AJ:28:VAL:HG11	6:AJ:41:VAL:HG11	1.86	0.58
33:Ag:26:ALA:O	33:Ag:30:LEU:HD23	2.04	0.58
42:BH:3:VAL:HG12	69:CA:120:ILE:HD13	1.86	0.58
72:CD:193:ASP:O	72:CD:193:ASP:OD1	2.22	0.58
4:AE:32:ASP:HA	4:AE:54:ARG:HD2	1.85	0.58
7:AK:95:ARG:O	7:AK:96:ARG:HG3	2.04	0.58
58:BX:93:ARG:O	58:BX:97:ILE:HD12	2.03	0.58
70:CB:106:THR:OG1	70:CB:109:GLU:OE1	2.13	0.58
3:AC:572:U:OP1	30:Ab:37:LYS:HG3	2.02	0.58
14:AX:64:LEU:HD11	16:Af:106:TYR:CD2	2.38	0.58
30:Ab:90:ARG:HA	30:Ab:93:ARG:HD2	1.86	0.57
77:CI:472:C:H2'	77:CI:473:C:C6	2.39	0.57
3:AC:637:C:C4	3:AC:638:U:C4	2.92	0.57
24:AU:209:VAL:HB	24:AU:210:PRO:HD3	1.86	0.57
55:BU:87:ARG:HG3	55:BU:109:VAL:CG2	2.34	0.57
4:AE:198:ILE:O	4:AE:198:ILE:HG22	2.05	0.57
6:AJ:99:ILE:HG23	15:Ac:67:LEU:HD22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AM:100:VAL:HG12	9:AM:101:ASP:H	1.68	0.57
24:AU:166:ARG:HB2	24:AU:248:TYR:CE1	2.39	0.57
5:AH:79:GLU:CD	5:AH:80:ARG:H	2.11	0.57
13:AT:134:THR:HG22	13:AT:134:THR:O	2.02	0.57
37:BC:144:ILE:HG21	37:BC:150:LEU:CD2	2.35	0.57
57:BW:48:ALA:HB3	57:BW:104:MET:HE2	1.87	0.57
25:AV:215:LYS:O	25:AV:219:GLU:OE1	2.23	0.57
69:CA:147:LEU:HD22	69:CA:152:ILE:HD11	1.86	0.57
3:AC:120:U:H1'	18:AF:33:THR:HG23	1.85	0.57
9:AM:116:ASP:OD1	9:AM:118:THR:HG22	2.03	0.57
34:Ah:43:ILE:HD11	34:Ah:60:LEU:HD21	1.86	0.57
26:AW:84:ILE:HD11	26:AW:148:ILE:HG21	1.86	0.57
77:CI:1685:OMG:O2'	77:CI:1686:C:P	2.62	0.57
3:AC:439:G:N2	3:AC:456:A:C2	2.73	0.57
3:AC:1589:A:H2'	3:AC:1590:A:C8	2.40	0.57
6:AJ:138:ALA:HB2	6:AJ:203:ASN:OD1	2.05	0.57
19:AG:90:ARG:HD2	19:AG:109:MET:HE3	1.87	0.57
64:Bd:80:PRO:O	64:Bd:84:GLN:OE1	2.23	0.57
77:CI:739:A:H62	77:CI:827:G:H21	1.52	0.57
77:CI:1122:C:H2'	77:CI:1123:C:C6	2.40	0.56
9:AM:6:PRO:C	9:AM:7:LEU:HD23	2.30	0.56
73:CE:12:MET:CE	78:CJ:51:G:H21	2.19	0.56
77:CI:1153:U:H2'	77:CI:1154:C:C6	2.40	0.56
3:AC:102:A:H4'	3:AC:104:A:C8	2.40	0.56
31:Ad:67:THR:HG21	31:Ad:72:ARG:NH1	2.20	0.56
38:BD:4:VAL:HG11	77:CI:3902:G:H5'	1.87	0.56
33:Ag:69:LEU:O	33:Ag:73:GLN:HG3	2.06	0.56
64:Bd:109:ASN:ND2	77:CI:1749:U:H2'	2.20	0.56
77:CI:2447:U:C2	77:CI:2448:U:C5	2.93	0.56
4:AE:113:LEU:HD11	4:AE:117:ARG:HD2	1.86	0.56
12:AP:97:ILE:O	12:AP:97:ILE:HG22	2.05	0.56
30:Ab:34:THR:HG21	30:Ab:62:THR:OG1	2.05	0.56
3:AC:1204:G:H2'	3:AC:1205:A:C8	2.41	0.56
67:Bg:42:CYS:HB3	67:Bg:60:CYS:SG	2.46	0.56
3:AC:1228:G:C2	3:AC:1229:A:C8	2.93	0.56
22:AR:28:LYS:HE2	22:AR:32:LEU:HD22	1.88	0.56
30:Ab:94:HIS:CE1	30:Ab:96:LEU:HD12	2.41	0.56
29:Aa:47:ILE:HD11	29:Aa:65:LEU:HD23	1.87	0.56
33:Ag:43:LEU:HD22	33:Ag:72:PHE:CD1	2.41	0.56
3:AC:1661:C:H4'	3:AC:1664:A:H62	1.71	0.55
13:AT:129:ILE:HG22	13:AT:142:VAL:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BH:42:THR:HA	42:BH:45:GLN:OE1	2.04	0.55
72:CD:48:LEU:HB2	72:CD:142:LEU:HD23	1.87	0.55
13:AT:191:HIS:CD2	13:AT:195:LEU:HD21	2.41	0.55
26:AW:84:ILE:HG23	26:AW:86:VAL:HG13	1.88	0.55
27:AY:31:ASP:O	27:AY:35:GLU:HG2	2.07	0.55
73:CE:39:VAL:HA	73:CE:123:ILE:HD11	1.89	0.55
3:AC:368:U:H4'	3:AC:372:A:C8	2.42	0.55
6:AJ:68:ILE:CD1	6:AJ:151:ILE:HD11	2.36	0.55
7:AK:50:GLN:O	7:AK:53:LYS:HG2	2.07	0.55
47:BM:91:LYS:O	47:BM:92:ASP:CG	2.49	0.55
26:AW:84:ILE:HD11	26:AW:148:ILE:CG2	2.37	0.55
30:Ab:20:ARG:HD2	30:Ab:74:MET:CG	2.36	0.55
9:AM:52:LEU:O	9:AM:56:LEU:HD23	2.07	0.55
27:AY:115:LEU:O	27:AY:119:GLU:HG3	2.07	0.55
43:BI:48:GLY:O	43:BI:51:ILE:HD11	2.07	0.55
54:BT:38:ILE:HD11	54:BT:46:VAL:HG21	1.89	0.55
25:AV:208:GLU:O	25:AV:211:LYS:HG2	2.07	0.55
3:AC:982:A:H2'	3:AC:983:G:C8	2.42	0.55
13:AT:54:ILE:HG23	13:AT:55:PRO:HD2	1.89	0.55
39:BE:78:ARG:O	53:BS:116:LEU:HD22	2.07	0.55
7:AK:27:VAL:HG13	7:AK:43:LEU:HD13	1.89	0.55
25:AV:197:GLN:O	25:AV:200:LYS:HG2	2.07	0.55
26:AW:63:LEU:HD11	26:AW:69:ARG:HH12	1.71	0.55
4:AE:7:LYS:O	4:AE:10:LYS:HG2	2.07	0.54
6:AJ:32:ASP:OD2	6:AJ:35:LEU:HD13	2.07	0.54
6:AJ:68:ILE:HD11	6:AJ:151:ILE:HD11	1.88	0.54
13:AT:173:LEU:HD23	13:AT:175:LYS:HE3	1.88	0.54
13:AT:309:VAL:HG13	13:AT:309:VAL:O	2.07	0.54
35:BA:219:ILE:HG22	35:BA:221:LYS:O	2.07	0.54
46:BL:47:ILE:HG21	46:BL:56:LEU:HD13	1.87	0.54
1:AA:45:ASN:O	6:AJ:139:VAL:HG13	2.07	0.54
17:AD:103:MET:HG2	17:AD:215:VAL:HB	1.90	0.54
34:Ah:113:TYR:HD2	34:Ah:121:LEU:HD22	1.73	0.54
37:BC:153:VAL:HG22	37:BC:257:PHE:CE2	2.42	0.54
46:BL:91:LEU:HD12	46:BL:96:LEU:HB3	1.88	0.54
73:CE:26:VAL:CG2	73:CE:33:LEU:HD23	2.36	0.54
77:CI:2234:C:C5	77:CI:2235:G:C8	2.95	0.54
6:AJ:25:THR:O	6:AJ:28:VAL:HG12	2.07	0.54
37:BC:345:ARG:O	37:BC:349:LEU:HD13	2.07	0.54
77:CI:938:U:H2'	77:CI:939:C:C6	2.43	0.54
77:CI:939:C:H2'	77:CI:940:C:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:1140:A2M:H2'	77:CI:1141:C:C6	2.43	0.54
77:CI:4056:G:H2'	77:CI:4057:C:H6	1.72	0.54
36:BB:57:VAL:HG12	36:BB:73:VAL:HG22	1.89	0.54
56:BV:66:THR:O	56:BV:66:THR:HG22	2.07	0.54
77:CI:3568:OMC:C5	77:CI:3569:C:C5	2.95	0.54
5:AH:87:GLU:HG2	5:AH:88:VAL:HG23	1.89	0.54
18:AF:184:THR:O	18:AF:184:THR:HG22	2.07	0.54
36:BB:60:VAL:HG21	36:BB:67:VAL:HG13	1.88	0.54
77:CI:4290:A:H3'	77:CI:4291:PSU:H4'	1.90	0.54
11:AO:114:GLU:OE1	11:AO:124:THR:HG22	2.07	0.54
46:BL:17:GLN:HG3	46:BL:18:VAL:H	1.73	0.54
61:Ba:39:TYR:HB3	61:Ba:40:PRO:HD3	1.89	0.54
69:CA:147:LEU:HD22	69:CA:152:ILE:CD1	2.38	0.54
74:CF:55:ILE:HG22	74:CF:96:ILE:HA	1.90	0.54
15:Ac:58:LEU:HD12	15:Ac:62:VAL:HG21	1.90	0.54
24:AU:69:LEU:O	24:AU:72:ASP:OD1	2.26	0.54
27:AY:11:LEU:O	27:AY:11:LEU:HD23	2.08	0.54
1:AA:59:LEU:HD21	6:AJ:122:ARG:CZ	2.38	0.54
18:AF:20:LEU:HD21	18:AF:46:ILE:HD12	1.90	0.54
11:AO:127:GLY:O	11:AO:131:LEU:HD13	2.08	0.54
18:AF:184:THR:C	18:AF:189:LEU:HD13	2.33	0.54
36:BB:58:ARG:HD2	36:BB:363:ILE:HG23	1.91	0.53
46:BL:56:LEU:HD12	46:BL:61:VAL:CG2	2.36	0.53
77:CI:1146:C:H2'	77:CI:1147:A:H8	1.71	0.53
3:AC:116:OMU:O5'	3:AC:116:OMU:H6	2.09	0.53
3:AC:1619:C:H4'	8:AL:50:ARG:HH22	1.73	0.53
9:AM:102:GLU:OE1	13:AT:55:PRO:HB2	2.07	0.53
17:AD:44:ILE:HD11	17:AD:86:LEU:HD12	1.90	0.53
46:BL:82:TYR:CD1	77:CI:2387:U:H2'	2.43	0.53
77:CI:2388:U:C2	77:CI:2389:U:C5	2.97	0.53
30:Ab:117:VAL:HG23	30:Ab:121:ALA:CB	2.39	0.53
34:Ah:62:VAL:HG11	34:Ah:75:LYS:CE	2.39	0.53
36:BB:217:ILE:HD12	36:BB:347:LEU:HB3	1.90	0.53
73:CE:50:PHE:HD1	73:CE:70:VAL:HG12	1.73	0.53
77:CI:1874:C:C2	77:CI:1875:C:C5	2.97	0.53
3:AC:1229:A:H2'	3:AC:1230:G:C8	2.44	0.53
3:AC:1293:C:C2	3:AC:1294:A:C8	2.97	0.53
23:AS:49:ALA:O	23:AS:53:ILE:HD12	2.08	0.53
25:AV:193:ALA:O	25:AV:197:GLN:HG3	2.09	0.53
36:BB:223:THR:HG22	36:BB:338:VAL:CG2	2.39	0.53
42:BH:176:ARG:O	52:BR:56:VAL:HG21	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:CA:52:VAL:HG11	77:CI:1085:C:O2	2.08	0.53
76:CH:165:THR:HG22	76:CH:166:SER:N	2.23	0.53
3:AC:818:G:N2	3:AC:819:A:H62	2.07	0.53
38:BD:93:THR:HG22	38:BD:93:THR:O	2.08	0.53
77:CI:3915:U:H2'	77:CI:3916:C:C6	2.44	0.53
8:AL:70:MET:HG3	8:AL:70:MET:O	2.08	0.53
25:AV:32:MET:SD	25:AV:54:GLY:HA2	2.48	0.53
15:Ac:58:LEU:HD21	15:Ac:87:ALA:HB1	1.91	0.53
25:AV:41:LEU:HD12	25:AV:41:LEU:O	2.09	0.53
71:CC:120:GLU:HG2	77:CI:4266:A:H2	1.73	0.53
72:CD:30:LYS:HG2	72:CD:66:GLU:OE1	2.09	0.53
77:CI:1128:C:O2'	77:CI:1129:C:P	2.67	0.53
5:AH:17:ILE:HD12	5:AH:58:MET:HE2	1.90	0.53
39:BE:162:THR:HG22	57:BW:106:TYR:CE1	2.43	0.53
17:AD:66:VAL:HG13	17:AD:101:HIS:NE2	2.24	0.52
36:BB:303:ALA:HB2	36:BB:314:ILE:HD13	1.91	0.52
39:BE:262:ASP:HA	39:BE:265:ILE:HG22	1.90	0.52
68:Bh:85:ASN:HD22	77:CI:696:C:H4'	1.72	0.52
77:CI:433:A:C2	77:CI:3526:A2M:H4'	2.45	0.52
3:AC:1278:C:H2'	3:AC:1279:A:H8	1.72	0.52
3:AC:1317:C:C2	3:AC:1318:C:C5	2.97	0.52
37:BC:211:TYR:CE2	37:BC:214:ASP:OD1	2.62	0.52
44:BJ:93:MET:HG2	77:CI:1754:G:H4'	1.91	0.52
67:Bg:89:LEU:O	67:Bg:92:GLN:O	2.27	0.52
17:AD:46:LYS:HE3	28:AZ:21:VAL:HG12	1.91	0.52
20:AI:134:LEU:HD22	20:AI:144:THR:HG21	1.90	0.52
42:BH:178:ARG:HD3	52:BR:53:PHE:HB2	1.91	0.52
73:CE:108:GLY:O	73:CE:109:ILE:HD13	2.08	0.52
77:CI:1131:U:C6	77:CI:1131:U:OP1	2.62	0.52
3:AC:573:U:H5'	30:Ab:60:PHE:O	2.10	0.52
45:BK:80:VAL:HG13	45:BK:80:VAL:O	2.09	0.52
53:BS:26:SER:HG	77:CI:1607:A:H2	1.55	0.52
24:AU:210:PRO:HD3	24:AU:236:PHE:HE2	1.74	0.52
26:AW:87:LEU:CD1	26:AW:100:LEU:HD21	2.39	0.52
60:BZ:23:LYS:HE3	74:CF:82:ARG:HH12	1.75	0.52
75:CG:56:GLN:NE2	75:CG:91:TRP:CZ2	2.77	0.52
77:CI:3748:G:C2	77:CI:3749:C:C5	2.98	0.52
3:AC:96:C:H2'	3:AC:97:U:C6	2.44	0.52
5:AH:20:TYR:CD2	5:AH:38:ILE:HD12	2.45	0.52
75:CG:56:GLN:HE22	77:CI:4517:OMG:H2'	1.75	0.52
76:CH:46:ASP:O	76:CH:49:ARG:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:218:C:C2	3:AC:219:A:C8	2.98	0.52
25:AV:41:LEU:HD12	25:AV:45:TRP:CD1	2.44	0.52
25:AV:147:LEU:HD22	25:AV:151:ASP:OD2	2.10	0.52
29:Aa:51:GLU:OE1	31:Ad:8:LEU:HD13	2.09	0.52
67:Bg:16:THR:HG22	77:CI:2632:G:C8	2.45	0.52
77:CI:4282:U:C2	77:CI:4283:PSU:C6	2.98	0.52
3:AC:858:U:H2'	3:AC:859:A:C8	2.44	0.52
14:AX:64:LEU:HD11	16:Af:106:TYR:CG	2.44	0.52
20:AI:158:ASP:OD2	21:AQ:32:ILE:HD13	2.09	0.52
25:AV:5:ILE:CG2	25:AV:113:ILE:HD11	2.40	0.52
70:CB:252:LYS:O	70:CB:255:LYS:HG2	2.09	0.52
3:AC:1825:A:H2'	77:CI:3419:A:H61	1.75	0.52
77:CI:3566:G:N3	77:CI:3568:OMC:C4	2.78	0.52
3:AC:1619:C:H4'	8:AL:50:ARG:HH12	1.73	0.52
12:AP:46:LYS:O	12:AP:46:LYS:HG3	2.09	0.52
17:AD:103:MET:SD	17:AD:188:LEU:HD11	2.50	0.52
77:CI:1128:C:O2'	77:CI:1129:C:C6	2.54	0.52
77:CI:3395:A:H2'	77:CI:3396:A:C8	2.44	0.52
3:AC:322:C:C2	3:AC:323:C:C5	2.98	0.51
73:CE:94:LEU:HD12	73:CE:166:PHE:CZ	2.45	0.51
8:AL:97:TYR:CZ	8:AL:99:GLY:O	2.64	0.51
9:AM:28:GLY:HA3	9:AM:67:ASP:OD2	2.10	0.51
24:AU:266:TYR:O	24:AU:270:THR:HG22	2.10	0.51
39:BE:100:VAL:HG22	39:BE:117:LEU:HD21	1.91	0.51
77:CI:1437:G:H21	77:CI:1455:A:H1'	1.76	0.51
79:CK:83:C:H4'	79:CK:84:A:OP2	2.10	0.51
4:AE:142:LEU:HD13	4:AE:150:MET:HE2	1.91	0.51
33:Ag:40:LEU:HA	33:Ag:43:LEU:HB2	1.91	0.51
72:CD:55:ASP:OD1	72:CD:55:ASP:O	2.28	0.51
77:CI:2240:A:H61	77:CI:2248:C:H42	1.56	0.51
1:AA:44:ARG:CD	1:AA:58:LEU:HD11	2.41	0.51
46:BL:42:PHE:CZ	46:BL:46:ARG:HD3	2.45	0.51
74:CF:64:VAL:HA	74:CF:67:HIS:HD2	1.75	0.51
20:AI:13:GLU:O	20:AI:17:LYS:HG3	2.11	0.51
77:CI:153:G:H2'	77:CI:154:G:H8	1.75	0.51
77:CI:3415:A:H61	77:CI:3427:U:H3	1.57	0.51
3:AC:1537:G:H2'	3:AC:1538:A:H8	1.75	0.51
7:AK:3:MET:HE2	7:AK:44:HIS:HA	1.93	0.51
24:AU:166:ARG:HB3	24:AU:247:THR:HB	1.93	0.51
51:BQ:29:ILE:HD13	51:BQ:98:LYS:HZ1	1.75	0.51
70:CB:137[A]:ARG:HG2	70:CB:142:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:1121:A:H2'	77:CI:1122:C:H6	1.74	0.51
77:CI:4192:C:H2'	77:CI:4193:G:H8	1.75	0.51
2:AB:13:LYS:HG3	2:AB:14:PHE:CE2	2.45	0.51
3:AC:1165:G:O2'	3:AC:1166:G:H5'	2.11	0.51
24:AU:267:GLN:O	24:AU:270:THR:HG23	2.11	0.51
56:BV:129:LEU:HD23	56:BV:129:LEU:H	1.76	0.51
73:CE:57:VAL:HG11	73:CE:60:PHE:CD2	2.46	0.51
77:CI:1141:C:H2'	77:CI:1142:G:C8	2.46	0.51
77:CI:1682:G:H8	77:CI:1683:C:H2'	1.75	0.51
77:CI:3377:A2M:H2'	77:CI:3378:A:C8	2.46	0.51
77:CI:4114:U:H2'	77:CI:4115:U:C6	2.46	0.51
77:CI:4150:G:C2	77:CI:4151:A:N7	2.79	0.51
2:AB:24:CYS:SG	2:AB:39:CYS:HB3	2.50	0.51
3:AC:1680:A:P	6:AJ:60:ARG:HE	2.34	0.51
10:AN:71:MET:HG2	10:AN:99:LEU:HD13	1.91	0.51
13:AT:17:TRP:CE2	13:AT:303:THR:HG23	2.46	0.51
13:AT:189:ILE:HG13	13:AT:189:ILE:O	2.10	0.51
25:AV:181:THR:HG23	25:AV:182:PRO:HD2	1.91	0.51
30:Ab:9:THR:OG1	30:Ab:23:MET:HB2	2.11	0.51
64:Bd:109:ASN:OD1	64:Bd:119:ASN:HB3	2.11	0.51
77:CI:2221:C:H2'	77:CI:2222:G:O4'	2.11	0.51
5:AH:119:VAL:HG13	5:AH:119:VAL:O	2.11	0.51
19:AG:77:VAL:HG22	19:AG:86:ILE:HD12	1.93	0.51
38:BD:104:LEU:HD13	38:BD:247:ILE:HG23	1.93	0.51
39:BE:112:THR:C	39:BE:113:ARG:HD2	2.36	0.51
71:CC:63:ASN:OD1	71:CC:66:GLU:OE1	2.29	0.51
77:CI:2415:A:C2	77:CI:2432:A:C8	2.99	0.51
3:AC:1061:A:H1'	3:AC:1063:A:N7	2.25	0.50
5:AH:24:LEU:HB2	5:AH:58:MET:HE3	1.92	0.50
35:BA:112:ILE:HG23	35:BA:133:TYR:CD1	2.46	0.50
66:Bf:9:ARG:HD3	77:CI:3945:U:OP1	2.11	0.50
77:CI:1446:G:H5'	77:CI:1447:A:OP1	2.12	0.50
3:AC:1713:A:H2'	3:AC:1714:C:C6	2.47	0.50
5:AH:6:THR:OG1	5:AH:8:THR:HG22	2.11	0.50
5:AH:89:SER:HB3	20:AI:198:MET:HE3	1.93	0.50
18:AF:173:ILE:HD11	18:AF:230:LYS:HA	1.93	0.50
19:AG:126:VAL:HG12	19:AG:145:VAL:HG22	1.93	0.50
70:CB:164:ILE:CG2	76:CH:22:LEU:HD11	2.41	0.50
71:CC:45:LEU:CD2	71:CC:57:VAL:HG22	2.42	0.50
3:AC:929:G:H2'	3:AC:930:G:C8	2.46	0.50
3:AC:1316:U:C2	3:AC:1317:C:C6	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AM:4:LYS:HA	9:AM:27:ARG:HH12	1.76	0.50
11:AO:28:LEU:HD13	11:AO:110:LEU:HD11	1.92	0.50
26:AW:130:ILE:HG21	26:AW:145:PRO:HA	1.92	0.50
30:Ab:118:ARG:HG3	30:Ab:119:GLY:H	1.76	0.50
37:BC:10:VAL:HG13	37:BC:153:VAL:HG12	1.93	0.50
44:BJ:106:VAL:HG13	44:BJ:126:ILE:CD1	2.41	0.50
75:CG:104:MET:HE3	75:CG:109:ARG:CG	2.38	0.50
77:CI:2234:C:C6	77:CI:2235:G:C8	2.99	0.50
33:Ag:43:LEU:HB3	33:Ag:72:PHE:HE1	1.76	0.50
37:BC:144:ILE:HG21	37:BC:150:LEU:HD23	1.94	0.50
55:BU:26:THR:HG21	77:CI:4645:G:OP1	2.11	0.50
77:CI:472:C:C2	77:CI:473:C:C5	2.99	0.50
11:AO:104:LEU:HD13	11:AO:121:ARG:HD2	1.94	0.50
25:AV:216:ARG:HA	25:AV:219:GLU:OE1	2.11	0.50
72:CD:89:VAL:HG22	72:CD:136:MET:HE2	1.93	0.50
77:CI:4061:U:C2	77:CI:4062:G:C8	2.99	0.50
3:AC:1680:A:H2'	6:AJ:60:ARG:HD2	1.93	0.50
5:AH:114:LEU:O	5:AH:117:LEU:HD22	2.12	0.50
14:AX:52:LEU:HD21	14:AX:65:VAL:CG1	2.41	0.50
25:AV:181:THR:HG22	25:AV:183:ARG:H	1.77	0.50
70:CB:58:PRO:HG2	70:CB:61:ILE:HD12	1.93	0.50
77:CI:4517:OMG:HM22	77:CI:4517:OMG:O3'	2.12	0.50
77:CI:4552:C:C4	77:CI:4553:C:C5	3.00	0.50
10:AN:108:ARG:O	10:AN:112:GLU:HG2	2.12	0.50
13:AT:59:LEU:HD23	13:AT:90:TRP:CD2	2.47	0.50
26:AW:74:GLY:O	26:AW:78:LEU:HD13	2.11	0.50
36:BB:285:TYR:CE1	36:BB:363:ILE:HD13	2.46	0.50
73:CE:33:LEU:HD11	73:CE:67:LYS:O	2.12	0.50
77:CI:4346:A:N1	77:CI:4355:A:C8	2.80	0.50
16:Af:118:ARG:HE	16:Af:119:ARG:H	1.60	0.50
20:AI:173:LEU:HD11	20:AI:177:MET:HE2	1.94	0.50
24:AU:207:ALA:O	24:AU:211:LYS:HG3	2.12	0.50
30:Ab:40:ILE:O	30:Ab:44:LEU:HD13	2.12	0.50
77:CI:2540:C:C2	77:CI:2541:C:C5	3.00	0.50
78:CJ:111:C:H2'	78:CJ:112:U:O4'	2.12	0.50
13:AT:224:GLY:O	13:AT:225:LYS:HE2	2.12	0.49
37:BC:292:ILE:O	37:BC:298:ILE:HD12	2.12	0.49
77:CI:3444:A2M:H2	77:CI:4206:U:O2	2.12	0.49
3:AC:1828:U:C2	3:AC:1829:C:C5	3.00	0.49
11:AO:7:LYS:NZ	11:AO:66:LEU:HD22	2.28	0.49
26:AW:80:ARG:O	26:AW:83:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:3893:G:H2'	77:CI:3894:A:H8	1.76	0.49
25:AV:25:ARG:HA	25:AV:28:TYR:HD2	1.77	0.49
34:Ah:29:LEU:C	34:Ah:29:LEU:HD12	2.37	0.49
40:BF:194:GLU:O	40:BF:198:THR:HG23	2.12	0.49
50:BP:74:TYR:HE2	50:BP:77:LYS:HG3	1.77	0.49
67:Bg:16:THR:HG22	77:CI:2632:G:N7	2.26	0.49
77:CI:4192:C:H2'	77:CI:4193:G:C8	2.48	0.49
13:AT:207:CYS:SG	13:AT:221:LEU:HD21	2.53	0.49
3:AC:1537:G:H2'	3:AC:1538:A:C8	2.47	0.49
8:AL:52:LYS:CD	8:AL:80:LEU:HD21	2.42	0.49
9:AM:102:GLU:HG2	9:AM:105:LYS:HD3	1.93	0.49
77:CI:424:U:H2'	77:CI:425:U:H6	1.77	0.49
77:CI:2168:A:H2'	77:CI:2169:U:C6	2.48	0.49
6:AJ:193:LYS:O	6:AJ:197:GLU:HG2	2.13	0.49
13:AT:42:MET:HE2	13:AT:57:ARG:HG2	1.94	0.49
28:AZ:20:GLN:O	28:AZ:20:GLN:HG2	2.12	0.49
30:Ab:56:PHE:CE1	30:Ab:94:HIS:CD2	3.00	0.49
48:BN:46:PRO:HA	48:BN:49:ILE:HD13	1.94	0.49
77:CI:2542:B9H:O2'	77:CI:2543:A:OP2	2.30	0.49
3:AC:289:G:H1	3:AC:296:C:H42	1.60	0.49
3:AC:912:C:O2'	3:AC:913:C:H5'	2.13	0.49
5:AH:34:VAL:O	5:AH:38:ILE:HG12	2.12	0.49
36:BB:268:ARG:HH21	77:CI:3554:G:N2	2.11	0.49
69:CA:154:MET:HA	69:CA:157:ILE:HD12	1.95	0.49
71:CC:113:GLU:HG2	71:CC:125:ARG:HG2	1.94	0.49
77:CI:50:C:C2	77:CI:51:A:C8	3.00	0.49
79:CK:92:U:H2'	79:CK:93:C:O4'	2.13	0.49
3:AC:1019:U:C2	3:AC:1020:C:C5	3.00	0.49
9:AM:102:GLU:O	9:AM:105:LYS:HG2	2.12	0.49
22:AR:49:GLY:HA2	22:AR:75:ILE:HD12	1.94	0.49
24:AU:210:PRO:HD3	24:AU:236:PHE:CE2	2.48	0.49
33:Ag:69:LEU:HD11	33:Ag:132:ASP:OD1	2.13	0.49
73:CE:31:ASP:O	73:CE:35:ARG:HG3	2.12	0.49
77:CI:4266:A:C2	77:CI:4267:C:C5	3.01	0.49
79:CK:14:OMU:HM22	79:CK:15:G:O4'	2.13	0.49
3:AC:854:C:C2	3:AC:855:A:C8	3.01	0.49
3:AC:1271:G:C2	3:AC:1272:C:C5	3.01	0.49
17:AD:97:LEU:HD13	17:AD:229:MET:HE1	1.95	0.49
25:AV:5:ILE:HG22	25:AV:113:ILE:HD11	1.94	0.49
38:BD:50:ARG:NH1	38:BD:52:ILE:HG13	2.27	0.49
70:CB:42:GLY:O	70:CB:43:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:CE:39:VAL:HG22	73:CE:123:ILE:HD11	1.94	0.49
77:CI:2167:C:H2'	77:CI:2168:A:H8	1.78	0.49
77:CI:2383:C:C2	77:CI:2384:U:C6	3.01	0.49
33:Ag:50:GLU:OE2	33:Ag:58:LYS:HD2	2.12	0.49
38:BD:204:VAL:O	38:BD:208:MET:HG3	2.13	0.49
42:BH:125:GLN:O	42:BH:129:GLU:HG3	2.13	0.49
71:CC:18:ILE:HG12	71:CC:27:VAL:HG22	1.95	0.49
3:AC:1438:C:O2'	3:AC:1439:A:P	2.71	0.48
34:Ah:113:TYR:CD2	34:Ah:121:LEU:HD22	2.48	0.48
35:BA:101:VAL:HG22	35:BA:165:VAL:HG22	1.95	0.48
35:BA:102:LEU:HB2	35:BA:107:MET:HE2	1.95	0.48
36:BB:348:ARG:HD2	36:BB:349:LYS:O	2.13	0.48
77:CI:233:U:H1'	77:CI:234:G:C8	2.48	0.48
77:CI:1039:C:N4	77:CI:1040:C:H41	2.11	0.48
10:AN:98:VAL:HG11	10:AN:106:LYS:HD2	1.95	0.48
18:AF:182:MET:HB2	18:AF:228:ILE:HD12	1.95	0.48
24:AU:202:THR:HG23	26:AW:58:ARG:HH22	1.78	0.48
77:CI:1687:G:N2	77:CI:1710:A:N3	2.61	0.48
77:CI:2449:G:H2'	77:CI:2450:G:N2	2.28	0.48
77:CI:3893:G:H2'	77:CI:3894:A:C8	2.48	0.48
3:AC:637:C:H2'	3:AC:638:U:O4'	2.13	0.48
3:AC:1799:C:H2'	3:AC:1800:G:O4'	2.13	0.48
15:Ac:50:PHE:HZ	15:Ac:87:ALA:HB2	1.78	0.48
18:AF:47:PHE:CE2	18:AF:52:LEU:HD11	2.48	0.48
36:BB:348:ARG:NH1	36:BB:351:LEU:HG	2.28	0.48
38:BD:286:SER:O	38:BD:289:ARG:HG2	2.13	0.48
41:BG:33:ALA:HA	41:BG:36:ILE:HG22	1.94	0.48
42:BH:41:SER:O	42:BH:45:GLN:OE1	2.31	0.48
52:BR:134:GLU:O	52:BR:138:LYS:HG2	2.13	0.48
69:CA:242:MET:HB3	69:CA:254:ASP:OD1	2.13	0.48
77:CI:424:U:H2'	77:CI:425:U:C6	2.49	0.48
77:CI:3929:A:H2'	77:CI:3930:G:C8	2.48	0.48
77:CI:4502:G:H2'	77:CI:4503:G:O4'	2.13	0.48
3:AC:805:U:H2'	3:AC:806:U:C6	2.49	0.48
3:AC:1124:C:C2	3:AC:1125:C:C6	3.01	0.48
3:AC:1825:A:N1	3:AC:1827:G:N7	2.61	0.48
4:AE:172:VAL:HG22	4:AE:185:LYS:HG2	1.95	0.48
17:AD:52:THR:HG22	17:AD:58:ALA:H	1.77	0.48
41:BG:41:ILE:HD11	41:BG:99:GLU:CG	2.43	0.48
77:CI:2501:A:H2'	77:CI:2502:A:C8	2.49	0.48
3:AC:997:A:H2'	3:AC:998:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AT:64:HIS:CG	13:AT:65:PHE:H	2.32	0.48
56:BV:84:GLU:O	56:BV:87:VAL:HG22	2.14	0.48
57:BW:4:ARG:NH2	57:BW:8:LYS:HG3	2.29	0.48
77:CI:1121:A:H2'	77:CI:1122:C:C6	2.47	0.48
77:CI:1323:G:H2'	77:CI:1324:C:C6	2.49	0.48
77:CI:2112:U:H5'	79:CK:14:OMU:HM21	1.94	0.48
5:AH:66:VAL:O	5:AH:68:GLY:N	2.47	0.48
26:AW:67:ASP:O	26:AW:71:LEU:HD23	2.13	0.48
29:Aa:38:LEU:HD23	29:Aa:41:MET:HE3	1.94	0.48
59:BY:33:VAL:O	59:BY:37:THR:HG23	2.13	0.48
73:CE:50:PHE:CD1	73:CE:70:VAL:HG12	2.47	0.48
77:CI:944:G:H1	77:CI:1040:C:H42	1.62	0.48
3:AC:219:A:C5	3:AC:220:U:C5	3.02	0.48
3:AC:457:C:N3	3:AC:458:C:C5	2.82	0.48
3:AC:811:A:H3'	3:AC:812:A:C5'	2.44	0.48
3:AC:1149:A:H4'	3:AC:1150:A:O4'	2.14	0.48
3:AC:1843:4AC:O5'	3:AC:1843:4AC:H6	2.12	0.48
18:AF:139:LEU:HD12	18:AF:139:LEU:C	2.38	0.48
28:AZ:137:SER:O	28:AZ:138:ASP:OD1	2.31	0.48
73:CE:85:LYS:O	73:CE:88:LYS:HG2	2.13	0.48
77:CI:1390:G:O2'	77:CI:1425:G:H4'	2.13	0.48
77:CI:4113:C:H2'	77:CI:4114:U:C6	2.48	0.48
3:AC:68:A:N6	3:AC:82:G:C2	2.82	0.48
9:AM:55:VAL:HG22	9:AM:63:PHE:CE2	2.49	0.48
11:AO:18:LEU:HD13	11:AO:134:ILE:HD12	1.95	0.48
13:AT:104:HIS:NE2	13:AT:122:SER:OG	2.45	0.48
18:AF:44:LEU:HD21	18:AF:72:ILE:HD11	1.95	0.48
23:AS:58:VAL:HG13	28:AZ:125:LYS:HB3	1.95	0.48
30:Ab:18:LEU:HD13	30:Ab:20:ARG:CZ	2.44	0.48
50:BP:115:ARG:HA	50:BP:118:ILE:HG12	1.96	0.48
51:BQ:54:THR:H	51:BQ:57:MET:HE3	1.79	0.48
3:AC:1257:G:H8	12:AP:66:ARG:HG2	1.79	0.48
3:AC:1538:A:O2'	3:AC:1605:G:H4'	2.14	0.48
17:AD:143:THR:HB	17:AD:205:TYR:CE2	2.49	0.48
18:AF:97:GLU:OE2	18:AF:113:ARG:HG2	2.14	0.48
29:Aa:32:LYS:O	29:Aa:35:VAL:HG22	2.14	0.48
36:BB:293:ILE:HD11	36:BB:298:LEU:HD13	1.96	0.48
38:BD:62:CYS:HB3	38:BD:105:LEU:HD22	1.95	0.48
3:AC:115:U:H2'	3:AC:116:OMU:C6	2.43	0.48
3:AC:943:G:N2	28:AZ:138:ASP:OD2	2.47	0.48
15:Ac:79:ILE:HD11	15:Ac:83:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BT:40:GLN:HG2	54:BT:42:LYS:HE3	1.95	0.48
77:CI:220:C:O2	77:CI:220:C:H2'	2.14	0.48
1:AA:59:LEU:HD11	6:AJ:122:ARG:HB2	1.96	0.47
3:AC:29:G:H2'	3:AC:30:C:C6	2.49	0.47
12:AP:79:ARG:HG3	12:AP:79:ARG:O	2.14	0.47
36:BB:218:ASP:OD2	36:BB:348:ARG:NH1	2.47	0.47
40:BF:48:TYR:HE1	40:BF:52:LEU:HD11	1.79	0.47
62:Bb:47:ILE:HD11	62:Bb:56:LEU:HD22	1.96	0.47
77:CI:2446:C:H2'	77:CI:2447:U:H6	1.78	0.47
77:CI:3532:G:H2'	77:CI:3533:G:C8	2.49	0.47
77:CI:3749:C:H2'	77:CI:3750:G:O4'	2.14	0.47
77:CI:3935:A:N3	77:CI:3935:A:H2'	2.29	0.47
12:AP:68:THR:HG23	12:AP:70:CYS:O	2.14	0.47
15:Ac:99:LEU:HA	15:Ac:109:TYR:HD1	1.78	0.47
18:AF:19:MET:SD	18:AF:108:ARG:HD2	2.54	0.47
28:AZ:34:PHE:CD1	28:AZ:98:ARG:NH1	2.82	0.47
35:BA:196:TRP:HB3	35:BA:197:PRO:HD3	1.95	0.47
74:CF:60:ARG:HD2	74:CF:67:HIS:O	2.14	0.47
77:CI:3376:A:H2'	77:CI:3377:A2M:C8	2.44	0.47
3:AC:128:U:O4'	3:AC:217:G:C8	2.68	0.47
3:AC:442:C:H2'	3:AC:443:C:C6	2.49	0.47
11:AO:116:ASP:OD1	11:AO:121:ARG:CA	2.62	0.47
36:BB:93:VAL:HG13	36:BB:102:PHE:HB2	1.95	0.47
42:BH:4:ASP:HB2	69:CA:120:ILE:HG21	1.97	0.47
46:BL:87:THR:O	46:BL:91:LEU:HD23	2.14	0.47
69:CA:204:PHE:CD1	69:CA:222:ARG:HG2	2.49	0.47
73:CE:57:VAL:HG11	73:CE:60:PHE:CE2	2.49	0.47
77:CI:201:C:C2	77:CI:202:C:C5	3.02	0.47
77:CI:286:U:H2'	77:CI:287:U:C6	2.48	0.47
3:AC:496:U:H2'	3:AC:497:C:O4'	2.14	0.47
6:AJ:136:ARG:HB3	6:AJ:203:ASN:HD22	1.79	0.47
9:AM:44:PRO:HB2	9:AM:81:ILE:HD11	1.95	0.47
20:AI:182:VAL:O	20:AI:186:ARG:HG3	2.14	0.47
24:AU:65:LYS:NZ	24:AU:273:LEU:HD21	2.29	0.47
31:Ad:48:SER:O	31:Ad:49:HIS:HB2	2.14	0.47
33:Ag:158:LEU:HD12	33:Ag:189:PHE:CE2	2.49	0.47
42:BH:178:ARG:HA	42:BH:184:ARG:O	2.13	0.47
77:CI:473:C:C2	77:CI:474:C:C5	3.03	0.47
3:AC:12:U:H2'	3:AC:13:C:C6	2.50	0.47
3:AC:838:A:H61	30:Ab:9:THR:CG2	2.27	0.47
3:AC:1554:C:OP1	3:AC:1554:C:H3'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AD:46:LYS:CE	28:AZ:21:VAL:HG12	2.44	0.47
36:BB:16:PHE:O	36:BB:19:ARG:HG3	2.15	0.47
36:BB:56:ILE:HD12	36:BB:365:LEU:CD2	2.41	0.47
71:CC:47:LEU:C	71:CC:48:LEU:HD22	2.39	0.47
77:CI:236:G:C2'	77:CI:237:B9B:OP1	2.62	0.47
3:AC:1375:C:H2'	3:AC:1376:G:O4'	2.15	0.47
3:AC:1446:U:O2'	3:AC:1447:A:H8	1.97	0.47
3:AC:1541:G:OP2	11:AO:43:LYS:CE	2.63	0.47
5:AH:13:ALA:O	5:AH:17:ILE:HG12	2.15	0.47
20:AI:147:LEU:HD11	20:AI:163:CYS:SG	2.54	0.47
33:Ag:23:ILE:HG23	33:Ag:24:SER:N	2.29	0.47
50:BP:47:MET:HE1	50:BP:118:ILE:HD12	1.97	0.47
60:BZ:33:LEU:HD13	60:BZ:41:ARG:NH2	2.30	0.47
73:CE:120:ASP:HB3	73:CE:123:ILE:HG22	1.95	0.47
77:CI:717:A:H2'	77:CI:718:C:C6	2.49	0.47
77:CI:1159:G:H2'	77:CI:1160:C:C6	2.49	0.47
77:CI:1682:G:OP2	77:CI:1683:C:H3'	2.15	0.47
3:AC:85:A:H5''	30:Ab:118:ARG:HE	1.79	0.47
3:AC:1629:C:H2'	3:AC:1630:C:C6	2.50	0.47
4:AE:142:LEU:CD1	4:AE:150:MET:HE2	2.45	0.47
6:AJ:200:ALA:O	6:AJ:203:ASN:OD1	2.33	0.47
9:AM:31:LEU:HD21	9:AM:33:LYS:CG	2.45	0.47
17:AD:131:ASP:OD2	17:AD:180:ASP:HB2	2.14	0.47
18:AF:37:LYS:HB2	18:AF:40:GLU:HG2	1.97	0.47
33:Ag:51:ILE:HD11	33:Ag:176:VAL:HG22	1.97	0.47
34:Ah:174:CYS:HB2	34:Ah:190:LEU:HD21	1.97	0.47
36:BB:67:VAL:O	36:BB:67:VAL:HG22	2.15	0.47
38:BD:236:MET:O	38:BD:239:MET:HG2	2.13	0.47
46:BL:63:ILE:HA	46:BL:71:THR:O	2.14	0.47
47:BM:90:ARG:HD3	47:BM:124:GLU:OE2	2.15	0.47
70:CB:146:LEU:O	70:CB:149:ASN:OD1	2.33	0.47
71:CC:167:VAL:CG2	71:CC:172:ILE:HG22	2.44	0.47
77:CI:672:G:H2'	77:CI:672:G:N3	2.30	0.47
77:CI:1131:U:O4'	77:CI:1471:G:OP2	2.33	0.47
77:CI:3323:G:H2'	77:CI:3324:G:H8	1.80	0.47
78:CJ:17:C:H2'	78:CJ:18:C:C6	2.49	0.47
3:AC:1274:C:H1'	3:AC:1276:G:OP1	2.15	0.47
40:BF:147:TRP:CZ2	40:BF:149:TYR:O	2.68	0.47
48:BN:37:GLU:O	48:BN:41:LEU:HD13	2.15	0.47
77:CI:204:U:H2'	77:CI:205:C:H6	1.79	0.47
77:CI:241:G:C5	77:CI:242:U:C5	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:2541:C:C5	77:CI:2542:B9H:N4	2.83	0.47
13:AT:234:ASP:CG	13:AT:235:ILE:H	2.22	0.47
27:AY:89:TYR:CE1	27:AY:150:VAL:HG23	2.50	0.47
42:BH:29:VAL:O	42:BH:33:ARG:HG3	2.14	0.47
43:BI:28:GLU:HG3	43:BI:49:LEU:HD22	1.97	0.47
67:Bg:61:MET:HE3	77:CI:2408:G:H22	1.79	0.47
77:CI:1660:A:C2	77:CI:1661:C:C5	3.03	0.47
3:AC:107:A:H2'	3:AC:108:G:C8	2.50	0.47
3:AC:352:G:C2	3:AC:353:U:C6	3.02	0.47
3:AC:823:PSU:C4	3:AC:828:A:C6	3.01	0.47
3:AC:1273:C:O2'	3:AC:1274:C:H6	1.97	0.47
9:AM:100:VAL:HG12	9:AM:101:ASP:N	2.30	0.47
13:AT:104:HIS:HE2	13:AT:122:SER:HG	1.62	0.47
30:Ab:37:LYS:O	30:Ab:41:ARG:HG3	2.14	0.47
34:Ah:103:LEU:HD23	34:Ah:172:LEU:HD23	1.97	0.47
36:BB:104:THR:HG22	77:CI:4379:A:O2'	2.15	0.47
45:BK:92:ARG:HB3	45:BK:94:GLU:OE1	2.15	0.47
50:BP:89:LYS:HD2	50:BP:95:VAL:HG11	1.96	0.47
71:CC:59:LYS:HE3	71:CC:66:GLU:HG3	1.96	0.47
77:CI:162:A:H2'	77:CI:163:A:C8	2.50	0.47
77:CI:1040:C:C2	77:CI:1041:G:C8	3.03	0.47
77:CI:1475:C:H2'	77:CI:1476:C:C6	2.50	0.47
3:AC:494:A:C2	3:AC:495:C:C6	3.03	0.46
3:AC:561:A:N6	3:AC:589:G:O6	2.49	0.46
3:AC:1406:A:H2'	3:AC:1407:G:O4'	2.16	0.46
5:AH:17:ILE:CD1	5:AH:58:MET:HE2	2.45	0.46
11:AO:99:VAL:O	11:AO:103:VAL:HG23	2.14	0.46
13:AT:178:ASN:C	13:AT:178:ASN:OD1	2.58	0.46
15:Ac:88:LEU:HD23	15:Ac:109:TYR:CD2	2.51	0.46
20:AI:11:LYS:O	20:AI:15:VAL:HG23	2.14	0.46
22:AR:87:ASN:OD1	22:AR:134:TYR:CE1	2.68	0.46
25:AV:3:LEU:HD22	25:AV:111:LEU:CD1	2.45	0.46
26:AW:44:TRP:O	26:AW:47:LYS:HG2	2.14	0.46
41:BG:36:ILE:HD11	41:BG:44:ALA:CB	2.45	0.46
41:BG:124:LYS:HB3	41:BG:140:MET:HE3	1.97	0.46
46:BL:80:LYS:HG2	46:BL:110:TYR:CE1	2.50	0.46
53:BS:100:PRO:HA	53:BS:107:ARG:HH22	1.80	0.46
73:CE:175:LEU:HB2	73:CE:176:PRO:HD2	1.97	0.46
74:CF:78:LEU:O	74:CF:82:ARG:HG3	2.16	0.46
77:CI:174:C:N3	77:CI:175:C:C5	2.83	0.46
3:AC:458:C:C2	3:AC:459:A:C8	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:1706:C:H2'	3:AC:1707:G:C8	2.50	0.46
3:AC:1794:A:C2	3:AC:1795:C:C5	3.02	0.46
4:AE:85:GLU:OE1	4:AE:87:TYR:CE2	2.68	0.46
5:AH:33:ARG:HG3	13:AT:125:ARG:NH1	2.30	0.46
6:AJ:76:MET:HB2	6:AJ:89:THR:HG21	1.97	0.46
36:BB:58:ARG:HB3	36:BB:365:LEU:HD23	1.96	0.46
36:BB:141:THR:O	36:BB:144:LYS:HG2	2.15	0.46
57:BW:104:MET:O	57:BW:105:LEU:HB3	2.16	0.46
77:CI:716:G:H2'	77:CI:717:A:H8	1.80	0.46
77:CI:3946:G:H5''	77:CI:3948:PSU:C6	2.50	0.46
77:CI:4108:C:C2	77:CI:4184:G:C2	3.03	0.46
3:AC:513:A:C2	3:AC:514:G:C8	3.03	0.46
3:AC:1688:C:C2	3:AC:1689:C:C5	3.03	0.46
13:AT:73:SER:O	13:AT:74:ASP:HB2	2.15	0.46
26:AW:88:ASP:O	26:AW:92:MET:HE3	2.16	0.46
58:BX:5:LEU:HD11	58:BX:22:LEU:HD22	1.96	0.46
77:CI:2112:U:H5''	79:CK:14:OMU:HM21	1.96	0.46
77:CI:2255:C:C2	77:CI:2256:U:C6	3.03	0.46
3:AC:1008:C:H2'	3:AC:1009:A:C8	2.51	0.46
3:AC:1598:C:H4'	3:AC:1604:G:O6	2.15	0.46
10:AN:4:VAL:C	10:AN:5:ILE:HG13	2.40	0.46
38:BD:4:VAL:HG11	77:CI:3902:G:C5'	2.45	0.46
69:CA:221:LYS:O	69:CA:222:ARG:HB2	2.15	0.46
38:BD:216:GLU:O	38:BD:220:LYS:HG3	2.15	0.46
39:BE:187:LEU:HD21	77:CI:4586:G:C6	2.51	0.46
45:BK:18:PRO:HB2	45:BK:21:LYS:HG3	1.96	0.46
46:BL:60:VAL:HG13	46:BL:75:GLU:OE2	2.15	0.46
71:CC:91:LYS:HG2	71:CC:145:ILE:CD1	2.46	0.46
73:CE:26:VAL:HG22	73:CE:33:LEU:HD23	1.98	0.46
77:CI:7:C:H2'	77:CI:8:U:C6	2.51	0.46
77:CI:1475:C:H2'	77:CI:1476:C:H6	1.81	0.46
77:CI:1836:G:H2'	77:CI:1837:C:C6	2.51	0.46
11:AO:39:LEU:HD13	11:AO:47:PRO:HG3	1.96	0.46
13:AT:83:TRP:HA	13:AT:107:ASP:HA	1.96	0.46
35:BA:125:LYS:HD3	77:CI:3340:G:O6	2.16	0.46
37:BC:150:LEU:HB2	37:BC:151:PRO:HD3	1.96	0.46
39:BE:187:LEU:HD21	77:CI:4586:G:C5	2.51	0.46
40:BF:48:TYR:CE1	40:BF:52:LEU:HD11	2.51	0.46
60:BZ:43:MET:HE1	70:CB:176:LYS:CG	2.43	0.46
77:CI:1281:C:H2'	77:CI:1282:C:H6	1.80	0.46
77:CI:2300:G:N7	79:CK:126:C:N4	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:4651:U:H2'	77:CI:4652:C:C6	2.51	0.46
2:AB:13:LYS:HG3	2:AB:14:PHE:CD2	2.51	0.46
12:AP:28:ASN:OD1	12:AP:28:ASN:O	2.34	0.46
14:AX:51:VAL:O	14:AX:108:CYS:HA	2.16	0.46
18:AF:44:LEU:HD11	18:AF:72:ILE:HD11	1.97	0.46
21:AQ:64:GLU:HG3	31:Ad:3:LEU:HG	1.98	0.46
24:AU:262:THR:HG22	24:AU:263:LYS:N	2.30	0.46
36:BB:356:LYS:HG3	36:BB:359:ALA:H	1.80	0.46
72:CD:3:ARG:NH2	77:CI:4086:U:OP2	2.49	0.46
77:CI:938:U:H2'	77:CI:939:C:H6	1.78	0.46
77:CI:2141:U:C2	77:CI:2142:U:C5	3.04	0.46
77:CI:4099:C:C2	77:CI:4100:U:C5	3.03	0.46
79:CK:19:C:H2'	79:CK:20:A:C8	2.51	0.46
3:AC:295:U:H3'	3:AC:296:C:C5'	2.45	0.46
3:AC:394:U:HO2'	3:AC:395:G:H8	1.61	0.46
3:AC:1395:G:H2'	3:AC:1396:C:O2	2.16	0.46
12:AP:32:LEU:HD21	12:AP:87:ARG:HG2	1.98	0.46
34:Ah:103:LEU:HD13	34:Ah:170:LYS:HD3	1.98	0.46
47:BM:85:ARG:HD3	77:CI:2603:G:OP1	2.16	0.46
51:BQ:100:VAL:HG13	51:BQ:106:LEU:C	2.40	0.46
59:BY:64:THR:O	59:BY:67:GLU:HG2	2.15	0.46
69:CA:57:LYS:O	69:CA:61:LEU:HG	2.15	0.46
70:CB:159:HIS:CE1	70:CB:185:LYS:HD3	2.50	0.46
71:CC:71:ARG:HG2	77:CI:4346:A:H4'	1.96	0.46
77:CI:1128:C:H41	77:CI:1138:A:C5'	2.29	0.46
77:CI:1875:C:C2	77:CI:1876:C:C5	3.04	0.46
77:CI:3566:G:C2	77:CI:3568:OMC:C4	2.89	0.46
1:AA:8:PRO:HB2	1:AA:10:LYS:HE3	1.97	0.46
7:AK:27:VAL:O	7:AK:27:VAL:HG12	2.16	0.46
10:AN:18:THR:O	10:AN:20:ILE:HD12	2.16	0.46
17:AD:71:LEU:HD13	17:AD:84:PHE:CD2	2.51	0.46
35:BA:135:THR:HB	35:BA:149:LYS:HG2	1.98	0.46
35:BA:245:ARG:NH1	77:CI:3315:A:H5''	2.31	0.46
39:BE:78:ARG:NH1	77:CI:881:U:C5	2.84	0.46
43:BI:135:LYS:HG2	43:BI:139:MET:HE3	1.97	0.46
60:BZ:34:THR:HG21	77:CI:276:C:H5'	1.98	0.46
61:Ba:86:PRO:O	61:Ba:87:LYS:C	2.58	0.46
77:CI:2432:A:OP1	77:CI:2432:A:O4'	2.34	0.46
77:CI:4615:A:H2'	77:CI:4616:A:C8	2.51	0.46
3:AC:1846:A:H2'	3:AC:1847:G:C8	2.51	0.46
4:AE:200:PRO:O	4:AE:201:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AK:5:LYS:O	7:AK:9:ILE:HG12	2.16	0.46
9:AM:97:GLN:HB3	9:AM:105:LYS:CE	2.46	0.46
10:AN:36:VAL:HG13	10:AN:40:TYR:HD2	1.81	0.46
10:AN:85:ASN:H	10:AN:97:GLN:HG2	1.81	0.46
20:AI:29:ASN:O	20:AI:150:THR:HG23	2.16	0.46
53:BS:111:ALA:O	53:BS:115:ARG:HG2	2.16	0.46
57:BW:48:ALA:CB	57:BW:104:MET:HE2	2.46	0.46
77:CI:1708:U:H2'	77:CI:1709:A:H8	1.81	0.46
77:CI:2048:C:H2'	77:CI:2049:U:C6	2.51	0.46
77:CI:2611:G:C2'	77:CI:2612:C:OP2	2.64	0.46
3:AC:1798:U:H2'	3:AC:1799:C:C6	2.50	0.45
9:AM:32:ILE:HG21	9:AM:39:LEU:HD11	1.96	0.45
15:Ac:79:ILE:HD11	15:Ac:83:LEU:HD23	1.98	0.45
16:Af:121:CYS:SG	16:Af:146:LEU:HD23	2.56	0.45
20:AI:110:ASN:O	20:AI:113:GLN:OE1	2.34	0.45
22:AR:47:ALA:O	22:AR:102:VAL:HG22	2.16	0.45
25:AV:2:LYS:HG2	25:AV:17:GLU:OE1	2.16	0.45
37:BC:209:ILE:HB	37:BC:229:LEU:HD13	1.97	0.45
77:CI:2167:C:H2'	77:CI:2168:A:C8	2.51	0.45
77:CI:4308:C:C2	77:CI:4309:C:C5	3.04	0.45
3:AC:1316:U:C4	3:AC:1317:C:C5	3.05	0.45
3:AC:1396:C:C2	3:AC:1475:A:C2	3.04	0.45
3:AC:1534:A:C2	3:AC:1537:G:N3	2.84	0.45
5:AH:75:GLU:O	5:AH:79:GLU:HB2	2.16	0.45
13:AT:62:HIS:HD2	13:AT:82:SER:HB2	1.81	0.45
18:AF:103:TYR:CD2	18:AF:189:LEU:HD11	2.51	0.45
25:AV:113:ILE:H	25:AV:113:ILE:HD12	1.81	0.45
27:AY:99:ARG:NH2	27:AY:119:GLU:OE2	2.49	0.45
37:BC:350:ARG:O	37:BC:354:LEU:HD23	2.16	0.45
77:CI:1430:G:H1'	77:CI:2269:A:N6	2.31	0.45
1:AA:60:GLU:HG2	6:AJ:204:ARG:HD3	1.98	0.45
3:AC:593:C:H3'	3:AC:594:C:H5''	1.98	0.45
10:AN:84:LEU:HD22	10:AN:97:GLN:HG3	1.97	0.45
13:AT:32:LEU:HD13	13:AT:71:ILE:HD11	1.97	0.45
15:Ac:73:VAL:HG21	15:Ac:88:LEU:HD11	1.99	0.45
26:AW:82:VAL:HG22	26:AW:92:MET:HE1	1.98	0.45
28:AZ:80:ASP:C	28:AZ:80:ASP:OD1	2.59	0.45
33:Ag:128:ALA:HA	33:Ag:131:GLU:HG2	1.97	0.45
52:BR:34:ASN:O	77:CI:94:A:H5''	2.15	0.45
74:CF:91:ALA:HB1	74:CF:96:ILE:HB	1.97	0.45
77:CI:1523:G:H2'	77:CI:1524:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:2655:C:H2'	77:CI:2656:U:C6	2.51	0.45
77:CI:3343:G:H2'	77:CI:3344:C:C6	2.51	0.45
77:CI:3918:C:H2'	77:CI:3919:G:O4'	2.17	0.45
2:AB:24:CYS:SG	2:AB:26:ASN:HB3	2.57	0.45
13:AT:64:HIS:ND1	13:AT:83:TRP:HB2	2.32	0.45
17:AD:57:ILE:HD12	70:CB:260:GLU:OE2	2.16	0.45
19:AG:55:TYR:CD2	19:AG:115:PRO:HG2	2.50	0.45
33:Ag:8:ILE:HG22	33:Ag:8:ILE:O	2.17	0.45
34:Ah:158:ILE:CG2	34:Ah:162:LEU:HD23	2.39	0.45
38:BD:41:LYS:HE2	38:BD:41:LYS:HA	1.99	0.45
77:CI:174:C:C2	77:CI:175:C:C6	3.04	0.45
77:CI:3259:G:H2'	77:CI:3260:C:H6	1.81	0.45
77:CI:3526:A2M:HM'2	77:CI:3526:A2M:H1'	1.81	0.45
77:CI:4193:G:H2'	77:CI:4194:U:C6	2.51	0.45
3:AC:1309:U:HO2'	3:AC:1310:C:H6	1.57	0.45
31:Ad:47:PHE:CE1	31:Ad:48:SER:O	2.70	0.45
41:BG:5:SER:HA	79:CK:11:C:O2'	2.16	0.45
41:BG:29:THR:HG21	41:BG:146:ILE:HD11	1.98	0.45
58:BX:93:ARG:O	58:BX:97:ILE:CD1	2.64	0.45
77:CI:1128:C:H41	77:CI:1138:A:H5''	1.82	0.45
77:CI:1146:C:H2'	77:CI:1147:A:C8	2.50	0.45
77:CI:2542:B9H:N3	77:CI:2542:B9H:C5	2.57	0.45
3:AC:1857:C:H2'	3:AC:1858:G:C8	2.52	0.45
24:AU:206:SER:HB3	24:AU:224:THR:CG2	2.46	0.45
71:CC:118:LEU:CD1	71:CC:167:VAL:HG12	2.46	0.45
13:AT:248:LEU:HD23	13:AT:259:TRP:HE3	1.81	0.45
29:Aa:104:LEU:HD23	29:Aa:125:ILE:HA	1.98	0.45
43:BI:51:ILE:HG22	43:BI:52:ARG:N	2.31	0.45
77:CI:3315:A:H2'	77:CI:3316:U:H6	1.81	0.45
77:CI:3352:U:C2	77:CI:3353:U:C6	3.05	0.45
77:CI:3571:U:O2'	77:CI:3572:G:H5'	2.16	0.45
77:CI:4249:U:C2	77:CI:4250:G:C8	3.05	0.45
3:AC:906:C:H2'	3:AC:907:U:C6	2.52	0.45
3:AC:959:G:H2'	3:AC:960:G:C8	2.51	0.45
3:AC:1628:C:H2'	3:AC:1629:C:H6	1.82	0.45
13:AT:229:THR:C	13:AT:230:LEU:HD12	2.42	0.45
19:AG:65:ASN:CG	19:AG:65:ASN:O	2.60	0.45
36:BB:82:PRO:HG3	36:BB:171:LEU:HD21	1.99	0.45
37:BC:109:ARG:HD2	37:BC:111:TRP:CH2	2.52	0.45
77:CI:1697:G:H2'	77:CI:1698:A:O4'	2.17	0.45
3:AC:350:A:H2'	3:AC:351:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:986:G:C1'	28:AZ:138:ASP:OD2	2.65	0.45
3:AC:1390:C:C2	3:AC:1391:U:C5	3.05	0.45
3:AC:1830:G:H2'	3:AC:1831:UR3:C6	2.47	0.45
4:AE:58:VAL:HG12	4:AE:66:ILE:HD11	1.99	0.45
24:AU:164:PRO:HB2	24:AU:248:TYR:CE2	2.46	0.45
39:BE:214:VAL:HG13	39:BE:264:GLN:CD	2.42	0.45
70:CB:231:ASP:O	70:CB:235:ARG:HG3	2.17	0.45
77:CI:3376:A:H2'	77:CI:3377:A2M:H8	1.98	0.45
2:AB:14:PHE:HA	3:AC:1557:A:N1	2.32	0.45
3:AC:334:G:OP2	25:AV:190:ARG:CD	2.65	0.45
3:AC:438:G:C6	3:AC:439:G:C6	3.04	0.45
3:AC:570:A:H2'	3:AC:571:C:O4'	2.17	0.45
3:AC:1047:U:H2'	3:AC:1048:C:C6	2.51	0.45
6:AJ:76:MET:HB2	6:AJ:89:THR:CG2	2.47	0.45
13:AT:129:ILE:CG2	13:AT:142:VAL:HB	2.47	0.45
13:AT:260:ASP:OD1	13:AT:262:GLU:OE1	2.35	0.45
18:AF:136:ILE:O	18:AF:136:ILE:HG13	2.17	0.45
34:Ah:6:ASP:OD2	34:Ah:8:TRP:NE1	2.50	0.45
36:BB:280:ILE:HD13	77:CI:4332:U:C4	2.52	0.45
37:BC:61:GLN:O	61:Ba:52:LYS:CE	2.65	0.45
37:BC:268:ARG:HD3	77:CI:662:C:OP1	2.17	0.45
77:CI:3950:U:H2'	77:CI:3951:U:H5'	1.98	0.45
77:CI:4246:U:H2'	77:CI:4247:C:C6	2.52	0.45
77:CI:4618:C:C2	77:CI:4619:A:C8	3.05	0.45
6:AJ:179:ASN:HB3	6:AJ:186:ASN:OD1	2.17	0.44
10:AN:83:PHE:CD1	10:AN:83:PHE:O	2.70	0.44
17:AD:124:HIS:HA	17:AD:137:LEU:O	2.17	0.44
18:AF:52:LEU:HD23	18:AF:54:TYR:CE1	2.52	0.44
33:Ag:72:PHE:O	33:Ag:76:GLN:HG3	2.17	0.44
44:BJ:15:ARG:HB3	44:BJ:27:LEU:HD23	1.99	0.44
50:BP:74:TYR:HD2	50:BP:77:LYS:HB2	1.82	0.44
67:Bg:47:MET:SD	67:Bg:57:CYS:HB2	2.56	0.44
73:CE:32:ARG:HG3	73:CE:126:TYR:OH	2.16	0.44
75:CG:127:VAL:O	75:CG:131:GLN:HG3	2.17	0.44
77:CI:272:U:H2'	77:CI:273:U:C6	2.52	0.44
77:CI:4615:A:H2'	77:CI:4616:A:H8	1.82	0.44
3:AC:349:A:H2'	3:AC:350:A:C8	2.52	0.44
3:AC:527:A:H61	3:AC:560:G:H22	1.64	0.44
3:AC:1349:G:C8	3:AC:1350:G:C8	3.06	0.44
6:AJ:156:THR:HG23	6:AJ:188:TYR:CE1	2.52	0.44
13:AT:261:LEU:N	13:AT:261:LEU:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AQ:51:LYS:CD	21:AQ:76:ASP:OD1	2.64	0.44
25:AV:198:ARG:O	25:AV:201:LYS:HG2	2.17	0.44
26:AW:81:LEU:HD12	26:AW:97:ILE:HD12	2.00	0.44
42:BH:94:GLU:N	42:BH:94:GLU:OE2	2.51	0.44
46:BL:72:VAL:O	46:BL:72:VAL:HG12	2.17	0.44
60:BZ:94:LEU:O	60:BZ:98:ARG:HG3	2.17	0.44
77:CI:423:G:H2'	77:CI:424:U:C6	2.52	0.44
77:CI:660:C:C2	77:CI:661:C:C5	3.05	0.44
77:CI:1122:C:C2	77:CI:1123:C:C5	3.05	0.44
77:CI:2446:C:H2'	77:CI:2447:U:C6	2.52	0.44
77:CI:2559:U:H2'	77:CI:2560:OMC:H6	1.82	0.44
77:CI:4280:C:O2'	77:CI:4281:A:H5'	2.17	0.44
77:CI:4552:C:C2	77:CI:4553:C:C6	3.05	0.44
3:AC:220:U:C2	3:AC:221:U:C5	3.05	0.44
3:AC:1533:C:H5'	3:AC:1605:G:H21	1.82	0.44
12:AP:112:VAL:O	12:AP:112:VAL:HG23	2.17	0.44
13:AT:304:ASP:O	13:AT:304:ASP:OD1	2.35	0.44
24:AU:191:VAL:HG11	24:AU:236:PHE:HA	1.99	0.44
57:BW:4:ARG:O	77:CI:4593:G:O6	2.35	0.44
69:CA:112:ALA:HB2	69:CA:147:LEU:HD21	1.99	0.44
74:CF:50:PRO:O	74:CF:51:ALA:HB3	2.17	0.44
77:CI:392:U:C2	77:CI:393:U:C5	3.06	0.44
77:CI:1360:A:C2	77:CI:2569:A:H8	2.36	0.44
77:CI:1403:C:H5''	77:CI:1404:U:O5'	2.17	0.44
77:CI:3928:A:H2'	77:CI:3929:A:C8	2.52	0.44
79:CK:62:A:H4'	79:CK:63:U:O5'	2.18	0.44
4:AE:7:LYS:HE2	12:AP:25:THR:HG21	1.99	0.44
5:AH:91:LEU:HD21	20:AI:17:LYS:HB3	1.98	0.44
13:AT:25:PRO:HA	13:AT:293:ALA:HB1	1.99	0.44
19:AG:82:MET:HE3	19:AG:85:THR:HG22	1.99	0.44
25:AV:112:VAL:O	25:AV:112:VAL:HG13	2.17	0.44
36:BB:101:THR:HG21	77:CI:4378:A:N3	2.32	0.44
51:BQ:87:VAL:CG1	51:BQ:89:ILE:HD12	2.47	0.44
69:CA:215:GLU:OE2	69:CA:221:LYS:O	2.35	0.44
71:CC:37:ASP:O	71:CC:37:ASP:OD1	2.36	0.44
73:CE:78:LYS:O	73:CE:81:GLU:HG2	2.18	0.44
77:CI:947:G:C2	77:CI:1038:G:N1	2.86	0.44
77:CI:1534:C:O2'	77:CI:1535:G:H5'	2.17	0.44
77:CI:2477:G:H2'	77:CI:2478:G:C8	2.53	0.44
77:CI:3867:A:H4'	77:CI:3868:A:N3	2.33	0.44
3:AC:1229:A:H2'	3:AC:1230:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:1541:G:OP2	11:AO:43:LYS:HE3	2.17	0.44
3:AC:1546:A:H2'	3:AC:1547:G:C8	2.52	0.44
5:AH:11:LYS:O	5:AH:14:ARG:HG2	2.17	0.44
6:AJ:98:GLU:OE1	15:Ac:101:SER:OG	2.34	0.44
33:Ag:48:ALA:C	33:Ag:49:LYS:HD3	2.43	0.44
46:BL:85:TYR:CD2	77:CI:2388:U:C5	3.05	0.44
71:CC:41:ILE:HG22	71:CC:43:VAL:HG13	1.99	0.44
75:CG:91:TRP:CD1	77:CI:4517:OMG:O5'	2.70	0.44
77:CI:669:G:O6	77:CI:670:G:C6	2.71	0.44
77:CI:2240:A:N6	77:CI:2248:C:H42	2.16	0.44
77:CI:2600:A:O2'	77:CI:4286:G:H4'	2.17	0.44
79:CK:127:U:H5'	79:CK:128:C:OP1	2.16	0.44
3:AC:350:A:H2'	3:AC:351:C:H6	1.83	0.44
3:AC:637:C:H2'	3:AC:638:U:C6	2.53	0.44
3:AC:943:G:H2'	3:AC:944:U:C6	2.52	0.44
4:AE:137:VAL:HG22	4:AE:151:LYS:HG3	1.99	0.44
16:Af:101:ALA:O	16:Af:102:VAL:HG13	2.17	0.44
17:AD:180:ASP:OD1	17:AD:183:GLU:OE1	2.36	0.44
25:AV:32:MET:HE1	25:AV:64:LYS:C	2.43	0.44
34:Ah:130:THR:O	34:Ah:134:GLU:OE1	2.36	0.44
35:BA:207:VAL:HG13	35:BA:208:GLU:OE1	2.17	0.44
39:BE:171:VAL:HG21	39:BE:265:ILE:CD1	2.47	0.44
41:BG:108:ASP:N	41:BG:152:GLU:OE2	2.51	0.44
47:BM:121:VAL:HG21	47:BM:136:ALA:HB2	1.99	0.44
54:BT:28:VAL:HG21	54:BT:37:MET:HG3	1.99	0.44
55:BU:84:ILE:HD11	55:BU:108:TYR:CE1	2.53	0.44
76:CH:126:THR:HG23	76:CH:127:TYR:CD2	2.53	0.44
77:CI:1129:C:N4	77:CI:1138:A:P	2.91	0.44
77:CI:1140:A2M:HM'3	77:CI:1140:A2M:H1'	1.89	0.44
77:CI:1606:A:O4'	77:CI:1608:G:C8	2.71	0.44
77:CI:3742:G:H2'	77:CI:3743:G:O4'	2.18	0.44
77:CI:3888:A:C4	77:CI:3890:G:N7	2.85	0.44
77:CI:3969:C:C2	77:CI:3970:A:C8	3.04	0.44
77:CI:4517:OMG:O4'	77:CI:4517:OMG:OP2	2.35	0.44
3:AC:1628:C:C2	3:AC:1629:C:C5	3.06	0.44
12:AP:22:ILE:HG12	12:AP:114:VAL:HG22	1.99	0.44
15:Ac:69:THR:HG1	15:Ac:72:VAL:HG23	1.80	0.44
24:AU:272:HIS:CE1	24:AU:276:THR:CG2	3.00	0.44
40:BF:185:VAL:O	40:BF:189:ILE:HG12	2.18	0.44
41:BG:36:ILE:HD11	41:BG:44:ALA:HA	2.00	0.44
55:BU:65:ASP:OD2	55:BU:67:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:162:A:H2'	77:CI:163:A:H8	1.83	0.44
77:CI:4056:G:O2'	77:CI:4057:C:P	2.76	0.44
1:AA:24:GLN:HB2	1:AA:26:GLN:NE2	2.33	0.44
8:AL:107:ILE:O	8:AL:111:MET:SD	2.76	0.44
13:AT:201:SER:OG	13:AT:202:PRO:HD2	2.17	0.44
20:AI:144:THR:O	20:AI:158:ASP:HB2	2.18	0.44
24:AU:166:ARG:CB	24:AU:248:TYR:CE1	3.01	0.44
24:AU:202:THR:HG23	26:AW:58:ARG:NH2	2.32	0.44
29:Aa:3:ARG:HH12	29:Aa:28:ARG:HE	1.64	0.44
36:BB:293:ILE:CD1	36:BB:298:LEU:HD13	2.48	0.44
40:BF:105:LEU:HD12	40:BF:109:PRO:HG2	1.99	0.44
46:BL:101:ARG:NH1	46:BL:103:VAL:HG21	2.32	0.44
74:CF:66:TYR:O	74:CF:69:LYS:HG2	2.18	0.44
74:CF:136:LYS:HG3	74:CF:136:LYS:O	2.17	0.44
77:CI:37:U:H2'	77:CI:38:A:O4'	2.17	0.44
77:CI:112:C:C2	77:CI:113:A:C8	3.06	0.44
3:AC:335:C:OP2	25:AV:190:ARG:NH2	2.50	0.44
3:AC:457:C:C2	3:AC:458:C:C5	3.06	0.44
3:AC:528:C:H41	3:AC:559:G:H1	1.66	0.44
3:AC:830:C:OP1	18:AF:21:ASP:OD1	2.36	0.44
3:AC:1026:U:H2'	3:AC:1027:C:O4'	2.18	0.44
3:AC:1280:C:C2	3:AC:1281:G:C8	3.05	0.44
3:AC:1827:G:C5	3:AC:1828:U:C5	3.06	0.44
9:AM:61:GLU:OE2	9:AM:62:ARG:HG3	2.18	0.44
11:AO:42:HIS:NE2	11:AO:43:LYS:NZ	2.66	0.44
17:AD:71:LEU:HD13	17:AD:84:PHE:HE2	1.79	0.44
19:AG:96:ILE:HD11	19:AG:103:GLU:HG2	1.99	0.44
37:BC:350:ARG:HD2	77:CI:730:C:OP1	2.17	0.44
40:BF:105:LEU:N	40:BF:105:LEU:HD23	2.33	0.44
47:BM:15:ARG:HB2	77:CI:4273:G:H5'	2.00	0.44
47:BM:91:LYS:O	47:BM:92:ASP:OD1	2.36	0.44
56:BV:76:LYS:HE3	56:BV:98:GLU:OE1	2.18	0.44
77:CI:205:C:O2	77:CI:209:U:O4	2.36	0.44
77:CI:240:G:H2'	77:CI:241:G:O4'	2.18	0.44
77:CI:4610:C:H2'	77:CI:4611:G:C8	2.52	0.44
3:AC:1752:C:O2	3:AC:1785:G:O6	2.36	0.43
12:AP:20:ILE:HD11	12:AP:114:VAL:HG13	2.00	0.43
14:AX:35:ILE:HD12	14:AX:61:TYR:HE1	1.83	0.43
35:BA:124:GLY:O	35:BA:125:LYS:HB2	2.17	0.43
41:BG:36:ILE:HD11	41:BG:44:ALA:HB1	2.00	0.43
52:BR:87:ARG:CG	52:BR:120:GLN:HE22	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bf:5:PRO:HD3	77:CI:3887:U:C2	2.53	0.43
75:CG:38:VAL:HG21	75:CG:50:MET:SD	2.57	0.43
77:CI:25:A:C8	77:CI:341:G:C8	3.06	0.43
77:CI:472:C:H2'	77:CI:473:C:H6	1.82	0.43
77:CI:1108:A:HO2'	77:CI:1109:U:H6	1.62	0.43
77:CI:1351:U:C2	77:CI:1352:G:C8	3.06	0.43
77:CI:4048:G:O4'	77:CI:4102:5MC:HM53	2.18	0.43
78:CJ:24:C:H2'	78:CJ:25:G:O4'	2.18	0.43
3:AC:636:G:C6	3:AC:637:C:C4	3.06	0.43
3:AC:638:U:N3	3:AC:639:C:C5	2.87	0.43
4:AE:106:ARG:CG	4:AE:175:VAL:HG22	2.40	0.43
7:AK:76:ILE:HG22	7:AK:80:ARG:NH1	2.33	0.43
13:AT:290:ALA:C	13:AT:298:LEU:HD12	2.42	0.43
17:AD:126:ASP:OD1	17:AD:136:ARG:HD3	2.18	0.43
19:AG:120:VAL:HG13	19:AG:124:ASP:OD2	2.19	0.43
23:AS:45:VAL:HG21	23:AS:64:LEU:HD13	2.00	0.43
38:BD:50:ARG:NH1	38:BD:147:ASP:OD1	2.50	0.43
70:CB:63:LEU:HD21	76:CH:29:GLN:HG3	2.00	0.43
72:CD:180:GLU:O	72:CD:184:LYS:HG3	2.18	0.43
77:CI:1287:C:H2'	77:CI:1288:G:O4'	2.18	0.43
1:AA:17:VAL:HG23	1:AA:17:VAL:O	2.17	0.43
3:AC:508:G:OP2	30:Ab:104:ARG:NH2	2.50	0.43
4:AE:7:LYS:CE	12:AP:25:THR:HG21	2.48	0.43
10:AN:99:LEU:O	10:AN:100:ALA:C	2.60	0.43
13:AT:207:CYS:SG	13:AT:219:TRP:HB2	2.57	0.43
13:AT:208:ALA:HB1	13:AT:239:LEU:HD21	1.99	0.43
21:AQ:23:ILE:HD11	24:AU:251:LEU:HA	2.00	0.43
22:AR:105:PHE:HD1	22:AR:121:LYS:HB3	1.82	0.43
28:AZ:77:ALA:O	28:AZ:81:VAL:HG23	2.18	0.43
33:Ag:169:LYS:O	33:Ag:172:THR:HG22	2.17	0.43
34:Ah:67:TRP:O	34:Ah:191:GLU:OE2	2.36	0.43
38:BD:33:ARG:O	38:BD:37:VAL:HG22	2.17	0.43
45:BK:28:ALA:O	45:BK:32:ARG:HG2	2.18	0.43
45:BK:130:ARG:O	77:CI:1639:A:H4'	2.18	0.43
58:BX:43:LYS:HE2	58:BX:52:ARG:CZ	2.49	0.43
62:Bb:2:PRO:HB2	77:CI:2448:U:O2	2.18	0.43
69:CA:247:THR:HG22	69:CA:248:HIS:N	2.32	0.43
70:CB:162:ASP:HB2	70:CB:163:PRO:CD	2.48	0.43
77:CI:1129:C:H2'	77:CI:1130:G:H8	1.79	0.43
77:CI:1281:C:C2	77:CI:1282:C:C5	3.07	0.43
3:AC:1124:C:C4	3:AC:1125:C:C5	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AM:8:GLN:HG3	9:AM:99:TYR:CZ	2.53	0.43
25:AV:178:ARG:HG2	25:AV:178:ARG:O	2.18	0.43
30:Ab:91:LEU:HA	30:Ab:94:HIS:NE2	2.33	0.43
44:BJ:99:ASP:OD1	44:BJ:100:LEU:N	2.52	0.43
44:BJ:107:THR:O	44:BJ:111:ARG:HG2	2.18	0.43
71:CC:36:ARG:HD3	71:CC:38:PHE:CZ	2.53	0.43
77:CI:3259:G:H2'	77:CI:3260:C:C6	2.53	0.43
77:CI:3948:PSU:N3	77:CI:3949:C:C5	2.87	0.43
77:CI:4652:C:H2'	77:CI:4653:G:O4'	2.19	0.43
3:AC:1273:C:HO2'	3:AC:1274:C:H6	1.59	0.43
35:BA:108:PRO:HD3	67:Bg:90:LYS:HE3	2.01	0.43
37:BC:159:GLU:O	37:BC:214:ASP:O	2.36	0.43
77:CI:321:U:H2'	77:CI:322:C:C6	2.54	0.43
77:CI:1659:C:H2'	77:CI:1660:A:H8	1.82	0.43
77:CI:3913:C:C2	77:CI:3914:C:C5	3.06	0.43
7:AK:64:TRP:O	7:AK:65:ARG:HB2	2.19	0.43
13:AT:232:GLY:HA2	13:AT:259:TRP:HZ2	1.84	0.43
15:Ac:113:THR:O	15:Ac:113:THR:CG2	2.67	0.43
23:AS:45:VAL:HG21	23:AS:64:LEU:CD1	2.48	0.43
34:Ah:101:ILE:HD12	34:Ah:190:LEU:HD11	2.01	0.43
42:BH:180:ARG:C	42:BH:181:ARG:HG3	2.44	0.43
43:BI:60:ARG:O	43:BI:64:ARG:HG3	2.18	0.43
62:Bb:17:ARG:NH2	62:Bb:38:CYS:SG	2.92	0.43
67:Bg:17:ARG:O	67:Bg:18:TYR:CD1	2.72	0.43
77:CI:3867:A:H4'	77:CI:3868:A:O5'	2.19	0.43
77:CI:3999:U:H2'	77:CI:4000:C:C6	2.52	0.43
77:CI:4190:A:H2'	77:CI:4191:OMC:H6	1.82	0.43
79:CK:108:A:C2	79:CK:112:G:C6	3.06	0.43
3:AC:329:U:O2'	3:AC:330:G:P	2.76	0.43
6:AJ:173:LEU:O	6:AJ:177:LEU:HG	2.18	0.43
20:AI:105:PRO:HA	20:AI:136:GLU:OE2	2.19	0.43
38:BD:83:LEU:N	38:BD:84:PRO:HD2	2.33	0.43
55:BU:22:THR:HB	55:BU:122:VAL:CG2	2.49	0.43
74:CF:64:VAL:HA	74:CF:67:HIS:CD2	2.54	0.43
76:CH:203:TYR:C	76:CH:204:ARG:HD3	2.43	0.43
77:CI:199:G:O3'	77:CI:200:U:H4'	2.19	0.43
77:CI:424:U:C2	77:CI:425:U:C5	3.06	0.43
77:CI:1361:G:O2'	77:CI:2568:A:H8	2.01	0.43
77:CI:2032:A:H2'	77:CI:2033:C:O4'	2.19	0.43
77:CI:3552:C:H2'	77:CI:3553:A:C8	2.53	0.43
77:CI:4322:C:H2'	77:CI:4323:U:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:CJ:16:A:H2'	78:CJ:17:C:O4'	2.18	0.43
3:AC:863:A:H8	29:Aa:105:THR:OG1	2.02	0.43
3:AC:1843:4AC:O7	3:AC:1843:4AC:H5	2.18	0.43
5:AH:66:VAL:O	5:AH:66:VAL:HG23	2.18	0.43
6:AJ:78:MET:O	6:AJ:79:HIS:HB2	2.19	0.43
13:AT:14:HIS:CE1	13:AT:35:SER:HB2	2.54	0.43
24:AU:233:LEU:HD23	24:AU:233:LEU:C	2.44	0.43
25:AV:38:ALA:HB2	25:AV:50:VAL:HG22	2.00	0.43
35:BA:137:ILE:HB	35:BA:147:ARG:HG3	2.01	0.43
36:BB:283:LYS:HE3	36:BB:363:ILE:HD12	2.00	0.43
49:BO:129:ARG:CG	49:BO:130:PRO:HD2	2.49	0.43
64:Bd:109:ASN:HD22	77:CI:1749:U:H2'	1.83	0.43
77:CI:129:C:H2'	77:CI:130:G:H8	1.82	0.43
77:CI:943:C:C2	77:CI:944:G:C8	3.07	0.43
77:CI:1614:C:C2	77:CI:1615:U:C5	3.07	0.43
77:CI:1873:A:C2	77:CI:1874:C:C6	3.07	0.43
77:CI:2107:C:O2	77:CI:2107:C:H2'	2.19	0.43
3:AC:986:G:H1'	28:AZ:138:ASP:OD2	2.18	0.43
5:AH:99:ASP:O	5:AH:102:THR:HG22	2.19	0.43
13:AT:191:HIS:CE1	13:AT:217:MET:SD	3.12	0.43
18:AF:86:PHE:CE1	18:AF:102:ILE:HD12	2.54	0.43
18:AF:173:ILE:HD13	18:AF:227:VAL:CG1	2.48	0.43
29:Aa:76:SER:HB2	29:Aa:77:PRO:HD3	2.01	0.43
30:Ab:9:THR:HG1	30:Ab:23:MET:HB2	1.83	0.43
36:BB:29:VAL:HG11	36:BB:32:PHE:CZ	2.54	0.43
37:BC:140:LYS:O	37:BC:140:LYS:HG2	2.19	0.43
38:BD:65:ALA:HB2	38:BD:74:ILE:HD13	2.01	0.43
40:BF:34:VAL:HG22	40:BF:103:LYS:CG	2.48	0.43
41:BG:4:TYR:CE1	41:BG:18:ARG:HD2	2.54	0.43
69:CA:109:PRO:HG3	69:CA:166:TYR:CE2	2.54	0.43
69:CA:261:GLN:OE1	69:CA:264:ARG:HD2	2.19	0.43
77:CI:1350:A:H2'	77:CI:1351:U:C6	2.53	0.43
3:AC:164:A:H2'	3:AC:165:G:C8	2.54	0.43
3:AC:321:G:H2'	3:AC:322:C:H6	1.83	0.43
3:AC:954:C:H2'	3:AC:955:U:O4'	2.19	0.43
13:AT:14:HIS:NE2	13:AT:35:SER:HB2	2.33	0.43
18:AF:147:ILE:HD11	18:AF:162:ILE:HD12	2.01	0.43
19:AG:16:ILE:O	19:AG:16:ILE:HG13	2.18	0.43
38:BD:79:TYR:O	38:BD:82:GLU:HG2	2.18	0.43
50:BP:50:ARG:HH21	79:CK:83:C:N4	2.17	0.43
51:BQ:100:VAL:O	51:BQ:100:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:718:C:C2	77:CI:719:C:C5	3.07	0.43
77:CI:4079:A:N7	77:CI:4130:G:C6	2.87	0.43
3:AC:1534:A:H2	3:AC:1537:G:N3	2.17	0.42
28:AZ:78:ALA:HB3	28:AZ:118:ALA:HB3	2.01	0.42
34:Ah:46:VAL:HG21	34:Ah:56:ARG:HE	1.84	0.42
34:Ah:76:THR:HG22	34:Ah:108:PRO:HG2	2.00	0.42
34:Ah:103:LEU:HD13	34:Ah:170:LYS:CD	2.49	0.42
37:BC:140:LYS:HD2	37:BC:248:ARG:HA	2.00	0.42
45:BK:141:VAL:HG13	45:BK:141:VAL:O	2.19	0.42
77:CI:1483:G:OP1	77:CI:1484:U:C5	2.72	0.42
77:CI:2046:C:C2	77:CI:2047:G:C8	3.07	0.42
77:CI:3512:U:C2	77:CI:3513:C:C5	3.07	0.42
77:CI:4070:1MA:H2'	77:CI:4071:G:O4'	2.19	0.42
77:CI:4364:U:C2	77:CI:4365:C:C6	3.06	0.42
3:AC:946:U:H2'	3:AC:947:U:C6	2.54	0.42
3:AC:1588:G:C6	11:AO:67:ARG:HD3	2.54	0.42
5:AH:29:HIS:O	5:AH:32:LYS:HG2	2.19	0.42
9:AM:107:GLU:HG3	9:AM:108:ILE:N	2.34	0.42
17:AD:91:VAL:HG22	17:AD:96:CYS:SG	2.59	0.42
18:AF:11:ARG:HD3	18:AF:28:ALA:HB2	2.00	0.42
21:AQ:51:LYS:HE3	21:AQ:76:ASP:OD1	2.19	0.42
26:AW:81:LEU:CD1	26:AW:97:ILE:HD12	2.49	0.42
45:BK:107:LYS:HE2	45:BK:107:LYS:HA	2.00	0.42
46:BL:102:VAL:HG22	46:BL:112:LEU:CD2	2.49	0.42
49:BO:89:LYS:HE3	49:BO:137:TYR:CE1	2.54	0.42
55:BU:22:THR:HA	55:BU:88:LEU:O	2.19	0.42
75:CG:46:ARG:NH1	77:CI:834:U:C5	2.87	0.42
77:CI:745:G:C2	77:CI:746:G:N7	2.87	0.42
77:CI:756:U:C2	77:CI:757:G:C8	3.07	0.42
77:CI:1317:G:H2'	77:CI:1318:C:C6	2.54	0.42
77:CI:1687:G:O2'	77:CI:1709:A:N6	2.51	0.42
77:CI:2571:A:H2'	77:CI:2572:G:C8	2.54	0.42
77:CI:3380:U:H2'	77:CI:3381:G:H8	1.84	0.42
77:CI:4191:OMC:HM22	77:CI:4192:C:O4'	2.19	0.42
79:CK:5:U:H2'	79:CK:6:C:H6	1.84	0.42
3:AC:953:G:H2'	3:AC:954:C:C6	2.54	0.42
3:AC:1629:C:H2'	3:AC:1630:C:H6	1.84	0.42
4:AE:54:ARG:HG3	4:AE:54:ARG:O	2.19	0.42
4:AE:65:ARG:O	4:AE:69:LEU:HD13	2.18	0.42
7:AK:48:ALA:O	7:AK:52:LEU:HD13	2.19	0.42
9:AM:50:LYS:HA	9:AM:53:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AN:40:TYR:CE2	10:AN:44:VAL:HG21	2.54	0.42
10:AN:51:ASP:O	10:AN:51:ASP:OD1	2.37	0.42
24:AU:174:ILE:O	24:AU:200:ARG:NH2	2.53	0.42
28:AZ:34:PHE:HB3	28:AZ:41:PHE:HB2	2.00	0.42
33:Ag:36:LEU:HA	33:Ag:39:GLN:OE1	2.19	0.42
34:Ah:130:THR:OG1	34:Ah:131:PRO:HD3	2.18	0.42
35:BA:101:VAL:C	35:BA:102:LEU:HD12	2.44	0.42
35:BA:138:SER:OG	35:BA:147:ARG:HG2	2.19	0.42
39:BE:153:THR:OG1	39:BE:154:PRO:HD2	2.19	0.42
44:BJ:70:LYS:O	77:CI:739:A:H4'	2.18	0.42
44:BJ:84:TYR:OH	44:BJ:93:MET:HE3	2.19	0.42
50:BP:110:LYS:O	50:BP:115:ARG:HD3	2.19	0.42
69:CA:195:SER:O	69:CA:199:ARG:HG3	2.19	0.42
73:CE:41:GLU:OE1	73:CE:47:THR:HA	2.19	0.42
77:CI:353:A:C4	77:CI:379:G:N7	2.87	0.42
77:CI:1114:G:H2'	77:CI:1115:C:C5	2.53	0.42
77:CI:1672:C:H2'	77:CI:1673:A2M:H8	2.02	0.42
77:CI:2411:C:C2	77:CI:2412:U:C5	3.07	0.42
77:CI:3723:U:H2'	77:CI:3724:U:C6	2.54	0.42
77:CI:4307:G:H2'	77:CI:4308:C:H6	1.83	0.42
77:CI:4427:C:O2	77:CI:4427:C:H2'	2.18	0.42
77:CI:4428:C:H2'	77:CI:4429:C:H6	1.84	0.42
3:AC:369:U:H2'	3:AC:370:C:H2'	2.01	0.42
3:AC:567:U:H2'	3:AC:568:C:O4'	2.18	0.42
24:AU:183:LYS:HA	24:AU:195:LEU:O	2.19	0.42
25:AV:29:GLU:HG3	25:AV:29:GLU:O	2.19	0.42
25:AV:69:THR:HG21	25:AV:73:VAL:HG11	2.01	0.42
34:Ah:161:LEU:H	34:Ah:161:LEU:HD12	1.84	0.42
37:BC:319:LEU:HD13	69:CA:174:GLU:OE1	2.20	0.42
77:CI:385:A:H4'	77:CI:386:A:OP1	2.19	0.42
77:CI:2383:C:H42	77:CI:4304:G:H1	1.66	0.42
77:CI:3352:U:C4	77:CI:3353:U:C5	3.07	0.42
77:CI:3782:G:H2'	77:CI:3783:C:O4'	2.18	0.42
77:CI:3889:A:N7	77:CI:3926:A:C2	2.88	0.42
77:CI:4113:C:H2'	77:CI:4114:U:H6	1.83	0.42
79:CK:5:U:C2	79:CK:6:C:C5	3.08	0.42
3:AC:94:G:O2'	3:AC:509:A:O2'	2.36	0.42
3:AC:943:G:N2	28:AZ:138:ASP:HB2	2.35	0.42
3:AC:1379:A:H4'	3:AC:1380:A:O5'	2.19	0.42
3:AC:1403:A:N1	3:AC:1406:A:C2	2.86	0.42
13:AT:304:ASP:OD1	13:AT:304:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AR:22:TRP:HE3	22:AR:28:LYS:HD2	1.85	0.42
34:Ah:158:ILE:HG22	34:Ah:159:SER:H	1.84	0.42
37:BC:114:ARG:HG3	76:CH:203:TYR:HB3	2.00	0.42
39:BE:173:LEU:HD12	39:BE:182:LEU:CD2	2.50	0.42
42:BH:46:VAL:O	42:BH:49:LYS:HG2	2.20	0.42
61:Ba:75:ARG:NH2	77:CI:343:C:O2'	2.52	0.42
71:CC:126:VAL:HG11	71:CC:161:ILE:HG12	2.02	0.42
77:CI:723:U:H2'	77:CI:724:C:C6	2.54	0.42
77:CI:851:C:O2'	77:CI:852:G:H5'	2.19	0.42
77:CI:1129:C:O2'	77:CI:2104:G:N2	2.52	0.42
77:CI:2168:A:H2'	77:CI:2169:U:H6	1.84	0.42
77:CI:3747:G:N7	77:CI:3748:G:C8	2.88	0.42
77:CI:4428:C:C2	77:CI:4429:C:C5	3.08	0.42
77:CI:4640:G:H2'	77:CI:4641:G:C8	2.54	0.42
1:AA:60:GLU:HG2	6:AJ:204:ARG:CD	2.50	0.42
3:AC:1159:G:H5''	29:Aa:76:SER:OG	2.19	0.42
3:AC:1729:U:O3'	34:Ah:17:LYS:NZ	2.53	0.42
4:AE:38:GLU:OE1	4:AE:40:ARG:HG3	2.20	0.42
5:AH:24:LEU:CB	5:AH:58:MET:HE3	2.49	0.42
5:AH:25:GLY:O	5:AH:58:MET:HG3	2.18	0.42
5:AH:45:LYS:O	5:AH:49:LYS:HG3	2.20	0.42
25:AV:52:ILE:HG23	25:AV:109:LEU:HD11	2.01	0.42
25:AV:121:ILE:HD12	25:AV:124:LEU:HD21	2.01	0.42
30:Ab:53:ASP:O	30:Ab:53:ASP:OD1	2.37	0.42
35:BA:11:GLY:HA3	77:CI:3326:C:O2'	2.19	0.42
42:BH:177:ALA:O	42:BH:178:ARG:C	2.62	0.42
53:BS:37:PRO:O	53:BS:41:ARG:HG2	2.19	0.42
54:BT:77:ASN:OD1	54:BT:77:ASN:C	2.62	0.42
69:CA:81:LYS:O	69:CA:85:GLN:HG3	2.18	0.42
73:CE:151:ILE:HD11	73:CE:156:ARG:HG3	2.01	0.42
75:CG:124:LYS:O	75:CG:127:VAL:HG22	2.20	0.42
77:CI:420:A:C8	77:CI:421:C:C5	3.07	0.42
77:CI:660:C:H2'	77:CI:661:C:H6	1.84	0.42
77:CI:842:U:C2	77:CI:843:C:C5	3.08	0.42
77:CI:1465:U:HO2'	77:CI:1466:A:P	2.42	0.42
77:CI:3398:C:C2	77:CI:3399:G:C8	3.07	0.42
77:CI:3570:C:C2	77:CI:3571:U:C5	3.07	0.42
7:AK:14:LEU:HD22	7:AK:35:LEU:HD21	2.01	0.42
13:AT:21:ILE:HD13	13:AT:299:PHE:HB3	2.02	0.42
18:AF:63:LYS:NZ	30:Ab:85:ASN:HA	2.35	0.42
18:AF:139:LEU:HD23	18:AF:150:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AS:37:LYS:HD3	23:AS:70:LYS:HE2	2.02	0.42
25:AV:67:VAL:HG12	25:AV:69:THR:HG22	2.02	0.42
25:AV:137:ARG:HB3	25:AV:140:ARG:HG3	2.01	0.42
26:AW:60:LEU:HD22	26:AW:70:ARG:HA	2.02	0.42
34:Ah:89:GLU:O	34:Ah:93:THR:HG23	2.20	0.42
37:BC:10:VAL:HG22	37:BC:153:VAL:CG1	2.48	0.42
44:BJ:165:PRO:O	44:BJ:166:ARG:HB3	2.18	0.42
67:Bg:17:ARG:O	77:CI:3294:A:N1	2.52	0.42
77:CI:1131:U:O4'	77:CI:1131:U:P	2.78	0.42
77:CI:1660:A:N3	77:CI:1661:C:C5	2.87	0.42
77:CI:1685:OMG:O6	77:CI:1698:A:N3	2.52	0.42
77:CI:1873:A:C4	77:CI:1874:C:C5	3.08	0.42
77:CI:3747:G:C8	77:CI:3748:G:C8	3.07	0.42
77:CI:3775:G:O2'	77:CI:3776:C:OP1	2.35	0.42
3:AC:120:U:C2	3:AC:121:U:C5	3.08	0.42
3:AC:171:A:OP1	3:AC:171:A:H4'	2.18	0.42
3:AC:582:U:H1'	30:Ab:62:THR:HG21	2.00	0.42
3:AC:651:A:OP2	22:AR:108:LYS:HD2	2.19	0.42
3:AC:1234:G:C6	3:AC:1527:G:C6	3.08	0.42
3:AC:1715:U:H2'	3:AC:1716:A:C8	2.55	0.42
31:Ad:7:LEU:O	31:Ad:24:LEU:HD11	2.19	0.42
31:Ad:57:VAL:O	31:Ad:57:VAL:HG12	2.19	0.42
33:Ag:159:ASP:O	33:Ag:160:LYS:HB3	2.18	0.42
35:BA:178:PRO:HG2	67:Bg:26:VAL:CG2	2.50	0.42
35:BA:247:ARG:N	35:BA:247:ARG:HD2	2.35	0.42
38:BD:36:LEU:HG	38:BD:50:ARG:HD3	2.02	0.42
39:BE:132:LYS:HD2	77:CI:855:G:C4	2.55	0.42
44:BJ:161:ARG:HD3	77:CI:1723:C:C6	2.54	0.42
46:BL:23:LEU:HD23	46:BL:110:TYR:HB2	2.02	0.42
48:BN:46:PRO:HG2	48:BN:54:LEU:HD23	2.01	0.42
62:Bb:64:LEU:HD23	62:Bb:64:LEU:H	1.84	0.42
72:CD:31:ILE:HG22	72:CD:62:SER:HB2	2.02	0.42
77:CI:2415:A:C2	77:CI:2432:A:N9	2.88	0.42
77:CI:2446:C:C2	77:CI:2447:U:C6	3.08	0.42
3:AC:16:G:H2'	3:AC:17:C:C6	2.54	0.42
3:AC:126:G:OP1	25:AV:198:ARG:HD2	2.20	0.42
3:AC:642:A:H2'	3:AC:643:U:O4'	2.20	0.42
3:AC:1202:U:H2'	3:AC:1203:U:C6	2.55	0.42
3:AC:1688:C:H2'	3:AC:1689:C:H6	1.85	0.42
35:BA:54:ARG:HD2	35:BA:56:ALA:O	2.20	0.42
38:BD:91:GLY:O	38:BD:94:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:BX:48:VAL:HG23	58:BX:49:CYS:N	2.34	0.42
70:CB:158:ALA:HB2	70:CB:190:LEU:HD12	2.01	0.42
74:CF:80:GLU:OE1	74:CF:113:ASN:CB	2.68	0.42
77:CI:1044:G:C2	77:CI:1045:G:C8	3.08	0.42
77:CI:1609:C:H2'	77:CI:1610:C:H6	1.84	0.42
77:CI:2296:C:C2	77:CI:2297:G:C8	3.08	0.42
77:CI:2410:C:C2	77:CI:2411:C:C5	3.08	0.42
77:CI:3349:U:H2'	77:CI:3350:G:O4'	2.20	0.42
77:CI:3368:U:O2	77:CI:3369:G:N7	2.53	0.42
77:CI:4284:U:C2	77:CI:4285:G:C8	3.08	0.42
77:CI:4365:C:H2'	77:CI:4366:C:C6	2.55	0.42
77:CI:4599:G:C2	77:CI:4600:U:C6	3.07	0.42
3:AC:562:A:N6	3:AC:588:A:C8	2.88	0.42
3:AC:818:G:H22	3:AC:819:A:H62	1.68	0.42
3:AC:875:G:H2'	3:AC:876:A:H8	1.85	0.42
3:AC:1343:U:H1'	3:AC:1344:U:H5	1.84	0.42
3:AC:1729:U:H2'	3:AC:1730:U:O4'	2.20	0.42
3:AC:1737:G:H2'	3:AC:1738:G:C8	2.54	0.42
5:AH:30:THR:O	5:AH:34:VAL:HG23	2.20	0.42
6:AJ:18:LYS:HE2	6:AJ:22:LYS:C	2.44	0.42
13:AT:248:LEU:HD23	13:AT:259:TRP:CE3	2.55	0.42
22:AR:73:GLN:NE2	22:AR:78:GLY:HA2	2.34	0.42
24:AU:82:TYR:CE2	24:AU:164:PRO:HD3	2.55	0.42
24:AU:98:LEU:HB3	24:AU:102:LEU:HG	2.02	0.42
34:Ah:103:LEU:CD2	34:Ah:172:LEU:HD23	2.50	0.42
34:Ah:121:LEU:N	34:Ah:121:LEU:HD23	2.35	0.42
38:BD:289:ARG:HD2	77:CI:1011:U:OP2	2.20	0.42
40:BF:101:ARG:O	40:BF:101:ARG:HG2	2.19	0.42
49:BO:129:ARG:HG2	49:BO:130:PRO:HD2	2.02	0.42
50:BP:50:ARG:HG2	50:BP:51:LYS:N	2.34	0.42
52:BR:21:ARG:HB3	77:CI:1132:C:OP2	2.19	0.42
55:BU:38:PHE:CE2	55:BU:78:ARG:NH2	2.88	0.42
72:CD:30:LYS:CD	72:CD:63:GLU:HG3	2.50	0.42
79:CK:141:C:H2'	79:CK:142:U:C6	2.55	0.42
3:AC:819:A:C4	3:AC:820:G:C8	3.08	0.41
3:AC:1846:A:H2'	3:AC:1847:G:H8	1.85	0.41
3:AC:1850:G:C4	77:CI:3426:C:OP1	2.72	0.41
4:AE:69:LEU:HA	4:AE:72:VAL:HG22	2.01	0.41
6:AJ:47:LYS:NZ	9:AM:115:TYR:O	2.53	0.41
13:AT:213:ASP:HB3	13:AT:215:GLN:OE1	2.19	0.41
17:AD:87:ILE:HB	17:AD:101:HIS:CD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AF:169:ILE:HD12	18:AF:169:ILE:H	1.85	0.41
18:AF:228:ILE:O	18:AF:228:ILE:HG22	2.20	0.41
34:Ah:158:ILE:HG22	34:Ah:159:SER:N	2.35	0.41
39:BE:224:TYR:OH	39:BE:254:ARG:HD3	2.19	0.41
41:BG:95:LEU:O	41:BG:99:GLU:HG3	2.20	0.41
43:BI:89:MET:HE3	43:BI:90:PRO:HD2	2.02	0.41
44:BJ:52:LYS:O	44:BJ:53:LYS:C	2.62	0.41
53:BS:45:PHE:O	53:BS:48:LYS:HG2	2.20	0.41
58:BX:44:SER:HA	58:BX:53:LEU:HD11	2.02	0.41
70:CB:185:LYS:HG3	70:CB:185:LYS:O	2.20	0.41
77:CI:1291:C:O2	77:CI:1291:C:H2'	2.20	0.41
77:CI:1361:G:O2'	77:CI:2568:A:C8	2.73	0.41
77:CI:1700:C:H5''	77:CI:1873:A:OP1	2.19	0.41
77:CI:2034:G:H4'	77:CI:2035:A:OP2	2.20	0.41
77:CI:3381:G:H2'	77:CI:3382:A2M:C8	2.48	0.41
77:CI:4067:C:C2	77:CI:4068:C:C5	3.08	0.41
79:CK:71:A:C2	79:CK:88:A:C1'	3.03	0.41
3:AC:345:U:H2'	3:AC:346:U:C6	2.55	0.41
3:AC:1037:A:C5	3:AC:1038:G:C8	3.09	0.41
3:AC:1060:G:C6	3:AC:1061:A:N7	2.88	0.41
7:AK:86:PRO:HB2	7:AK:88:GLU:OE1	2.20	0.41
9:AM:61:GLU:OE2	9:AM:62:ARG:CG	2.68	0.41
12:AP:23:THR:HB	12:AP:113:GLU:CD	2.45	0.41
12:AP:110:VAL:O	12:AP:110:VAL:HG13	2.19	0.41
19:AG:33:LEU:HG	19:AG:33:LEU:O	2.20	0.41
24:AU:78:LEU:HD21	24:AU:82:TYR:OH	2.20	0.41
37:BC:122:TYR:CD1	37:BC:280:PRO:HG3	2.54	0.41
39:BE:110:GLY:CA	39:BE:113:ARG:HH12	2.33	0.41
52:BR:103:VAL:HG22	52:BR:125:LYS:O	2.20	0.41
67:Bg:26:VAL:O	67:Bg:26:VAL:HG12	2.20	0.41
73:CE:46:GLN:HG3	78:CJ:39:C:O2'	2.20	0.41
77:CI:64:A:C4	77:CI:109:G:N7	2.88	0.41
77:CI:140:G:H2'	77:CI:141:C:O4'	2.20	0.41
77:CI:153:G:H2'	77:CI:154:G:C8	2.54	0.41
77:CI:241:G:C4	77:CI:242:U:C6	3.08	0.41
77:CI:386:A:H3'	77:CI:387:G:H5''	2.02	0.41
77:CI:1881:G:H2'	77:CI:1882:U:C6	2.55	0.41
77:CI:3775:G:O3'	77:CI:3776:C:O4'	2.38	0.41
77:CI:4193:G:H2'	77:CI:4194:U:H6	1.85	0.41
77:CI:4364:U:O2	77:CI:4364:U:H2'	2.20	0.41
79:CK:91:A:H2'	79:CK:92:U:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:849:U:H2'	3:AC:850:A:H8	1.85	0.41
3:AC:1304:C:C2	3:AC:1305:U:C6	3.08	0.41
3:AC:1617:U:H2'	3:AC:1618:G:O4'	2.20	0.41
3:AC:1628:C:H5''	11:AO:41:LYS:HD2	2.02	0.41
3:AC:1840:U:H2'	3:AC:1841:U:C6	2.55	0.41
3:AC:1855:U:H2'	3:AC:1856:G:H8	1.85	0.41
8:AL:64:LYS:HE3	8:AL:92:SER:HB3	2.03	0.41
12:AP:21:ARG:HD3	12:AP:90:ASP:OD1	2.20	0.41
13:AT:57:ARG:HB2	13:AT:94:THR:HG23	2.02	0.41
13:AT:300:ALA:HB2	13:AT:310:TRP:HH2	1.85	0.41
17:AD:72:ALA:HB3	28:AZ:128:ARG:NH2	2.35	0.41
36:BB:19:ARG:NH1	36:BB:235:TRP:CZ3	2.88	0.41
38:BD:15:ARG:HD2	77:CI:1545:A:O4'	2.20	0.41
39:BE:76:TYR:CD1	39:BE:77:LYS:HG3	2.55	0.41
60:BZ:2:ALA:O	60:BZ:3:LEU:HB2	2.19	0.41
61:Ba:11:ARG:HH11	61:Ba:11:ARG:HG3	1.85	0.41
63:Bc:27:ILE:H	63:Bc:27:ILE:HD12	1.85	0.41
69:CA:124:SER:O	69:CA:128:ARG:HG3	2.20	0.41
75:CG:123:ILE:O	75:CG:127:VAL:HG13	2.20	0.41
77:CI:341:G:C6	77:CI:342:G:N7	2.89	0.41
77:CI:373:OMG:HM21	77:CI:1458:C:O3'	2.21	0.41
77:CI:1546:U:C4	77:CI:1547:G:N7	2.88	0.41
77:CI:3260:C:C2	77:CI:3261:C:C6	3.09	0.41
77:CI:3361:A:C5	77:CI:3362:G:C8	3.08	0.41
77:CI:4308:C:H2'	77:CI:4309:C:H6	1.85	0.41
77:CI:4392:G:H2'	77:CI:4393:C:C6	2.56	0.41
3:AC:1396:C:O2	3:AC:1396:C:O4'	2.38	0.41
3:AC:1626:U:N3	3:AC:1627:C:C5	2.88	0.41
8:AL:83:MET:HB3	8:AL:116:LEU:HD12	2.01	0.41
12:AP:20:ILE:HG22	12:AP:91:LEU:O	2.21	0.41
12:AP:106:ILE:HD12	12:AP:110:VAL:HG11	2.02	0.41
17:AD:97:LEU:CD1	17:AD:229:MET:HE1	2.49	0.41
18:AF:93:ASP:OD1	18:AF:93:ASP:O	2.37	0.41
24:AU:166:ARG:HG3	24:AU:248:TYR:HE1	1.84	0.41
25:AV:2:LYS:HD3	25:AV:15:LEU:HD21	2.03	0.41
26:AW:43:VAL:O	26:AW:46:VAL:HG22	2.20	0.41
34:Ah:43:ILE:HD13	34:Ah:57:ALA:HA	2.02	0.41
36:BB:92:TYR:HB3	36:BB:99:LEU:HD11	2.01	0.41
39:BE:173:LEU:HD11	39:BE:184:THR:CG2	2.50	0.41
49:BO:110:LYS:NZ	49:BO:121:VAL:O	2.53	0.41
74:CF:127:PHE:CD1	74:CF:143:GLU:OE2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:1695:C:H1'	77:CI:1739:C:O2	2.20	0.41
77:CI:3913:C:N3	77:CI:3914:C:C5	2.88	0.41
79:CK:4:C:H2'	79:CK:5:U:H6	1.84	0.41
2:AB:13:LYS:O	2:AB:14:PHE:CG	2.73	0.41
3:AC:512:U:H2'	3:AC:513:A:C8	2.55	0.41
3:AC:1186:C:C2	3:AC:1187:U:C6	3.09	0.41
9:AM:42:ILE:HG13	9:AM:44:PRO:HD2	2.03	0.41
11:AO:114:GLU:OE1	11:AO:124:THR:CG2	2.68	0.41
17:AD:184:VAL:O	17:AD:187:LYS:HG2	2.21	0.41
21:AQ:30:ALA:O	21:AQ:60:ARG:HD3	2.21	0.41
31:Ad:45:THR:O	31:Ad:45:THR:HG23	2.19	0.41
39:BE:182:LEU:HD23	39:BE:182:LEU:C	2.46	0.41
40:BF:110:PRO:N	40:BF:111:PRO:CD	2.83	0.41
44:BJ:154:LEU:HD13	44:BJ:157:ARG:CZ	2.50	0.41
71:CC:44:GLU:HG3	75:CG:2:VAL:HG12	2.02	0.41
73:CE:26:VAL:O	73:CE:26:VAL:HG23	2.19	0.41
76:CH:145:ASN:O	76:CH:149:GLN:HG3	2.20	0.41
77:CI:1581:U:H2'	77:CI:1582:A:C8	2.56	0.41
77:CI:3311:A:H2'	77:CI:3312:A:C8	2.56	0.41
3:AC:1667:C:H2'	3:AC:1668:U:O4'	2.21	0.41
6:AJ:136:ARG:CB	6:AJ:203:ASN:HD22	2.34	0.41
13:AT:62:HIS:H	13:AT:88:ARG:HD2	1.86	0.41
17:AD:137:LEU:HG	17:AD:215:VAL:HG22	2.03	0.41
36:BB:194:LEU:O	36:BB:198:ARG:HG3	2.20	0.41
40:BF:141:LEU:O	40:BF:145:VAL:HG22	2.21	0.41
57:BW:24:HIS:HA	57:BW:91:ASN:ND2	2.36	0.41
76:CH:16:SER:O	76:CH:20:ARG:HG3	2.20	0.41
77:CI:390:C:C2	77:CI:391:U:C5	3.09	0.41
77:CI:1106:C:H2'	77:CI:1107:G:O4'	2.19	0.41
77:CI:1873:A:N3	77:CI:1874:C:C6	2.88	0.41
77:CI:2501:A:H2'	77:CI:2502:A:H8	1.85	0.41
77:CI:2561:C:N4	77:CI:2562:A:N6	2.69	0.41
79:CK:4:C:C2	79:CK:5:U:C5	3.09	0.41
3:AC:17:C:H2'	3:AC:18:C:C6	2.55	0.41
3:AC:116:OMU:HM23	3:AC:116:OMU:H1'	1.93	0.41
3:AC:848:A:N7	3:AC:849:U:C2	2.89	0.41
3:AC:1048:C:H2'	3:AC:1049:G:O4'	2.20	0.41
3:AC:1445:U:C2'	3:AC:1446:U:H5'	2.50	0.41
3:AC:1554:C:OP1	3:AC:1555:C:OP2	2.39	0.41
3:AC:1658:G:O2'	3:AC:1659:G:H5'	2.21	0.41
6:AJ:74:ASN:HA	6:AJ:77:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AD:144:LYS:HG3	17:AD:208:HIS:ND1	2.35	0.41
25:AV:209:TYR:CZ	25:AV:213:LEU:HD21	2.56	0.41
33:Ag:38:ALA:HA	33:Ag:41:ARG:HG3	2.02	0.41
33:Ag:49:LYS:HE2	33:Ag:63:PHE:CE1	2.55	0.41
37:BC:33:ARG:HG3	37:BC:122:TYR:OH	2.21	0.41
44:BJ:11:LYS:HE2	44:BJ:29:ARG:HD2	2.02	0.41
58:BX:93:ARG:HG2	58:BX:97:ILE:HD13	2.02	0.41
73:CE:16:ARG:HH12	73:CE:137:PRO:HG3	1.86	0.41
73:CE:27:GLY:HA2	73:CE:68:ILE:HG23	2.02	0.41
77:CI:78:U:N3	77:CI:79:C:C5	2.89	0.41
77:CI:174:C:C2	77:CI:175:C:C5	3.08	0.41
77:CI:1128:C:H5	77:CI:1137:A:HO2'	1.69	0.41
77:CI:2044:G:C2	77:CI:2046:C:C5	3.09	0.41
77:CI:3367:C:H2'	77:CI:3368:U:C1'	2.50	0.41
77:CI:4005:C:C2	77:CI:4006:U:C5	3.09	0.41
3:AC:306:U:H3'	3:AC:307:C:C5'	2.51	0.41
3:AC:417:U:H2'	3:AC:418:C:O4'	2.21	0.41
3:AC:641:A:H2'	3:AC:642:A:C8	2.55	0.41
5:AH:77:GLU:O	5:AH:82:ASP:HB2	2.21	0.41
9:AM:7:LEU:HG	9:AM:7:LEU:O	2.21	0.41
18:AF:149:TYR:HD1	25:AV:205:GLU:OE1	2.04	0.41
25:AV:2:LYS:HB3	25:AV:15:LEU:HD11	2.03	0.41
26:AW:57:ALA:O	26:AW:61:LEU:HD23	2.21	0.41
27:AY:57:SER:O	27:AY:58:HIS:HB2	2.21	0.41
29:Aa:28:ARG:HB3	29:Aa:29:PRO:HD3	2.02	0.41
30:Ab:110:ARG:O	30:Ab:114:MET:HG3	2.20	0.41
36:BB:63:PRO:HA	36:BB:68:ASN:ND2	2.35	0.41
53:BS:61:ASN:OD1	77:CI:1631:G:H1'	2.20	0.41
73:CE:175:LEU:C	73:CE:175:LEU:HD12	2.45	0.41
77:CI:423:G:H2'	77:CI:424:U:H6	1.85	0.41
77:CI:951:C:N3	77:CI:1033:G:O6	2.53	0.41
77:CI:1147:A:H2'	77:CI:1148:A:C8	2.56	0.41
77:CI:1483:G:C8	77:CI:1657:G:C8	3.09	0.41
77:CI:1541:G:H5''	78:CJ:102:U:H1'	2.03	0.41
77:CI:1685:OMG:O2'	77:CI:1686:C:OP2	2.39	0.41
77:CI:3514:C:H2'	77:CI:3515:A:H8	1.86	0.41
77:CI:3735:G:H2'	77:CI:3736:U:C6	2.56	0.41
1:AA:12:ALA:HB1	1:AA:32:VAL:HB	2.03	0.41
3:AC:219:A:C6	3:AC:220:U:C5	3.09	0.41
3:AC:302:A:C2	34:Ah:73:THR:HG21	2.56	0.41
3:AC:430:C:C2	3:AC:431:C:C5	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:571:C:C4	3:AC:572:U:C4	3.08	0.41
3:AC:675:C:H2'	3:AC:676:U:C6	2.55	0.41
3:AC:953:G:C6	3:AC:976:G:C6	3.08	0.41
3:AC:1238:C:H2'	3:AC:1239:U:O4'	2.21	0.41
3:AC:1272:C:O2	3:AC:1272:C:H2'	2.20	0.41
3:AC:1630:C:H2'	3:AC:1631:A:O4'	2.20	0.41
3:AC:1829:C:H2'	3:AC:1830:G:O4'	2.20	0.41
5:AH:5:ARG:HD2	5:AH:9:VAL:HG11	2.02	0.41
9:AM:42:ILE:HD12	9:AM:42:ILE:HA	1.99	0.41
10:AN:36:VAL:HG21	10:AN:71:MET:SD	2.61	0.41
10:AN:71:MET:HG2	10:AN:99:LEU:CD1	2.50	0.41
11:AO:4:VAL:HB	11:AO:8:ASP:OD2	2.20	0.41
11:AO:39:LEU:HD13	11:AO:47:PRO:CG	2.51	0.41
11:AO:39:LEU:HD12	11:AO:39:LEU:N	2.36	0.41
13:AT:168:CYS:HB3	13:AT:198:VAL:HG21	2.02	0.41
15:Ac:50:PHE:CD2	15:Ac:55:TYR:HD1	2.39	0.41
16:Af:125:GLU:HG3	16:Af:125:GLU:O	2.21	0.41
17:AD:44:ILE:CD1	17:AD:86:LEU:HD12	2.50	0.41
20:AI:147:LEU:CD1	20:AI:163:CYS:SG	3.09	0.41
34:Ah:110:ARG:HD3	34:Ah:114:GLU:OE1	2.21	0.41
36:BB:247:GLY:HA2	77:CI:2594:G:H5'	2.02	0.41
36:BB:303:ALA:HB2	36:BB:314:ILE:CD1	2.50	0.41
42:BH:168:ARG:HG2	42:BH:169:SER:N	2.36	0.41
44:BJ:164:LYS:HB3	44:BJ:165:PRO:HD3	2.03	0.41
44:BJ:175:PHE:O	44:BJ:176:PHE:HB2	2.21	0.41
45:BK:38:ASP:C	45:BK:38:ASP:OD1	2.64	0.41
58:BX:2:VAL:HG12	58:BX:3:GLN:N	2.36	0.41
67:Bg:52:VAL:O	67:Bg:52:VAL:HG13	2.21	0.41
72:CD:75:TYR:CZ	72:CD:150:GLU:HG2	2.56	0.41
73:CE:120:ASP:O	73:CE:123:ILE:HG22	2.21	0.41
75:CG:56:GLN:NE2	75:CG:91:TRP:HZ2	2.17	0.41
77:CI:341:G:C2	77:CI:342:G:C8	3.09	0.41
77:CI:716:G:H2'	77:CI:717:A:C8	2.55	0.41
77:CI:935:C:C5	77:CI:1053:G:N2	2.89	0.41
77:CI:1169:G:H2'	77:CI:1170:U:C6	2.56	0.41
77:CI:2614:A:H2'	77:CI:2615:G:O4'	2.21	0.41
77:CI:3307:A:H1'	77:CI:3444:A2M:N6	2.36	0.41
77:CI:3452:U:C2	77:CI:3453:C:C5	3.09	0.41
77:CI:4057:C:C4	77:CI:4058:PSU:C2	3.09	0.41
77:CI:4386:G:H2'	77:CI:4386:G:N3	2.35	0.41
3:AC:71:G:H2'	3:AC:72:C:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:1114:A:H2'	3:AC:1115:U:C6	2.56	0.41
3:AC:1385:C:C2	3:AC:1386:G:C8	3.09	0.41
6:AJ:33:ILE:HD12	6:AJ:33:ILE:H	1.86	0.41
6:AJ:43:GLU:OE1	6:AJ:43:GLU:N	2.52	0.41
6:AJ:200:ALA:HA	6:AJ:203:ASN:OD1	2.21	0.41
7:AK:25:LYS:HG2	7:AK:25:LYS:O	2.21	0.41
11:AO:7:LYS:HZ3	11:AO:66:LEU:HD22	1.85	0.41
13:AT:67:SER:HB3	13:AT:83:TRP:CD1	2.55	0.41
20:AI:10:MET:HE3	20:AI:15:VAL:HG22	2.02	0.41
29:Aa:105:THR:O	29:Aa:105:THR:HG23	2.21	0.41
41:BG:126:ARG:HA	41:BG:140:MET:SD	2.61	0.41
42:BH:93:LEU:HB2	42:BH:94:GLU:OE2	2.20	0.41
72:CD:70:ILE:O	72:CD:74:LYS:HG3	2.21	0.41
77:CI:1128:C:O2'	77:CI:1129:C:O5'	2.37	0.41
77:CI:2241:U:N3	77:CI:2242:G:N7	2.69	0.41
77:CI:4115:U:H2'	77:CI:4116:C:H6	1.86	0.41
3:AC:1089:U:H4'	3:AC:1090:G:OP2	2.22	0.40
3:AC:1273:C:O2'	3:AC:1274:C:C6	2.71	0.40
3:AC:1569:C:H2'	3:AC:1570:A:C8	2.56	0.40
13:AT:60:ARG:O	13:AT:61:GLY:C	2.63	0.40
14:AX:52:LEU:HD21	14:AX:65:VAL:HB	2.04	0.40
18:AF:126:VAL:HG11	18:AF:129:ILE:HD11	2.03	0.40
23:AS:64:LEU:HA	23:AS:65:PRO:HD3	1.97	0.40
33:Ag:43:LEU:HD22	33:Ag:72:PHE:HE1	1.79	0.40
41:BG:132:ALA:O	77:CI:1413:A:OP2	2.38	0.40
47:BM:71:GLU:HG2	47:BM:72:LEU:HD12	2.02	0.40
65:Be:10:MET:HE1	65:Be:17:ARG:HH12	1.86	0.40
69:CA:239:ARG:HD3	77:CI:724:C:OP1	2.21	0.40
71:CC:128:MET:SD	71:CC:157:SER:HB3	2.61	0.40
77:CI:2008:G:H3'	77:CI:2009:G:C5'	2.51	0.40
77:CI:2254:C:N4	77:CI:2255:C:H41	2.19	0.40
77:CI:3351:A:C4	77:CI:3352:U:C6	3.09	0.40
77:CI:4501:G:H2'	77:CI:4502:G:O4'	2.20	0.40
3:AC:1345:A:H4'	3:AC:1346:G:OP1	2.21	0.40
9:AM:31:LEU:HB3	9:AM:67:ASP:OD1	2.21	0.40
9:AM:42:ILE:O	9:AM:42:ILE:CG2	2.69	0.40
23:AS:64:LEU:HD22	28:AZ:129:ILE:HD12	2.02	0.40
28:AZ:98:ARG:HB3	28:AZ:132:VAL:HG23	2.04	0.40
30:Ab:20:ARG:HA	30:Ab:75:ILE:O	2.20	0.40
33:Ag:126:HIS:CD2	33:Ag:181:THR:HB	2.57	0.40
44:BJ:48:VAL:HG11	44:BJ:54:MET:SD	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:BZ:94:LEU:O	60:BZ:97:MET:HG2	2.22	0.40
69:CA:170:LYS:O	69:CA:174:GLU:HG2	2.21	0.40
69:CA:258:ARG:HG3	69:CA:258:ARG:O	2.21	0.40
70:CB:98:LEU:HD12	70:CB:98:LEU:HA	1.97	0.40
73:CE:22:LEU:CD2	73:CE:130:PHE:CD1	3.04	0.40
77:CI:1668:UR3:C3U	77:CI:4060:G:C8	3.04	0.40
77:CI:3361:A:C6	77:CI:3362:G:C8	3.09	0.40
77:CI:4303:A:H2'	77:CI:4304:G:H8	1.86	0.40
3:AC:120:U:O2	3:AC:120:U:H2'	2.20	0.40
3:AC:596:U:H2'	3:AC:597:U:C6	2.57	0.40
3:AC:609:C:N3	3:AC:610:U:C4	2.90	0.40
3:AC:828:A:C6	3:AC:829:G:C5	3.10	0.40
3:AC:1273:C:O2'	3:AC:1274:C:P	2.79	0.40
3:AC:1317:C:H2'	3:AC:1318:C:H6	1.85	0.40
3:AC:1783:G:H2'	3:AC:1784:C:OP1	2.21	0.40
6:AJ:139:VAL:HG12	6:AJ:140:ASP:N	2.36	0.40
13:AT:201:SER:HB2	13:AT:206:LEU:HB2	2.02	0.40
20:AI:84:GLN:O	20:AI:87:VAL:HG12	2.22	0.40
25:AV:146:ASN:ND2	25:AV:146:ASN:O	2.54	0.40
26:AW:138:ARG:O	26:AW:139:LYS:HB2	2.21	0.40
35:BA:63:PHE:HD2	35:BA:74:GLU:OE1	2.05	0.40
36:BB:258:HIS:HB3	36:BB:259:PRO:HD3	2.04	0.40
37:BC:163:LYS:O	37:BC:166:GLU:HG2	2.21	0.40
40:BF:74:ARG:O	40:BF:142:ALA:HB1	2.21	0.40
46:BL:91:LEU:HB3	46:BL:97:ARG:HG2	2.03	0.40
57:BW:4:ARG:HH22	57:BW:8:LYS:HG3	1.87	0.40
75:CG:74:ARG:O	75:CG:78:GLU:HG3	2.22	0.40
77:CI:100:C:C2	77:CI:101:A:C8	3.09	0.40
77:CI:108:A:H4'	77:CI:109:G:OP1	2.21	0.40
77:CI:422:C:H2'	77:CI:423:G:H8	1.87	0.40
77:CI:719:C:C2	77:CI:720:G:C8	3.09	0.40
77:CI:1001:G:O6	77:CI:1024:C:N3	2.54	0.40
77:CI:1746:A:N6	77:CI:1841:G:N2	2.69	0.40
77:CI:2451:A:H1'	77:CI:2453:A:N7	2.36	0.40
79:CK:82:A:OP2	79:CK:82:A:H4'	2.21	0.40
1:AA:14:VAL:HG13	1:AA:30:VAL:HB	2.03	0.40
1:AA:35:MET:CE	1:AA:55:VAL:HG13	2.52	0.40
2:AB:14:PHE:HB2	3:AC:1662:A:O4'	2.21	0.40
3:AC:4:C:C2	3:AC:5:U:C5	3.10	0.40
3:AC:155:G:H4'	25:AV:15:LEU:HD22	2.04	0.40
3:AC:319:A:C2	3:AC:334:G:C6	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:1047:U:O2'	3:AC:1048:C:OP1	2.37	0.40
3:AC:1538:A:H2'	3:AC:1539:C:H6	1.86	0.40
13:AT:135:LEU:HG	13:AT:135:LEU:O	2.21	0.40
17:AD:167:LYS:HD3	17:AD:200:ALA:HB1	2.03	0.40
17:AD:188:LEU:O	17:AD:188:LEU:HD23	2.21	0.40
22:AR:94:ILE:HG12	22:AR:125:VAL:HG21	2.03	0.40
44:BJ:90:THR:HG23	45:BK:156:TYR:CD2	2.56	0.40
61:Ba:36:LYS:HE2	77:CI:372:A:OP1	2.21	0.40
70:CB:58:PRO:CG	70:CB:61:ILE:HD12	2.51	0.40
77:CI:78:U:C2	77:CI:79:C:C6	3.09	0.40
77:CI:1006:G:H2'	77:CI:1007:A:O4'	2.21	0.40
77:CI:1122:C:H2'	77:CI:1123:C:H6	1.85	0.40
77:CI:1354:U:H3	77:CI:1431:G:H1	1.70	0.40
77:CI:2239:G:N3	77:CI:2252:G:C2	2.90	0.40
77:CI:3364:G:H2'	77:CI:3365:C:H6	1.87	0.40
3:AC:527:A:O2'	3:AC:528:C:O5'	2.39	0.40
3:AC:823:PSU:H6	3:AC:825:C:OP2	2.04	0.40
3:AC:1324:U:H2'	3:AC:1325:G:C8	2.57	0.40
3:AC:1338:C:H4'	12:AP:67:LYS:HG2	2.04	0.40
3:AC:1822:U:H2'	3:AC:1823:A:C8	2.57	0.40
5:AH:12:ALA:O	5:AH:16:ILE:CD1	2.67	0.40
10:AN:16:LEU:O	10:AN:16:LEU:HG	2.22	0.40
11:AO:5:THR:O	11:AO:8:ASP:OD1	2.40	0.40
18:AF:11:ARG:HD2	18:AF:20:LEU:HB3	2.03	0.40
24:AU:69:LEU:HA	24:AU:72:ASP:OD1	2.21	0.40
30:Ab:91:LEU:HA	30:Ab:94:HIS:HE2	1.86	0.40
36:BB:242:ARG:NH2	77:CI:2612:C:O2	2.54	0.40
37:BC:109:ARG:HA	77:CI:1155:U:H5'	2.03	0.40
37:BC:170:LEU:C	37:BC:170:LEU:HD23	2.46	0.40
43:BI:31:GLU:OE2	43:BI:44:LEU:HD21	2.22	0.40
44:BJ:44:PHE:CZ	44:BJ:48:VAL:HG21	2.56	0.40
55:BU:54:MET:O	55:BU:57:MET:O	2.40	0.40
62:Bb:38:CYS:HB3	62:Bb:41:TYR:O	2.21	0.40
73:CE:144:LYS:HE3	73:CE:147:ARG:O	2.21	0.40
74:CF:77:SER:O	74:CF:80:GLU:HG2	2.22	0.40
77:CI:119:G:H4'	77:CI:120:A:OP2	2.22	0.40
77:CI:393:U:H3	77:CI:398:A2M:H62	1.70	0.40
77:CI:1128:C:O2	77:CI:3524:A:C4	2.75	0.40
77:CI:1170:U:H2'	77:CI:1171:C:C6	2.57	0.40
77:CI:1257:G:N1	77:CI:1258:U:C4	2.90	0.40
77:CI:1527:U:H2'	77:CI:1528:U:H6	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:1713:C:O2'	77:CI:1720:U:H5''	2.22	0.40
77:CI:2132:A:H2'	77:CI:2133:C:C6	2.56	0.40
77:CI:2173:A:C4	77:CI:2174:A:C8	3.10	0.40
77:CI:2175:C:C2	77:CI:2176:A:C8	3.10	0.40
77:CI:3504:A:H2'	77:CI:3505:C:H6	1.87	0.40
77:CI:3847:A:H2'	77:CI:3848:C:H6	1.86	0.40
77:CI:3885:C:O2	77:CI:3926:A:N6	2.55	0.40
77:CI:4599:G:C2	77:CI:4600:U:C5	3.10	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	AA	62/69 (90%)	59 (95%)	3 (5%)	0	100	100
2	AB	52/56 (93%)	51 (98%)	1 (2%)	0	100	100
4	AE	224/243 (92%)	218 (97%)	6 (3%)	0	100	100
5	AH	132/135 (98%)	129 (98%)	2 (2%)	1 (1%)	16	32
6	AJ	187/204 (92%)	180 (96%)	6 (3%)	1 (0%)	24	44
7	AK	95/165 (58%)	94 (99%)	1 (1%)	0	100	100
8	AL	121/145 (83%)	117 (97%)	4 (3%)	0	100	100
9	AM	142/146 (97%)	138 (97%)	4 (3%)	0	100	100
10	AN	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
11	AO	139/145 (96%)	139 (100%)	0	0	100	100
12	AP	100/119 (84%)	97 (97%)	3 (3%)	0	100	100
13	AT	311/317 (98%)	297 (96%)	14 (4%)	0	100	100
14	AX	83/132 (63%)	80 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	Ac	73/125 (58%)	72 (99%)	1 (1%)	0	100	100
16	Af	60/156 (38%)	56 (93%)	4 (7%)	0	100	100
17	AD	212/264 (80%)	209 (99%)	3 (1%)	0	100	100
18	AF	260/263 (99%)	259 (100%)	1 (0%)	0	100	100
19	AG	144/158 (91%)	139 (96%)	5 (4%)	0	100	100
20	AI	212/295 (72%)	207 (98%)	5 (2%)	0	100	100
21	AQ	81/83 (98%)	81 (100%)	0	0	100	100
22	AR	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
23	AS	99/115 (86%)	99 (100%)	0	0	100	100
24	AU	220/293 (75%)	215 (98%)	5 (2%)	0	100	100
25	AV	225/249 (90%)	217 (96%)	8 (4%)	0	100	100
26	AW	145/194 (75%)	143 (99%)	2 (1%)	0	100	100
27	AY	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
28	AZ	132/151 (87%)	131 (99%)	1 (1%)	0	100	100
29	Aa	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
30	Ab	119/133 (90%)	113 (95%)	5 (4%)	1 (1%)	16	32
31	Ad	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
32	Ae	11/133 (8%)	11 (100%)	0	0	100	100
33	Ag	179/194 (92%)	169 (94%)	10 (6%)	0	100	100
34	Ah	204/208 (98%)	199 (98%)	5 (2%)	0	100	100
35	BA	249/257 (97%)	240 (96%)	9 (4%)	0	100	100
36	BB	394/403 (98%)	388 (98%)	6 (2%)	0	100	100
37	BC	364/419 (87%)	358 (98%)	6 (2%)	0	100	100
38	BD	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
39	BE	212/296 (72%)	205 (97%)	6 (3%)	1 (0%)	24	44
40	BF	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
41	BG	151/184 (82%)	147 (97%)	3 (2%)	1 (1%)	18	36
42	BH	184/188 (98%)	179 (97%)	5 (3%)	0	100	100
43	BI	182/196 (93%)	182 (100%)	0	0	100	100
44	BJ	173/176 (98%)	170 (98%)	3 (2%)	0	100	100
45	BK	157/160 (98%)	156 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	BL	99/128 (77%)	94 (95%)	5 (5%)	0	100	100
47	BM	127/140 (91%)	126 (99%)	1 (1%)	0	100	100
48	BN	59/157 (38%)	58 (98%)	1 (2%)	0	100	100
49	BO	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
50	BP	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
51	BQ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
52	BR	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
53	BS	95/160 (59%)	92 (97%)	3 (3%)	0	100	100
54	BT	92/115 (80%)	89 (97%)	3 (3%)	0	100	100
55	BU	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
56	BV	106/135 (78%)	105 (99%)	1 (1%)	0	100	100
57	BW	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
58	BX	112/117 (96%)	112 (100%)	0	0	100	100
59	BY	118/123 (96%)	117 (99%)	1 (1%)	0	100	100
60	BZ	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
61	Ba	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
62	Bb	67/70 (96%)	67 (100%)	0	0	100	100
63	Bc	48/51 (94%)	48 (100%)	0	0	100	100
64	Bd	49/128 (38%)	49 (100%)	0	0	100	100
65	Be	23/25 (92%)	23 (100%)	0	0	100	100
66	Bf	101/106 (95%)	98 (97%)	3 (3%)	0	100	100
67	Bg	87/92 (95%)	85 (98%)	2 (2%)	0	100	100
68	Bh	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
69	CA	221/270 (82%)	215 (97%)	6 (3%)	0	100	100
70	CB	227/266 (85%)	221 (97%)	6 (3%)	0	100	100
71	CC	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
72	CD	204/214 (95%)	198 (97%)	6 (3%)	0	100	100
73	CE	166/178 (93%)	160 (96%)	6 (4%)	0	100	100
74	CF	205/211 (97%)	196 (96%)	9 (4%)	0	100	100
75	CG	137/217 (63%)	134 (98%)	3 (2%)	0	100	100
76	CH	201/204 (98%)	195 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	10994/12787 (86%)	10737 (98%)	252 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AH	67	ARG
41	BG	132	ALA
30	Ab	80	ASP
39	BE	110	GLY
6	AJ	79	HIS

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	AA	57/62 (92%)	57 (100%)	0	100	100
2	AB	48/49 (98%)	48 (100%)	0	100	100
4	AE	189/202 (94%)	189 (100%)	0	100	100
5	AH	120/121 (99%)	120 (100%)	0	100	100
6	AJ	159/170 (94%)	159 (100%)	0	100	100
7	AK	88/136 (65%)	88 (100%)	0	100	100
8	AL	109/130 (84%)	109 (100%)	0	100	100
9	AM	119/121 (98%)	119 (100%)	0	100	100
10	AN	125/132 (95%)	125 (100%)	0	100	100
11	AO	112/115 (97%)	112 (100%)	0	100	100
12	AP	93/107 (87%)	93 (100%)	0	100	100
13	AT	272/275 (99%)	272 (100%)	0	100	100
14	AX	74/108 (68%)	74 (100%)	0	100	100
15	Ac	66/103 (64%)	66 (100%)	0	100	100
16	Af	55/140 (39%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AD	195/229 (85%)	195 (100%)	0	100	100
18	AF	224/225 (100%)	224 (100%)	0	100	100
19	AG	133/142 (94%)	133 (100%)	0	100	100
20	AI	179/242 (74%)	179 (100%)	0	100	100
21	AQ	67/67 (100%)	67 (100%)	0	100	100
22	AR	113/115 (98%)	113 (100%)	0	100	100
23	AS	88/98 (90%)	88 (100%)	0	100	100
24	AU	188/224 (84%)	188 (100%)	0	100	100
25	AV	198/218 (91%)	198 (100%)	0	100	100
26	AW	133/168 (79%)	133 (100%)	0	100	100
27	AY	130/131 (99%)	130 (100%)	0	100	100
28	AZ	104/119 (87%)	104 (100%)	0	100	100
29	Aa	112/113 (99%)	112 (100%)	0	100	100
30	Ab	107/115 (93%)	107 (100%)	0	100	100
31	Ad	75/76 (99%)	75 (100%)	0	100	100
32	Ae	9/106 (8%)	9 (100%)	0	100	100
33	Ag	164/174 (94%)	164 (100%)	0	100	100
34	Ah	178/180 (99%)	178 (100%)	0	100	100
35	BA	193/199 (97%)	193 (100%)	0	100	100
36	BB	344/348 (99%)	344 (100%)	0	100	100
37	BC	307/347 (88%)	307 (100%)	0	100	100
38	BD	245/249 (98%)	245 (100%)	0	100	100
39	BE	196/256 (77%)	196 (100%)	0	100	100
40	BF	172/173 (99%)	172 (100%)	0	100	100
41	BG	134/163 (82%)	134 (100%)	0	100	100
42	BH	164/165 (99%)	164 (100%)	0	100	100
43	BI	163/175 (93%)	163 (100%)	0	100	100
44	BJ	155/156 (99%)	155 (100%)	0	100	100
45	BK	139/140 (99%)	139 (100%)	0	100	100
46	BL	91/114 (80%)	91 (100%)	0	100	100
47	BM	100/107 (94%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BN	54/126 (43%)	54 (100%)	0	100	100
49	BO	106/133 (80%)	106 (100%)	0	100	100
50	BP	124/135 (92%)	124 (100%)	0	100	100
51	BQ	117/118 (99%)	117 (100%)	0	100	100
52	BR	120/121 (99%)	120 (100%)	0	100	100
53	BS	85/124 (68%)	85 (100%)	0	100	100
54	BT	79/97 (81%)	79 (100%)	0	100	100
55	BU	98/110 (89%)	98 (100%)	0	100	100
56	BV	98/121 (81%)	98 (100%)	0	100	100
57	BW	88/89 (99%)	88 (100%)	0	100	100
58	BX	98/100 (98%)	98 (100%)	0	100	100
59	BY	108/110 (98%)	108 (100%)	0	100	100
60	BZ	86/89 (97%)	86 (100%)	0	100	100
61	Ba	73/80 (91%)	73 (100%)	0	100	100
62	Bb	64/65 (98%)	64 (100%)	0	100	100
63	Bc	47/48 (98%)	47 (100%)	0	100	100
64	Bd	47/115 (41%)	47 (100%)	0	100	100
65	Be	24/24 (100%)	24 (100%)	0	100	100
66	Bf	91/94 (97%)	91 (100%)	0	100	100
67	Bg	73/75 (97%)	73 (100%)	0	100	100
68	Bh	109/121 (90%)	109 (100%)	0	100	100
69	CA	194/234 (83%)	194 (100%)	0	100	100
70	CB	198/223 (89%)	198 (100%)	0	100	100
71	CC	169/171 (99%)	169 (100%)	0	100	100
72	CD	177/180 (98%)	177 (100%)	0	100	100
73	CE	142/149 (95%)	142 (100%)	0	100	100
74	CF	174/178 (98%)	174 (100%)	0	100	100
75	CG	118/157 (75%)	118 (100%)	0	100	100
76	CH	171/172 (99%)	171 (100%)	0	100	100
All	All	9618/10864 (88%)	9618 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	45	ASN
4	AE	57	ASN
4	AE	165	ASN
6	AJ	31	ASN
6	AJ	82	ASN
6	AJ	149	GLN
7	AK	73	ASN
7	AK	77	GLN
8	AL	103	ASN
8	AL	104	GLN
9	AM	11	GLN
9	AM	77	HIS
10	AN	73	ASN
10	AN	76	GLN
11	AO	63	HIS
12	AP	81	GLN
13	AT	117	ASN
13	AT	119	GLN
13	AT	159	ASN
13	AT	181	ASN
13	AT	191	HIS
15	Ac	106	GLN
16	Af	151	ASN
17	AD	157	GLN
18	AF	67	GLN
18	AF	157	ASN
18	AF	201	HIS
18	AF	209	HIS
19	AG	18	GLN
19	AG	19	ASN
19	AG	112	HIS
22	AR	87	ASN
22	AR	97	ASN
23	AS	72	HIS
24	AU	115	GLN
25	AV	197	GLN
25	AV	202	ASN
27	AY	5	HIS
27	AY	123	HIS
29	Aa	56	HIS
29	Aa	70	ASN

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Mol	Chain	Res	Type
29	Aa	92	ASN
30	Ab	94	HIS
31	Ad	9	HIS
31	Ad	51	GLN
33	Ag	126	HIS
33	Ag	157	HIS
33	Ag	168	HIS
34	Ah	35	ASN
34	Ah	138	ASN
35	BA	83	HIS
35	BA	205	ASN
35	BA	217	GLN
36	BB	11	HIS
36	BB	145	GLN
36	BB	179	HIS
36	BB	204	GLN
36	BB	213	GLN
36	BB	258	HIS
37	BC	43	ASN
37	BC	169	GLN
37	BC	329	ASN
38	BD	291	GLN
39	BE	50	HIS
39	BE	165	HIS
39	BE	253	GLN
40	BF	50	ASN
40	BF	63	ASN
40	BF	150	GLN
41	BG	56	GLN
41	BG	133	HIS
43	BI	66	ASN
44	BJ	37	HIS
45	BK	144	ASN
46	BL	41	GLN
46	BL	94	ASN
49	BO	69	ASN
49	BO	73	HIS
50	BP	18	HIS
50	BP	20	ASN
51	BQ	127	ASN
52	BR	19	HIS
52	BR	60	HIS

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Mol	Chain	Res	Type
52	BR	93	ASN
53	BS	6	ASN
53	BS	50	ASN
53	BS	114	GLN
54	BT	72	HIS
54	BT	73	HIS
56	BV	101	HIS
58	BX	100	GLN
58	BX	112	GLN
59	BY	98	HIS
60	BZ	15	HIS
60	BZ	20	ASN
60	BZ	92	ASN
61	Ba	57	ASN
63	Bc	17	GLN
63	Bc	33	ASN
67	Bg	56	HIS
68	Bh	36	ASN
68	Bh	100	ASN
69	CA	102	ASN
69	CA	132	GLN
70	CB	46	GLN
70	CB	100	HIS
70	CB	112	GLN
70	CB	159	HIS
70	CB	206	GLN
70	CB	208	ASN
70	CB	225	ASN
71	CC	98	HIS
71	CC	106	GLN
71	CC	188	GLN
72	CD	73	ASN
72	CD	166	HIS
74	CF	19	GLN
74	CF	149	GLN
75	CG	20	HIS
75	CG	34	ASN
76	CH	117	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	AC	1686/1871 (90%)	312 (18%)	2 (0%)
77	CI	3541/4731 (74%)	664 (18%)	16 (0%)
78	CJ	119/121 (98%)	8 (6%)	0
79	CK	155/156 (99%)	28 (18%)	2 (1%)
All	All	5501/6879 (79%)	1012 (18%)	20 (0%)

All (1012) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	AC	17	C
3	AC	33	G
3	AC	46	A
3	AC	56	G
3	AC	58	C
3	AC	59	U
3	AC	65	C
3	AC	67	C
3	AC	72	C
3	AC	74	G
3	AC	75	G
3	AC	78	C
3	AC	103	A
3	AC	113	G
3	AC	115	U
3	AC	126	G
3	AC	143	U
3	AC	151	C
3	AC	155	G
3	AC	160	U
3	AC	161	U
3	AC	171	A
3	AC	182	C
3	AC	184	G
3	AC	191	A
3	AC	198	U
3	AC	199	U
3	AC	202	C
3	AC	203	G
3	AC	205	G
3	AC	206	G
3	AC	207	G
3	AC	213	G
3	AC	214	C

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Mol	Chain	Res	Type
3	AC	294	C
3	AC	295	U
3	AC	296	C
3	AC	303	A
3	AC	306	U
3	AC	307	C
3	AC	308	G
3	AC	309	G
3	AC	310	G
3	AC	320	C
3	AC	325	C
3	AC	326	C
3	AC	327	C
3	AC	328	G
3	AC	329	U
3	AC	330	G
3	AC	331	G
3	AC	340	A
3	AC	341	C
3	AC	348	G
3	AC	361	A
3	AC	363	C
3	AC	365	A
3	AC	369	U
3	AC	370	C
3	AC	371	G
3	AC	386	G
3	AC	387	C
3	AC	393	A
3	AC	395	G
3	AC	410	C
3	AC	449	A
3	AC	450	A
3	AC	451	C
3	AC	452	G
3	AC	465	A
3	AC	471	G
3	AC	472	G
3	AC	473	C
3	AC	475	G
3	AC	483	G
3	AC	488	U

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Mol	Chain	Res	Type
3	AC	493	C
3	AC	517	A
3	AC	526	A
3	AC	527	A
3	AC	528	C
3	AC	560	G
3	AC	561	A
3	AC	562	A
3	AC	564	G
3	AC	565	A
3	AC	570	A
3	AC	573	U
3	AC	577	A
3	AC	582	U
3	AC	583	U
3	AC	584	A
3	AC	588	A
3	AC	590	G
3	AC	592	U
3	AC	594	C
3	AC	608	U
3	AC	613	PSU
3	AC	615	C
3	AC	618	G
3	AC	629	A
3	AC	630	A
3	AC	632	U
3	AC	633	C
3	AC	644	A
3	AC	656	A
3	AC	661	C
3	AC	669	A2M
3	AC	670	A
3	AC	672	A
3	AC	673	A
3	AC	689	U
3	AC	691	G
3	AC	693	G
3	AC	694	A
3	AC	695	G
3	AC	696	C
3	AC	697	G

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Mol	Chain	Res	Type
3	AC	698	G
3	AC	699	G
3	AC	732	G
3	AC	733	U
3	AC	734	C
3	AC	736	C
3	AC	737	C
3	AC	738	G
3	AC	739	C
3	AC	749	C
3	AC	750	U
3	AC	751	C
3	AC	752	G
3	AC	753	G
3	AC	754	C
3	AC	789	G
3	AC	790	G
3	AC	791	C
3	AC	792	C
3	AC	793	C
3	AC	796	A
3	AC	798	C
3	AC	800	U
3	AC	802	U
3	AC	812	A
3	AC	822	G
3	AC	823	PSU
3	AC	824	PSU
3	AC	831	A
3	AC	837	G
3	AC	838	A
3	AC	840	C
3	AC	841	C
3	AC	842	G
3	AC	848	A
3	AC	860	G
3	AC	863	A
3	AC	870	A
3	AC	871	A
3	AC	872	U
3	AC	878	C
3	AC	888	U

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Mol	Chain	Res	Type
3	AC	897	U
3	AC	898	U
3	AC	900	U
3	AC	908	G
3	AC	914	A
3	AC	921	A
3	AC	923	A
3	AC	934	G
3	AC	935	G
3	AC	972	G
3	AC	991	A
3	AC	993	A
3	AC	1002	A
3	AC	1018	U
3	AC	1024	A
3	AC	1048	C
3	AC	1062	U
3	AC	1063	A
3	AC	1084	A
3	AC	1086	C
3	AC	1116	U
3	AC	1117	C
3	AC	1118	C
3	AC	1120	A
3	AC	1122	G
3	AC	1134	A
3	AC	1139	C
3	AC	1154	C
3	AC	1155	U
3	AC	1172	G
3	AC	1196	A
3	AC	1208	G
3	AC	1216	C
3	AC	1218	A
3	AC	1222	G
3	AC	1225	G
3	AC	1239	U
3	AC	1243	U
3	AC	1244	PSU
3	AC	1249	B8N
3	AC	1252	A
3	AC	1254	A

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Mol	Chain	Res	Type
3	AC	1257	G
3	AC	1258	G
3	AC	1260	A
3	AC	1274	C
3	AC	1275	G
3	AC	1276	G
3	AC	1295	G
3	AC	1301	U
3	AC	1303	G
3	AC	1304	C
3	AC	1309	U
3	AC	1321	G
3	AC	1323	G
3	AC	1342	C
3	AC	1343	U
3	AC	1345	A
3	AC	1372	U
3	AC	1379	A
3	AC	1397	A
3	AC	1398	U
3	AC	1399	G
3	AC	1405	U
3	AC	1407	G
3	AC	1418	C
3	AC	1420	C
3	AC	1421	G
3	AC	1422	A
3	AC	1423	G
3	AC	1424	C
3	AC	1434	C
3	AC	1435	C
3	AC	1436	C
3	AC	1437	C
3	AC	1438	C
3	AC	1439	A
3	AC	1443	U
3	AC	1446	U
3	AC	1447	A
3	AC	1455	A
3	AC	1463	U
3	AC	1464	U
3	AC	1491	G

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Mol	Chain	Res	Type
3	AC	1498	G
3	AC	1499	A
3	AC	1509	A
3	AC	1521	G
3	AC	1522	C
3	AC	1523	A
3	AC	1534	A
3	AC	1549	G
3	AC	1554	C
3	AC	1556	U
3	AC	1580	A
3	AC	1581	A
3	AC	1588	G
3	AC	1589	A
3	AC	1602	A
3	AC	1622	U
3	AC	1624	A
3	AC	1625	U
3	AC	1640	G
3	AC	1649	G
3	AC	1655	G
3	AC	1664	A
3	AC	1665	A
3	AC	1666	G
3	AC	1672	G
3	AC	1681	G
3	AC	1710	G
3	AC	1713	A
3	AC	1716	A
3	AC	1718	C
3	AC	1722	U
3	AC	1723	G
3	AC	1724	G
3	AC	1727	G
3	AC	1729	U
3	AC	1745	G
3	AC	1746	A
3	AC	1747	U
3	AC	1749	G
3	AC	1753	C
3	AC	1756	C
3	AC	1773	C

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Mol	Chain	Res	Type
3	AC	1774	C
3	AC	1775	C
3	AC	1779	C
3	AC	1783	G
3	AC	1784	C
3	AC	1785	G
3	AC	1787	U
3	AC	1802	A
3	AC	1808	C
3	AC	1813	U
3	AC	1814	A
3	AC	1817	G
3	AC	1820	A
3	AC	1825	A
3	AC	1826	A
3	AC	1830	G
3	AC	1836	A
3	AC	1839	U
3	AC	1850	G
3	AC	1852	A
3	AC	1853	C
3	AC	1862	G
3	AC	1863	G
3	AC	1864	A
3	AC	1865	U
3	AC	1866	C
77	CI	2	G
77	CI	18	C
77	CI	25	A
77	CI	39	A
77	CI	42	A
77	CI	48	G
77	CI	59	A
77	CI	64	A
77	CI	65	A
77	CI	66	A
77	CI	91	G
77	CI	104	G
77	CI	108	A
77	CI	109	G
77	CI	119	G
77	CI	120	A

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Mol	Chain	Res	Type
77	CI	127	G
77	CI	133	C
77	CI	134	G
77	CI	136	C
77	CI	137	G
77	CI	139	G
77	CI	144	G
77	CI	159	C
77	CI	160	G
77	CI	172	C
77	CI	177	G
77	CI	178	C
77	CI	182	G
77	CI	183	C
77	CI	184	U
77	CI	185	C
77	CI	186	G
77	CI	188	G
77	CI	189	G
77	CI	200	U
77	CI	217	C
77	CI	218	A
77	CI	219	G
77	CI	220	C
77	CI	233	U
77	CI	234	G
77	CI	237	B9B
77	CI	241	G
77	CI	246	G
77	CI	254	G
77	CI	265	U
77	CI	266	C
77	CI	267	G
77	CI	276	C
77	CI	277	G
77	CI	278	G
77	CI	280	G
77	CI	295	A
77	CI	297	U
77	CI	315	G
77	CI	316	U
77	CI	340	C

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Mol	Chain	Res	Type
77	CI	383	A
77	CI	387	G
77	CI	401	G
77	CI	407	A
77	CI	409	G
77	CI	410	A
77	CI	412	G
77	CI	413	G
77	CI	440	U
77	CI	449	C
77	CI	451	C
77	CI	452	A
77	CI	453	G
77	CI	454	U
77	CI	457	G
77	CI	461	G
77	CI	469	C
77	CI	470	A
77	CI	487	C
77	CI	488	C
77	CI	489	G
77	CI	491	C
77	CI	499	G
77	CI	500	U
77	CI	501	G
77	CI	502	G
77	CI	503	U
77	CI	504	C
77	CI	505	C
77	CI	506	G
77	CI	507	G
77	CI	512	U
77	CI	514	U
77	CI	515	U
77	CI	516	U
77	CI	668	C
77	CI	672	G
77	CI	673	A
77	CI	674	C
77	CI	680	G
77	CI	687	G
77	CI	688	G

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Mol	Chain	Res	Type
77	CI	692	A
77	CI	702	U
77	CI	703	G
77	CI	710	C
77	CI	727	G
77	CI	737	G
77	CI	746	G
77	CI	747	U
77	CI	748	G
77	CI	755	G
77	CI	762	G
77	CI	766	G
77	CI	769	G
77	CI	813	A
77	CI	815	A
77	CI	818	C
77	CI	823	G
77	CI	836	G
77	CI	841	A
77	CI	842	U
77	CI	856	A
77	CI	857	A
77	CI	871	C
77	CI	877	2MG
77	CI	881	U
77	CI	883	C
77	CI	885	U
77	CI	887	U
77	CI	923	G
77	CI	925	G
77	CI	927	C
77	CI	928	G
77	CI	929	G
77	CI	934	C
77	CI	935	C
77	CI	937	C
77	CI	942	A
77	CI	1000	G
77	CI	1001	G
77	CI	1010	G
77	CI	1011	U
77	CI	1012	C

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Mol	Chain	Res	Type
77	CI	1013	C
77	CI	1015	C
77	CI	1019	G
77	CI	1031	U
77	CI	1032	C
77	CI	1038	G
77	CI	1040	C
77	CI	1043	C
77	CI	1044	G
77	CI	1048	C
77	CI	1064	G
77	CI	1066	C
77	CI	1068	C
77	CI	1070	C
77	CI	1072	U
77	CI	1082	A
77	CI	1083	A
77	CI	1086	C
77	CI	1087	G
77	CI	1089	G
77	CI	1094	C
77	CI	1098	G
77	CI	1099	U
77	CI	1101	G
77	CI	1108	A
77	CI	1116	U
77	CI	1117	A
77	CI	1118	C
77	CI	1126	A
77	CI	1127	C
77	CI	1129	C
77	CI	1130	G
77	CI	1131	U
77	CI	1132	C
77	CI	1140	A2M
77	CI	1152	G
77	CI	1168	A
77	CI	1172	A
77	CI	1173	G
77	CI	1180	G
77	CI	1191	G
77	CI	1193	C

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Mol	Chain	Res	Type
77	CI	1194	G
77	CI	1195	U
77	CI	1201	A
77	CI	1208	G
77	CI	1211	A
77	CI	1213	G
77	CI	1220	G
77	CI	1222	C
77	CI	1224	G
77	CI	1233	A
77	CI	1255	C
77	CI	1259	C
77	CI	1276	C
77	CI	1281	C
77	CI	1294	C
77	CI	1295	G
77	CI	1296	C
77	CI	1299	C
77	CI	1311	G
77	CI	1315	G
77	CI	1331	A
77	CI	1347	A2M
77	CI	1360	A
77	CI	1378	A
77	CI	1379	C
77	CI	1391	U
77	CI	1399	G
77	CI	1404	U
77	CI	1409	U
77	CI	1413	A
77	CI	1418	G7M
77	CI	1423	C
77	CI	1437	G
77	CI	1438	OMG
77	CI	1439	G
77	CI	1443	A
77	CI	1444	A
77	CI	1445	A
77	CI	1446	G
77	CI	1447	A
77	CI	1451	A
77	CI	1453	C

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Mol	Chain	Res	Type
77	CI	1454	G
77	CI	1455	A
77	CI	1464	G
77	CI	1466	A
77	CI	1467	G
77	CI	1474	C
77	CI	1476	C
77	CI	1483	G
77	CI	1489	C
77	CI	1490	PSU
77	CI	1493	G
77	CI	1510	G
77	CI	1512	U
77	CI	1522	C
77	CI	1523	G
77	CI	1527	U
77	CI	1536	G
77	CI	1538	A
77	CI	1540	A
77	CI	1544	A
77	CI	1552	G
77	CI	1589	A
77	CI	1606	A
77	CI	1621	G
77	CI	1623	G
77	CI	1624	U
77	CI	1625	G
77	CI	1631	G
77	CI	1635	G
77	CI	1638	G
77	CI	1639	A
77	CI	1644	G
77	CI	1657	G
77	CI	1665	U
77	CI	1671	G
77	CI	1682	G
77	CI	1683	C
77	CI	1684	U
77	CI	1685	OMG
77	CI	1686	C
77	CI	1687	G
77	CI	1688	G

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Mol	Chain	Res	Type
77	CI	1689	G
77	CI	1693	A
77	CI	1698	A
77	CI	1700	C
77	CI	1701	G
77	CI	1718	G
77	CI	1720	U
77	CI	1721	G
77	CI	1722	C
77	CI	1723	C
77	CI	1724	G
77	CI	1727	G
77	CI	1733	C
77	CI	1734	A
77	CI	1742	G
77	CI	1750	G
77	CI	1753	G
77	CI	1829	U
77	CI	1836	G
77	CI	1848	G
77	CI	1850	U
77	CI	1857	G
77	CI	1858	G
77	CI	1871	A
77	CI	1873	A
77	CI	1886	C
77	CI	1887	G
77	CI	1893	C
77	CI	1894	G
77	CI	1895	G
77	CI	1900	G
77	CI	1902	A
77	CI	1915	G
77	CI	2010	G
77	CI	2011	C
77	CI	2014	C
77	CI	2015	G
77	CI	2016	C
77	CI	2017	G
77	CI	2023	U
77	CI	2035	A
77	CI	2036	G

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Mol	Chain	Res	Type
77	CI	2045	C
77	CI	2056	A
77	CI	2057	G
77	CI	2069	A
77	CI	2070	G
77	CI	2078	G
77	CI	2089	G
77	CI	2104	G
77	CI	2107	C
77	CI	2120	OMG
77	CI	2121	OMC
77	CI	2135	A
77	CI	2151	A
77	CI	2153	G
77	CI	2172	G
77	CI	2173	A
77	CI	2178	OMC
77	CI	2182	U
77	CI	2185	A
77	CI	2192	U
77	CI	2195	G
77	CI	2203	U
77	CI	2204	G
77	CI	2225	C
77	CI	2227	G
77	CI	2230	G
77	CI	2232	G
77	CI	2234	C
77	CI	2238	C
77	CI	2245	C
77	CI	2246	U
77	CI	2247	C
77	CI	2248	C
77	CI	2259	G
77	CI	2260	C
77	CI	2262	G
77	CI	2263	A
77	CI	2268	A
77	CI	2269	A
77	CI	2276	C
77	CI	2285	A
77	CI	2302	G

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Mol	Chain	Res	Type
77	CI	2315	G
77	CI	2329	A
77	CI	2332	G
77	CI	2342	G
77	CI	2343	A
77	CI	2345	C
77	CI	2347	A
77	CI	2357	A
77	CI	2383	C
77	CI	2384	U
77	CI	2387	U
77	CI	2409	C
77	CI	2415	A
77	CI	2418	G
77	CI	2425	C
77	CI	2432	A
77	CI	2437	G
77	CI	2443	U
77	CI	2444	G
77	CI	2450	G
77	CI	2451	A
77	CI	2452	A
77	CI	2464	U
77	CI	2466	C
77	CI	2467	G
77	CI	2470	G
77	CI	2475	C
77	CI	2482	G
77	CI	2491	G
77	CI	2495	C
77	CI	2499	A
77	CI	2511	A
77	CI	2512	G
77	CI	2516	G
77	CI	2519	U
77	CI	2525	U
77	CI	2526	C
77	CI	2529	OMG
77	CI	2543	A
77	CI	2544	U
77	CI	2546	U
77	CI	2552	G

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Mol	Chain	Res	Type
77	CI	2553	C
77	CI	2554	A
77	CI	2570	C
77	CI	2582	U
77	CI	2583	G
77	CI	2585	U
77	CI	2590	C
77	CI	2591	A
77	CI	2594	G
77	CI	2611	G
77	CI	2612	C
77	CI	2613	A
77	CI	2633	G
77	CI	2644	G
77	CI	2652	G
77	CI	2653	G
77	CI	2659	G
77	CI	3244	G
77	CI	3246	C
77	CI	3247	C
77	CI	3251	G
77	CI	3252	C
77	CI	3253	C
77	CI	3256	G
77	CI	3257	C
77	CI	3259	G
77	CI	3274	G
77	CI	3284	G
77	CI	3285	G
77	CI	3294	A
77	CI	3303	U
77	CI	3305	A
77	CI	3307	A
77	CI	3320	G
77	CI	3321	A
77	CI	3332	C
77	CI	3333	G
77	CI	3351	A
77	CI	3355	C
77	CI	3370	A
77	CI	3371	A
77	CI	3374	PSU

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Mol	Chain	Res	Type
77	CI	3376	A
77	CI	3404	U
77	CI	3409	G
77	CI	3415	A
77	CI	3418	A
77	CI	3419	A
77	CI	3420	C
77	CI	3426	C
77	CI	3430	C
77	CI	3432	U
77	CI	3433	A
77	CI	3434	A
77	CI	3435	G
77	CI	3436	G
77	CI	3444	A2M
77	CI	3445	U
77	CI	3448	C
77	CI	3461	U
77	CI	3470	G
77	CI	3473	U
77	CI	3476	A
77	CI	3477	U
77	CI	3478	G
77	CI	3481	U
77	CI	3483	A
77	CI	3497	U
77	CI	3499	U
77	CI	3524	A
77	CI	3526	A2M
77	CI	3527	G
77	CI	3528	OMC
77	CI	3536	A
77	CI	3537	C
77	CI	3538	G
77	CI	3539	P7G
77	CI	3546	OMC
77	CI	3547	G
77	CI	3549	A
77	CI	3554	G
77	CI	3556	G
77	CI	3560	A
77	CI	3565	A

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Mol	Chain	Res	Type
77	CI	3566	G
77	CI	3567	A
77	CI	3574	U
77	CI	3585	C
77	CI	3597	G
77	CI	3598	G
77	CI	3729	G
77	CI	3737	G
77	CI	3738	A
77	CI	3739	G
77	CI	3743	G
77	CI	3752	G
77	CI	3758	A
77	CI	3759	G
77	CI	3760	G
77	CI	3761	G
77	CI	3764	U
77	CI	3768	G
77	CI	3769	C
77	CI	3770	U
77	CI	3771	U
77	CI	3772	C
77	CI	3775	G
77	CI	3776	C
77	CI	3780	A
77	CI	3781	A
77	CI	3790	C
77	CI	3791	C
77	CI	3792	C
77	CI	3797	G
77	CI	3803	G
77	CI	3818	U
77	CI	3825	A
77	CI	3838	G
77	CI	3839	G
77	CI	3846	G
77	CI	3858	A
77	CI	3869	A
77	CI	3877	G
77	CI	3884	U
77	CI	3888	A
77	CI	3898	C

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Mol	Chain	Res	Type
77	CI	3904	G
77	CI	3906	A
77	CI	3909	G
77	CI	3913	C
77	CI	3920	U
77	CI	3928	A
77	CI	3935	A
77	CI	3936	A
77	CI	3946	G
77	CI	3948	PSU
77	CI	3951	U
77	CI	3957	U
77	CI	3960	G
77	CI	3961	OMU
77	CI	3985	G
77	CI	4005	C
77	CI	4021	A
77	CI	4024	A
77	CI	4025	OMG
77	CI	4028	G
77	CI	4032	G
77	CI	4033	A
77	CI	4036	A
77	CI	4042	C
77	CI	4049	A
77	CI	4050	U
77	CI	4057	C
77	CI	4074	U
77	CI	4075	U
77	CI	4081	C
77	CI	4099	C
77	CI	4102	5MC
77	CI	4103	G
77	CI	4104	A
77	CI	4105	PSU
77	CI	4107	U
77	CI	4108	C
77	CI	4119	A
77	CI	4121	C
77	CI	4130	G
77	CI	4147	U
77	CI	4160	C

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Mol	Chain	Res	Type
77	CI	4167	U
77	CI	4168	A
77	CI	4174	C
77	CI	4179	G
77	CI	4183	G
77	CI	4186	PSU
77	CI	4187	U
77	CI	4200	G
77	CI	4203	A
77	CI	4204	G
77	CI	4216	C
77	CI	4222	G
77	CI	4224	U
77	CI	4227	U
77	CI	4228	G
77	CI	4244	A
77	CI	4245	A
77	CI	4255	G
77	CI	4265	A
77	CI	4272	G
77	CI	4275	OMU
77	CI	4291	PSU
77	CI	4292	OMG
77	CI	4311	A
77	CI	4318	G
77	CI	4325	C
77	CI	4327	A
77	CI	4350	C
77	CI	4354	U
77	CI	4355	A
77	CI	4363	A
77	CI	4364	U
77	CI	4375	C
77	CI	4388	C
77	CI	4395	G
77	CI	4396	A
77	CI	4397	G
77	CI	4406	G
77	CI	4409	G
77	CI	4412	C
77	CI	4414	C
77	CI	4416	G

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Mol	Chain	Res	Type
77	CI	4420	G
77	CI	4426	U
77	CI	4427	C
77	CI	4436	U
77	CI	4443	U
77	CI	4493	C
77	CI	4499	U
77	CI	4500	C
77	CI	4504	A
77	CI	4505	C
77	CI	4510	G
77	CI	4514	G
77	CI	4516	U
77	CI	4517	OMG
77	CI	4518	C
77	CI	4519	2MG
77	CI	4522	G
77	CI	4530	C
77	CI	4533	C
77	CI	4540	A
77	CI	4542	C
77	CI	4543	G
77	CI	4550	G
77	CI	4552	C
77	CI	4554	G
77	CI	4556	A
77	CI	4559	G
77	CI	4571	C
77	CI	4572	U
77	CI	4573	C
77	CI	4584	U
77	CI	4585	U
77	CI	4589	G
77	CI	4591	A
77	CI	4593	G
77	CI	4601	G
77	CI	4605	C
77	CI	4611	G
77	CI	4614	A
77	CI	4615	A
77	CI	4624	U
77	CI	4636	U

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Mol	Chain	Res	Type
77	CI	4637	U
77	CI	4639	U
77	CI	4645	G
77	CI	4655	A
77	CI	4661	C
77	CI	4662	A
77	CI	4664	A
77	CI	4665	G
77	CI	4668	G
77	CI	4669	C
77	CI	4673	C
77	CI	4682	A
77	CI	4689	G
77	CI	4698	C
77	CI	4701	U
77	CI	4703	G
77	CI	4709	A
77	CI	4717	U
78	CJ	7	G
78	CJ	18	C
78	CJ	33	U
78	CJ	53	U
78	CJ	64	G
78	CJ	100	A
78	CJ	110	G
78	CJ	120	U
79	CK	14	OMU
79	CK	23	C
79	CK	34	U
79	CK	35	C
79	CK	52	A
79	CK	62	A
79	CK	63	U
79	CK	79	G
79	CK	80	A
79	CK	82	A
79	CK	84	A
79	CK	85	U
79	CK	87	G
79	CK	94	G
79	CK	103	A
79	CK	105	C

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Mol	Chain	Res	Type
79	CK	110	U
79	CK	111	U
79	CK	114	G
79	CK	121	G
79	CK	122	G
79	CK	123	U
79	CK	124	U
79	CK	125	C
79	CK	126	C
79	CK	127	U
79	CK	128	C
79	CK	129	C

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	AC	1047	U
3	AC	1438	C
77	CI	143	U
77	CI	1403	C
77	CI	1446	G
77	CI	1465	U
77	CI	1683	C
77	CI	1685	OMG
77	CI	2383	C
77	CI	2431	G
77	CI	2611	G
77	CI	2612	C
77	CI	3332	C
77	CI	3775	G
77	CI	4056	G
77	CI	4074	U
77	CI	4354	U
77	CI	4517	OMG
79	CK	83	C
79	CK	127	U

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

100 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$
77	PSU	CI	3374	77	18,21,22	1.08	1 (5%)	22,30,33	1.90	5 (22%)
77	A2M	CI	3382	77	22,25,26	3.41	10 (45%)	31,36,39	2.58	10 (32%)
77	PSU	CI	3388	77	18,21,22	1.11	1 (5%)	22,30,33	1.85	5 (22%)
77	E7G	CI	2053	77	24,27,28	5.56	11 (45%)	30,40,43	2.18	9 (30%)
77	OMG	CI	4278	77	23,26,27	0.50	0	33,38,41	0.50	0
3	A2M	AC	166	3	22,25,26	3.42	8 (36%)	31,36,39	2.66	12 (38%)
3	PSU	AC	824	3	18,21,22	1.11	1 (5%)	22,30,33	1.76	4 (18%)
77	E7G	CI	1599	77	24,27,28	5.61	11 (45%)	30,40,43	2.22	9 (30%)
77	MHG	CI	4026	77	29,32,33	5.57	11 (37%)	34,46,49	2.55	11 (32%)
77	OMG	CI	2529	77	23,26,27	0.52	0	33,38,41	0.46	0
77	2MG	CI	1330	77	23,26,27	0.50	0	32,38,41	0.55	0
77	5MC	CI	4102	77	18,22,23	0.52	0	26,32,35	0.64	0
77	B8W	CI	3840	77	23,26,27	1.85	4 (17%)	33,38,41	2.54	14 (42%)
3	OMC	AC	518	3	19,22,23	0.53	0	26,31,34	0.59	0
77	A2M	CI	3484	77	22,25,26	3.40	9 (40%)	31,36,39	2.64	12 (38%)
77	PSU	CI	4105	77	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
3	A2M	AC	1032	3	22,25,26	3.41	9 (40%)	31,36,39	2.63	12 (38%)
77	PSU	CI	1496	77	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
77	1MA	CI	4070	77	21,25,26	0.51	0	31,37,40	0.78	1 (3%)
77	2MG	CI	877	77	23,26,27	0.48	0	32,38,41	0.50	0
77	OMC	CI	2617	77	19,22,23	0.51	0	26,31,34	0.65	0
77	A2M	CI	3377	77	22,25,26	3.41	9 (40%)	31,36,39	2.58	11 (35%)
77	A2M	CI	4226	77	22,25,26	3.41	9 (40%)	31,36,39	2.57	11 (35%)
3	A2M	AC	669	3	22,25,26	3.35	9 (40%)	31,36,39	2.56	11 (35%)
77	I4U	CI	1472	77	21,24,25	3.55	9 (42%)	27,34,37	0.97	1 (3%)
77	PSU	CI	1395	77	18,21,22	1.10	1 (5%)	22,30,33	1.63	3 (13%)
77	B9B	CI	1387	77	25,28,29	1.74	6 (24%)	35,40,43	2.97	11 (31%)
77	OMG	CI	3451	77	23,26,27	0.51	0	33,38,41	0.43	0
77	A2M	CI	3526	77	22,25,26	3.43	10 (45%)	31,36,39	2.63	12 (38%)
77	PSU	CI	4291	77	18,21,22	1.06	1 (5%)	22,30,33	1.84	5 (22%)
77	UR3	CI	4252	77	19,22,23	3.05	8 (42%)	26,32,35	1.35	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
77	G7M	CI	2278	77	23,26,27	2.94	9 (39%)	35,39,42	2.52	10 (28%)
77	OMG	CI	4517	77	23,26,27	1.58	5 (21%)	33,38,41	1.74	9 (27%)
77	6MZ	CI	3875	77	22,25,26	3.80	9 (40%)	30,36,39	2.40	10 (33%)
3	PSU	AC	613	3	18,21,22	1.03	1 (5%)	22,30,33	1.98	5 (22%)
77	B8T	CI	4138	77	19,22,23	3.24	8 (42%)	26,31,34	0.80	1 (3%)
77	A2M	CI	2157	77	22,25,26	3.39	9 (40%)	31,36,39	2.67	12 (38%)
77	OMC	CI	2560	77	19,22,23	0.53	0	26,31,34	0.61	0
3	PSU	AC	823	3	18,21,22	1.02	1 (5%)	22,30,33	1.81	4 (18%)
3	A2M	AC	27	3	22,25,26	3.40	9 (40%)	31,36,39	2.64	13 (41%)
79	OMU	CK	14	79	19,22,23	3.61	8 (42%)	26,31,34	1.77	6 (23%)
77	PSU	CI	4097	77	18,21,22	1.08	1 (5%)	22,30,33	1.75	5 (22%)
77	OMG	CI	1685	77	23,26,27	0.53	0	33,38,41	0.57	0
77	B8Q	CI	1269	77	17,22,23	4.65	5 (29%)	22,32,35	2.05	6 (27%)
77	A2M	CI	1337	77	22,25,26	3.42	9 (40%)	31,36,39	2.70	12 (38%)
77	OMG	CI	1335	77	23,26,27	0.52	0	33,38,41	0.56	0
77	P7G	CI	1711	77,78	24,28,29	5.13	9 (37%)	27,41,44	1.08	1 (3%)
77	PSU	CI	1490	77	18,21,22	1.10	1 (5%)	22,30,33	1.80	5 (22%)
3	PSU	AC	1082	3	18,21,22	1.03	1 (5%)	22,30,33	1.84	5 (22%)
77	P7G	CI	3539	77	24,28,29	5.20	9 (37%)	27,41,44	1.73	3 (11%)
77	A2M	CI	1673	77	22,25,26	3.43	10 (45%)	31,36,39	2.61	11 (35%)
3	4AC	AC	1843	3	21,24,25	3.77	10 (47%)	29,34,37	0.99	4 (13%)
77	G7M	CI	1418	77	23,26,27	2.95	9 (39%)	35,39,42	2.47	10 (28%)
77	B9H	CI	2542	77	20,25,26	4.80	4 (20%)	22,35,38	1.53	4 (18%)
77	5MC	CI	3990	77	18,22,23	0.55	0	26,32,35	0.55	0
77	OMG	CI	2120	77	23,26,27	0.50	0	33,38,41	0.50	0
77	OMC	CI	3546	77	19,22,23	0.59	0	26,31,34	0.75	0
77	OMG	CI	4149	77	23,26,27	0.50	0	33,38,41	0.49	0
77	A2M	CI	3444	77	22,25,26	3.34	10 (45%)	31,36,39	2.64	12 (38%)
77	OMU	CI	3961	77	19,22,23	3.53	8 (42%)	26,31,34	1.69	5 (19%)
77	PSU	CI	4058	77	18,21,22	1.05	1 (5%)	22,30,33	1.86	4 (18%)
77	A2M	CI	2119	77	22,25,26	3.41	9 (40%)	31,36,39	2.58	11 (35%)
77	G7M	CI	4205	77	23,26,27	2.96	9 (39%)	35,39,42	2.49	10 (28%)
77	PSU	CI	4283	77	18,21,22	1.00	1 (5%)	22,30,33	1.69	4 (18%)
77	OMC	CI	3360	77	19,22,23	0.53	0	26,31,34	0.60	0
77	PSU	CI	3423	77	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
3	B8N	AC	1249	3	24,29,30	3.29	6 (25%)	29,42,45	1.84	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
77	OMG	CI	4025	77	23,26,27	0.49	0	33,38,41	0.50	0
77	A2M	CI	398	77	22,25,26	3.40	10 (45%)	31,36,39	2.64	13 (41%)
77	OMC	CI	3528	77	19,22,23	0.54	0	26,31,34	0.64	0
64	MLZ	Bd	98	64	8,9,10	0.75	0	4,9,11	0.65	0
77	B9B	CI	237	77	25,28,29	1.76	6 (24%)	35,40,43	2.83	12 (34%)
3	OMU	AC	116	3	19,22,23	3.55	8 (42%)	26,31,34	1.62	5 (19%)
77	PSU	CI	4155	77	18,21,22	1.10	1 (5%)	22,30,33	1.85	4 (18%)
77	PSU	CI	3948	77	18,21,22	1.05	1 (5%)	22,30,33	1.80	5 (22%)
77	E6G	CI	4010	77	24,27,28	2.11	5 (20%)	34,39,42	5.93	16 (47%)
77	A2M	CI	1140	77	22,25,26	3.38	9 (40%)	31,36,39	2.59	10 (32%)
77	I4U	CI	3849	77	21,24,25	3.53	9 (42%)	27,34,37	0.93	1 (3%)
77	PSU	CI	4186	77	18,21,22	1.12	1 (5%)	22,30,33	1.84	5 (22%)
77	OMG	CI	4292	77	23,26,27	0.49	0	33,38,41	0.45	0
77	OMG	CI	1438	77	23,26,27	0.49	0	33,38,41	0.49	0
77	OMC	CI	2121	77	19,22,23	0.59	0	26,31,34	1.27	4 (15%)
77	5MC	CI	3441	77	18,22,23	0.59	0	26,32,35	0.49	0
77	OMG	CI	1852	77	23,26,27	0.52	0	33,38,41	0.44	0
77	OMC	CI	2178	77	19,22,23	0.55	0	26,31,34	0.54	0
77	A2M	CI	1347	77	22,25,26	3.42	9 (40%)	31,36,39	2.61	10 (32%)
77	OMG	CI	373	77	23,26,27	0.49	0	33,38,41	0.50	0
3	PSU	AC	1244	3	18,21,22	1.08	1 (5%)	22,30,33	1.82	5 (22%)
77	OMC	CI	4191	77	19,22,23	0.54	0	26,31,34	0.65	0
3	OMG	AC	645	3	23,26,27	0.50	0	33,38,41	0.46	0
77	OMC	CI	3568	77	19,22,23	0.53	0	26,31,34	0.87	1 (3%)
37	MLZ	BC	333	37	8,9,10	0.82	0	4,9,11	0.67	0
3	OMG	AC	684	3	23,26,27	0.50	0	33,38,41	0.55	0
77	OMG	CI	2180	77	23,26,27	0.52	0	33,38,41	0.46	0
77	2MG	CI	4519	77	23,26,27	0.47	0	32,38,41	0.59	0
3	UR3	AC	1831	3	19,22,23	3.03	8 (42%)	26,32,35	1.37	3 (11%)
77	OMG	CI	3851	77	23,26,27	0.50	0	33,38,41	0.43	0
77	OMU	CI	4275	77	19,22,23	3.49	8 (42%)	26,31,34	1.58	5 (19%)
77	UR3	CI	1668	77	19,22,23	3.01	8 (42%)	26,32,35	1.29	3 (11%)
77	PSU	CI	2264	77	18,21,22	1.05	1 (5%)	22,30,33	1.95	5 (22%)

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
77	PSU	CI	3374	77	-	2/7/25/26	0/2/2/2
77	A2M	CI	3382	77	-	1/9/27/28	0/3/3/3
77	PSU	CI	3388	77	-	2/7/25/26	0/2/2/2
77	E7G	CI	2053	77	-	0/9/39/40	0/3/3/3
77	OMG	CI	4278	77	-	0/9/27/28	0/3/3/3
3	A2M	AC	166	3	-	0/9/27/28	0/3/3/3
3	PSU	AC	824	3	-	0/7/25/26	0/2/2/2
77	E7G	CI	1599	77	-	1/9/39/40	0/3/3/3
77	MHG	CI	4026	77	-	5/16/46/47	0/3/3/3
77	OMG	CI	2529	77	-	2/9/27/28	0/3/3/3
77	2MG	CI	1330	77	-	0/9/27/28	0/3/3/3
77	5MC	CI	4102	77	-	6/7/25/26	0/2/2/2
77	B8W	CI	3840	77	-	2/9/27/28	0/3/3/3
3	OMC	AC	518	3	-	0/9/27/28	0/2/2/2
77	A2M	CI	3484	77	-	1/9/27/28	0/3/3/3
77	PSU	CI	4105	77	-	5/7/25/26	0/2/2/2
3	A2M	AC	1032	3	-	0/9/27/28	0/3/3/3
77	PSU	CI	1496	77	-	0/7/25/26	0/2/2/2
77	1MA	CI	4070	77	-	0/7/25/26	0/3/3/3
77	2MG	CI	877	77	-	2/9/27/28	0/3/3/3
77	OMC	CI	2617	77	-	0/9/27/28	0/2/2/2
77	A2M	CI	3377	77	-	2/9/27/28	0/3/3/3
77	A2M	CI	4226	77	-	0/9/27/28	0/3/3/3
3	A2M	AC	669	3	-	4/9/27/28	0/3/3/3
77	I4U	CI	1472	77	-	0/9/29/30	0/2/2/2
77	PSU	CI	1395	77	-	1/7/25/26	0/2/2/2
77	B9B	CI	1387	77	-	2/11/29/30	0/3/3/3
77	OMG	CI	3451	77	-	0/9/27/28	0/3/3/3
77	A2M	CI	3526	77	-	3/9/27/28	0/3/3/3
77	PSU	CI	4291	77	-	6/7/25/26	0/2/2/2
77	UR3	CI	4252	77	-	0/7/25/26	0/2/2/2
77	G7M	CI	2278	77	-	0/7/25/26	0/3/3/3
77	OMG	CI	4517	77	-	4/9/27/28	0/3/3/3
77	6MZ	CI	3875	77	-	0/9/27/28	0/3/3/3
3	PSU	AC	613	3	-	2/7/25/26	0/2/2/2
77	B8T	CI	4138	77	-	0/7/27/28	0/2/2/2
77	A2M	CI	2157	77	-	0/9/27/28	0/3/3/3
77	OMC	CI	2560	77	-	1/9/27/28	0/2/2/2
3	PSU	AC	823	3	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	AC	27	3	-	1/9/27/28	0/3/3/3
79	OMU	CK	14	79	-	5/9/27/28	0/2/2/2
77	PSU	CI	4097	77	-	0/7/25/26	0/2/2/2
77	OMG	CI	1685	77	-	2/9/27/28	0/3/3/3
77	B8Q	CI	1269	77	-	0/7/42/43	0/2/2/2
77	A2M	CI	1337	77	-	1/9/27/28	0/3/3/3
77	OMG	CI	1335	77	-	0/9/27/28	0/3/3/3
77	P7G	CI	1711	77,78	-	0/10/40/41	0/3/3/3
77	PSU	CI	1490	77	-	1/7/25/26	0/2/2/2
3	PSU	AC	1082	3	-	0/7/25/26	0/2/2/2
77	P7G	CI	3539	77	-	2/10/40/41	0/3/3/3
77	A2M	CI	1673	77	-	1/9/27/28	0/3/3/3
3	4AC	AC	1843	3	-	0/11/29/30	0/2/2/2
77	G7M	CI	1418	77	-	2/7/25/26	0/3/3/3
77	B9H	CI	2542	77	-	2/12/47/48	0/2/2/2
77	5MC	CI	3990	77	-	0/7/25/26	0/2/2/2
77	OMG	CI	2120	77	-	2/9/27/28	0/3/3/3
77	OMC	CI	3546	77	-	3/9/27/28	0/2/2/2
77	OMG	CI	4149	77	-	2/9/27/28	0/3/3/3
77	A2M	CI	3444	77	-	1/9/27/28	0/3/3/3
77	OMU	CI	3961	77	-	3/9/27/28	0/2/2/2
77	PSU	CI	4058	77	-	0/7/25/26	0/2/2/2
77	A2M	CI	2119	77	-	0/9/27/28	0/3/3/3
77	G7M	CI	4205	77	-	2/7/25/26	0/3/3/3
77	PSU	CI	4283	77	-	0/7/25/26	0/2/2/2
77	OMC	CI	3360	77	-	4/9/27/28	0/2/2/2
77	PSU	CI	3423	77	-	1/7/25/26	0/2/2/2
3	B8N	AC	1249	3	-	6/16/34/35	0/2/2/2
77	OMG	CI	4025	77	-	2/9/27/28	0/3/3/3
77	A2M	CI	398	77	-	1/9/27/28	0/3/3/3
77	OMC	CI	3528	77	-	2/9/27/28	0/2/2/2
64	MLZ	Bd	98	64	-	1/7/8/10	-
77	B9B	CI	237	77	-	6/11/29/30	0/3/3/3
3	OMU	AC	116	3	-	0/9/27/28	0/2/2/2
77	PSU	CI	4155	77	-	1/7/25/26	0/2/2/2
77	PSU	CI	3948	77	-	2/7/25/26	0/2/2/2
77	E6G	CI	4010	77	-	3/10/28/29	0/3/3/3
77	A2M	CI	1140	77	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	I4U	CI	3849	77	-	2/9/29/30	0/2/2/2
77	PSU	CI	4186	77	-	2/7/25/26	0/2/2/2
77	OMG	CI	4292	77	-	1/9/27/28	0/3/3/3
77	OMG	CI	1438	77	-	2/9/27/28	0/3/3/3
77	OMC	CI	2121	77	-	2/9/27/28	0/2/2/2
77	5MC	CI	3441	77	-	0/7/25/26	0/2/2/2
77	OMG	CI	1852	77	-	0/9/27/28	0/3/3/3
77	OMC	CI	2178	77	-	1/9/27/28	0/2/2/2
77	A2M	CI	1347	77	-	2/9/27/28	0/3/3/3
77	OMG	CI	373	77	-	0/9/27/28	0/3/3/3
3	PSU	AC	1244	3	-	3/7/25/26	0/2/2/2
77	OMC	CI	4191	77	-	0/9/27/28	0/2/2/2
3	OMG	AC	645	3	-	1/9/27/28	0/3/3/3
77	OMC	CI	3568	77	-	0/9/27/28	0/2/2/2
37	MLZ	BC	333	37	-	1/7/8/10	-
3	OMG	AC	684	3	-	0/9/27/28	0/3/3/3
77	OMG	CI	2180	77	-	0/9/27/28	0/3/3/3
77	2MG	CI	4519	77	-	2/9/27/28	0/3/3/3
3	UR3	AC	1831	3	-	0/7/25/26	0/2/2/2
77	OMG	CI	3851	77	-	0/9/27/28	0/3/3/3
77	OMU	CI	4275	77	-	0/9/27/28	0/2/2/2
77	UR3	CI	1668	77	-	0/7/25/26	0/2/2/2
77	PSU	CI	2264	77	-	0/7/25/26	0/2/2/2

All (397) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	1599	E7G	C8-N9	22.70	1.58	1.46
77	CI	2053	E7G	C8-N9	22.56	1.58	1.46
77	CI	4026	MHG	C8-N9	19.70	1.57	1.46
77	CI	3539	P7G	C8-N9	18.35	1.56	1.46
77	CI	1711	P7G	C8-N9	17.85	1.55	1.46
77	CI	2542	B9H	C4-N3	14.31	1.70	1.48
77	CI	3875	6MZ	C6-N6	11.57	1.46	1.34
77	CI	4026	MHG	C8-N7	11.36	1.56	1.45
77	CI	1269	B8Q	C4-N3	11.30	1.65	1.48
77	CI	2542	B9H	C6-C5	11.15	1.58	1.33
77	CI	4026	MHG	C2-N3	10.90	1.52	1.31
77	CI	1472	I4U	C4-N3	10.76	1.45	1.31
77	CI	1269	B8Q	C6-C5	10.72	1.57	1.33
77	CI	3849	I4U	C4-N3	10.59	1.45	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	3539	P7G	C8-N7	10.49	1.55	1.45
77	CI	1711	P7G	C8-N7	10.43	1.55	1.45
77	CI	1599	E7G	C5-N7	9.59	1.46	1.35
77	CI	2053	E7G	C5-N7	9.39	1.46	1.35
77	CI	1269	B8Q	C2-N1	9.32	1.51	1.38
3	AC	1249	B8N	C4-N3	-9.21	1.23	1.40
77	CI	4026	MHG	C2-N2	8.88	1.53	1.33
3	AC	166	A2M	O4'-C1'	8.70	1.62	1.42
79	CK	14	OMU	C2-N3	8.66	1.53	1.38
77	CI	3382	A2M	O4'-C1'	8.64	1.62	1.42
77	CI	2119	A2M	C2'-C1'	-8.62	1.30	1.53
3	AC	1032	A2M	C2'-C1'	-8.61	1.30	1.53
3	AC	166	A2M	C2'-C1'	-8.61	1.30	1.53
77	CI	1347	A2M	C2'-C1'	-8.60	1.30	1.53
77	CI	3377	A2M	O4'-C1'	8.58	1.62	1.42
77	CI	1673	A2M	C2'-C1'	-8.58	1.31	1.53
77	CI	4226	A2M	O4'-C1'	8.57	1.62	1.42
3	AC	1032	A2M	O4'-C1'	8.55	1.62	1.42
77	CI	1140	A2M	C2'-C1'	-8.55	1.31	1.53
77	CI	1337	A2M	O4'-C1'	8.55	1.62	1.42
77	CI	1347	A2M	O4'-C1'	8.54	1.62	1.42
77	CI	398	A2M	O4'-C1'	8.53	1.62	1.42
77	CI	1673	A2M	O4'-C1'	8.52	1.62	1.42
77	CI	1337	A2M	C2'-C1'	-8.52	1.31	1.53
77	CI	3377	A2M	C2'-C1'	-8.51	1.31	1.53
77	CI	3484	A2M	C2'-C1'	-8.51	1.31	1.53
3	AC	116	OMU	C2-N3	8.51	1.53	1.38
3	AC	27	A2M	O4'-C1'	8.51	1.62	1.42
77	CI	3444	A2M	C2'-C1'	-8.48	1.31	1.53
77	CI	2119	A2M	O4'-C1'	8.48	1.62	1.42
77	CI	4226	A2M	C2'-C1'	-8.47	1.31	1.53
77	CI	2157	A2M	O4'-C1'	8.46	1.62	1.42
77	CI	3484	A2M	O4'-C1'	8.45	1.62	1.42
77	CI	3382	A2M	C2'-C1'	-8.45	1.31	1.53
77	CI	2157	A2M	C2'-C1'	-8.44	1.31	1.53
77	CI	3526	A2M	O4'-C1'	8.43	1.62	1.42
77	CI	398	A2M	C2'-C1'	-8.43	1.31	1.53
77	CI	3526	A2M	C2'-C1'	-8.40	1.31	1.53
3	AC	27	A2M	C2'-C1'	-8.38	1.31	1.53
77	CI	3961	OMU	C2-N3	8.31	1.52	1.38
77	CI	4275	OMU	C2-N3	8.27	1.52	1.38
77	CI	1140	A2M	O4'-C1'	8.27	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AC	669	A2M	O4'-C1'	8.25	1.61	1.42
77	CI	2542	B9H	C2-N3	-8.21	1.27	1.37
77	CI	3444	A2M	O4'-C1'	8.11	1.61	1.42
77	CI	3875	6MZ	O4'-C1'	8.10	1.61	1.42
77	CI	4026	MHG	C2-N1	8.08	1.49	1.36
79	CK	14	OMU	C2-N1	8.04	1.51	1.38
3	AC	669	A2M	C2'-C1'	-7.97	1.32	1.53
3	AC	1843	4AC	C6-C5	7.81	1.53	1.35
3	AC	1843	4AC	C4-N3	7.80	1.46	1.32
77	CI	3961	OMU	C2-N1	7.76	1.50	1.38
3	AC	116	OMU	C2-N1	7.72	1.50	1.38
77	CI	4275	OMU	C2-N1	7.67	1.50	1.38
3	AC	1249	B8N	C6-N1	7.45	1.55	1.36
77	CI	1711	P7G	C2-N1	7.44	1.51	1.33
77	CI	2542	B9H	C2-N1	7.42	1.49	1.38
77	CI	3539	P7G	C2-N1	7.42	1.51	1.33
3	AC	1831	UR3	C2-N1	7.27	1.49	1.38
77	CI	4252	UR3	C2-N1	7.24	1.48	1.38
77	CI	1668	UR3	C2-N1	7.19	1.48	1.38
77	CI	4205	G7M	C4-N3	7.07	1.51	1.34
3	AC	1249	B8N	C6-C5	7.06	1.44	1.34
77	CI	4138	B8T	C4-N3	7.05	1.45	1.32
77	CI	1711	P7G	C5-C4	7.03	1.51	1.37
77	CI	1418	G7M	C4-N3	7.01	1.50	1.34
77	CI	2278	G7M	C4-N3	6.99	1.50	1.34
3	AC	1843	4AC	C2-N3	6.97	1.50	1.36
77	CI	3539	P7G	C5-C4	6.87	1.51	1.37
3	AC	669	A2M	O4'-C4'	-6.73	1.30	1.45
77	CI	4252	UR3	C6-C5	6.71	1.50	1.35
3	AC	1831	UR3	C6-C5	6.69	1.50	1.35
77	CI	1668	UR3	C6-C5	6.65	1.50	1.35
77	CI	4205	G7M	C2-N2	6.57	1.49	1.34
77	CI	4010	E6G	O6-C6	6.56	1.45	1.35
77	CI	1418	G7M	C2-N2	6.55	1.49	1.34
77	CI	2278	G7M	C2-N2	6.48	1.49	1.34
77	CI	3526	A2M	O4'-C4'	-6.45	1.30	1.45
3	AC	1249	B8N	C2-N1	6.40	1.58	1.39
77	CI	1337	A2M	O4'-C4'	-6.40	1.30	1.45
77	CI	1140	A2M	O4'-C4'	-6.39	1.30	1.45
3	AC	27	A2M	O4'-C4'	-6.34	1.30	1.45
77	CI	398	A2M	O4'-C4'	-6.34	1.30	1.45
77	CI	1347	A2M	O4'-C4'	-6.33	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	2119	A2M	O4'-C4'	-6.33	1.30	1.45
77	CI	3484	A2M	O4'-C4'	-6.33	1.30	1.45
77	CI	4138	B8T	C2-N3	6.32	1.49	1.36
77	CI	1673	A2M	O4'-C4'	-6.31	1.30	1.45
77	CI	3849	I4U	C6-C5	6.28	1.49	1.35
77	CI	3382	A2M	O4'-C4'	-6.28	1.31	1.45
77	CI	3444	A2M	O4'-C4'	-6.28	1.31	1.45
77	CI	2157	A2M	O4'-C4'	-6.24	1.31	1.45
77	CI	4226	A2M	O4'-C4'	-6.24	1.31	1.45
3	AC	1032	A2M	O4'-C4'	-6.21	1.31	1.45
77	CI	3377	A2M	O4'-C4'	-6.20	1.31	1.45
3	AC	166	A2M	O4'-C4'	-6.09	1.31	1.45
77	CI	1472	I4U	C2-N3	6.09	1.48	1.36
77	CI	1472	I4U	C6-C5	6.08	1.49	1.35
3	AC	116	OMU	C6-C5	6.08	1.49	1.35
77	CI	3961	OMU	C6-C5	6.07	1.49	1.35
77	CI	4275	OMU	C6-C5	6.07	1.49	1.35
77	CI	4138	B8T	C6-C5	6.06	1.49	1.35
77	CI	1418	G7M	C2-N3	6.05	1.47	1.33
77	CI	1599	E7G	C2-N3	6.03	1.47	1.33
77	CI	3849	I4U	C2-N3	5.97	1.48	1.36
77	CI	4205	G7M	C2-N3	5.96	1.47	1.33
77	CI	3875	6MZ	O4'-C4'	-5.95	1.31	1.45
77	CI	4010	E6G	C2-N2	5.94	1.45	1.33
79	CK	14	OMU	C6-C5	5.92	1.48	1.35
77	CI	2053	E7G	C2-N3	5.92	1.47	1.33
77	CI	2278	G7M	C2-N3	5.92	1.47	1.33
77	CI	4252	UR3	C2-N3	5.90	1.50	1.39
77	CI	4026	MHG	C4-N3	5.85	1.48	1.34
77	CI	3539	P7G	C4-N3	5.82	1.47	1.37
77	CI	1711	P7G	C4-N3	5.79	1.47	1.37
3	AC	1831	UR3	C2-N3	5.77	1.50	1.39
77	CI	237	B9B	C2-N2	5.75	1.45	1.33
77	CI	1668	UR3	C2-N3	5.66	1.50	1.39
77	CI	1387	B9B	C2-N2	5.65	1.45	1.33
77	CI	3875	6MZ	C2'-C1'	-5.57	1.35	1.53
77	CI	3840	B8W	C2-N2	5.50	1.44	1.33
77	CI	1599	E7G	C4-N3	5.36	1.47	1.34
77	CI	1269	B8Q	C2-N3	-5.29	1.26	1.35
77	CI	4026	MHG	C6-N1	5.28	1.48	1.38
77	CI	2053	E7G	C4-N3	5.27	1.46	1.34
3	AC	1843	4AC	C7-N4	5.19	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	3840	B8W	O6-C6	5.01	1.43	1.35
77	CI	3539	P7G	C2-N3	4.96	1.49	1.37
3	AC	1843	4AC	C4-N4	4.89	1.46	1.39
77	CI	1711	P7G	C2-N3	4.84	1.49	1.37
77	CI	1599	E7G	C2-N2	4.73	1.45	1.34
77	CI	4138	B8T	C4-N4	4.72	1.45	1.35
77	CI	2278	G7M	O6-C6	-4.71	1.14	1.23
77	CI	3849	I4U	C5-C4	4.70	1.49	1.43
77	CI	1472	I4U	C5-C4	4.70	1.49	1.43
3	AC	1843	4AC	C2-N1	4.70	1.50	1.40
77	CI	1418	G7M	O6-C6	-4.68	1.14	1.23
77	CI	4205	G7M	O6-C6	-4.64	1.14	1.23
77	CI	2053	E7G	C2-N2	4.63	1.45	1.34
77	CI	1140	A2M	C6-N6	4.52	1.45	1.34
3	AC	27	A2M	C6-N6	4.52	1.45	1.34
77	CI	1337	A2M	C6-N6	4.52	1.45	1.34
77	CI	3484	A2M	C6-N6	4.51	1.45	1.34
3	AC	166	A2M	C6-N6	4.51	1.45	1.34
77	CI	2157	A2M	C6-N6	4.51	1.45	1.34
77	CI	3382	A2M	C6-N6	4.50	1.45	1.34
77	CI	3526	A2M	C6-N6	4.49	1.45	1.34
77	CI	4226	A2M	C6-N6	4.49	1.45	1.34
3	AC	1032	A2M	C6-N6	4.48	1.45	1.34
77	CI	398	A2M	C6-N6	4.48	1.45	1.34
3	AC	669	A2M	C6-N6	4.48	1.45	1.34
77	CI	1347	A2M	C6-N6	4.47	1.45	1.34
77	CI	3377	A2M	C6-N6	4.47	1.45	1.34
77	CI	2119	A2M	C6-N6	4.45	1.45	1.34
77	CI	1673	A2M	C6-N6	4.43	1.45	1.34
79	CK	14	OMU	C4-N3	4.43	1.46	1.38
77	CI	4026	MHG	C5-C4	4.35	1.52	1.38
77	CI	3444	A2M	C6-N6	4.35	1.45	1.34
3	AC	1843	4AC	C5-C4	4.33	1.50	1.40
3	AC	116	OMU	C4-N3	4.27	1.46	1.38
77	CI	2053	E7G	C2-N1	4.24	1.48	1.37
77	CI	1599	E7G	C2-N1	4.20	1.48	1.37
77	CI	1711	P7G	C6-N1	4.19	1.45	1.38
77	CI	4138	B8T	C2-N1	4.18	1.49	1.40
77	CI	3849	I4U	C2-N1	4.16	1.49	1.40
77	CI	3539	P7G	C6-N1	4.14	1.45	1.38
77	CI	1472	I4U	C2-N1	4.14	1.49	1.40
77	CI	3539	P7G	C2-N2	4.11	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	4275	OMU	C4-N3	4.09	1.45	1.38
77	CI	3961	OMU	C4-N3	4.09	1.45	1.38
77	CI	1711	P7G	C2-N2	4.07	1.43	1.34
77	CI	4205	G7M	C5-C6	3.94	1.54	1.43
77	CI	4517	OMG	O3'-C3'	3.94	1.52	1.43
3	AC	1843	4AC	O2-C2	-3.91	1.16	1.23
77	CI	1668	UR3	C6-N1	3.89	1.47	1.38
77	CI	2278	G7M	C5-C6	3.89	1.54	1.43
77	CI	4252	UR3	C6-N1	3.88	1.47	1.38
77	CI	1418	G7M	C5-C6	3.87	1.54	1.43
77	CI	4138	B8T	C5-C4	3.83	1.49	1.40
3	AC	1831	UR3	C6-N1	3.79	1.47	1.38
79	CK	14	OMU	C6-N1	3.79	1.47	1.38
77	CI	3961	OMU	C6-N1	3.78	1.47	1.38
77	CI	237	B9B	O6-C6	3.75	1.40	1.35
77	CI	3961	OMU	C5-C4	3.72	1.51	1.43
77	CI	1599	E7G	C6-N1	3.71	1.45	1.38
3	AC	116	OMU	C5-C4	3.71	1.51	1.43
3	AC	116	OMU	C6-N1	3.68	1.46	1.38
77	CI	4186	PSU	C6-C5	3.65	1.39	1.35
77	CI	1490	PSU	C6-C5	3.65	1.39	1.35
77	CI	2053	E7G	C6-N1	3.61	1.45	1.38
77	CI	1395	PSU	C6-C5	3.60	1.39	1.35
79	CK	14	OMU	C5-C4	3.60	1.51	1.43
3	AC	824	PSU	C6-C5	3.57	1.39	1.35
79	CK	14	OMU	O4-C4	-3.55	1.17	1.24
77	CI	4275	OMU	C6-N1	3.54	1.46	1.38
77	CI	4155	PSU	C6-C5	3.54	1.39	1.35
77	CI	4275	OMU	C5-C4	3.53	1.51	1.43
3	AC	1843	4AC	C6-N1	3.50	1.46	1.38
77	CI	1496	PSU	C6-C5	3.49	1.39	1.35
77	CI	3388	PSU	C6-C5	3.49	1.39	1.35
77	CI	3961	OMU	O4-C4	-3.47	1.17	1.24
77	CI	4291	PSU	C6-C5	3.46	1.39	1.35
77	CI	4026	MHG	C5-C6	3.46	1.52	1.43
3	AC	1244	PSU	C6-C5	3.46	1.39	1.35
77	CI	4275	OMU	O4-C4	-3.45	1.17	1.24
77	CI	4105	PSU	C6-C5	3.45	1.39	1.35
77	CI	4097	PSU	C6-C5	3.45	1.39	1.35
77	CI	4275	OMU	O2-C2	-3.45	1.16	1.23
3	AC	116	OMU	O2-C2	-3.44	1.16	1.23
77	CI	4026	MHG	O6-C6	-3.44	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	3961	OMU	O2-C2	-3.44	1.16	1.23
77	CI	3423	PSU	C6-C5	3.41	1.39	1.35
77	CI	1387	B9B	O6-C6	3.41	1.40	1.35
77	CI	3374	PSU	C6-C5	3.41	1.39	1.35
79	CK	14	OMU	O2-C2	-3.39	1.16	1.23
3	AC	116	OMU	O4-C4	-3.35	1.18	1.24
77	CI	1418	G7M	C5-N7	-3.35	1.35	1.39
77	CI	2264	PSU	C6-C5	3.28	1.39	1.35
77	CI	4058	PSU	C6-C5	3.28	1.39	1.35
3	AC	823	PSU	C6-C5	3.27	1.39	1.35
77	CI	1673	A2M	O3'-C3'	-3.22	1.35	1.43
77	CI	3849	I4U	C6-N1	3.21	1.45	1.38
77	CI	1599	E7G	C5-C6	3.20	1.51	1.43
77	CI	1472	I4U	C6-N1	3.17	1.45	1.38
77	CI	3948	PSU	C6-C5	3.13	1.39	1.35
77	CI	4252	UR3	C4-N3	3.13	1.47	1.40
77	CI	3526	A2M	O3'-C3'	-3.12	1.35	1.43
77	CI	1668	UR3	C4-N3	3.12	1.47	1.40
77	CI	4138	B8T	C6-N1	3.12	1.45	1.38
3	AC	613	PSU	C6-C5	3.12	1.39	1.35
77	CI	4283	PSU	C6-C5	3.12	1.39	1.35
3	AC	1831	UR3	C4-N3	3.12	1.47	1.40
3	AC	27	A2M	O2'-C2'	3.11	1.50	1.42
77	CI	2053	E7G	C5-C6	3.11	1.51	1.43
3	AC	166	A2M	O3'-C3'	-3.10	1.35	1.43
77	CI	3526	A2M	O2'-C2'	3.10	1.50	1.42
77	CI	4205	G7M	C5-N7	-3.09	1.35	1.39
3	AC	1082	PSU	C6-C5	3.09	1.38	1.35
77	CI	3377	A2M	O2'-C2'	3.08	1.50	1.42
77	CI	1472	I4U	O4-C41	-3.08	1.40	1.47
77	CI	2278	G7M	C5-N7	-3.06	1.35	1.39
77	CI	3875	6MZ	O3'-C3'	-3.06	1.35	1.43
77	CI	1337	A2M	O3'-C3'	-3.06	1.35	1.43
77	CI	1140	A2M	O2'-C2'	3.04	1.50	1.42
77	CI	398	A2M	O3'-C3'	-3.04	1.35	1.43
3	AC	1032	A2M	O3'-C3'	-3.02	1.35	1.43
77	CI	3444	A2M	C5-C4	-3.00	1.33	1.39
3	AC	166	A2M	O2'-C2'	3.00	1.50	1.42
3	AC	1032	A2M	O2'-C2'	3.00	1.50	1.42
77	CI	3849	I4U	O4-C41	-2.99	1.40	1.47
77	CI	2157	A2M	O2'-C2'	2.98	1.50	1.42
77	CI	3484	A2M	O3'-C3'	-2.97	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	2157	A2M	O3'-C3'	-2.97	1.36	1.43
3	AC	27	A2M	O3'-C3'	-2.96	1.36	1.43
3	AC	669	A2M	O2'-C2'	2.95	1.50	1.42
77	CI	3484	A2M	O2'-C2'	2.95	1.50	1.42
77	CI	1673	A2M	C5-C4	-2.95	1.33	1.39
77	CI	3382	A2M	O2'-C2'	2.94	1.50	1.42
77	CI	1347	A2M	O3'-C3'	-2.94	1.36	1.43
77	CI	2119	A2M	O3'-C3'	-2.94	1.36	1.43
77	CI	3526	A2M	C5-C4	-2.94	1.33	1.39
77	CI	1387	B9B	C5-C4	-2.92	1.33	1.39
77	CI	1347	A2M	C5-C4	-2.92	1.33	1.39
77	CI	4226	A2M	O2'-C2'	2.91	1.50	1.42
77	CI	398	A2M	O2'-C2'	2.90	1.50	1.42
3	AC	669	A2M	O3'-C3'	-2.90	1.36	1.43
77	CI	3377	A2M	O3'-C3'	-2.90	1.36	1.43
77	CI	4205	G7M	C6-N1	2.90	1.44	1.38
77	CI	1337	A2M	C5-C4	-2.90	1.33	1.39
77	CI	4226	A2M	O3'-C3'	-2.88	1.36	1.43
77	CI	1418	G7M	C6-N1	2.87	1.44	1.38
77	CI	2119	A2M	C5-C4	-2.86	1.33	1.39
77	CI	2119	A2M	O2'-C2'	2.85	1.49	1.42
77	CI	3382	A2M	O3'-C3'	-2.85	1.36	1.43
77	CI	4026	MHG	C72-C71	2.84	1.58	1.52
77	CI	2278	G7M	C6-N1	2.83	1.44	1.38
77	CI	3484	A2M	C5-C4	-2.82	1.33	1.39
77	CI	1673	A2M	O2'-C2'	2.81	1.49	1.42
77	CI	2157	A2M	C5-C4	-2.80	1.33	1.39
3	AC	669	A2M	C5-C4	-2.80	1.33	1.39
77	CI	4226	A2M	C5-C4	-2.80	1.33	1.39
77	CI	237	B9B	C5-C4	-2.78	1.33	1.39
77	CI	3377	A2M	C5-N7	-2.77	1.33	1.39
3	AC	27	A2M	C5-C4	-2.76	1.33	1.39
77	CI	1337	A2M	O2'-C2'	2.76	1.49	1.42
77	CI	1472	I4U	O2-C2	-2.75	1.18	1.23
77	CI	1347	A2M	O2'-C2'	2.75	1.49	1.42
3	AC	1032	A2M	C5-C4	-2.73	1.33	1.39
77	CI	3444	A2M	O2'-C2'	2.73	1.49	1.42
77	CI	3382	A2M	C5-N7	-2.71	1.33	1.39
77	CI	3377	A2M	C5-C4	-2.71	1.34	1.39
77	CI	4138	B8T	O2-C2	-2.70	1.18	1.23
77	CI	4252	UR3	O2-C2	-2.70	1.17	1.22
77	CI	398	A2M	C5-C4	-2.70	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	1140	A2M	C5-C4	-2.67	1.34	1.39
3	AC	166	A2M	C5-C4	-2.66	1.34	1.39
77	CI	3849	I4U	O2-C2	-2.66	1.18	1.23
77	CI	3875	6MZ	C5-C4	-2.66	1.34	1.39
3	AC	1831	UR3	O2-C2	-2.64	1.17	1.22
77	CI	3444	A2M	O3'-C3'	-2.64	1.36	1.43
3	AC	1831	UR3	O4-C4	-2.64	1.17	1.23
77	CI	3382	A2M	C5-C4	-2.62	1.34	1.39
77	CI	1140	A2M	C5-N7	-2.61	1.34	1.39
77	CI	4226	A2M	C5-N7	-2.60	1.34	1.39
77	CI	1668	UR3	O2-C2	-2.60	1.17	1.22
77	CI	2053	E7G	O6-C6	-2.59	1.18	1.23
77	CI	1140	A2M	O3'-C3'	-2.58	1.36	1.43
77	CI	3484	A2M	C5-N7	-2.57	1.34	1.39
77	CI	1668	UR3	O4-C4	-2.57	1.18	1.23
77	CI	1673	A2M	C5-N7	-2.57	1.34	1.39
3	AC	1032	A2M	C5-N7	-2.57	1.34	1.39
77	CI	398	A2M	C5-N7	-2.56	1.34	1.39
77	CI	3526	A2M	C5-N7	-2.56	1.34	1.39
77	CI	2119	A2M	C5-N7	-2.55	1.34	1.39
77	CI	2157	A2M	C5-N7	-2.55	1.34	1.39
3	AC	27	A2M	C5-N7	-2.54	1.34	1.39
77	CI	1347	A2M	C5-N7	-2.54	1.34	1.39
77	CI	4252	UR3	O4-C4	-2.54	1.18	1.23
3	AC	1843	4AC	O7-C7	-2.54	1.17	1.23
77	CI	3840	B8W	C5-N7	-2.53	1.34	1.39
3	AC	669	A2M	C5-N7	-2.53	1.34	1.39
77	CI	3444	A2M	C5-N7	-2.53	1.34	1.39
77	CI	4205	G7M	C2-N1	2.53	1.43	1.37
77	CI	2053	E7G	C5-C4	2.53	1.46	1.38
77	CI	1418	G7M	C2-N1	2.52	1.43	1.37
77	CI	1337	A2M	C5-N7	-2.50	1.34	1.39
77	CI	1599	E7G	O6-C6	-2.49	1.18	1.23
3	AC	166	A2M	C5-N7	-2.48	1.34	1.39
77	CI	2278	G7M	C2-N1	2.47	1.43	1.37
77	CI	3875	6MZ	C5-N7	-2.46	1.34	1.39
77	CI	1599	E7G	C5-C4	2.45	1.46	1.38
77	CI	1387	B9B	C8-N9	-2.41	1.33	1.37
77	CI	4010	E6G	C8-N7	2.40	1.36	1.31
77	CI	2278	G7M	CN7-N7	2.40	1.51	1.46
77	CI	1673	A2M	O5'-C5'	-2.39	1.38	1.44
77	CI	3849	I4U	O4-C4	2.39	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	3840	B8W	C5-C4	-2.38	1.34	1.39
77	CI	237	B9B	C8-N9	-2.38	1.33	1.37
3	AC	1249	B8N	O4-C4	-2.36	1.18	1.23
77	CI	1472	I4U	O4-C4	2.35	1.40	1.35
77	CI	4517	OMG	C4-N3	-2.34	1.28	1.34
77	CI	3875	6MZ	O2'-C2'	2.32	1.48	1.43
77	CI	4010	E6G	C2-N1	2.30	1.39	1.35
77	CI	4226	A2M	C8-N9	-2.30	1.33	1.37
77	CI	3377	A2M	C8-N9	-2.28	1.33	1.37
77	CI	4205	G7M	CN7-N7	2.27	1.50	1.46
77	CI	4517	OMG	C6-N1	-2.25	1.34	1.38
77	CI	1418	G7M	CN7-N7	2.21	1.50	1.46
77	CI	4517	OMG	C3'-C4'	2.20	1.58	1.53
77	CI	1387	B9B	C5-N7	-2.20	1.34	1.39
77	CI	3382	A2M	C8-N9	-2.20	1.33	1.37
77	CI	3526	A2M	C8-N9	-2.18	1.33	1.37
77	CI	4010	E6G	C5-N7	-2.18	1.34	1.39
77	CI	4252	UR3	C5-C4	2.18	1.49	1.43
77	CI	1711	P7G	O6-C6	-2.17	1.20	1.23
77	CI	1269	B8Q	O2-C2	-2.17	1.18	1.22
77	CI	3539	P7G	O6-C6	-2.16	1.20	1.23
77	CI	4517	OMG	O6-C6	2.13	1.27	1.23
77	CI	237	B9B	C5-N7	-2.13	1.35	1.39
77	CI	1668	UR3	C5-C4	2.12	1.49	1.43
77	CI	1347	A2M	C8-N9	-2.12	1.33	1.37
77	CI	1387	B9B	C5-C6	-2.11	1.37	1.41
77	CI	2053	E7G	C4-N9	-2.11	1.35	1.37
77	CI	3484	A2M	C8-N9	-2.11	1.33	1.37
77	CI	2119	A2M	C8-N9	-2.10	1.33	1.37
3	AC	669	A2M	O5'-C5'	-2.10	1.39	1.44
77	CI	2157	A2M	C8-N9	-2.10	1.33	1.37
3	AC	1831	UR3	C5-C4	2.09	1.49	1.43
77	CI	1140	A2M	C8-N9	-2.08	1.33	1.37
77	CI	3526	A2M	O5'-C5'	-2.08	1.39	1.44
77	CI	398	A2M	O5'-C5'	-2.06	1.39	1.44
77	CI	1599	E7G	C4-N9	-2.05	1.35	1.37
77	CI	1673	A2M	C8-N9	-2.05	1.33	1.37
77	CI	1337	A2M	C8-N9	-2.05	1.33	1.37
3	AC	1249	B8N	C31-N3	2.04	1.52	1.47
77	CI	3444	A2M	C8-N9	-2.04	1.33	1.37
77	CI	237	B9B	C5-C6	-2.04	1.37	1.41
77	CI	3382	A2M	O5'-C5'	-2.04	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	3444	A2M	O5'-C5'	-2.02	1.39	1.44
77	CI	3875	6MZ	C8-N9	-2.02	1.33	1.37
3	AC	27	A2M	C8-N9	-2.02	1.33	1.37
3	AC	1032	A2M	C8-N9	-2.01	1.33	1.37
77	CI	398	A2M	C8-N9	-2.01	1.33	1.37

All (479) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	4010	E6G	O6-C6-C5	21.47	143.75	116.57
77	CI	4010	E6G	O6-C6-N1	-18.21	94.64	120.00
77	CI	4010	E6G	C1'-N9-C8	-9.98	104.59	127.14
77	CI	4010	E6G	C4-N9-C1'	8.74	147.42	126.59
77	CI	4010	E6G	N2-C2-N3	8.42	130.35	117.25
77	CI	1387	B9B	O6-C6-N1	7.62	130.60	120.00
77	CI	3539	P7G	C4-C5-N7	7.55	110.66	106.67
77	CI	237	B9B	O6-C6-N1	6.91	129.63	120.00
77	CI	4026	MHG	C4-C5-N7	6.87	111.02	104.91
77	CI	1387	B9B	O6-C6-C5	-6.85	107.89	116.57
77	CI	1387	B9B	N9-C8-N7	-6.64	104.83	113.91
77	CI	4026	MHG	C2-N3-C4	6.53	120.14	112.04
77	CI	3840	B8W	C5-C4-N3	-6.51	119.87	127.19
77	CI	2278	G7M	C1'-N9-C4	-6.47	107.30	126.50
77	CI	237	B9B	N9-C8-N7	-6.46	105.08	113.91
77	CI	1337	A2M	N6-C6-N1	-6.36	104.41	118.35
77	CI	1347	A2M	N6-C6-N1	-6.25	104.65	118.35
77	CI	3444	A2M	N6-C6-N1	-6.23	104.70	118.35
77	CI	3484	A2M	N6-C6-N1	-6.17	104.83	118.35
3	AC	166	A2M	N6-C6-N1	-6.15	104.87	118.35
77	CI	1387	B9B	C4-N9-C8	6.13	112.37	105.73
3	AC	669	A2M	N6-C6-N1	-6.12	104.95	118.35
77	CI	1140	A2M	N6-C6-N1	-6.12	104.95	118.35
77	CI	2119	A2M	N6-C6-N1	-6.11	104.96	118.35
3	AC	1032	A2M	N6-C6-N1	-6.11	104.97	118.35
77	CI	2157	A2M	N6-C6-N1	-6.10	104.99	118.35
77	CI	398	A2M	N6-C6-N1	-6.09	105.02	118.35
77	CI	1673	A2M	N6-C6-N1	-6.08	105.03	118.35
77	CI	3840	B8W	N2-C2-N3	6.07	126.69	117.25
3	AC	27	A2M	N6-C6-N1	-6.06	105.07	118.35
77	CI	3526	A2M	N6-C6-N1	-6.06	105.08	118.35
77	CI	1269	B8Q	N3-C2-N1	6.02	124.20	117.13
77	CI	3382	A2M	N6-C6-N1	-5.99	105.23	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	3377	A2M	N6-C6-N1	-5.98	105.26	118.35
77	CI	1418	G7M	CN7-N7-C5	5.95	134.16	126.77
77	CI	4205	G7M	C1'-N9-C4	-5.95	108.83	126.50
77	CI	237	B9B	C4-N9-C8	5.94	112.16	105.73
77	CI	4226	A2M	N6-C6-N1	-5.93	105.36	118.35
77	CI	4010	E6G	C5-C4-N3	-5.91	120.54	127.19
3	AC	1249	B8N	C5-C4-N3	5.90	127.09	116.17
77	CI	4205	G7M	CN7-N7-C5	5.86	134.04	126.77
77	CI	237	B9B	O6-C6-C5	-5.83	109.18	116.57
77	CI	2053	E7G	C4-C5-N7	5.81	110.08	104.91
77	CI	237	B9B	C5-C4-N3	-5.81	120.66	127.19
77	CI	3382	A2M	C5-C4-N3	-5.74	119.26	126.75
77	CI	1387	B9B	C5-C4-N3	-5.72	120.76	127.19
77	CI	2278	G7M	CN7-N7-C5	5.69	133.84	126.77
77	CI	1673	A2M	N3-C2-N1	-5.67	119.74	128.60
77	CI	1599	E7G	C4-C5-N7	5.61	109.90	104.91
77	CI	398	A2M	C5-C4-N3	-5.55	119.51	126.75
77	CI	3444	A2M	N3-C2-N1	-5.55	119.92	128.60
77	CI	1418	G7M	C1'-N9-C4	-5.53	110.08	126.50
77	CI	2119	A2M	N3-C2-N1	-5.51	119.98	128.60
77	CI	1337	A2M	C5-C6-N6	5.50	135.39	123.43
77	CI	1337	A2M	N3-C2-N1	-5.48	120.02	128.60
3	AC	166	A2M	C5-C4-N3	-5.47	119.61	126.75
3	AC	1032	A2M	C5-C4-N3	-5.45	119.64	126.75
77	CI	1140	A2M	C5-C4-N3	-5.45	119.64	126.75
77	CI	3377	A2M	C5-C4-N3	-5.45	119.64	126.75
77	CI	1347	A2M	N3-C2-N1	-5.44	120.09	128.60
77	CI	3484	A2M	C5-C4-N3	-5.42	119.68	126.75
3	AC	27	A2M	N3-C2-N1	-5.42	120.12	128.60
77	CI	398	A2M	N3-C2-N1	-5.41	120.14	128.60
77	CI	4226	A2M	N3-C2-N1	-5.41	120.15	128.60
3	AC	669	A2M	N3-C2-N1	-5.40	120.15	128.60
77	CI	3484	A2M	C5-C6-N6	5.38	135.14	123.43
77	CI	1140	A2M	N3-C2-N1	-5.37	120.20	128.60
77	CI	3875	6MZ	N1-C2-N3	-5.37	120.21	128.60
3	AC	1032	A2M	N3-C2-N1	-5.37	120.21	128.60
77	CI	1347	A2M	C5-C6-N6	5.36	135.10	123.43
3	AC	166	A2M	N3-C2-N1	-5.36	120.21	128.60
77	CI	2157	A2M	C5-C4-N3	-5.36	119.75	126.75
3	AC	27	A2M	C5-C4-N3	-5.35	119.77	126.75
77	CI	2157	A2M	N3-C2-N1	-5.35	120.23	128.60
77	CI	3382	A2M	N3-C2-N1	-5.34	120.25	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	669	A2M	C5-C6-N6	5.32	135.01	123.43
77	CI	3840	B8W	O6-C6-N1	5.32	126.34	119.01
77	CI	3484	A2M	N3-C2-N1	-5.31	120.30	128.60
77	CI	2119	A2M	C5-C6-N6	5.31	134.98	123.43
3	AC	166	A2M	C5-C6-N6	5.30	134.97	123.43
77	CI	1140	A2M	C5-C6-N6	5.30	134.97	123.43
3	AC	669	A2M	C5-C4-N3	-5.30	119.84	126.75
77	CI	2157	A2M	C5-C6-N6	5.29	134.95	123.43
77	CI	4010	E6G	N2-C2-N1	-5.29	109.02	117.25
3	AC	27	A2M	C5-C6-N6	5.29	134.94	123.43
77	CI	3377	A2M	C5-C6-N6	5.24	134.83	123.43
77	CI	2278	G7M	C1'-N9-C8	5.24	144.42	126.74
77	CI	3875	6MZ	C5-C4-N3	-5.23	119.92	126.75
77	CI	1673	A2M	C5-C6-N6	5.23	134.81	123.43
77	CI	3526	A2M	C5-C6-N6	5.23	134.81	123.43
77	CI	3526	A2M	N3-C2-N1	-5.23	120.42	128.60
3	AC	1032	A2M	C5-C6-N6	5.22	134.80	123.43
77	CI	3444	A2M	C5-C4-N3	-5.22	119.94	126.75
77	CI	237	B9B	N3-C4-N9	5.21	134.22	126.99
77	CI	4226	A2M	C5-C4-N3	-5.20	119.97	126.75
77	CI	398	A2M	C5-C6-N6	5.20	134.74	123.43
77	CI	3961	OMU	C4-N3-C2	-5.18	119.74	126.58
77	CI	1337	A2M	C5-C4-N3	-5.18	119.99	126.75
77	CI	3444	A2M	C5-C6-N6	5.17	134.69	123.43
77	CI	3382	A2M	C5-C6-N6	5.17	134.67	123.43
77	CI	1387	B9B	N3-C4-N9	5.15	134.13	126.99
77	CI	4226	A2M	C5-C6-N6	5.15	134.63	123.43
77	CI	3377	A2M	N3-C2-N1	-5.14	120.56	128.60
77	CI	1347	A2M	C5-C4-N3	-5.12	120.08	126.75
77	CI	2119	A2M	C5-C4-N3	-5.10	120.09	126.75
77	CI	2264	PSU	C4-N3-C2	-5.10	118.99	126.34
77	CI	3526	A2M	C5-C4-N3	-5.04	120.18	126.75
77	CI	1599	E7G	C5-C6-N1	5.03	119.86	110.99
3	AC	613	PSU	N1-C2-N3	5.03	120.83	115.13
77	CI	2542	B9H	C31-N3-C2	4.97	123.42	117.21
77	CI	1673	A2M	C5-C4-N3	-4.93	120.32	126.75
77	CI	2264	PSU	N1-C2-N3	4.92	120.71	115.13
3	AC	1831	UR3	C4-N3-C2	-4.91	119.94	124.56
77	CI	4026	MHG	C5-C6-N1	4.91	119.64	110.99
77	CI	4252	UR3	C4-N3-C2	-4.90	119.95	124.56
77	CI	3374	PSU	N1-C2-N3	4.90	120.69	115.13
3	AC	613	PSU	C4-N3-C2	-4.88	119.31	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	2053	E7G	C5-C6-N1	4.88	119.58	110.99
77	CI	4205	G7M	C1'-N9-C8	4.85	143.11	126.74
3	AC	116	OMU	C4-N3-C2	-4.83	120.21	126.58
77	CI	4058	PSU	N1-C2-N3	4.81	120.58	115.13
77	CI	3374	PSU	C4-N3-C2	-4.79	119.44	126.34
79	CK	14	OMU	C4-N3-C2	-4.77	120.28	126.58
77	CI	3388	PSU	C4-N3-C2	-4.75	119.49	126.34
77	CI	4058	PSU	C4-N3-C2	-4.75	119.49	126.34
77	CI	4291	PSU	C4-N3-C2	-4.75	119.49	126.34
77	CI	4155	PSU	C4-N3-C2	-4.75	119.50	126.34
77	CI	3388	PSU	N1-C2-N3	4.71	120.47	115.13
77	CI	4291	PSU	N1-C2-N3	4.71	120.46	115.13
77	CI	4026	MHG	C5-C4-N3	-4.70	119.17	128.13
77	CI	1418	G7M	C5-C4-N3	-4.70	119.13	128.15
77	CI	4186	PSU	N1-C2-N3	4.67	120.43	115.13
77	CI	4186	PSU	C4-N3-C2	-4.67	119.61	126.34
77	CI	1496	PSU	N1-C2-N3	4.67	120.42	115.13
77	CI	4105	PSU	C4-N3-C2	-4.64	119.65	126.34
3	AC	1244	PSU	C4-N3-C2	-4.63	119.67	126.34
77	CI	3423	PSU	C4-N3-C2	-4.63	119.67	126.34
77	CI	4155	PSU	N1-C2-N3	4.62	120.37	115.13
77	CI	1490	PSU	C4-N3-C2	-4.61	119.70	126.34
77	CI	1668	UR3	C4-N3-C2	-4.61	120.23	124.56
77	CI	3948	PSU	N1-C2-N3	4.60	120.35	115.13
77	CI	4283	PSU	C4-N3-C2	-4.58	119.74	126.34
3	AC	1244	PSU	N1-C2-N3	4.58	120.31	115.13
3	AC	823	PSU	C4-N3-C2	-4.57	119.75	126.34
77	CI	4205	G7M	C5-C4-N3	-4.57	119.38	128.15
77	CI	3526	A2M	N9-C8-N7	-4.57	107.66	113.91
77	CI	1599	E7G	C2-N3-C4	4.57	120.44	112.30
3	AC	824	PSU	C4-N3-C2	-4.57	119.76	126.34
3	AC	1082	PSU	C4-N3-C2	-4.55	119.78	126.34
3	AC	1082	PSU	N1-C2-N3	4.55	120.28	115.13
77	CI	1490	PSU	N1-C2-N3	4.55	120.28	115.13
77	CI	1347	A2M	N9-C8-N7	-4.53	107.72	113.91
77	CI	2278	G7M	C5-C4-N3	-4.52	119.49	128.15
77	CI	4097	PSU	C4-N3-C2	-4.52	119.83	126.34
77	CI	1269	B8Q	C31-N3-C4	4.51	121.05	114.25
77	CI	4010	E6G	N9-C8-N7	-4.50	107.76	113.91
77	CI	4205	G7M	C2-N3-C4	4.48	120.29	112.30
3	AC	824	PSU	N1-C2-N3	4.48	120.20	115.13
77	CI	1418	G7M	C1'-N9-C8	4.46	141.81	126.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	3948	PSU	C4-N3-C2	-4.45	119.92	126.34
77	CI	4105	PSU	N1-C2-N3	4.45	120.17	115.13
77	CI	2278	G7M	C2-N3-C4	4.45	120.23	112.30
77	CI	1496	PSU	C4-N3-C2	-4.44	119.94	126.34
77	CI	1418	G7M	CN7-N7-C8	-4.44	117.98	124.84
77	CI	1418	G7M	C2-N3-C4	4.44	120.21	112.30
77	CI	4205	G7M	CN7-N7-C8	-4.44	117.99	124.84
77	CI	4097	PSU	N1-C2-N3	4.44	120.16	115.13
77	CI	1673	A2M	N9-C8-N7	-4.43	107.86	113.91
77	CI	1395	PSU	C4-N3-C2	-4.43	119.96	126.34
77	CI	2157	A2M	N9-C8-N7	-4.38	107.93	113.91
77	CI	4275	OMU	C4-N3-C2	-4.37	120.81	126.58
77	CI	3444	A2M	N9-C8-N7	-4.36	107.95	113.91
77	CI	2053	E7G	C2-N3-C4	4.36	120.06	112.30
3	AC	166	A2M	N9-C8-N7	-4.34	107.97	113.91
77	CI	1337	A2M	N9-C8-N7	-4.34	107.98	113.91
77	CI	3875	6MZ	N9-C8-N7	-4.33	108.00	113.91
77	CI	2119	A2M	N9-C8-N7	-4.31	108.01	113.91
3	AC	823	PSU	N1-C2-N3	4.31	120.01	115.13
77	CI	3840	B8W	N9-C8-N7	-4.31	108.02	113.91
3	AC	27	A2M	N9-C8-N7	-4.31	108.02	113.91
77	CI	3423	PSU	N1-C2-N3	4.30	120.00	115.13
77	CI	3875	6MZ	C4-C5-C6	4.29	120.14	116.81
77	CI	2278	G7M	CN7-N7-C8	-4.28	118.23	124.84
77	CI	3484	A2M	N9-C8-N7	-4.28	108.06	113.91
77	CI	4010	E6G	C61-O6-C6	-4.25	113.45	117.59
77	CI	398	A2M	N9-C8-N7	-4.19	108.18	113.91
3	AC	1032	A2M	N9-C8-N7	-4.19	108.18	113.91
77	CI	1395	PSU	N1-C2-N3	4.18	119.86	115.13
3	AC	1249	B8N	C4-N3-C2	-4.17	120.19	125.46
77	CI	4026	MHG	C72-C71-N7	-4.16	108.31	112.41
77	CI	4283	PSU	N1-C2-N3	4.16	119.85	115.13
77	CI	1599	E7G	C5-C4-N3	-4.14	120.23	128.13
77	CI	4517	OMG	C2'-C1'-N9	4.10	122.19	114.22
3	AC	669	A2M	N9-C8-N7	-4.08	108.33	113.91
77	CI	2278	G7M	C5-C6-N1	4.05	120.25	111.79
77	CI	4205	G7M	C5-C6-N1	4.05	120.25	111.79
77	CI	2053	E7G	C5-C4-N3	-3.97	120.57	128.13
77	CI	1418	G7M	C5-C6-N1	3.96	120.07	111.79
77	CI	1140	A2M	N9-C8-N7	-3.95	108.51	113.91
77	CI	4226	A2M	N9-C8-N7	-3.93	108.54	113.91
77	CI	1418	G7M	N9-C4-N3	3.84	133.65	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	3961	OMU	N3-C2-N1	3.83	119.97	114.89
77	CI	4026	MHG	C2-N1-C6	-3.82	120.09	124.48
77	CI	1387	B9B	C5-N7-C8	3.77	108.86	103.51
77	CI	1387	B9B	C4-N9-C1'	-3.76	117.64	126.59
77	CI	237	B9B	C5-N7-C8	3.73	108.81	103.51
77	CI	3377	A2M	N9-C8-N7	-3.72	108.83	113.91
77	CI	3840	B8W	N3-C4-N9	3.71	132.14	126.99
77	CI	3382	A2M	C2-N3-C4	3.69	120.46	111.75
77	CI	1418	G7M	O6-C6-C5	-3.68	119.75	128.06
77	CI	4026	MHG	N9-C4-N3	3.66	130.94	125.47
3	AC	116	OMU	N3-C2-N1	3.61	119.68	114.89
77	CI	3444	A2M	C2-N3-C4	3.60	120.26	111.75
77	CI	398	A2M	C2-N3-C4	3.60	120.26	111.75
77	CI	4205	G7M	O6-C6-C5	-3.59	119.96	128.06
77	CI	1711	P7G	C4-C5-N7	3.58	108.56	106.67
77	CI	1140	A2M	C2-N3-C4	3.57	120.19	111.75
3	AC	166	A2M	C2-N3-C4	3.57	120.17	111.75
77	CI	4205	G7M	N9-C4-N3	3.56	133.08	125.94
3	AC	1032	A2M	C2-N3-C4	3.56	120.15	111.75
79	CK	14	OMU	C1'-N1-C2	3.56	124.01	117.57
77	CI	1337	A2M	C2-N3-C4	3.55	120.14	111.75
77	CI	2278	G7M	N9-C4-N3	3.54	133.04	125.94
3	AC	1032	A2M	N3-C4-N9	3.53	132.91	127.08
77	CI	2157	A2M	C2-N3-C4	3.53	120.08	111.75
77	CI	2119	A2M	C2-N3-C4	3.53	120.08	111.75
3	AC	669	A2M	C2-N3-C4	3.52	120.07	111.75
77	CI	1347	A2M	C2-N3-C4	3.52	120.06	111.75
3	AC	27	A2M	C2-N3-C4	3.51	120.05	111.75
77	CI	3484	A2M	C2-N3-C4	3.51	120.05	111.75
77	CI	3382	A2M	N9-C8-N7	-3.51	109.11	113.91
77	CI	1673	A2M	C2-N3-C4	3.49	120.00	111.75
77	CI	1472	I4U	C5-C4-N3	-3.47	119.62	124.91
77	CI	2157	A2M	C2'-C1'-N9	-3.47	107.69	113.53
77	CI	4226	A2M	C2-N3-C4	3.46	119.93	111.75
77	CI	398	A2M	N3-C4-N9	3.45	132.77	127.08
77	CI	2278	G7M	O6-C6-C5	-3.45	120.27	128.06
77	CI	3382	A2M	N3-C4-N9	3.44	132.76	127.08
3	AC	166	A2M	N3-C4-N9	3.44	132.75	127.08
77	CI	3875	6MZ	C2-N3-C4	3.42	119.84	111.75
77	CI	3377	A2M	C2-N3-C4	3.41	119.82	111.75
79	CK	14	OMU	C5-C4-N3	3.41	119.94	114.84
77	CI	3526	A2M	C2-N3-C4	3.40	119.78	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	4275	OMU	N3-C2-N1	3.39	119.39	114.89
3	AC	823	PSU	O2-C2-N1	-3.38	119.06	122.79
77	CI	4226	A2M	C2'-C1'-N9	-3.38	107.84	113.53
77	CI	1269	B8Q	O2-C2-N3	-3.38	117.99	122.95
77	CI	1140	A2M	N3-C4-N9	3.36	132.61	127.08
77	CI	2157	A2M	N3-C4-N9	3.33	132.57	127.08
77	CI	237	B9B	N3-C2-N1	-3.30	120.25	125.42
79	CK	14	OMU	O4-C4-C5	-3.30	119.36	125.16
3	AC	27	A2M	N3-C4-N9	3.30	132.51	127.08
77	CI	3961	OMU	C5-C4-N3	3.29	119.77	114.84
77	CI	3377	A2M	N3-C4-N9	3.28	132.50	127.08
77	CI	1347	A2M	C5-N7-C8	3.28	108.16	103.51
77	CI	3484	A2M	N3-C4-N9	3.27	132.48	127.08
77	CI	3875	6MZ	N3-C4-N9	3.26	132.46	127.08
77	CI	1673	A2M	C2'-C1'-N9	-3.26	108.04	113.53
77	CI	3849	I4U	C5-C4-N3	-3.26	119.95	124.91
77	CI	3840	B8W	C5-N7-C8	3.26	108.13	103.51
77	CI	3526	A2M	C5-N7-C8	3.25	108.12	103.51
77	CI	3875	6MZ	C9-N6-C6	-3.23	120.09	122.87
77	CI	3840	B8W	N1-C2-N3	-3.22	120.36	125.42
77	CI	2157	A2M	C5-N7-C8	3.22	108.08	103.51
3	AC	166	A2M	C5-N7-C8	3.21	108.08	103.51
77	CI	1387	B9B	N3-C2-N1	-3.19	120.42	125.42
77	CI	4226	A2M	N3-C4-N9	3.18	132.32	127.08
77	CI	3484	A2M	C5-N7-C8	3.17	108.02	103.51
77	CI	2121	OMC	C1'-N1-C2	3.17	125.50	118.42
77	CI	3875	6MZ	C5-N7-C8	3.16	108.00	103.51
77	CI	1337	A2M	C5-N7-C8	3.15	107.99	103.51
77	CI	2119	A2M	C5-N7-C8	3.15	107.98	103.51
77	CI	1418	G7M	C2-N1-C6	-3.15	119.36	125.10
3	AC	27	A2M	C5-N7-C8	3.15	107.98	103.51
77	CI	4517	OMG	C5-C4-N3	-3.15	123.36	128.46
77	CI	4205	G7M	C2-N1-C6	-3.12	119.40	125.10
77	CI	398	A2M	C5-N7-C8	3.12	107.95	103.51
79	CK	14	OMU	N3-C2-N1	3.11	119.02	114.89
77	CI	2278	G7M	C2-N1-C6	-3.11	119.43	125.10
77	CI	3444	A2M	N3-C4-N9	3.11	132.20	127.08
77	CI	1673	A2M	C5-N7-C8	3.11	107.92	103.51
3	AC	116	OMU	C5-C4-N3	3.11	119.49	114.84
77	CI	1599	E7G	O6-C6-C5	-3.10	119.94	127.54
3	AC	166	A2M	C2'-C1'-N9	-3.10	108.32	113.53
3	AC	1082	PSU	O2-C2-N1	-3.09	119.39	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	669	A2M	N3-C4-N9	3.09	132.17	127.08
77	CI	3444	A2M	C5-N7-C8	3.08	107.88	103.51
3	AC	1032	A2M	C5-N7-C8	3.07	107.86	103.51
77	CI	4010	E6G	N3-C2-N1	-3.06	120.62	125.42
77	CI	4010	E6G	C5-N7-C8	3.04	107.83	103.51
77	CI	3377	A2M	C2'-C1'-N9	-3.03	108.42	113.53
77	CI	1347	A2M	N3-C4-N9	3.03	132.08	127.08
3	AC	613	PSU	O2-C2-N1	-3.02	119.46	122.79
3	AC	669	A2M	C5-N7-C8	3.01	107.79	103.51
77	CI	1337	A2M	N3-C4-N9	3.01	132.03	127.08
77	CI	4275	OMU	C5-C4-N3	3.00	119.33	114.84
77	CI	3526	A2M	N3-C4-N9	3.00	132.02	127.08
77	CI	4026	MHG	O6-C6-C5	-2.99	120.22	127.54
77	CI	3374	PSU	O2-C2-N1	-2.98	119.51	122.79
77	CI	1140	A2M	C5-N7-C8	2.97	107.73	103.51
77	CI	1673	A2M	N3-C4-N9	2.97	131.98	127.08
77	CI	2119	A2M	N3-C4-N9	2.96	131.96	127.08
77	CI	2264	PSU	O2-C2-N1	-2.95	119.54	122.79
77	CI	4517	OMG	C6-C5-C4	2.95	123.32	118.77
77	CI	2053	E7G	O6-C6-C5	-2.94	120.33	127.54
77	CI	1599	E7G	C5-C4-N9	2.93	110.15	106.35
77	CI	1337	A2M	C2'-C1'-N9	-2.93	108.60	113.53
77	CI	4517	OMG	CM2-O2'-C2'	-2.92	106.85	114.52
77	CI	4226	A2M	C5-N7-C8	2.89	107.61	103.51
77	CI	3388	PSU	O2-C2-N1	-2.88	119.62	122.79
3	AC	1249	B8N	N3-C2-N1	2.88	120.82	116.76
77	CI	3377	A2M	C5-N7-C8	2.87	107.59	103.51
77	CI	2053	E7G	C5-C4-N9	2.87	110.07	106.35
77	CI	4010	E6G	N3-C4-N9	2.85	130.94	126.99
77	CI	4283	PSU	O2-C2-N1	-2.84	119.66	122.79
77	CI	1490	PSU	O2-C2-N1	-2.83	119.67	122.79
77	CI	3961	OMU	O4-C4-C5	-2.83	120.19	125.16
77	CI	3875	6MZ	C3'-C2'-C1'	2.82	106.79	101.43
77	CI	4275	OMU	O4-C4-C5	-2.81	120.22	125.16
3	AC	1249	B8N	O4-C4-N3	-2.81	115.21	119.98
77	CI	4155	PSU	O2-C2-N1	-2.81	119.70	122.79
3	AC	1244	PSU	O2-C2-N1	-2.80	119.70	122.79
77	CI	1269	B8Q	C1'-N1-C2	2.80	121.72	116.99
77	CI	237	B9B	C4-N9-C1'	-2.80	119.92	126.59
77	CI	1599	E7G	C2-N1-C6	-2.79	120.01	125.10
77	CI	1599	E7G	N9-C4-N3	2.77	129.62	125.47
77	CI	3840	B8W	N2-C2-N1	-2.77	112.94	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	3444	A2M	C4'-O4'-C1'	-2.76	103.39	109.47
77	CI	3382	A2M	C5-N7-C8	2.75	107.42	103.51
77	CI	3840	B8W	C5-C6-N1	-2.75	119.64	123.46
77	CI	4026	MHG	C5-C4-N9	2.73	109.90	106.35
3	AC	116	OMU	O4-C4-C5	-2.73	120.36	125.16
77	CI	3484	A2M	C2'-C1'-N9	-2.73	108.93	113.53
77	CI	4186	PSU	O2-C2-N1	-2.72	119.79	122.79
77	CI	2121	OMC	C1'-N1-C6	-2.67	115.03	120.84
77	CI	237	B9B	N2-C2-N3	2.65	121.37	117.25
77	CI	2053	E7G	C2-N1-C6	-2.65	120.28	125.10
77	CI	1269	B8Q	C31-N3-C2	2.64	121.63	117.79
77	CI	3526	A2M	C4'-O4'-C1'	-2.63	103.67	109.47
3	AC	613	PSU	C6-N1-C2	-2.61	120.01	122.68
77	CI	2053	E7G	N9-C4-N3	2.60	129.36	125.47
77	CI	4186	PSU	C6-C5-C4	2.59	120.01	118.20
77	CI	3374	PSU	C6-N1-C2	-2.59	120.04	122.68
77	CI	4058	PSU	O2-C2-N1	-2.58	119.95	122.79
77	CI	2121	OMC	O2-C2-N1	2.56	124.17	118.89
77	CI	3840	B8W	C2-N1-C6	2.55	119.98	115.93
77	CI	4517	OMG	O3'-C3'-C4'	-2.55	103.69	111.05
3	AC	613	PSU	C6-C5-C4	2.54	119.97	118.20
77	CI	2542	B9H	O2-C2-N1	-2.53	116.79	122.72
3	AC	1032	A2M	C2'-C1'-N9	-2.53	109.27	113.53
77	CI	1599	E7G	C8-N7-C71	2.53	126.51	120.50
77	CI	3948	PSU	C6-N1-C2	-2.52	120.10	122.68
3	AC	27	A2M	C2'-C1'-N9	-2.52	109.29	113.53
77	CI	4155	PSU	C6-C5-C4	2.52	119.96	118.20
3	AC	1082	PSU	C6-N1-C2	-2.51	120.11	122.68
77	CI	4105	PSU	O2-C2-N1	-2.51	120.03	122.79
77	CI	1496	PSU	O2-C2-N1	-2.50	120.03	122.79
77	CI	3526	A2M	C4-N9-C8	2.50	108.43	105.73
77	CI	3444	A2M	O4'-C1'-N9	2.49	112.97	108.06
77	CI	2264	PSU	C6-C5-C4	2.49	119.94	118.20
77	CI	3948	PSU	O2-C2-N1	-2.49	120.05	122.79
77	CI	2542	B9H	O2-C2-N3	-2.48	118.92	122.07
77	CI	2119	A2M	C2'-C1'-N9	-2.47	109.37	113.53
3	AC	1831	UR3	C6-N1-C2	-2.47	119.58	121.79
3	AC	1249	B8N	C31-N3-C4	2.46	120.93	117.31
77	CI	4097	PSU	O2-C2-N1	-2.45	120.09	122.79
77	CI	4138	B8T	C6-C5-C4	2.44	119.95	116.96
3	AC	824	PSU	O2-C2-N1	-2.44	120.10	122.79
77	CI	4070	1MA	N1-C6-N6	2.44	125.97	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	1496	PSU	C6-N1-C2	-2.43	120.20	122.68
77	CI	4058	PSU	C6-N1-C2	-2.43	120.20	122.68
77	CI	4291	PSU	O2-C2-N1	-2.42	120.12	122.79
3	AC	27	A2M	O2'-C2'-C1'	2.41	113.77	109.08
77	CI	4517	OMG	C2'-C3'-C4'	2.40	107.21	101.99
77	CI	3423	PSU	O2-C2-N1	-2.39	120.16	122.79
77	CI	1395	PSU	O2-C2-N1	-2.38	120.17	122.79
77	CI	1347	A2M	C4-N9-C8	2.38	108.31	105.73
77	CI	4105	PSU	C6-C5-C4	2.37	119.86	118.20
77	CI	2053	E7G	C8-N7-C71	2.36	126.12	120.50
77	CI	3377	A2M	C6-C5-C4	2.36	120.36	117.18
77	CI	3840	B8W	O6-C6-C5	-2.36	114.01	116.97
77	CI	1673	A2M	C4-N9-C8	2.35	108.27	105.73
77	CI	4010	E6G	C5-C4-N9	2.35	108.51	105.78
77	CI	3382	A2M	C3'-C2'-C1'	2.33	107.27	102.89
77	CI	2121	OMC	C4-N3-C2	2.32	124.00	120.25
77	CI	2157	A2M	C4-N9-C8	2.31	108.23	105.73
77	CI	1387	B9B	N2-C2-N3	2.31	120.85	117.25
3	AC	1032	A2M	C1'-N9-C8	-2.30	121.94	127.14
3	AC	1082	PSU	O4'-C1'-C2'	2.30	108.38	105.14
77	CI	4252	UR3	C1'-N1-C2	2.29	120.86	116.99
77	CI	4026	MHG	C21-N2-C2	-2.29	118.81	123.86
77	CI	3377	A2M	C3'-C2'-C1'	2.29	107.19	102.89
77	CI	4097	PSU	C6-N1-C2	-2.28	120.35	122.68
77	CI	3875	6MZ	C4-N9-C8	2.26	108.18	105.73
77	CI	3388	PSU	C6-C5-C4	2.26	119.78	118.20
77	CI	1140	A2M	C3'-C2'-C1'	2.26	107.13	102.89
3	AC	166	A2M	C4-N9-C8	2.25	108.17	105.73
77	CI	3382	A2M	C6-C5-C4	2.25	120.21	117.18
77	CI	1673	A2M	C5'-C4'-C3'	-2.25	106.76	115.18
77	CI	4291	PSU	C6-C5-C4	2.25	119.77	118.20
3	AC	1843	4AC	C6-C5-C4	2.23	119.69	116.96
77	CI	4026	MHG	N1-C2-N3	-2.22	120.52	123.95
77	CI	3840	B8W	C4-C5-N7	-2.22	107.92	110.62
77	CI	3948	PSU	C6-C5-C4	2.21	119.75	118.20
3	AC	27	A2M	C4-N9-C8	2.21	108.12	105.73
77	CI	3539	P7G	C5-C4-N3	-2.21	120.11	124.00
77	CI	3444	A2M	C4-N9-C8	2.20	108.12	105.73
3	AC	823	PSU	C6-C5-C4	2.20	119.74	118.20
3	AC	1843	4AC	CM7-C7-N4	2.20	119.10	115.29
3	AC	824	PSU	C6-N1-C2	-2.19	120.44	122.68
77	CI	3840	B8W	C2-N3-C4	2.19	119.95	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	3388	PSU	C6-N1-C2	-2.19	120.45	122.68
3	AC	1244	PSU	C6-N1-C2	-2.19	120.45	122.68
77	CI	1347	A2M	C4-C5-N7	-2.18	107.96	110.62
77	CI	4010	E6G	C4-C5-N7	-2.18	107.96	110.62
3	AC	1032	A2M	C4-N9-C8	2.18	108.09	105.73
3	AC	1244	PSU	C6-C5-C4	2.17	119.72	118.20
77	CI	2542	B9H	C2'-C1'-N1	-2.17	110.00	114.22
77	CI	4010	E6G	C2-N3-C4	2.17	119.89	113.89
77	CI	398	A2M	C1'-N9-C8	-2.16	122.25	127.14
77	CI	2119	A2M	C4-N9-C8	2.16	108.07	105.73
77	CI	2119	A2M	C4-C5-N7	-2.16	107.99	110.62
77	CI	3526	A2M	C4-C5-N7	-2.16	107.99	110.62
77	CI	4517	OMG	C6-C5-N7	-2.16	126.24	130.25
77	CI	3484	A2M	C6-C5-C4	2.15	120.08	117.18
3	AC	166	A2M	C6-C5-C4	2.14	120.07	117.18
3	AC	27	A2M	C6-C5-C4	2.14	120.06	117.18
77	CI	3539	P7G	O6-C6-C5	-2.14	119.59	125.59
77	CI	3374	PSU	C6-C5-C4	2.14	119.69	118.20
77	CI	237	B9B	C2-N3-C4	2.13	119.79	113.89
3	AC	116	OMU	O2-C2-N1	-2.13	119.95	122.79
77	CI	1337	A2M	C4-C5-N7	-2.13	108.02	110.62
3	AC	1843	4AC	N4-C4-N3	2.13	117.42	113.85
3	AC	1831	UR3	C1'-N1-C2	2.13	120.58	116.99
77	CI	3484	A2M	C4-N9-C8	2.12	108.03	105.73
77	CI	1337	A2M	C4-N9-C8	2.12	108.03	105.73
77	CI	2157	A2M	C6-C5-C4	2.12	120.03	117.18
77	CI	3484	A2M	C4-C5-N7	-2.12	108.04	110.62
77	CI	1668	UR3	C1'-N1-C2	2.11	120.56	116.99
77	CI	398	A2M	C6-C5-C4	2.11	120.02	117.18
77	CI	3444	A2M	O4'-C1'-C2'	-2.11	102.87	106.57
77	CI	1387	B9B	C2-N3-C4	2.10	119.71	113.89
77	CI	3526	A2M	C2'-C1'-N9	-2.10	109.99	113.53
3	AC	1032	A2M	C6-C5-C4	2.10	120.01	117.18
77	CI	398	A2M	C3'-C2'-C1'	2.10	106.84	102.89
77	CI	4226	A2M	C6-C5-C4	2.10	120.01	117.18
77	CI	1668	UR3	C6-N1-C2	-2.10	119.91	121.79
77	CI	1269	B8Q	O2-C2-N1	-2.10	117.81	122.72
77	CI	1140	A2M	C6-C5-C4	2.09	120.00	117.18
77	CI	1490	PSU	C6-C5-C4	2.09	119.66	118.20
77	CI	3568	OMC	C1'-N1-C2	2.09	123.08	118.42
77	CI	4291	PSU	C6-N1-C2	-2.09	120.55	122.68
77	CI	4186	PSU	C6-N1-C2	-2.09	120.55	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	2157	A2M	C4-C5-N7	-2.08	108.08	110.62
77	CI	237	B9B	C2-N1-C6	2.08	119.23	115.93
77	CI	4252	UR3	C6-N1-C2	-2.07	119.93	121.79
77	CI	4283	PSU	C6-N1-C2	-2.07	120.56	122.68
77	CI	398	A2M	C4-N9-C8	2.07	107.97	105.73
3	AC	669	A2M	C6-C5-C4	2.07	119.96	117.18
3	AC	669	A2M	C3'-C2'-C1'	2.07	106.77	102.89
77	CI	3423	PSU	C6-N1-C2	-2.06	120.58	122.68
77	CI	4517	OMG	C1'-N9-C4	-2.06	120.38	126.50
77	CI	4275	OMU	C2'-C1'-N1	-2.06	110.23	114.22
77	CI	4517	OMG	O4'-C1'-N9	2.06	113.06	108.36
77	CI	2264	PSU	C6-N1-C2	-2.05	120.59	122.68
77	CI	4226	A2M	C3'-C2'-C1'	2.05	106.74	102.89
3	AC	1843	4AC	C5-C4-N3	-2.05	119.30	122.59
77	CI	3840	B8W	C4-N9-C8	2.05	107.94	105.73
77	CI	1490	PSU	C6-N1-C2	-2.04	120.59	122.68
3	AC	166	A2M	C4-C5-N7	-2.04	108.14	110.62
79	CK	14	OMU	C1'-N1-C6	-2.03	116.41	120.84
77	CI	4010	E6G	C4-N9-C8	2.03	107.92	105.73
3	AC	669	A2M	C4-C5-N7	-2.02	108.16	110.62
3	AC	27	A2M	C4-C5-N7	-2.02	108.16	110.62
77	CI	1337	A2M	C4'-O4'-C1'	-2.01	105.03	109.47
77	CI	3961	OMU	O2-C2-N1	-2.01	120.11	122.79
3	AC	1249	B8N	O4'-C1'-C2'	2.01	107.97	105.14
77	CI	4097	PSU	O4'-C1'-C2'	2.00	107.97	105.14
77	CI	398	A2M	C4-C5-N7	-2.00	108.18	110.62

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
77	CI	237	B9B	C5-C6-O6-C61
77	CI	237	B9B	N1-C6-O6-C61
77	CI	237	B9B	C4'-C5'-O5'-P
77	CI	1140	A2M	C1'-C2'-O2'-CM'
77	CI	1438	OMG	O4'-C4'-C5'-O5'
77	CI	1438	OMG	C3'-C4'-C5'-O5'
77	CI	2120	OMG	O4'-C4'-C5'-O5'
77	CI	2529	OMG	O4'-C4'-C5'-O5'
77	CI	2529	OMG	C3'-C4'-C5'-O5'
77	CI	2542	B9H	C32-C31-N3-C2
77	CI	3374	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
77	CI	3374	PSU	O4'-C4'-C5'-O5'
77	CI	3377	A2M	C1'-C2'-O2'-CM'
77	CI	3484	A2M	C1'-C2'-O2'-CM'
77	CI	3526	A2M	O4'-C4'-C5'-O5'
77	CI	3526	A2M	C1'-C2'-O2'-CM'
77	CI	3528	OMC	C3'-C4'-C5'-O5'
77	CI	3528	OMC	O4'-C4'-C5'-O5'
77	CI	3546	OMC	C3'-C4'-C5'-O5'
77	CI	3840	B8W	C5-C6-O6-C61
77	CI	3840	B8W	N1-C6-O6-C61
77	CI	3961	OMU	C3'-C4'-C5'-O5'
77	CI	4010	E6G	C5-C6-O6-C61
77	CI	4010	E6G	N1-C6-O6-C61
77	CI	4010	E6G	C62-C61-O6-C6
77	CI	4025	OMG	O4'-C4'-C5'-O5'
77	CI	4026	MHG	C2'-C1'-N9-C8
77	CI	4026	MHG	C71-C72-C73-C75
77	CI	4102	5MC	C2'-C1'-N1-C2
77	CI	4102	5MC	C2'-C1'-N1-C6
77	CI	4105	PSU	C2'-C1'-C5-C4
77	CI	4291	PSU	C2'-C1'-C5-C4
77	CI	4291	PSU	C3'-C4'-C5'-O5'
77	CI	4517	OMG	C4'-C5'-O5'-P
77	CI	4517	OMG	C3'-C2'-O2'-CM2
77	CI	4519	2MG	O4'-C4'-C5'-O5'
79	CK	14	OMU	O4'-C1'-N1-C2
79	CK	14	OMU	O4'-C1'-N1-C6
3	AC	27	A2M	C1'-C2'-O2'-CM'
3	AC	669	A2M	C1'-C2'-O2'-CM'
3	AC	823	PSU	C2'-C1'-C5-C6
3	AC	823	PSU	O4'-C1'-C5-C6
3	AC	1244	PSU	C3'-C4'-C5'-O5'
3	AC	1249	B8N	O4'-C4'-C5'-O5'
3	AC	1249	B8N	C3'-C4'-C5'-O5'
3	AC	1249	B8N	O4'-C1'-C5-C6
3	AC	1249	B8N	O4'-C1'-C5-C4
77	CI	3360	OMC	C2'-C1'-N1-C6
77	CI	1347	A2M	O4'-C4'-C5'-O5'
77	CI	1347	A2M	C3'-C4'-C5'-O5'
77	CI	2120	OMG	C3'-C4'-C5'-O5'
77	CI	2121	OMC	O4'-C4'-C5'-O5'
77	CI	3526	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
77	CI	3948	PSU	O4'-C4'-C5'-O5'
77	CI	4025	OMG	C3'-C4'-C5'-O5'
77	CI	4102	5MC	O4'-C4'-C5'-O5'
77	CI	4105	PSU	C3'-C4'-C5'-O5'
77	CI	4517	OMG	C3'-C4'-C5'-O5'
77	CI	4519	2MG	C3'-C4'-C5'-O5'
3	AC	669	A2M	O4'-C4'-C5'-O5'
3	AC	669	A2M	C3'-C4'-C5'-O5'
3	AC	1244	PSU	O4'-C4'-C5'-O5'
77	CI	1685	OMG	O4'-C4'-C5'-O5'
77	CI	1685	OMG	C3'-C4'-C5'-O5'
77	CI	2121	OMC	C3'-C4'-C5'-O5'
77	CI	4105	PSU	O4'-C4'-C5'-O5'
77	CI	4291	PSU	O4'-C4'-C5'-O5'
3	AC	613	PSU	C3'-C4'-C5'-O5'
3	AC	613	PSU	O4'-C4'-C5'-O5'
64	Bd	98	MLZ	CD-CE-NZ-CM
77	CI	3360	OMC	C2'-C1'-N1-C2
77	CI	237	B9B	C3'-C4'-C5'-O5'
77	CI	3961	OMU	O4'-C4'-C5'-O5'
77	CI	3546	OMC	O4'-C4'-C5'-O5'
77	CI	3849	I4U	C3'-C4'-C5'-O5'
77	CI	3377	A2M	C3'-C2'-O2'-CM'
77	CI	2178	OMC	O4'-C4'-C5'-O5'
77	CI	237	B9B	O6-C61-C62-C63
77	CI	3948	PSU	C3'-C4'-C5'-O5'
77	CI	4517	OMG	O4'-C4'-C5'-O5'
77	CI	3849	I4U	O4'-C4'-C5'-O5'
77	CI	3546	OMC	C4'-C5'-O5'-P
77	CI	237	B9B	O4'-C4'-C5'-O5'
77	CI	4102	5MC	C3'-C4'-C5'-O5'
77	CI	4102	5MC	O4'-C1'-N1-C6
77	CI	4026	MHG	C71-C72-C73-C74
3	AC	645	OMG	C4'-C5'-O5'-P
77	CI	1140	A2M	C3'-C4'-C5'-O5'
77	CI	1673	A2M	C3'-C4'-C5'-O5'
77	CI	3388	PSU	C3'-C4'-C5'-O5'
77	CI	3539	P7G	C72-C71-N7-C8
77	CI	1387	B9B	C62-C61-O6-C6
79	CK	14	OMU	C3'-C2'-O2'-CM2
77	CI	3360	OMC	O4'-C1'-N1-C6
77	CI	1140	A2M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
37	BC	333	MLZ	N-CA-CB-CG
77	CI	877	2MG	C3'-C4'-C5'-O5'
77	CI	4205	G7M	C3'-C4'-C5'-O5'
77	CI	4292	OMG	C3'-C4'-C5'-O5'
3	AC	1249	B8N	C32-C33-C34-O36
3	AC	1249	B8N	C32-C33-C34-O35
77	CI	3360	OMC	O4'-C1'-N1-C2
77	CI	3961	OMU	C4'-C5'-O5'-P
77	CI	4155	PSU	C4'-C5'-O5'-P
79	CK	14	OMU	C3'-C4'-C5'-O5'
77	CI	1418	G7M	C4'-C5'-O5'-P
77	CI	1418	G7M	C3'-C4'-C5'-O5'
77	CI	1599	E7G	O4'-C4'-C5'-O5'
77	CI	3388	PSU	O4'-C4'-C5'-O5'
77	CI	398	A2M	C4'-C5'-O5'-P
77	CI	877	2MG	C4'-C5'-O5'-P
77	CI	4102	5MC	O4'-C1'-N1-C2
77	CI	4026	MHG	C2'-C1'-N9-C4
77	CI	1337	A2M	O4'-C1'-N9-C8
77	CI	4105	PSU	O4'-C1'-C5-C4
77	CI	4186	PSU	O4'-C1'-C5-C4
77	CI	4291	PSU	O4'-C1'-C5-C4
77	CI	4149	OMG	C3'-C2'-O2'-CM2
77	CI	4291	PSU	C4'-C5'-O5'-P
3	AC	1244	PSU	C4'-C5'-O5'-P
77	CI	2542	B9H	C32-C31-N3-C4
77	CI	3423	PSU	O4'-C4'-C5'-O5'
77	CI	3539	P7G	C3'-C4'-C5'-O5'
77	CI	4205	G7M	O4'-C4'-C5'-O5'
77	CI	3382	A2M	C1'-C2'-O2'-CM'
77	CI	4149	OMG	C1'-C2'-O2'-CM2
79	CK	14	OMU	C1'-C2'-O2'-CM2
77	CI	1490	PSU	O4'-C1'-C5-C6
77	CI	4105	PSU	O4'-C1'-C5-C6
77	CI	4186	PSU	O4'-C1'-C5-C6
77	CI	4291	PSU	O4'-C1'-C5-C6
77	CI	4026	MHG	O4'-C4'-C5'-O5'
77	CI	2560	OMC	C2'-C1'-N1-C2
77	CI	1140	A2M	O4'-C4'-C5'-O5'
77	CI	3444	A2M	O4'-C4'-C5'-O5'
77	CI	1387	B9B	C2'-C1'-N9-C8
3	AC	669	A2M	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
77	CI	1395	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

29 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	CI	3382	A2M	2	0
77	CI	4102	5MC	1	0
77	CI	4070	1MA	2	0
77	CI	3377	A2M	4	0
77	CI	4226	A2M	1	0
77	CI	3526	A2M	2	0
77	CI	4291	PSU	1	0
77	CI	4517	OMG	6	0
77	CI	2560	OMC	1	0
3	AC	823	PSU	2	0
79	CK	14	OMU	4	0
77	CI	1685	OMG	3	0
77	CI	1673	A2M	1	0
3	AC	1843	4AC	2	0
77	CI	2542	B9H	6	0
77	CI	3444	A2M	2	0
77	CI	4058	PSU	1	0
77	CI	4283	PSU	1	0
77	CI	398	A2M	1	0
77	CI	237	B9B	1	0
3	AC	116	OMU	3	0
77	CI	3948	PSU	2	0
77	CI	1140	A2M	2	0
77	CI	373	OMG	1	0
77	CI	4191	OMC	2	0
77	CI	3568	OMC	3	0
3	AC	1831	UR3	1	0
77	CI	4275	OMU	2	0
77	CI	1668	UR3	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

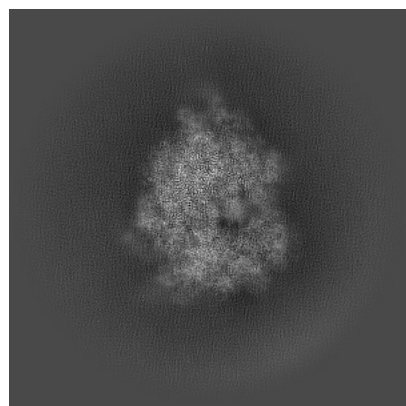
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-58362. These allow visual inspection of the internal detail of the map and identification of artifacts.

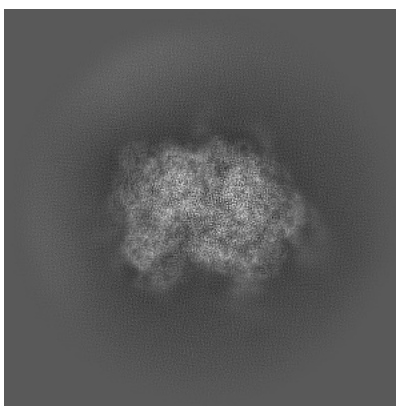
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

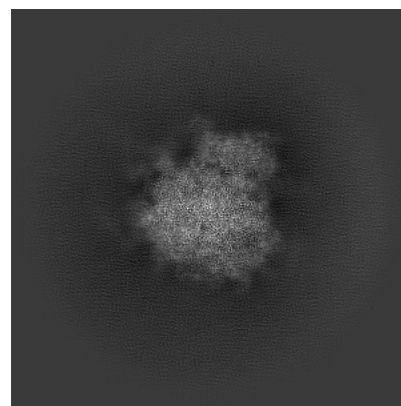
6.1.1 Primary map



X

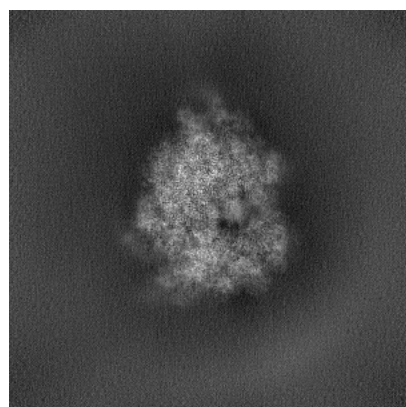


Y

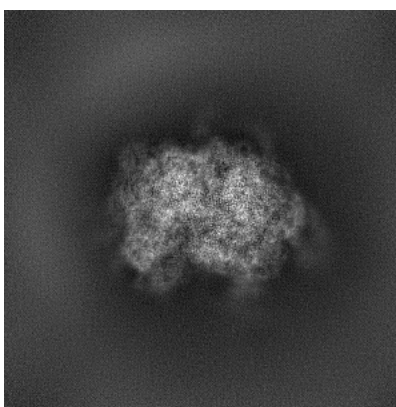


Z

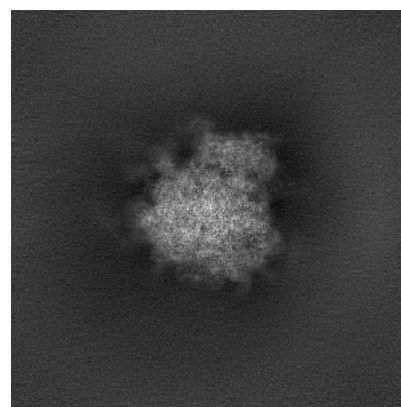
6.1.2 Raw map



X



Y

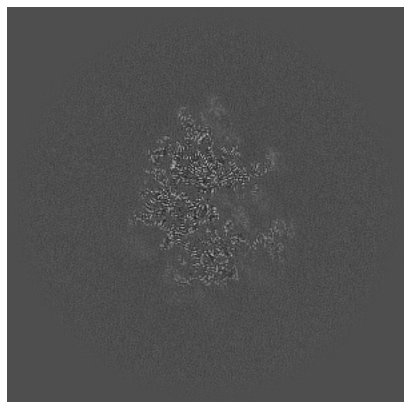


Z

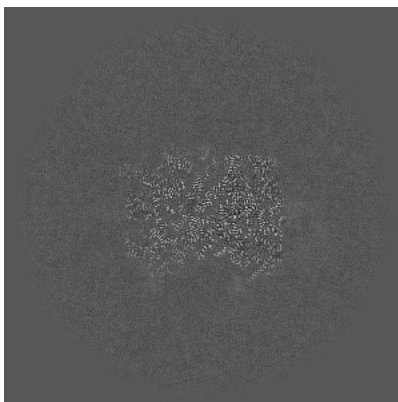
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

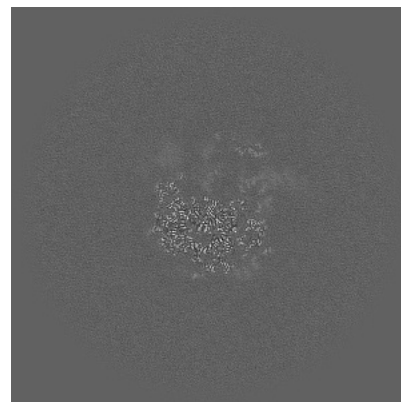
6.2.1 Primary map



X Index: 256

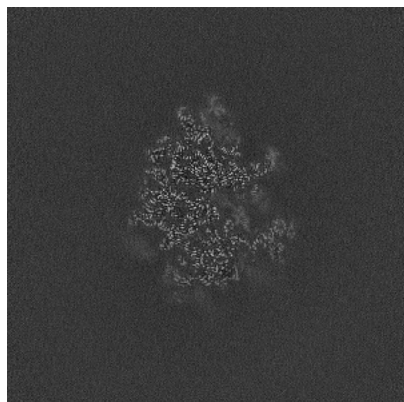


Y Index: 256

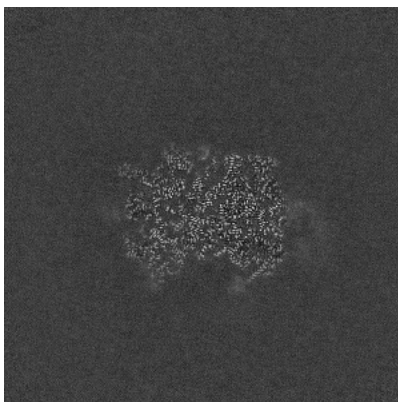


Z Index: 256

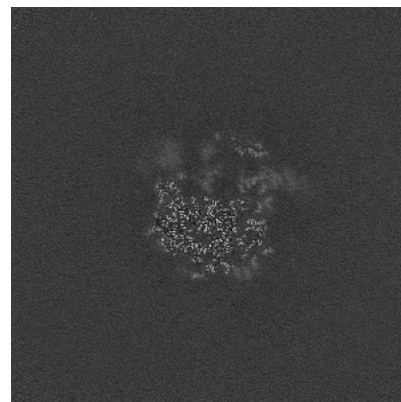
6.2.2 Raw map



X Index: 256



Y Index: 256

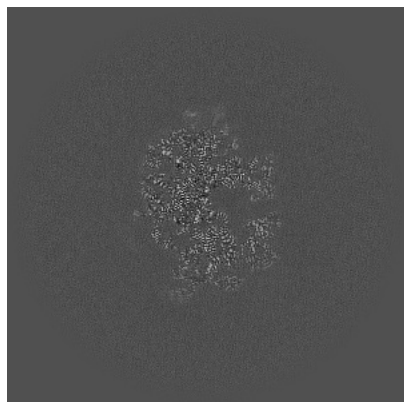


Z Index: 256

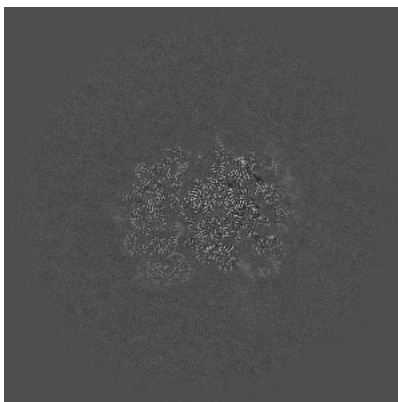
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

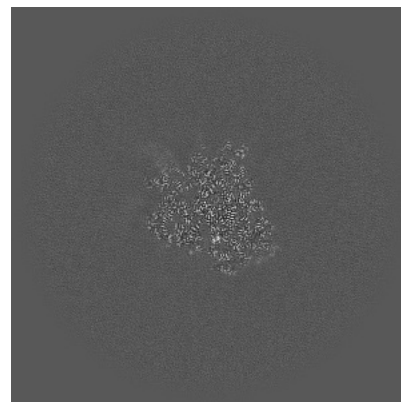
6.3.1 Primary map



X Index: 272

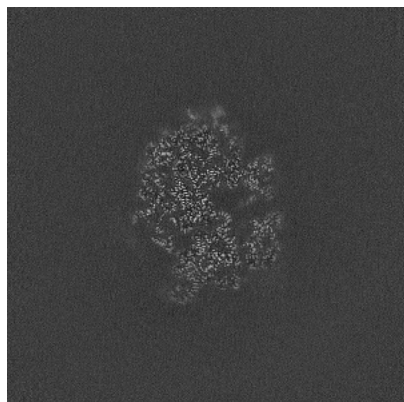


Y Index: 243

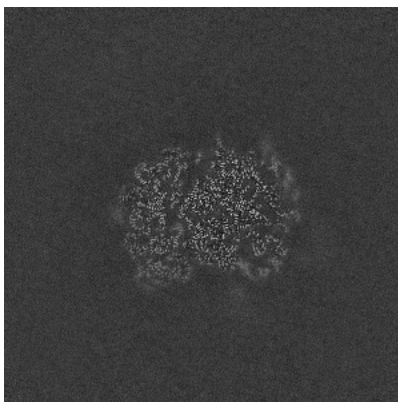


Z Index: 289

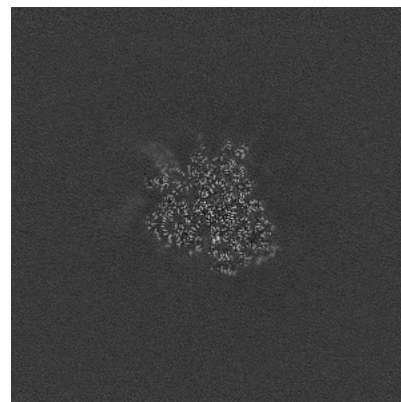
6.3.2 Raw map



X Index: 269



Y Index: 242

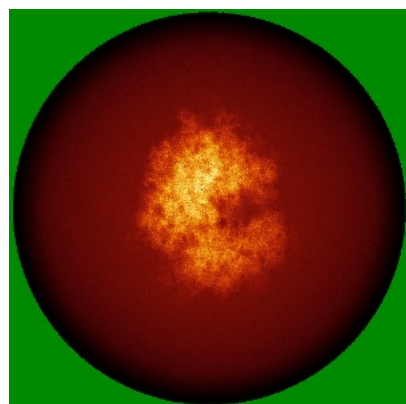


Z Index: 289

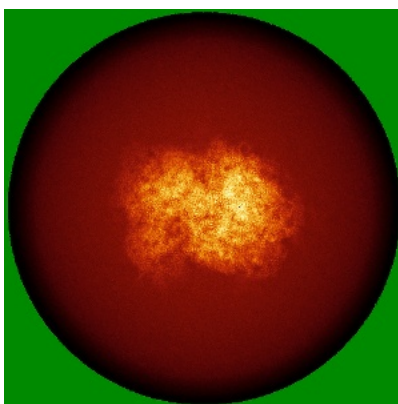
The images above show the largest variance slices of the map in three orthogonal directions.

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

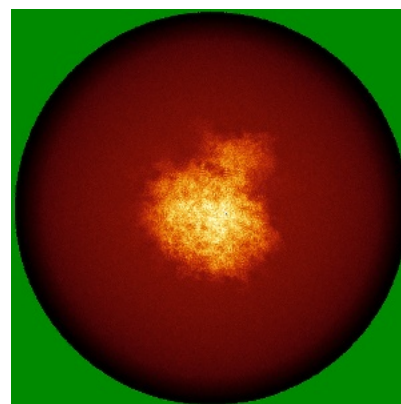
6.4.1 Primary map



X

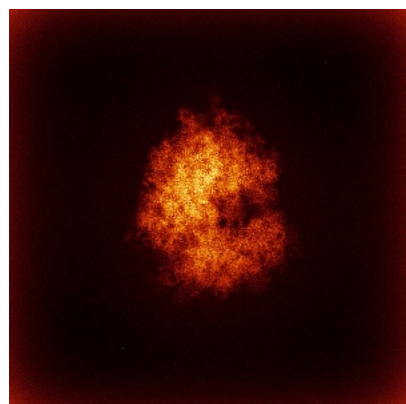


Y

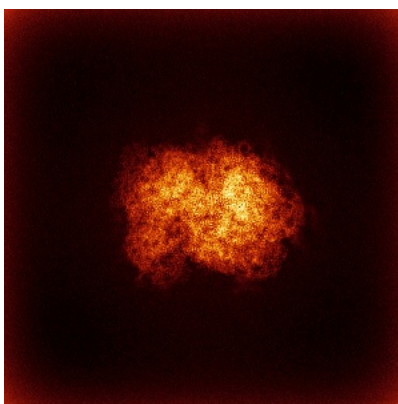


Z

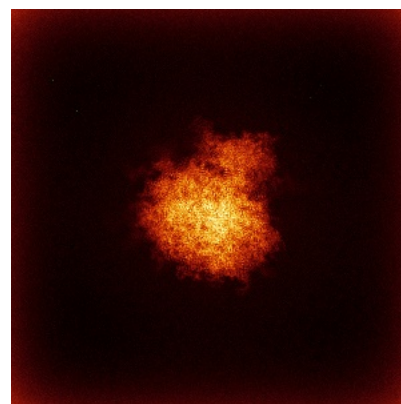
6.4.2 Raw map



X



Y

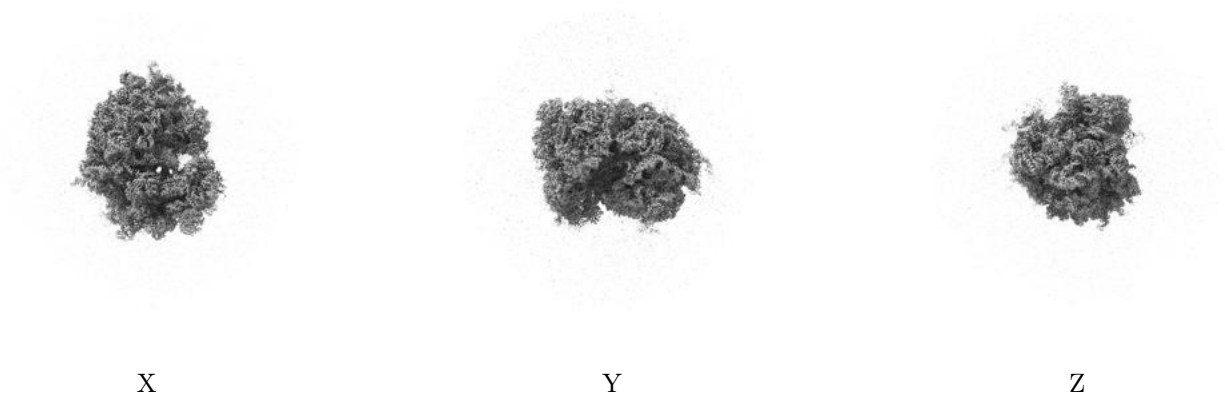


Z

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.

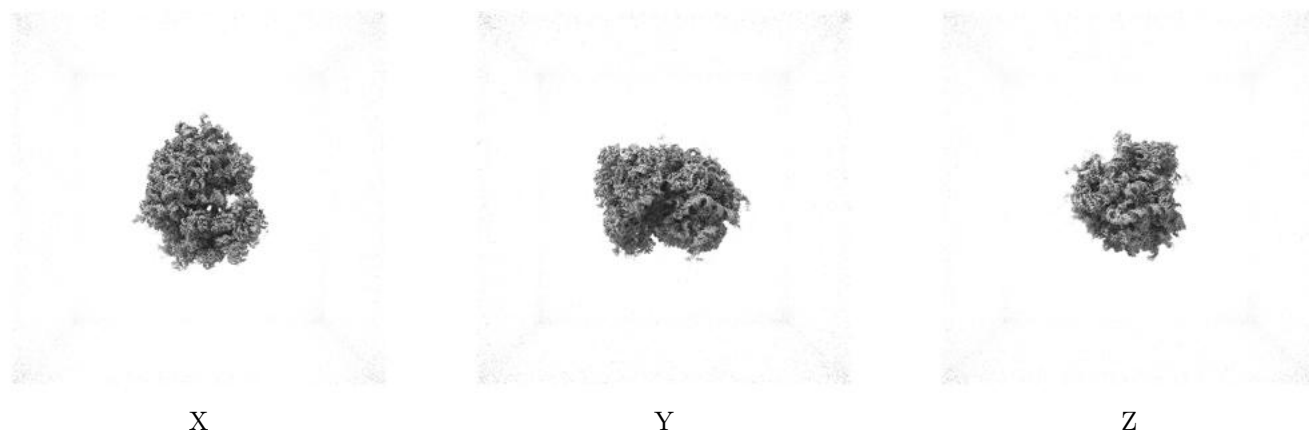
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

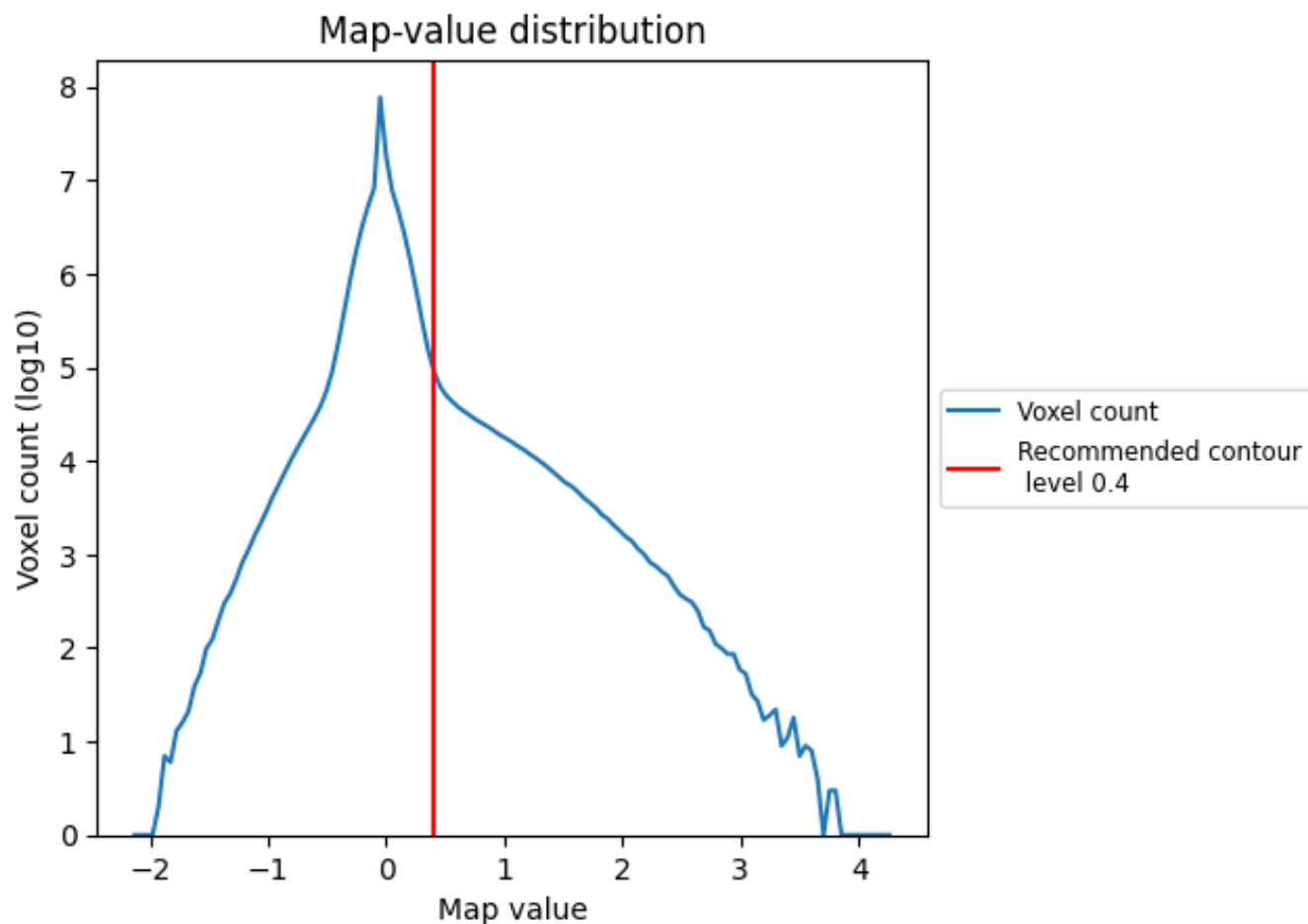
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

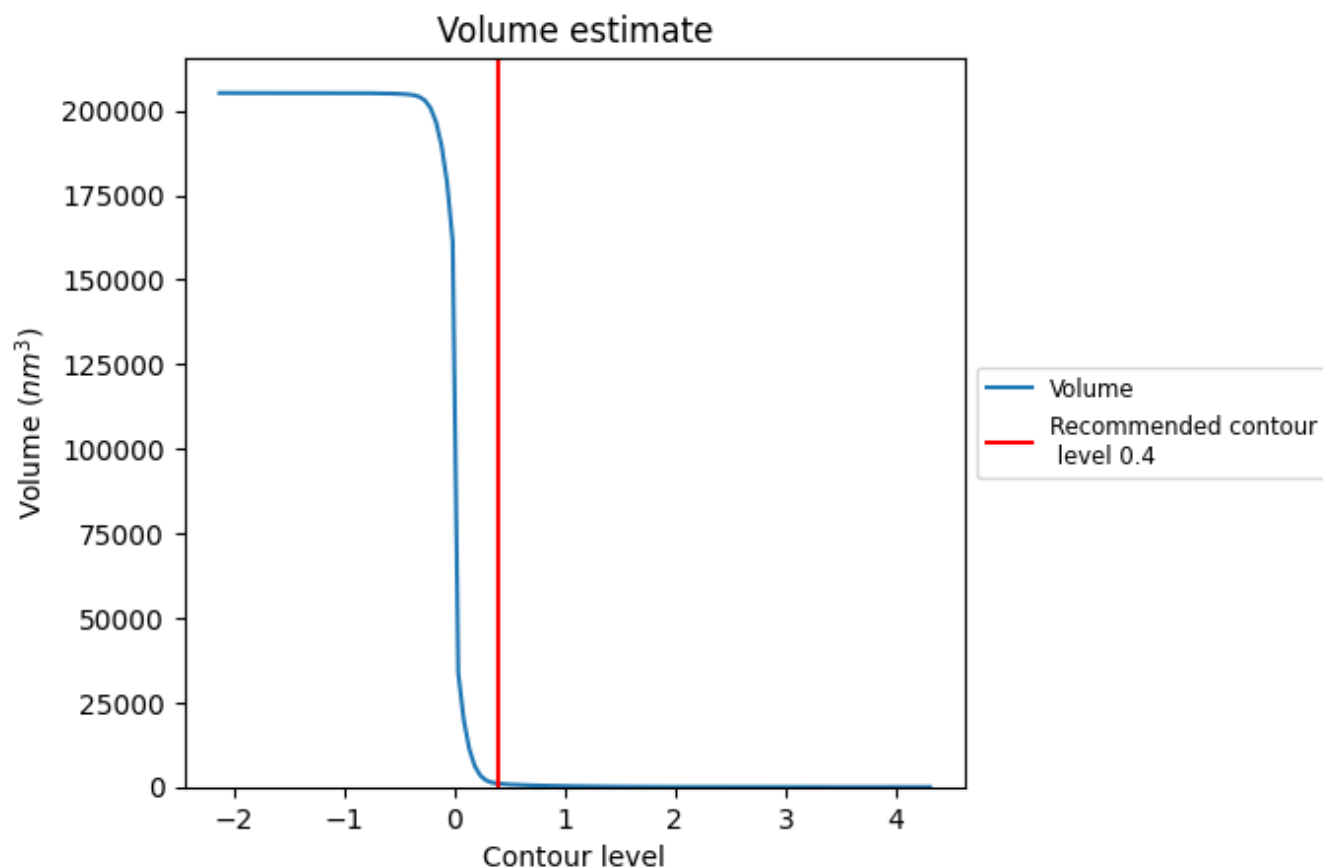
This section contains the results of statistical analysis of the map.

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.

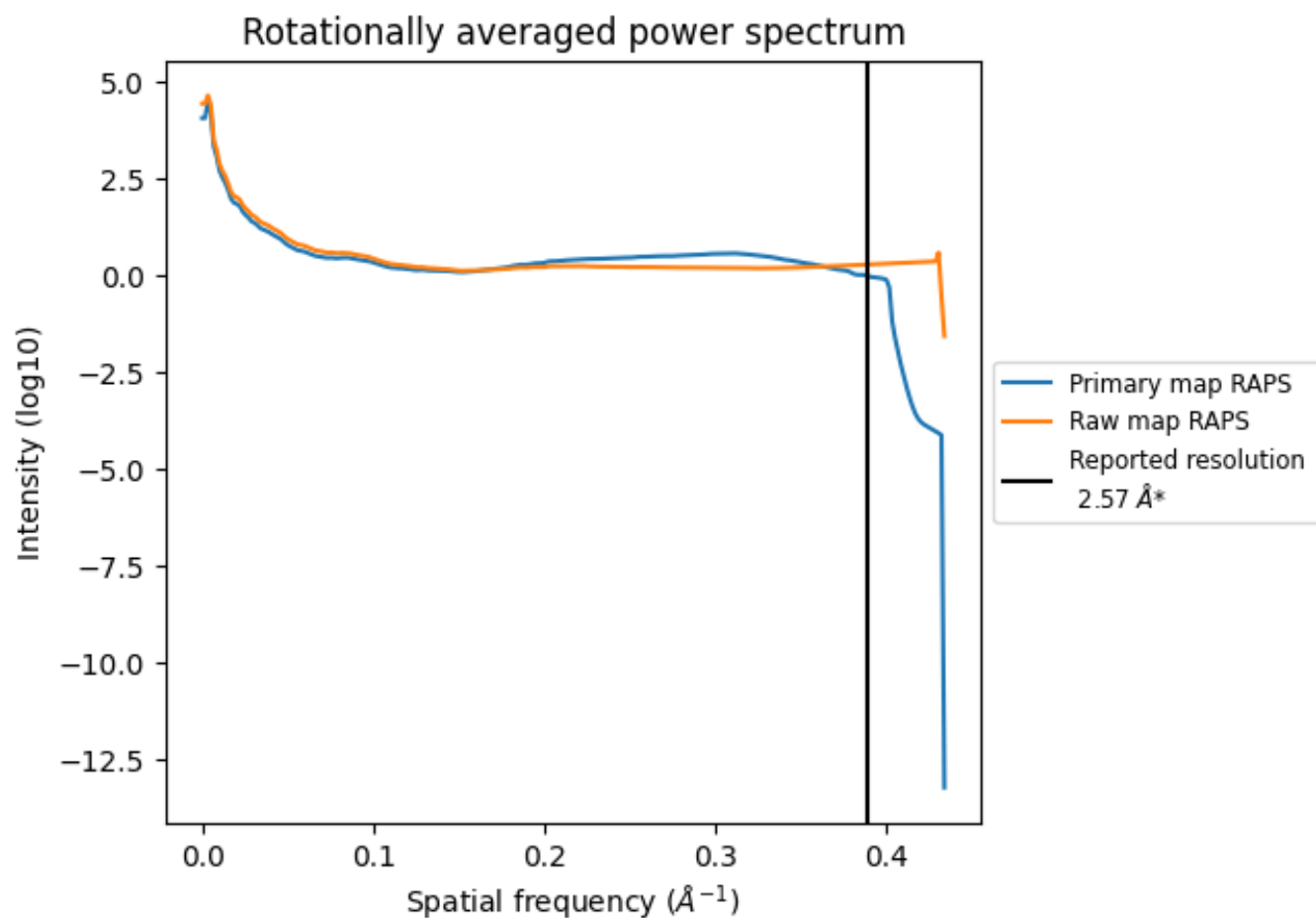
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 986 nm^3 ; this corresponds to an approximate mass of 890 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 ⓘ

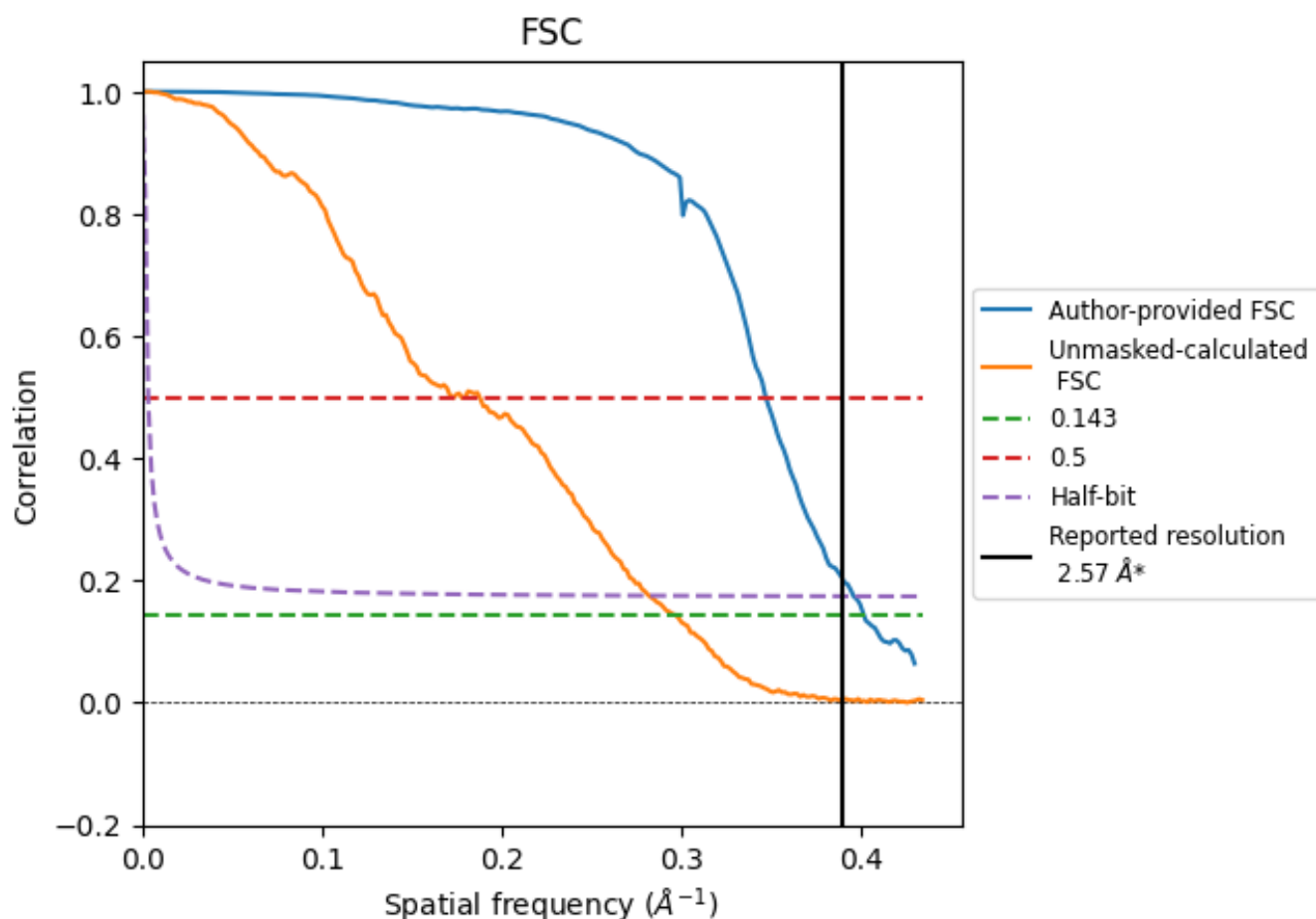


*Reported resolution corresponds to spatial frequency of 0.389 Å⁻¹

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 0.389 Å⁻¹

8.2 Resolution estimates [i](#)

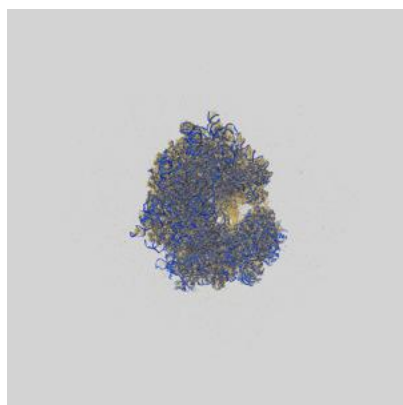
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	2.49	2.88	2.53
Unmasked-calculated*	3.37	5.80	3.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.37 differs from the reported value 2.57 by more than 10 %

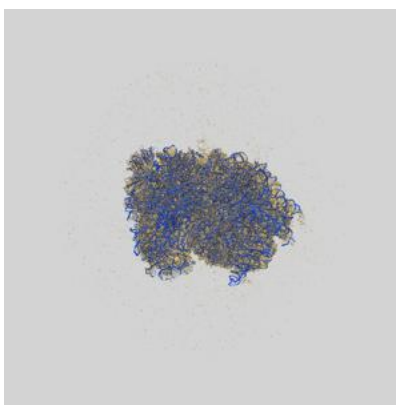
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-58362 and PDB model 31FY. Per-residue inclusion information can be found in section [3](#) on page [20](#).

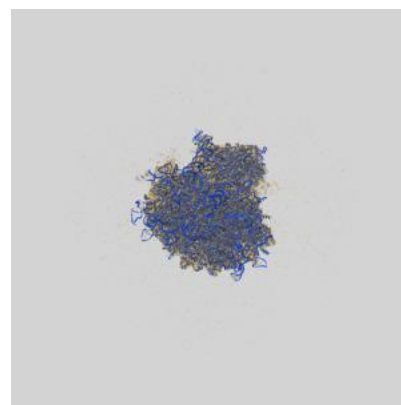
9.1 Map-model overlay [i](#)



X



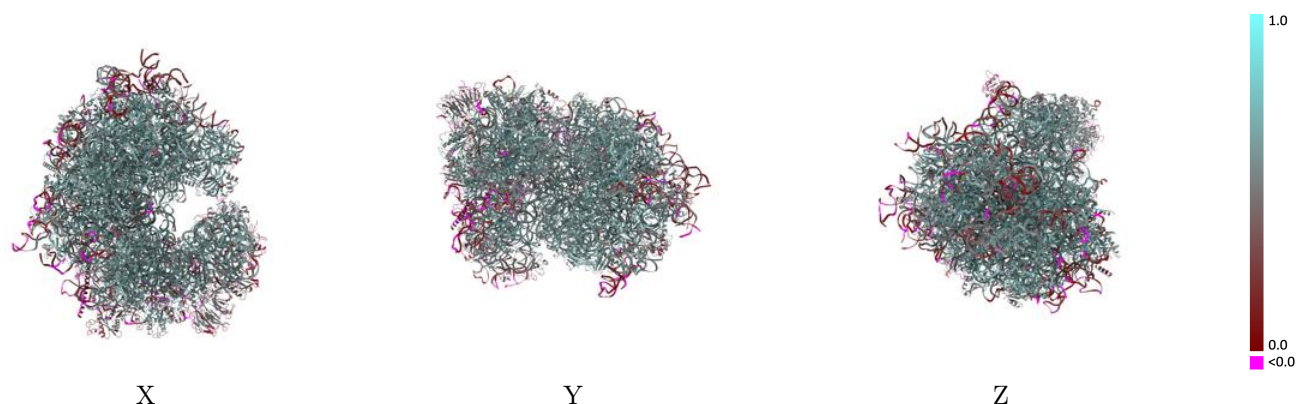
Y



Z

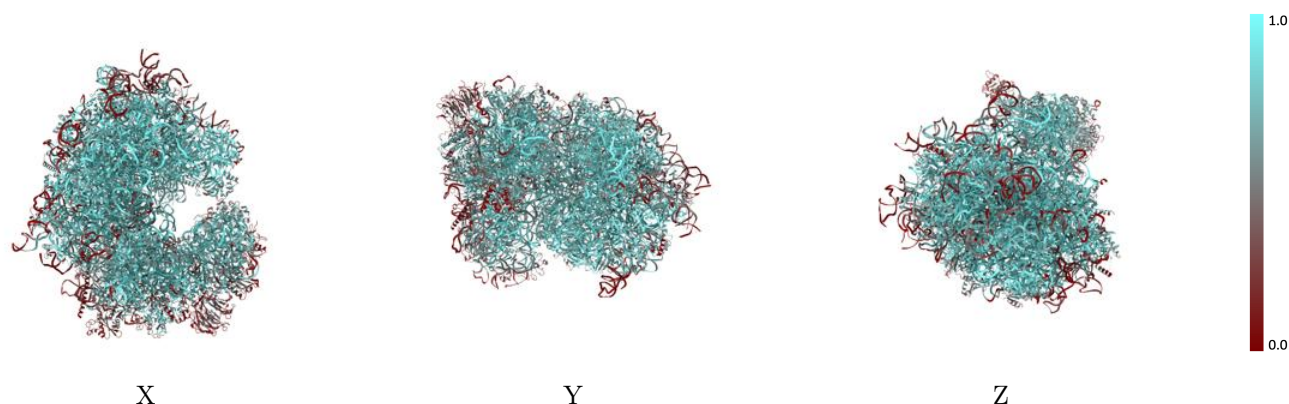
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



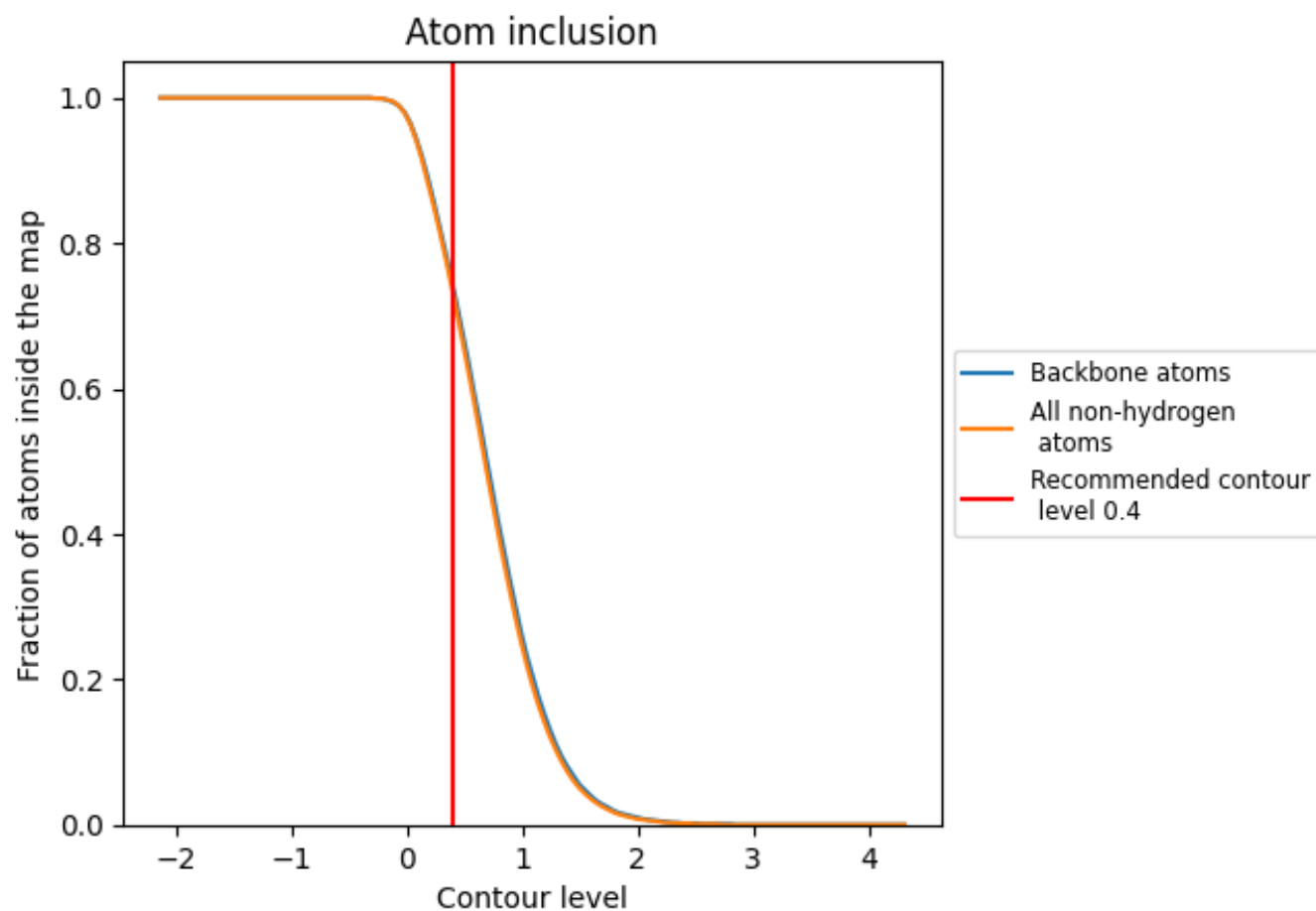
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 73% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7330	 0.5350
AA	 0.4420	 0.3940
AB	 0.7670	 0.5540
AC	 0.7610	 0.5270
AD	 0.7010	 0.5600
AE	 0.5210	 0.4650
AF	 0.5800	 0.4620
AG	 0.6710	 0.5080
AH	 0.4470	 0.4080
AI	 0.6560	 0.5390
AJ	 0.5930	 0.4980
AK	 0.4890	 0.4750
AL	 0.6110	 0.5100
AM	 0.6280	 0.5130
AN	 0.6250	 0.5020
AO	 0.6630	 0.5400
AP	 0.4480	 0.4440
AQ	 0.6540	 0.5610
AR	 0.7260	 0.5360
AS	 0.7620	 0.5830
AT	 0.2840	 0.3480
AU	 0.7320	 0.5710
AV	 0.4290	 0.3990
AW	 0.3300	 0.2040
AX	 0.0610	 0.1830
AY	 0.7090	 0.5660
AZ	 0.7070	 0.5550
Aa	 0.7930	 0.5970
Ab	 0.5350	 0.4390
Ac	 0.4990	 0.4410
Ad	 0.5340	 0.4650
Ae	 0.4270	 0.2130
Af	 0.0790	 0.1570
Ag	 0.3700	 0.3960
Ah	 0.5290	 0.4370



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Chain	Atom inclusion	Q-score
BA	 0.8700	 0.6120
BB	 0.8240	 0.5900
BC	 0.8100	 0.5850
BD	 0.7440	 0.5630
BE	 0.7030	 0.5470
BF	 0.8410	 0.6000
BG	 0.8350	 0.6040
BH	 0.8690	 0.6270
BI	 0.7040	 0.5050
BJ	 0.8500	 0.6020
BK	 0.7740	 0.5810
BL	 0.5300	 0.4700
BM	 0.8430	 0.6140
BN	 0.8190	 0.5960
BO	 0.7870	 0.5730
BP	 0.7850	 0.5690
BQ	 0.7420	 0.5680
BR	 0.8860	 0.6220
BS	 0.6750	 0.5230
BT	 0.7500	 0.5520
BU	 0.7630	 0.5590
BV	 0.8300	 0.6130
BW	 0.8780	 0.6180
BX	 0.7630	 0.5810
BY	 0.7580	 0.5800
BZ	 0.7320	 0.5740
Ba	 0.8770	 0.6110
Bb	 0.5700	 0.5060
Bc	 0.7870	 0.5890
Bd	 0.7770	 0.5870
Be	 0.7200	 0.5870
Bf	 0.7800	 0.5810
Bg	 0.8420	 0.6190
Bh	 0.8360	 0.5980
CA	 0.8270	 0.5990
CB	 0.6830	 0.5470
CC	 0.7490	 0.5790
CD	 0.7650	 0.5820
CE	 0.6830	 0.5170
CF	 0.7440	 0.5460
CG	 0.7560	 0.5510
CH	 0.8950	 0.6340

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Chain	Atom inclusion	Q-score
CI	 0.7830	 0.5400
CJ	 0.9370	 0.6250
CK	 0.8460	 0.5730