



Full wwPDB EM Validation Report ⓘ

Sep 13, 2026 – 09:56 am BST

PDB ID : 31FX / pdb_000031fx
EMDB ID : EMD-58361
Title : Mouse 80S ribosome, sgRNA control
Authors : Rabl, J.; Valdivia Francia, F.; Sendoel, A.
Deposited on : 2026-06-02
Resolution : 2.54 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

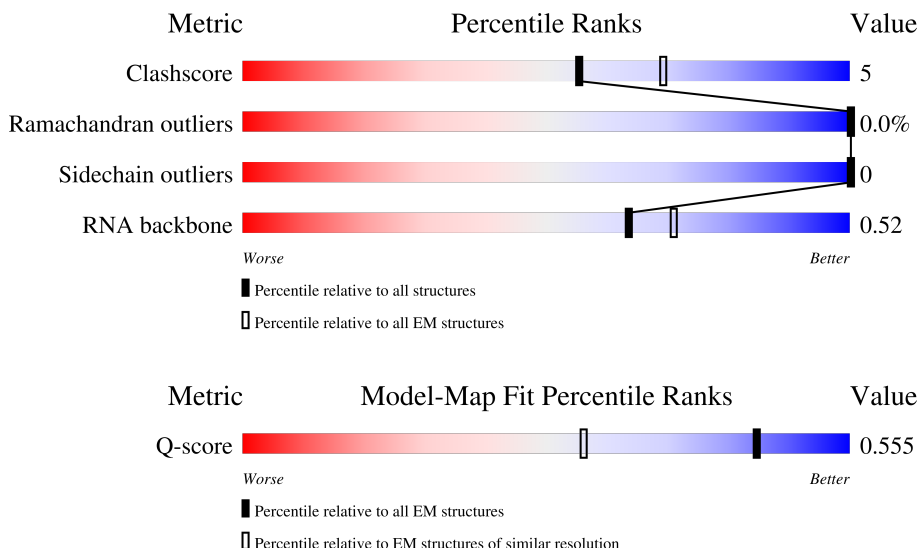
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.54 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	7403 (2.04 - 3.04)

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	51% 61% 32% 7%
2	AB	56	12% 77% 20% •
3	AC	1871	17% 58% 29% • 9%

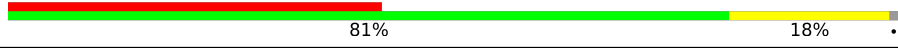
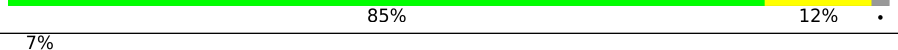
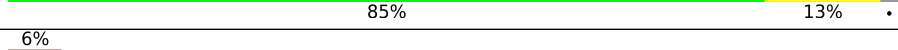
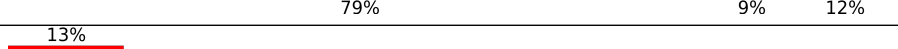
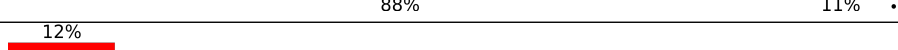
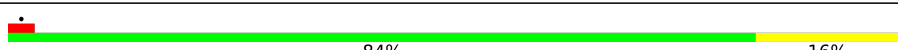
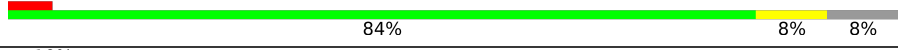
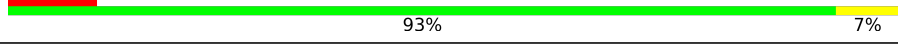
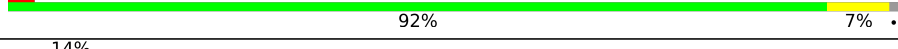
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Mol	Chain	Length	Quality of chain
4	AE	243	
5	AH	135	
6	AJ	204	
7	AK	165	
8	AL	145	
9	AM	146	
10	AN	152	
11	AO	145	
12	AP	119	
13	AT	317	
14	AX	132	
15	Ac	125	
16	Af	156	
17	AD	264	
18	AF	263	
19	AG	158	
20	AI	295	
21	AQ	83	
22	AR	143	
23	AS	115	
24	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	12% 69% 25% 5%

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 363043 atoms, of which 154658 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
			3043	934	1548	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

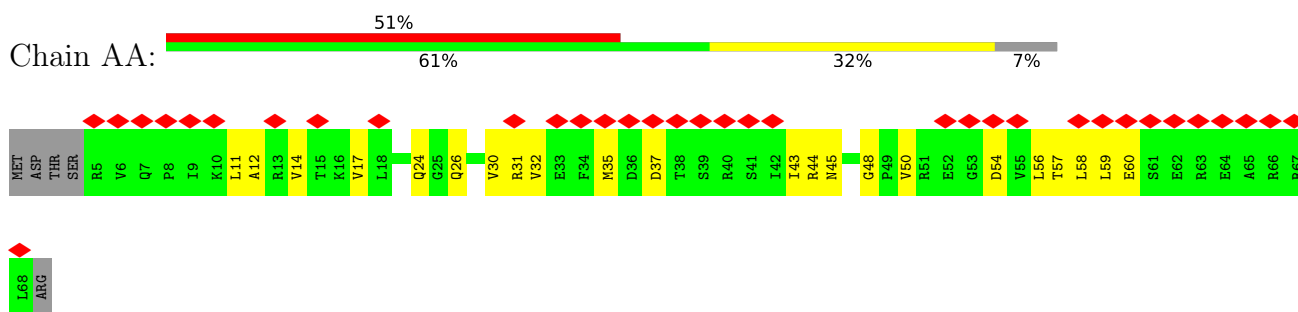
- Molecule 81 is water.

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

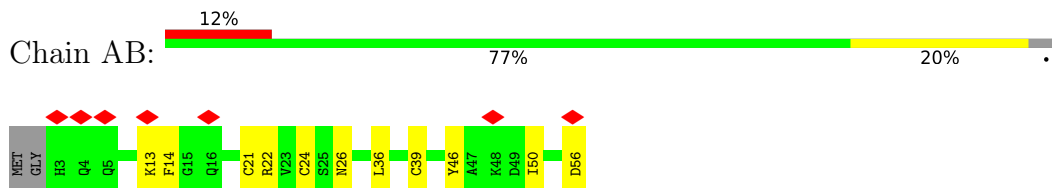
3 Residue-property plots [i](#)

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.

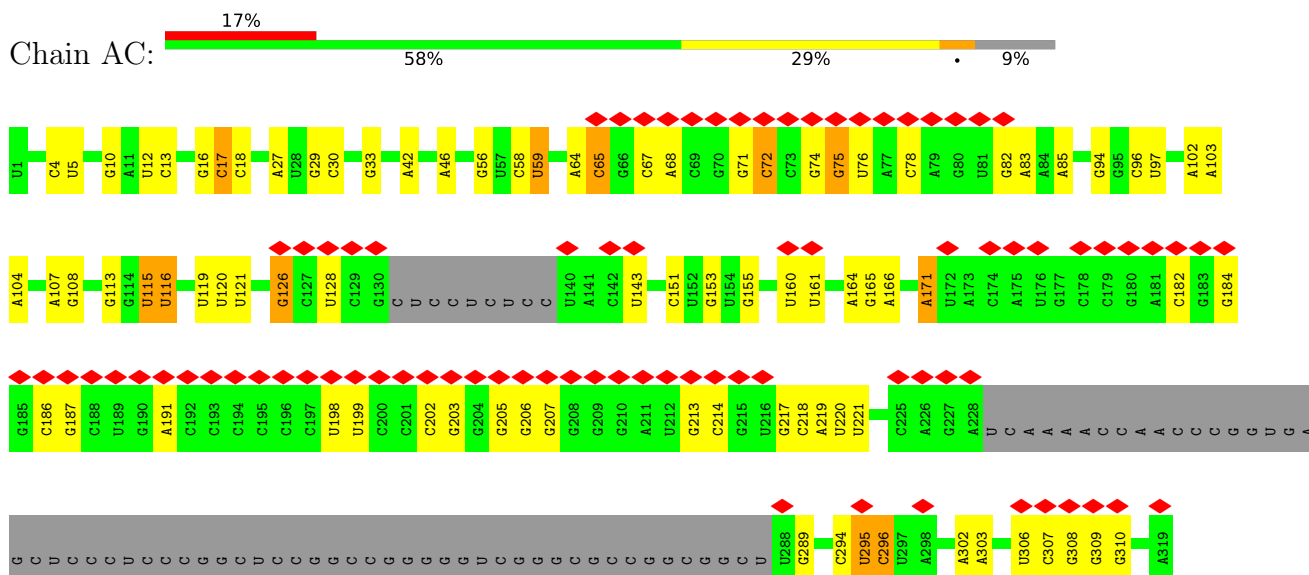
- Molecule 1: Small ribosomal subunit protein eS28



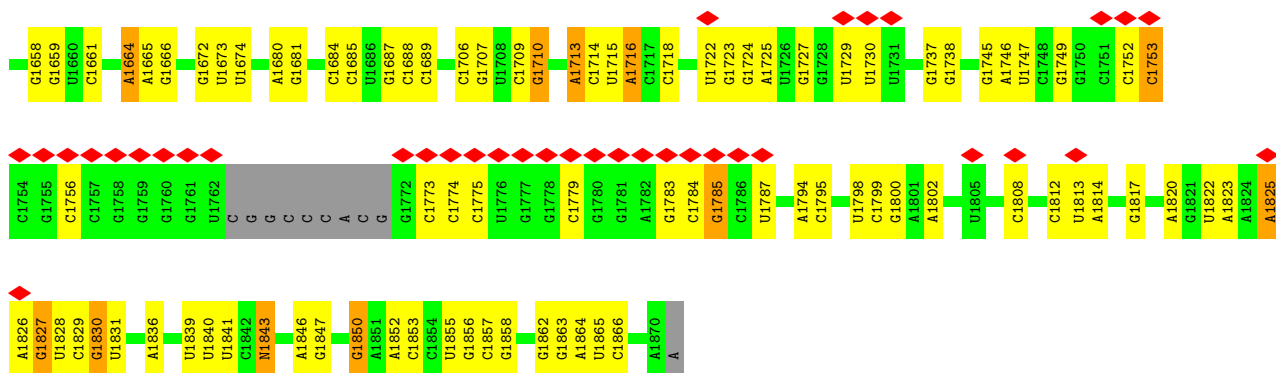
- Molecule 2: Small ribosomal subunit protein uS14



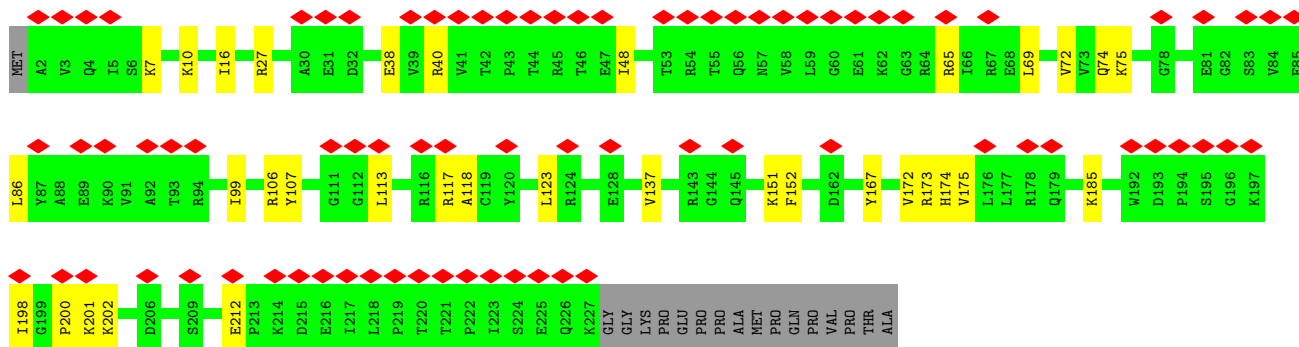
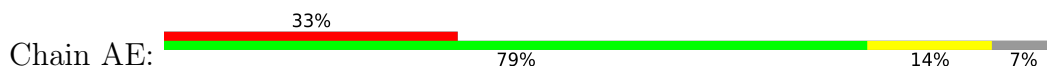
- Molecule 3: 18S rRNA



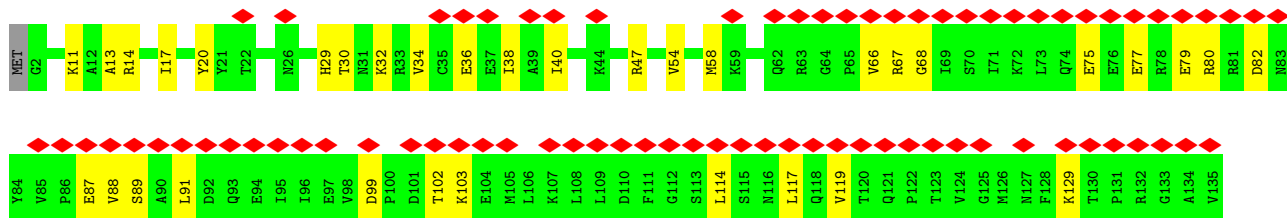
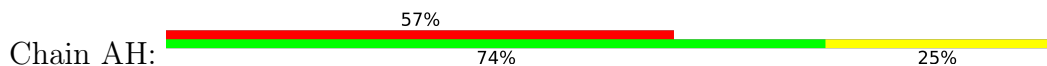




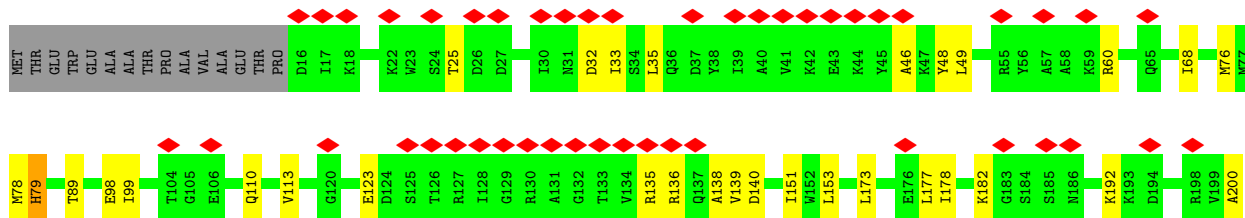
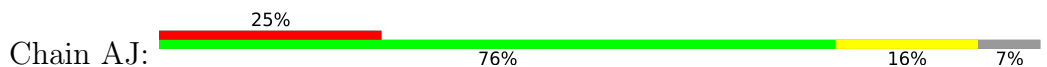
- Molecule 4: Small ribosomal subunit protein uS3



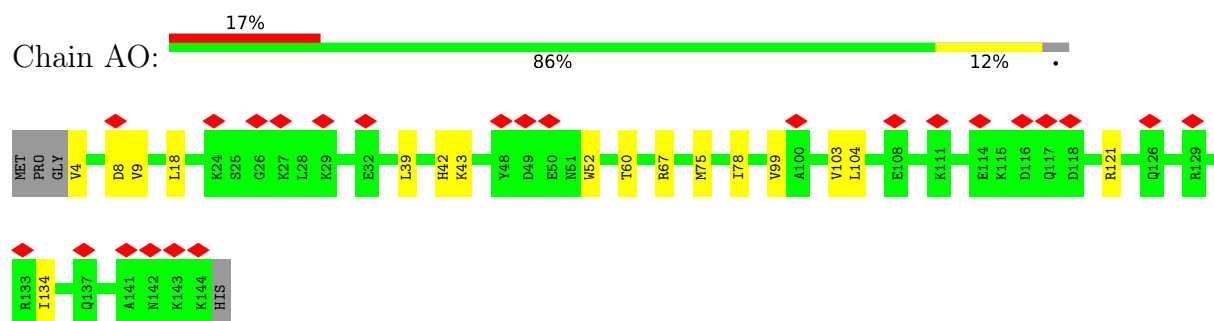
- Molecule 5: Small ribosomal subunit protein eS17



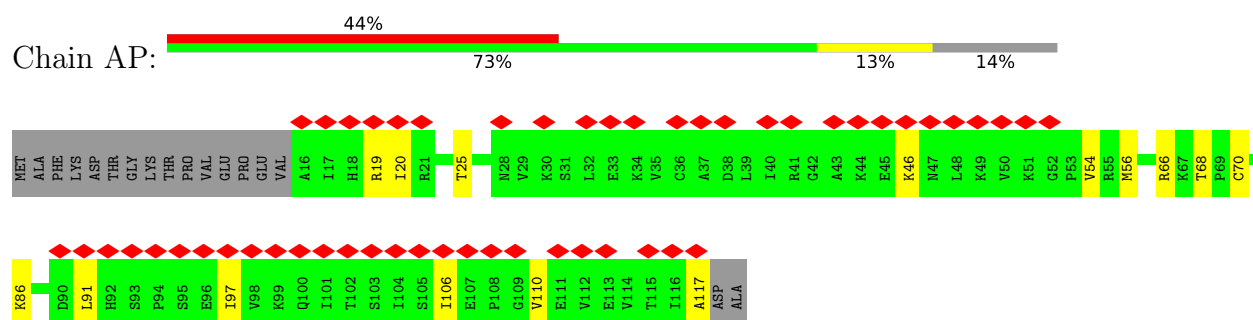
- Molecule 6: Small ribosomal subunit protein uS7



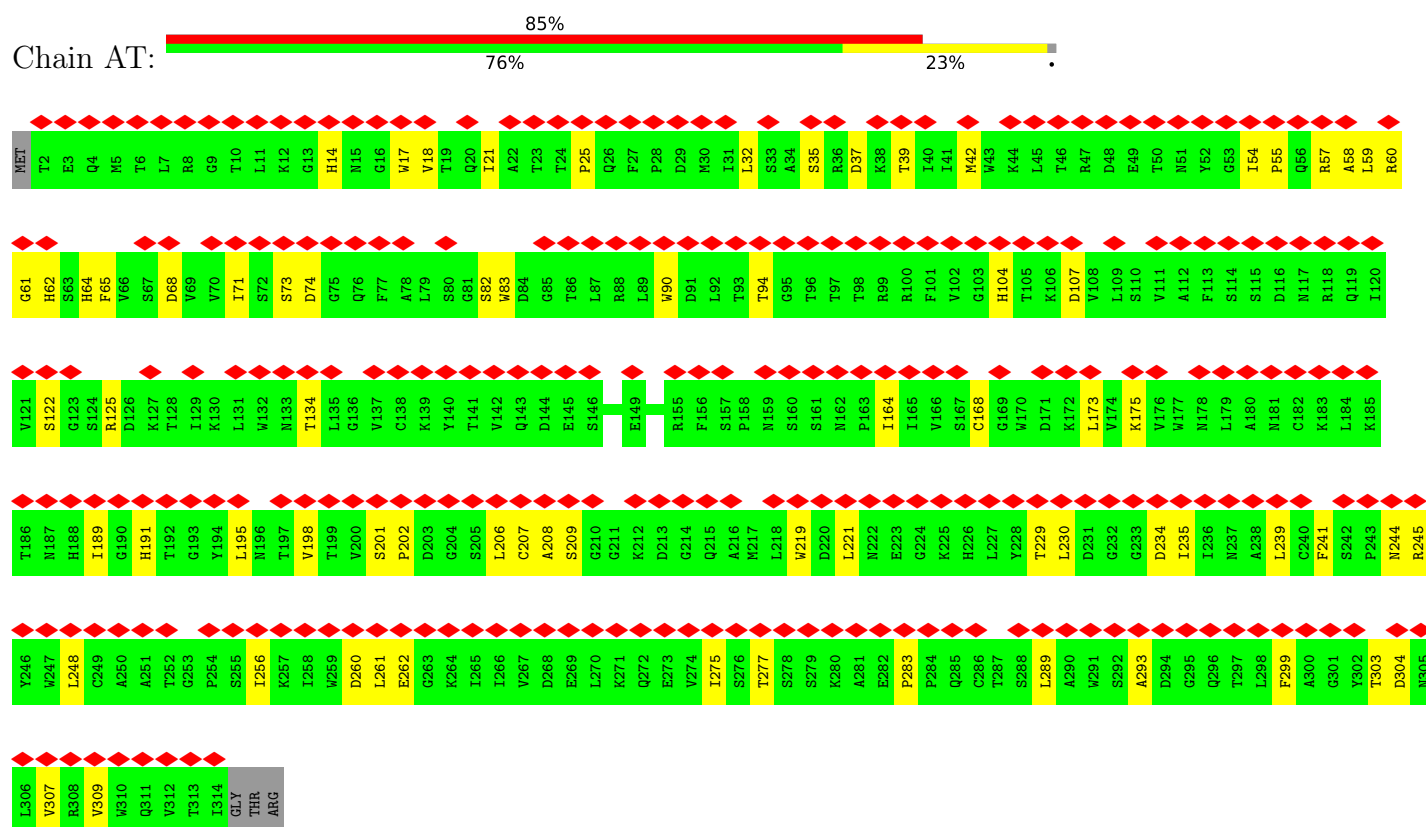
- Molecule 11: Small ribosomal subunit protein eS19



- Molecule 12: Small ribosomal subunit protein uS10



- Molecule 13: Small ribosomal subunit protein RACK1



- Molecule 14: Small ribosomal subunit protein eS12

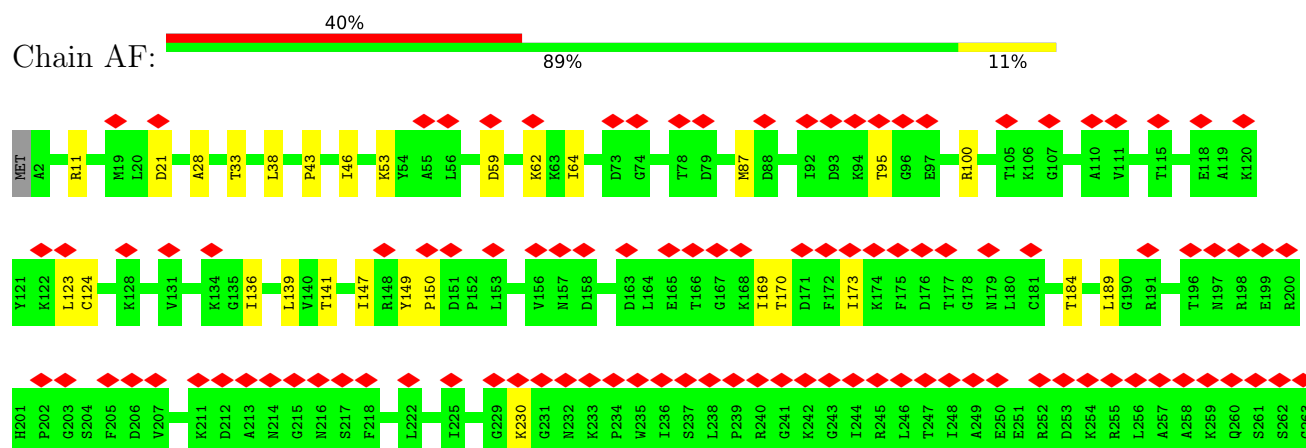
Lys	ASP	VAL	ILE	GLU	GLU	Tyr	PHE	CYS	Lys	Lys																																																	
V61	V62	K63	L64	V65	E66	A67	L68	C69	A70	H71	H72	Q73	I74	N75	L76	I77	K78	V79	D80	H81	H82	K83	K84	L85	G86	E87	H88	V89	GLY	LEU	CYS	LYS	ILE	ASP	ARG	GLU	GLY	LYS	PRO	ARG	LYS	VAL	VAL	GLY	C106	S107	C108	V109	V110	V111	K112	D113	TYR	GLY	LYS	GLU	SER	GLN	ALA
MET	ALA	GLU	GLY	ILE	ALA	ALA	GLY	GLY	V11	M12	D13	V14	N15	T16	A17	L18	Q19	E20	V21	L22	K23	T24	A25	L26	I27	H28	D29	G30	L31	A32	R33	G34	I35	R36	E37	A38	A39	K40	A41	L42	D43	K44	R45	Q46	A47	H48	L49	C50	V51	L52	A53	S54	N55	C56	D57	E58	P59	M60	

P63	P64	P65	P66	P67	P68	P69	P70	P71	P72	P73	P74	P75	P76	P77	P78	P79	P80	P81	P82	P83	P84	P85	P86	P87	P88	P89	P90	P91	P92	P93	P94	P95	P96	P97	P98	P99	P100	P101	P102	P103	P104	P105	P106	P107	P108	P109	P110	P111	P112	P113	P114	P115	P116	P117	P118	P119	P120	P121	P122	P123	P124	P125	P126	P127	P128	P129	P130	P131	P132	P133	P134	P135	P136	P137	P138	P139	P140	P141	P142	P143	P144	P145	P146	P147	P148	P149	P150	P151	P152	P153	P154	P155	P156	P157	P158	P159	P160	P161	P162	P163	P164	P165	P166	P167	P168	P169	P170	P171	P172	P173	P174	P175	P176	P177	P178	P179	P180	P181	P182	P183	P184	P185	P186	P187	P188	P189	P190	P191	P192	P193	P194	P195	P196	P197	P198	P199	P200	P201	P202	P203	P204	P205	P206	P207	P208	P209	P210	P211	P212	P213	P214	P215	P216	P217	P218	P219	P220	P221	P222	P223	P224	P225	P226	P227	P228	P229	P230	P231	P232	P233	P234	P235	P236	P237	P238	P239	P240	P241	P242	P243	P244	P245	P246	P247	P248	P249	P250	P251	P252	P253	P254	P255	P256	P257	P258	P259	P260	P261	P262	P263	P264	P265	P266	P267	P268	P269	P270	P271	P272	P273	P274	P275	P276	P277	P278	P279	P280	P281	P282	P283	P284	P285	P286	P287	P288	P289	P290	P291	P292	P293	P294	P295	P296	P297	P298	P299	P300	P301	P302	P303	P304	P305	P306	P307	P308	P309	P310	P311	P312	P313	P314	P315	P316	P317	P318	P319	P320	P321	P322	P323	P324	P325	P326	P327	P328	P329	P330	P331	P332	P333	P334	P335	P336	P337	P338	P339	P340	P341	P342	P343	P344	P345	P346	P347	P348	P349	P350	P351	P352	P353	P354	P355	P356	P357	P358	P359	P360	P361	P362	P363	P364	P365	P366	P367	P368	P369	P370	P371	P372	P373	P374	P375	P376	P377	P378	P379	P380	P381	P382	P383	P384	P385	P386	P387	P388	P389	P390	P391	P392	P393	P394	P395	P396	P397	P398	P399	P400	P401	P402	P403	P404	P405	P406	P407	P408	P409	P410	P411	P412	P413	P414	P415	P416	P417	P418	P419	P420	P421	P422	P423	P424	P425	P426	P427	P428	P429	P430	P431	P432	P433	P434	P435	P436	P437	P438	P439	P440	P441	P442	P443	P444	P445	P446	P447	P448	P449	P450	P451	P452	P453	P454	P455	P456	P457	P458	P459	P460	P461	P462	P463	P464	P465	P466	P467	P468	P469	P470	P471	P472	P473	P474	P475	P476	P477	P478	P479	P480	P481	P482	P483	P484	P485	P486	P487	P488	P489	P490	P491	P492	P493	P494	P495	P496	P497	P498	P499	P500	P501	P502	P503	P504	P505	P506	P507	P508	P509	P510	P511	P512	P513	P514	P515	P516	P517	P518	P519	P520	P521	P522	P523	P524	P525	P526	P527	P528	P529	P530	P531	P532	P533	P534	P535	P536	P537	P538	P539	P540	P541	P542	P543	P544	P545	P546	P547	P548	P549	P550	P551	P552	P553	P554	P555	P556	P557	P558	P559	P560	P561	P562	P563	P564	P565	P566	P567	P568	P569	P570	P571	P572	P573	P574	P575	P576	P577	P57
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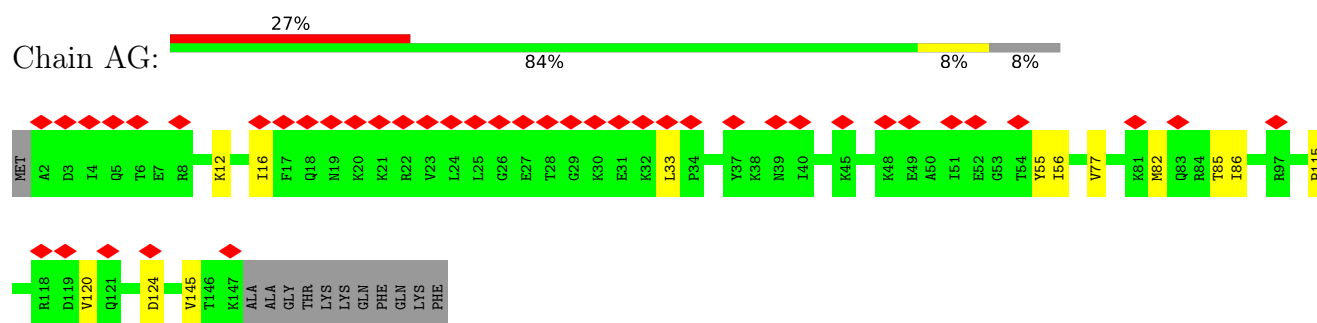
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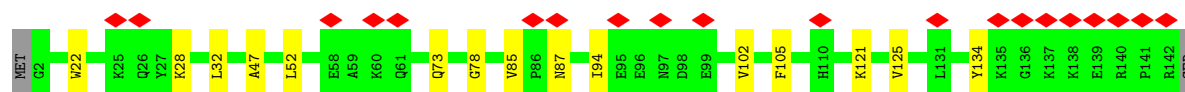
Protein	Position	Residue	Frequency	Conservation	Annotations
Protein A	1	GLY	0.00	0.00	
	2	SER	0.00	0.00	
	3	SER	0.00	0.00	
	4	GLY	0.00	0.00	
	5	LYS	0.00	0.00	
	6	ALA	0.00	0.00	
	7	ALA	0.00	0.00	
	8	GLY	0.00	0.00	
	9	ASP	0.00	0.00	
	10	GLU	0.00	0.00	
Protein B	11	THR	0.00	0.00	
	12	GLY	0.00	0.00	
	13	GLY	0.00	0.00	
	14	LYS	0.00	0.00	
	15	LYS	0.00	0.00	
	16	GLY	0.00	0.00	
	17	ALA	0.00	0.00	
	18	LYS	0.00	0.00	
	19	LYS	0.00	0.00	
	20	LYS	0.00	0.00	
Protein C	21	VAL	0.00	0.00	
	22	GLY	0.00	0.00	
	23	PRO	0.00	0.00	
	24	VAL	0.00	0.00	
	25	GLN	0.00	0.00	
	26	GLU	0.00	0.00	
	27	SER	0.00	0.00	
	28	VAL	0.00	0.00	
	29	GLY	0.00	0.00	
	30	GLY	0.00	0.00	
Protein D	31	ASP	0.00	0.00	
	32	ASP	0.00	0.00	
	33	TYR	0.00	0.00	
	34	GLU	0.00	0.00	
	35	PRO	0.00	0.00	
	36	PRO	0.00	0.00	
	37	VAL	0.00	0.00	
	38	GLN	0.00	0.00	
	39	GLU	0.00	0.00	
	40	SER	0.00	0.00	
Protein E	41	VAL	0.00	0.00	
	42	GLY	0.00	0.00	
	43	GLY	0.00	0.00	
	44	LYS	0.00	0.00	
	45	LYS	0.00	0.00	
	46	GLY	0.00	0.00	
	47	ALA	0.00	0.00	
	48	LYS	0.00	0.00	
	49	LYS	0.00	0.00	
	50	LYS	0.00	0.00	
Protein F	51	VAL	0.00	0.00	
	52	GLY	0.00	0.00	
	53	ASN	0.00	0.00	
	54	LYS	0.00	0.00	
	55	ARG	0.00	0.00	
	56	LEU	0.00	0.00	
	57	THR	0.00	0.00	
	58	LYS	0.00	0.00	
	59	GLY	0.00	0.00	
	60	GLY	0.00	0.00	
Protein G	61	LYS	0.00	0.00	
	62	LYS	0.00	0.00	
	63	VAL	0.00	0.00	
	64	VAL	0.00	0.00	
	65	GLY	0.00	0.00	
	66	GLY	0.00	0.00	
	67	LYS	0.00	0.00	
	68	LYS	0.00	0.00	
	69	LYS	0.00	0.00	
	70	LYS	0.00	0.00	
Protein H	71	VAL	0.00	0.00	
	72	VAL	0.00	0.00	
	73	GLY	0.00	0.00	
	74	GLY	0.00	0.00	
	75	ASN	0.00	0.00	
	76	LYS	0.00	0.00	
	77	LYS	0.00	0.00	
	78	ARG	0.00	0.00	
	79	LEU	0.00	0.00	
	80	THR	0.00	0.00	
Protein I	81	LYS	0.00	0.00	
	82	LYS	0.00	0.00	
	83	GLY			

- Molecule 18: Small ribosomal subunit protein eS4

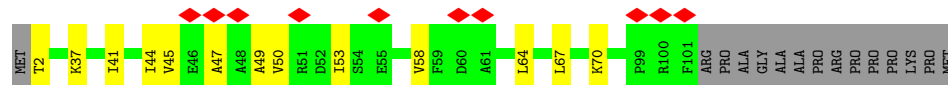
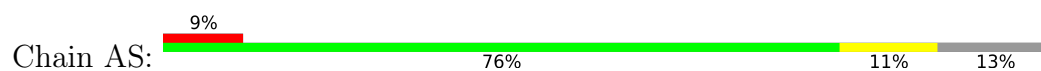


- Molecule 19: Small ribosomal subunit protein uS17

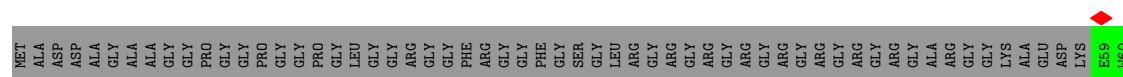




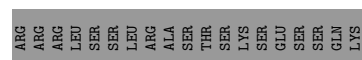
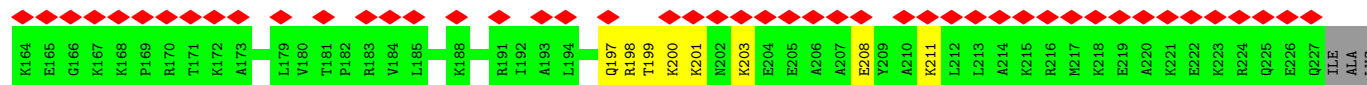
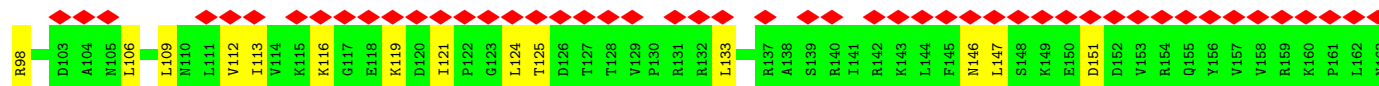
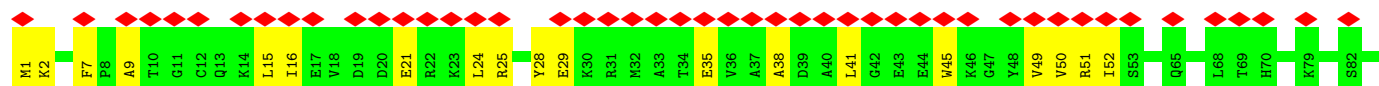
- Molecule 23: Small ribosomal subunit protein eS26



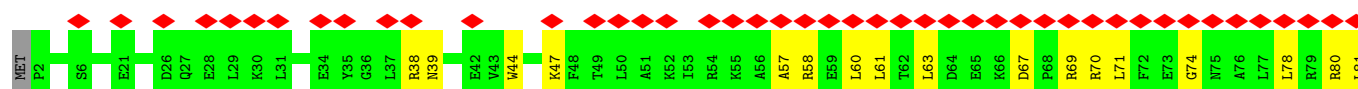
- Molecule 24: Small ribosomal subunit protein uS5

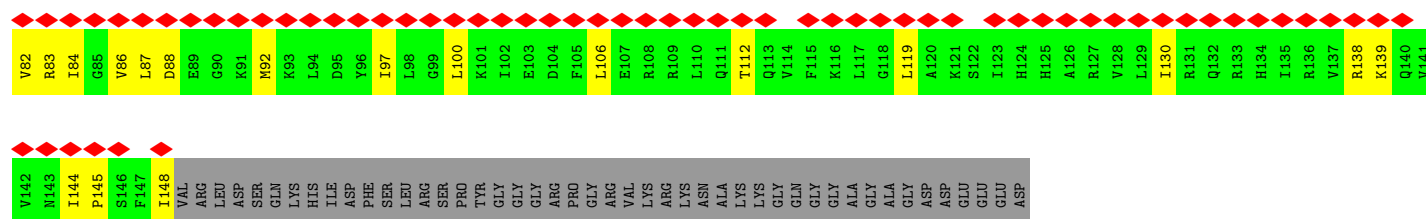


- Molecule 25: Small ribosomal subunit protein eS6

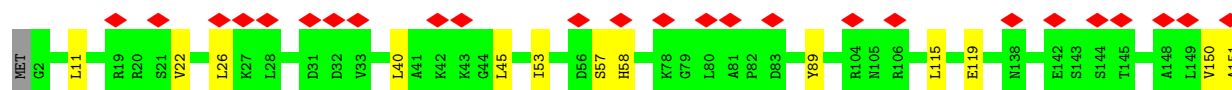
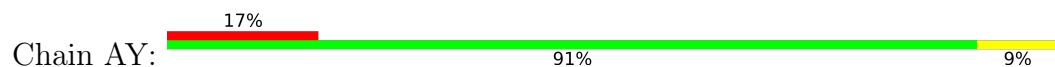


- Molecule 26: Small ribosomal subunit protein uS4

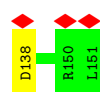
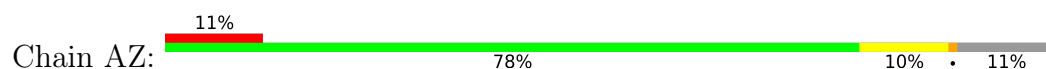




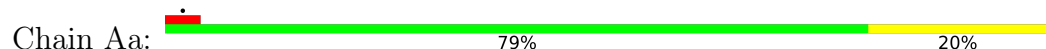
- Molecule 27: Small ribosomal subunit protein uS15



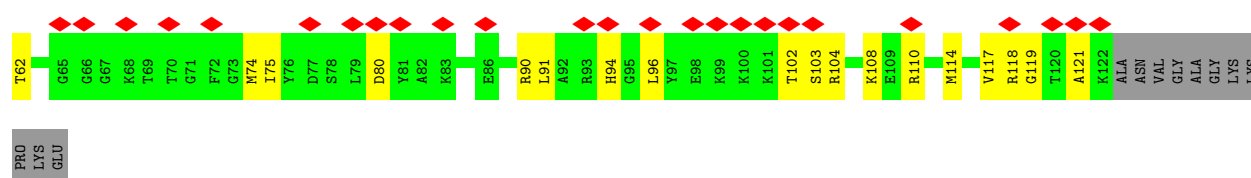
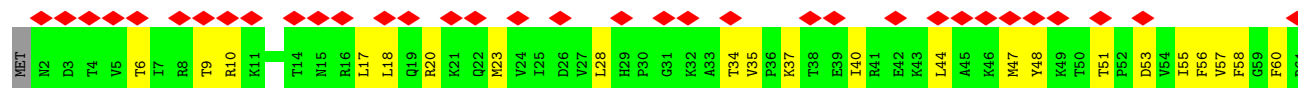
- Molecule 28: Small ribosomal subunit protein uS11



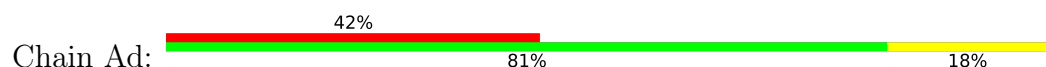
- Molecule 29: Small ribosomal subunit protein uS8

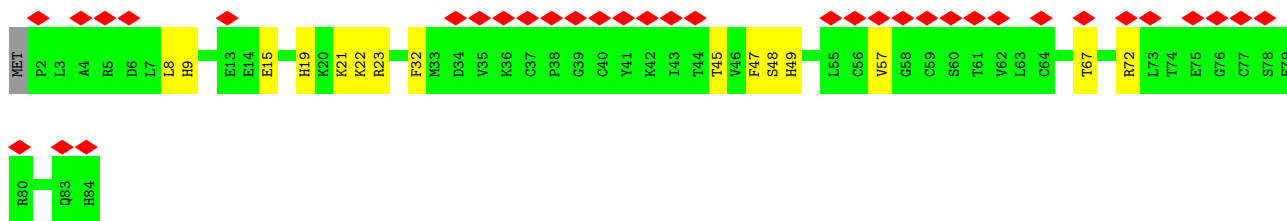


- Molecule 30: Small ribosomal subunit protein eS24

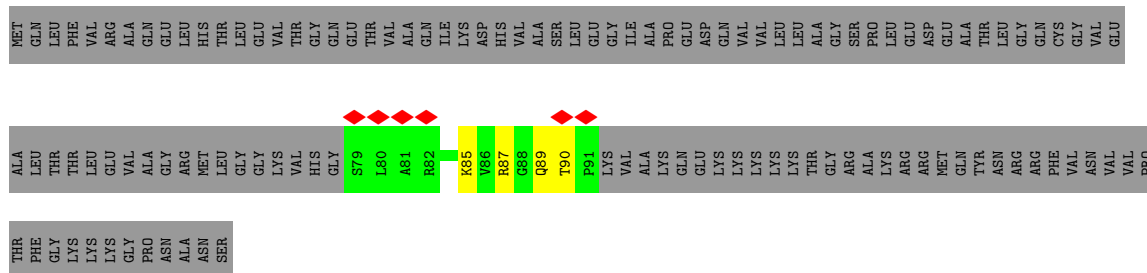


- Molecule 31: Small ribosomal subunit protein eS27-like

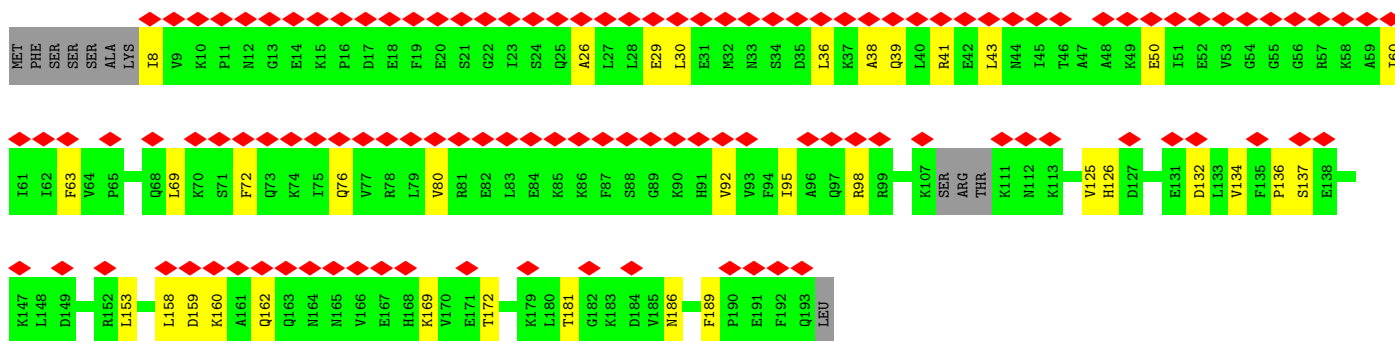
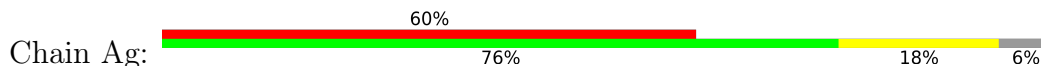




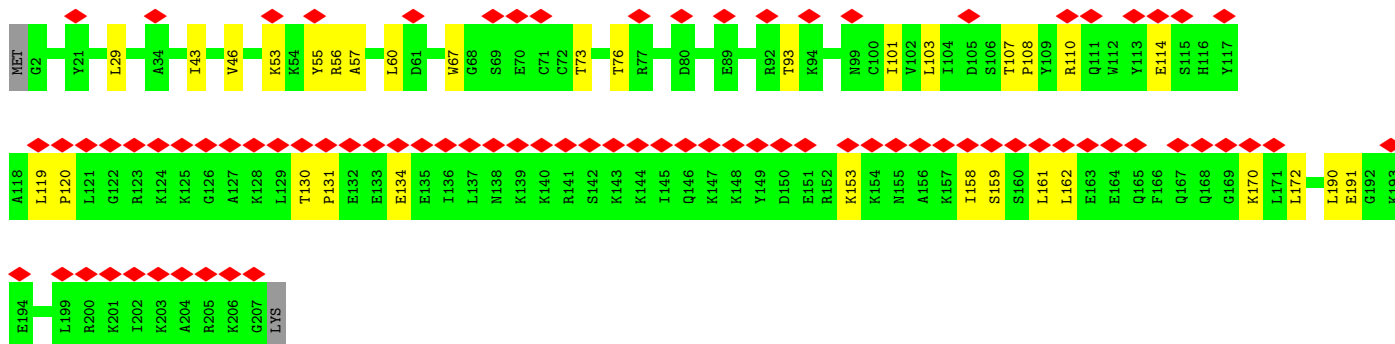
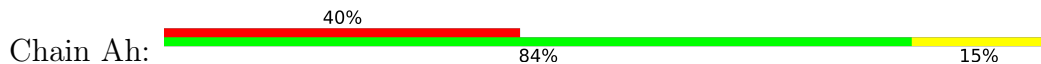
- Molecule 32: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



- Molecule 33: Small ribosomal subunit protein eS7

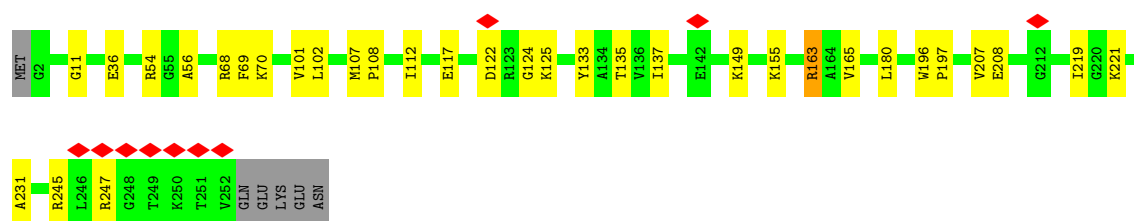


- Molecule 34: Small ribosomal subunit protein eS8



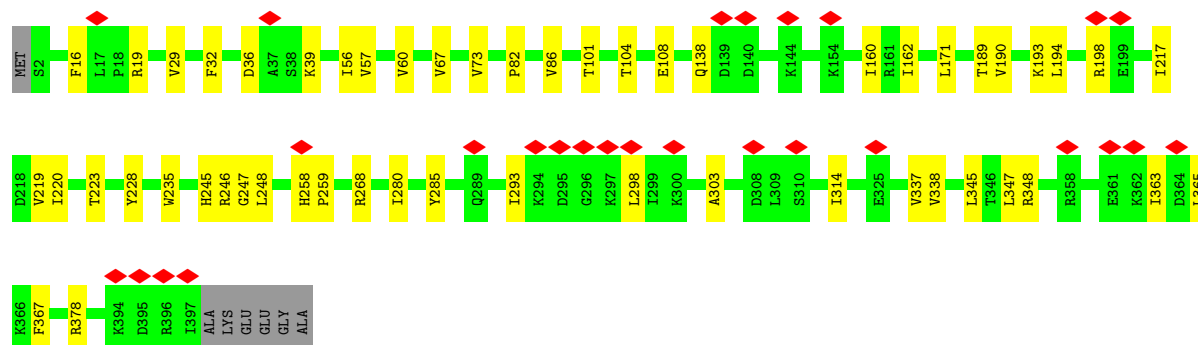
- Molecule 35: Large ribosomal subunit protein uL2

Chain BA: 



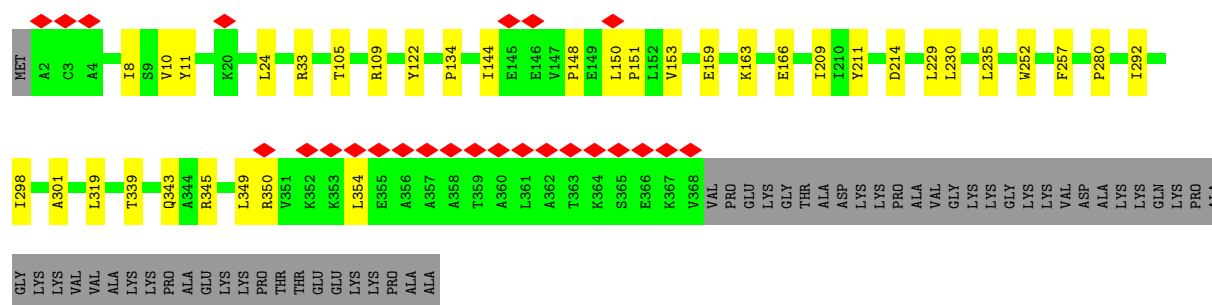
- Molecule 36: Large ribosomal subunit protein uL3

Chain BB: 



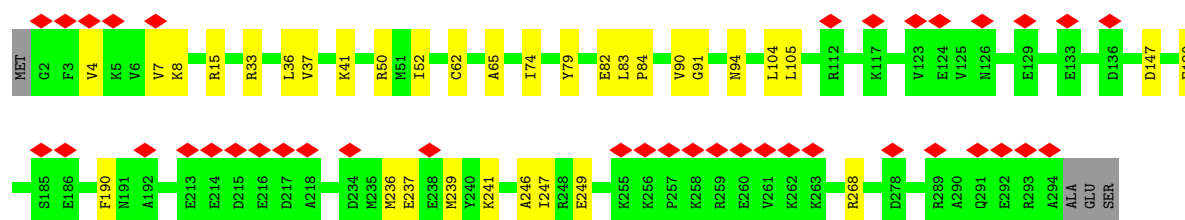
- Molecule 37: Large ribosomal subunit protein uL4

Chain BC: 

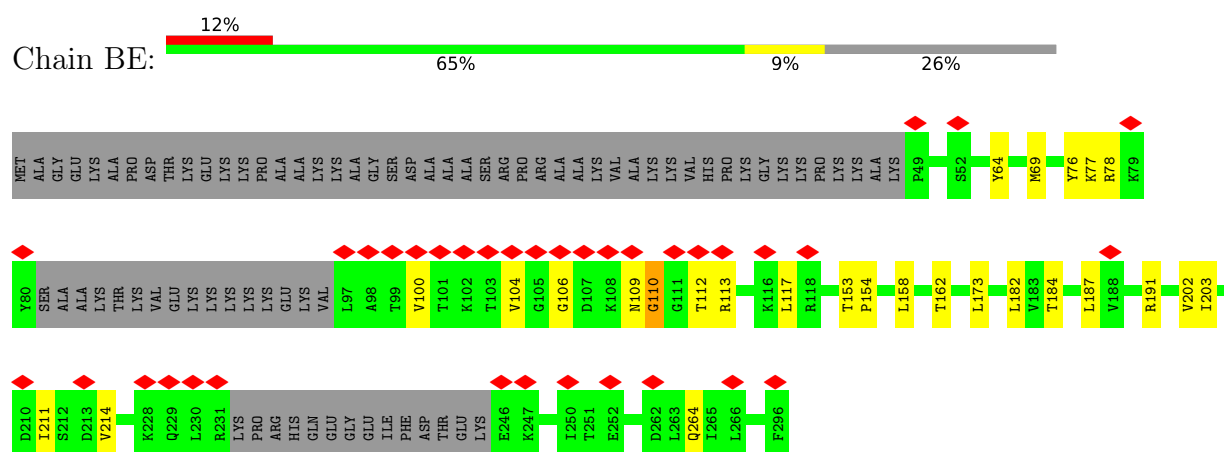


- Molecule 38: Large ribosomal subunit protein uL18

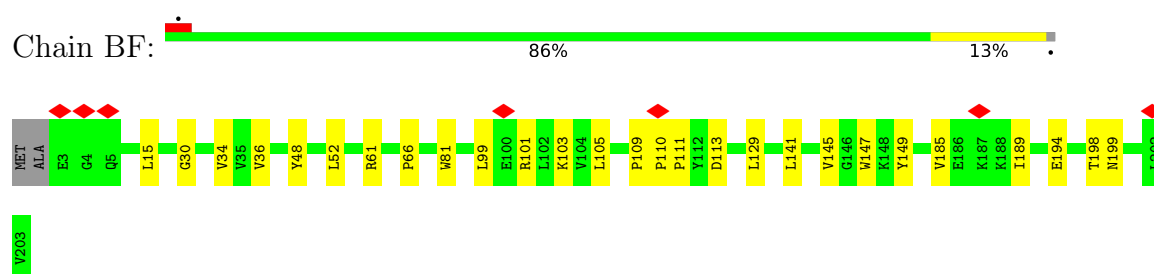
Chain BD: 



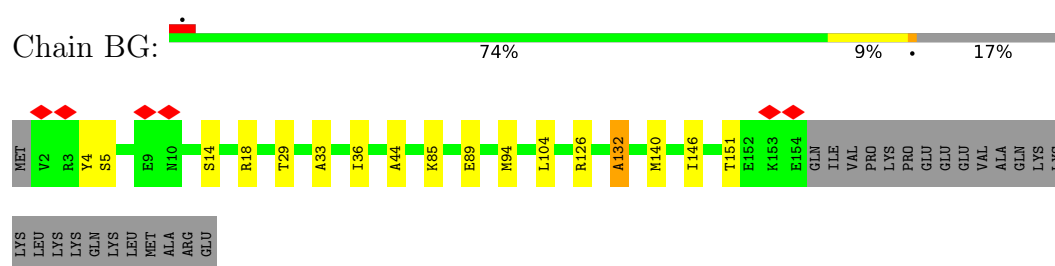
- Molecule 39: Large ribosomal subunit protein eL6



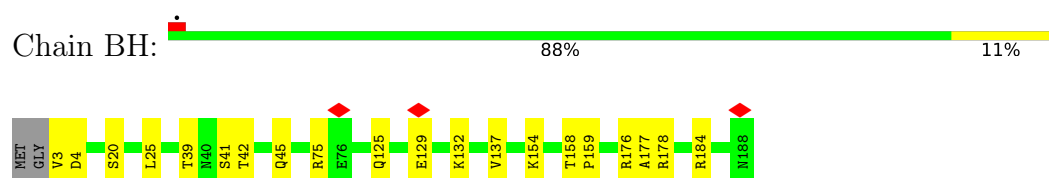
- Molecule 40: Large ribosomal subunit protein uL13



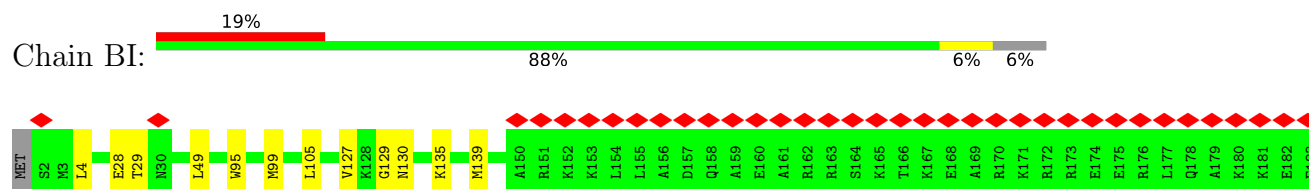
- Molecule 41: Large ribosomal subunit protein uL22

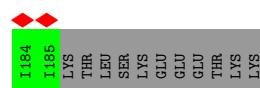


- Molecule 42: Large ribosomal subunit protein eL18

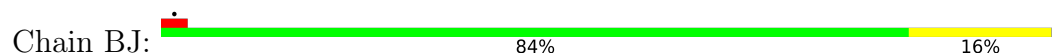


- Molecule 43: Large ribosomal subunit protein eL19

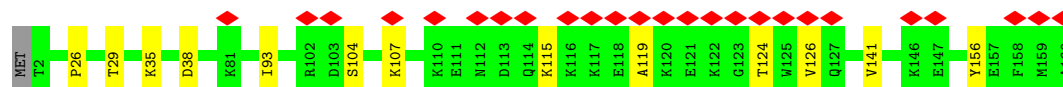




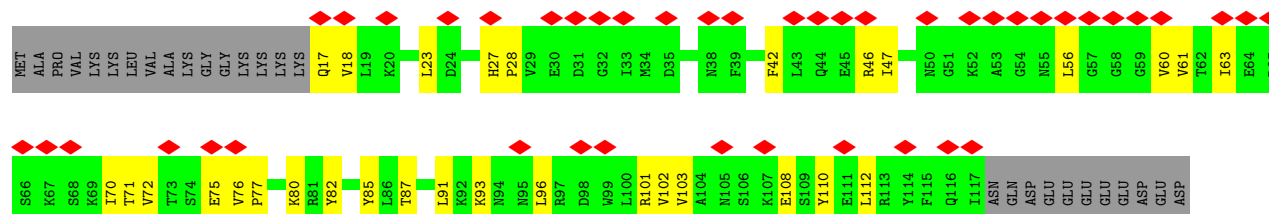
- Molecule 44: Large ribosomal subunit protein eL20



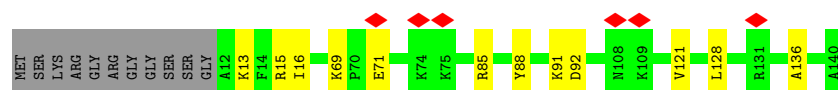
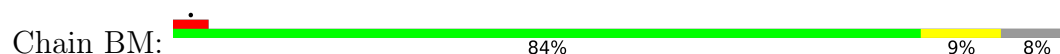
- Molecule 45: Large ribosomal subunit protein eL21



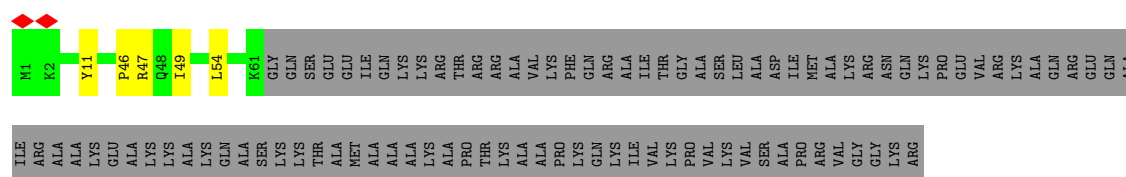
- Molecule 46: Large ribosomal subunit protein eL22



- Molecule 47: Large ribosomal subunit protein uL14

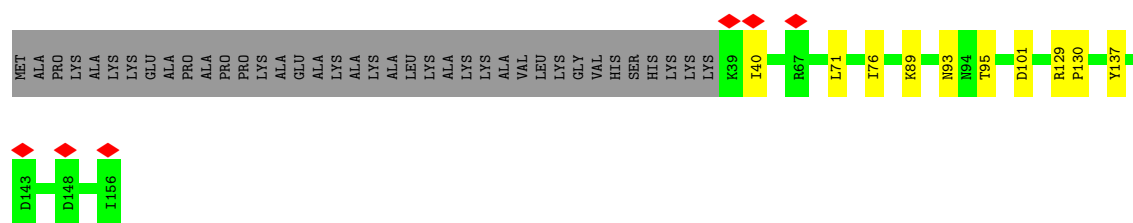


- Molecule 48: Large ribosomal subunit protein eL24



- Molecule 49: Large ribosomal subunit protein uL23

Chain BO: 

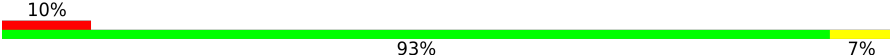


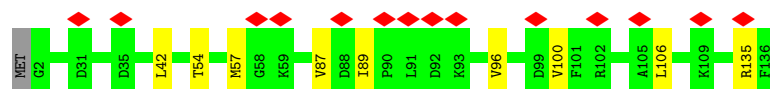
- Molecule 50: Large ribosomal subunit protein uL24

Chain BP: 

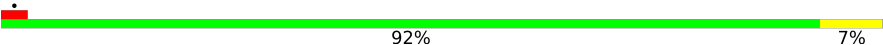


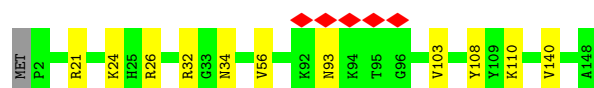
- Molecule 51: Large ribosomal subunit protein eL27

Chain BQ: 



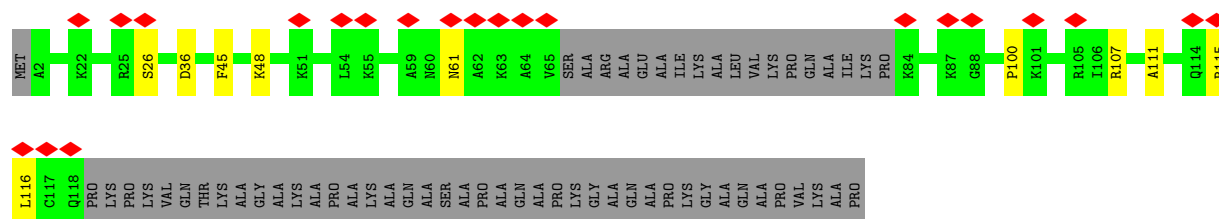
- Molecule 52: Large ribosomal subunit protein uL15

Chain BR: 



- Molecule 53: Large ribosomal subunit protein eL29

Chain BS: 

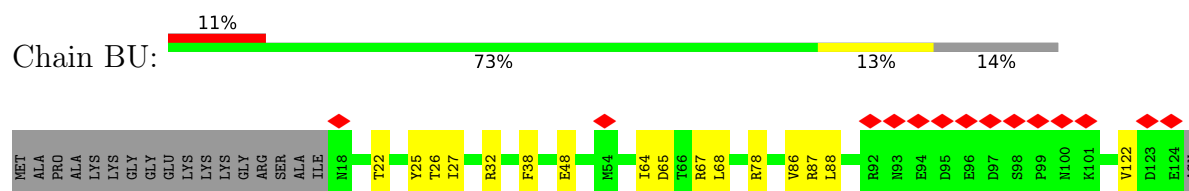


- Molecule 54: Large ribosomal subunit protein eL30

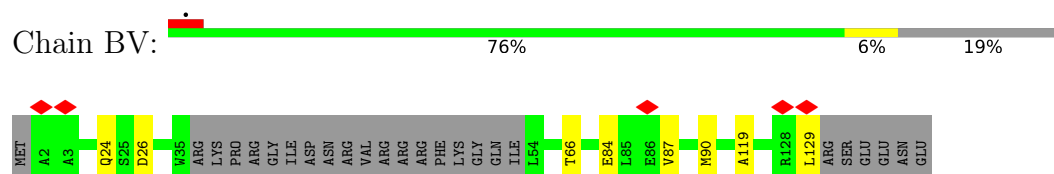
Chain BT: 



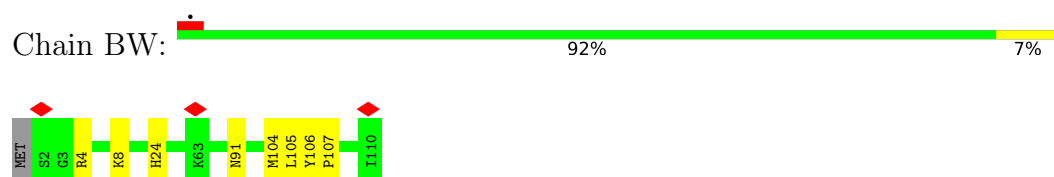
- Molecule 55: Large ribosomal subunit protein eL31



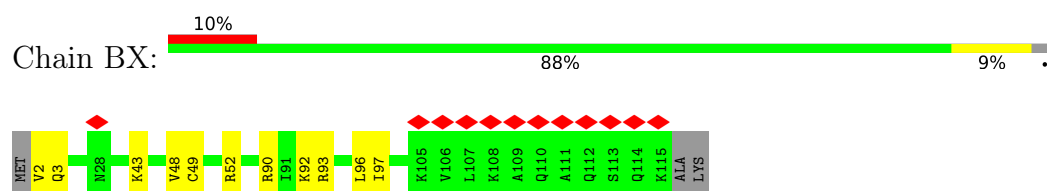
- Molecule 56: Large ribosomal subunit protein eL32



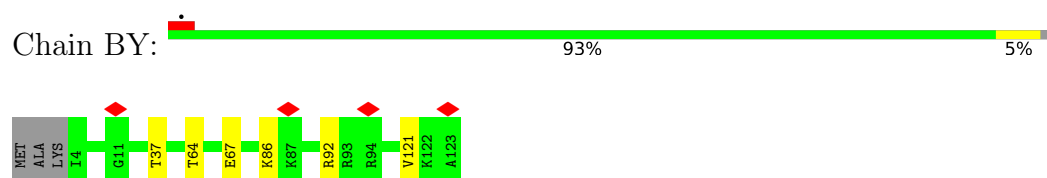
- Molecule 57: Large ribosomal subunit protein eL33



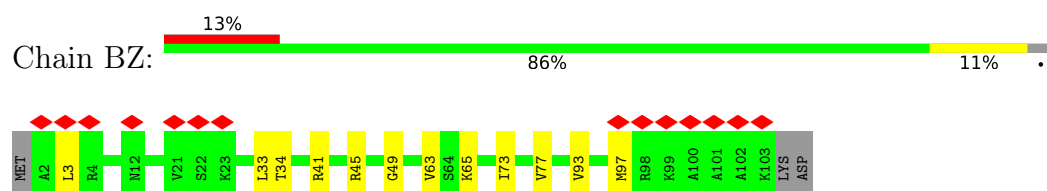
- Molecule 58: Large ribosomal subunit protein eL34



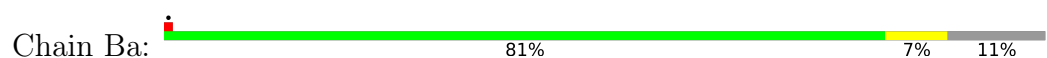
- Molecule 59: Large ribosomal subunit protein uL29

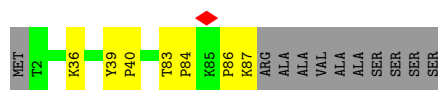


- Molecule 60: Large ribosomal subunit protein eL36

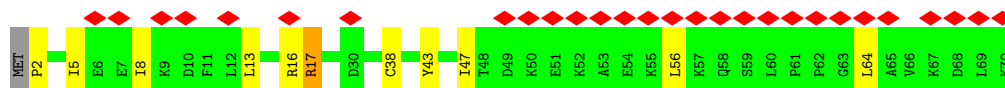
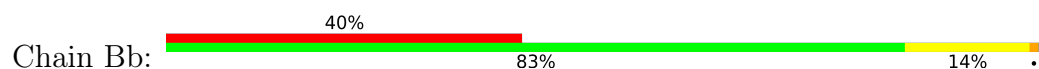


- Molecule 61: Large ribosomal subunit protein eL37

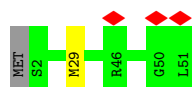




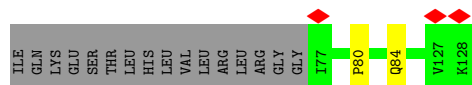
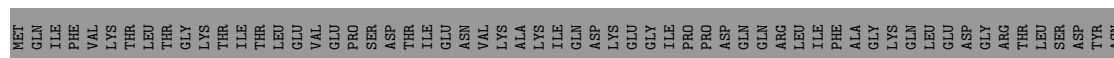
- Molecule 62: Large ribosomal subunit protein eL38



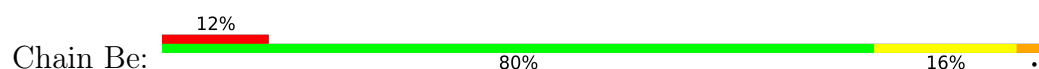
- Molecule 63: Large ribosomal subunit protein eL39



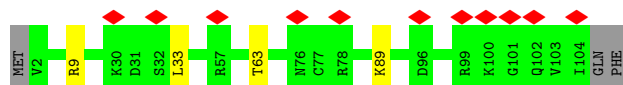
- Molecule 64: Ubiquitin-ribosomal protein eL40 fusion protein



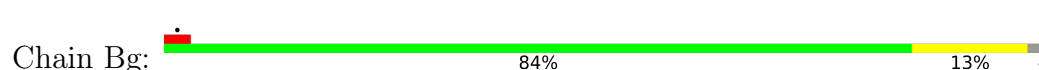
- Molecule 65: 60S ribosomal protein L41

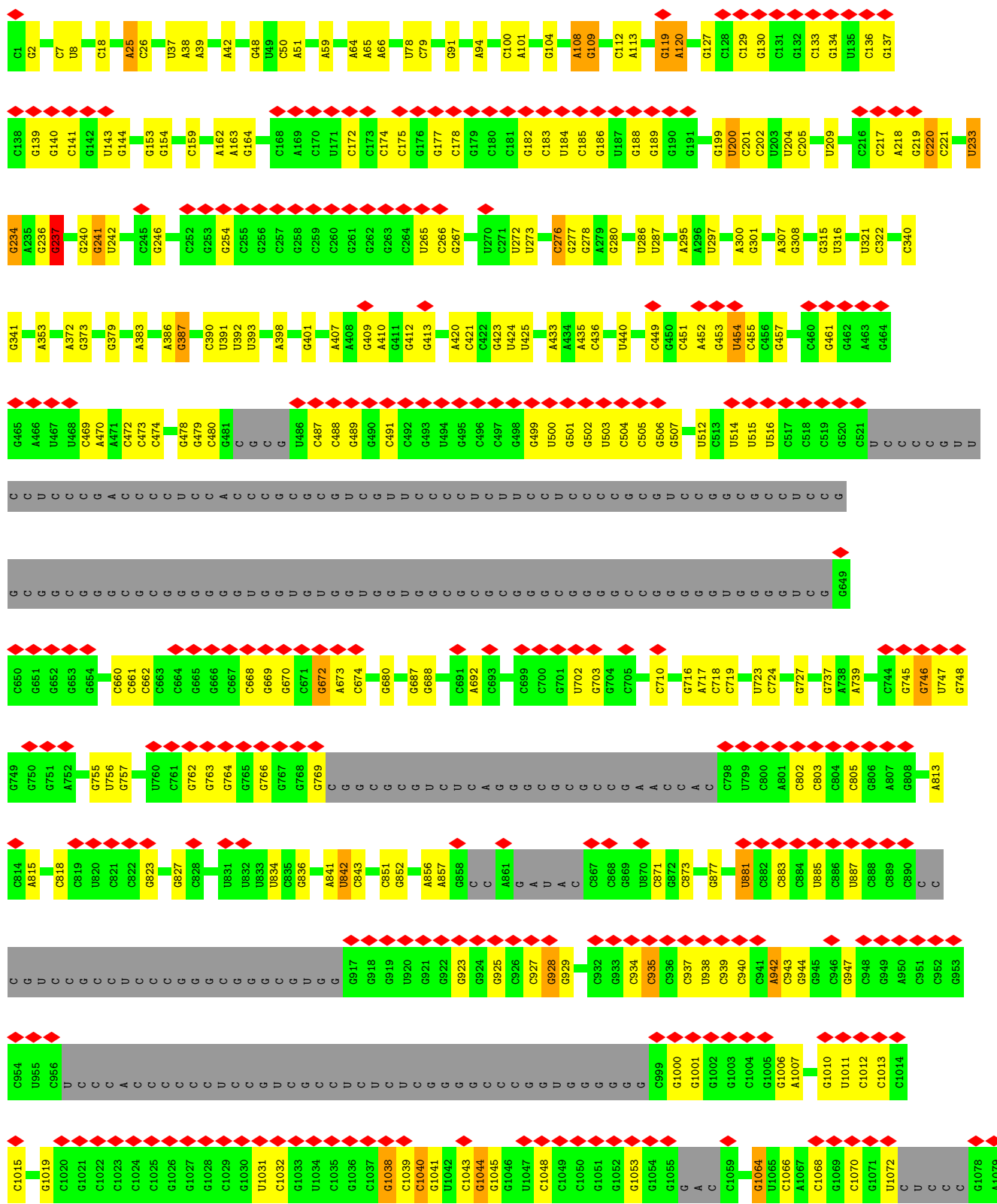


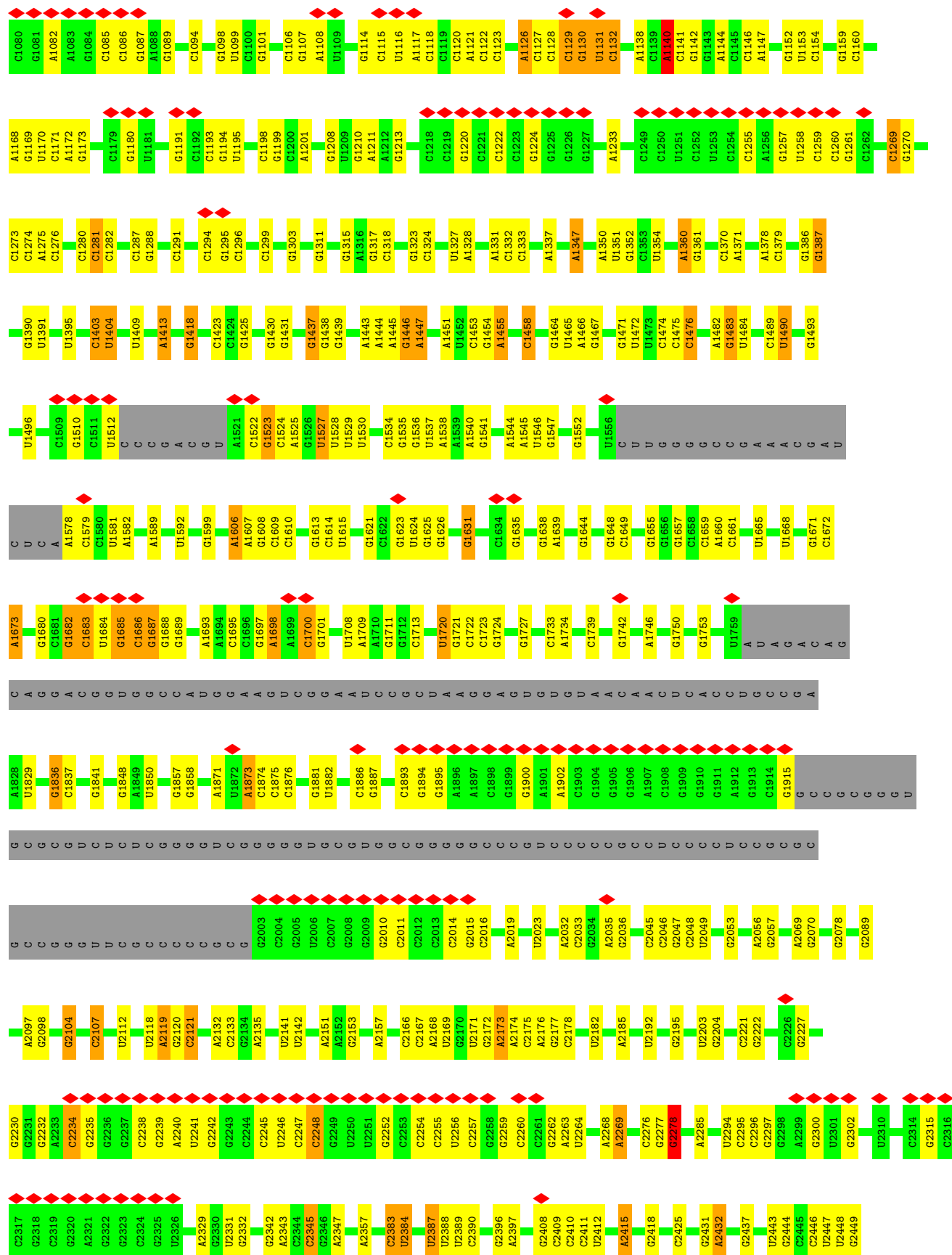
- Molecule 66: Large ribosomal subunit protein eL42



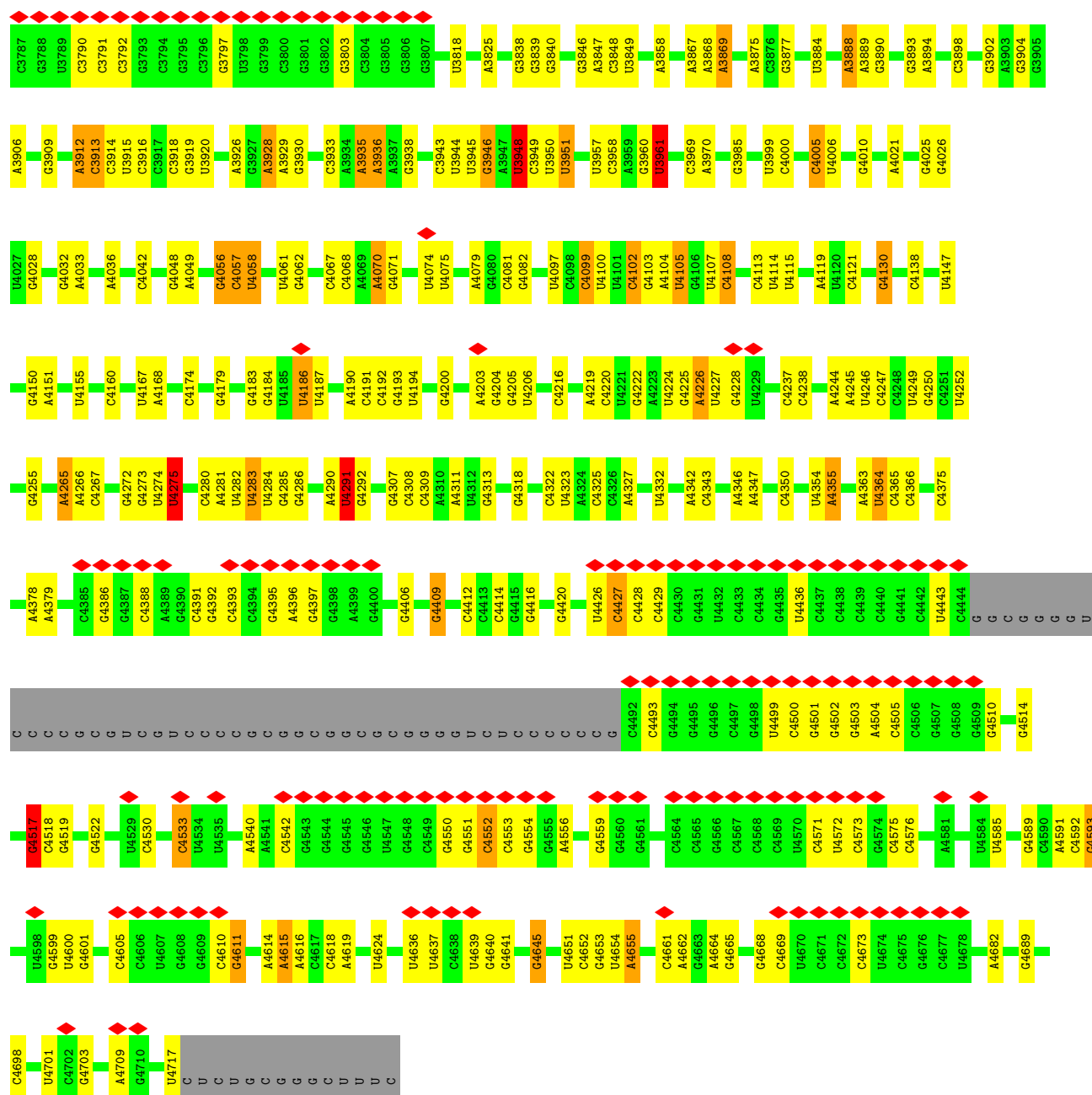
- Molecule 67: Large ribosomal subunit protein eL43









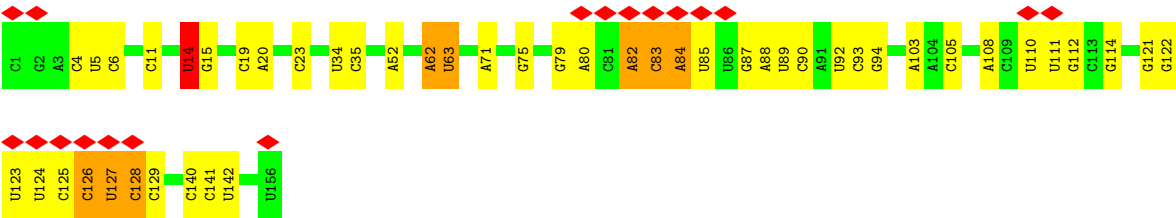


● Molecule 78: 5S rRNA

Chain CJ: 81% 17% ..

● Molecule 79: 5.8S rRNA

Chain CK: 12% 69% 25% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96948	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	4.696	Depositor
Minimum map value	-2.470	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	589.824, 589.824, 589.824	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: 4AC, UR3, MHG, E7G, B8T, B8N, 2MG, MLZ, B9H, E6G, B8W, 5MC, ZN, A2M, OMG, 6MZ, OMU, B8Q, 1MA, PSU, B9B, OMC, P7G, G7M, I4U

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	0.25	0/508	0.51	0/680
2	AB	0.22	0/466	0.47	0/618
3	AC	0.16	2/40063 (0.0%)	0.30	0/62440
4	AE	0.17	0/1784	0.43	0/2402
5	AH	0.18	0/1094	0.50	0/1469
6	AJ	0.18	0/1516	0.40	0/2037
7	AK	0.18	0/843	0.45	0/1137
8	AL	0.19	0/1026	0.44	0/1373
9	AM	0.20	0/1161	0.47	0/1553
10	AN	0.17	0/1208	0.43	0/1618
11	AO	0.15	0/1122	0.35	0/1503
12	AP	0.16	0/817	0.42	0/1097
13	AT	0.20	1/2493 (0.0%)	0.44	0/3394
14	AX	0.17	0/673	0.35	0/907
15	Ac	0.25	0/604	0.51	0/810
16	Af	0.12	0/515	0.37	0/682
17	AD	0.17	0/1765	0.38	0/2362
18	AF	0.14	0/2118	0.36	0/2849
19	AG	0.14	0/1220	0.33	0/1633
20	AI	0.19	0/1731	0.37	0/2352
21	AQ	0.18	0/645	0.34	0/863
22	AR	0.16	0/1116	0.43	0/1490
23	AS	0.18	0/828	0.43	0/1109
24	AU	0.19	0/1762	0.40	0/2382
25	AV	0.19	0/1863	0.43	0/2481
26	AW	0.18	0/1258	0.42	0/1683
27	AY	0.18	0/1232	0.36	0/1656
28	AZ	0.19	0/1015	0.44	0/1361
29	Aa	0.19	0/1051	0.39	0/1406
30	Ab	0.30	0/1015	0.52	0/1348
31	Ad	0.16	0/665	0.43	0/890

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ae	0.24	0/93	0.61	0/123
33	Ag	0.15	0/1499	0.38	0/2007
34	Ah	0.16	0/1715	0.40	0/2287
35	BA	0.18	0/1959	0.40	0/2627
36	BB	0.16	0/3264	0.38	0/4368
37	BC	0.18	0/2971	0.38	0/3987
38	BD	0.15	0/2431	0.37	0/3256
39	BE	0.18	0/1799	0.40	0/2413
40	BF	0.18	0/1670	0.39	0/2232
41	BG	0.17	0/1268	0.40	0/1700
42	BH	0.17	0/1535	0.38	0/2048
43	BI	0.19	0/1558	0.39	0/2059
44	BJ	0.18	0/1490	0.43	0/2000
45	BK	0.15	0/1327	0.34	0/1771
46	BL	0.16	0/839	0.40	0/1126
47	BM	0.16	0/983	0.36	0/1319
48	BN	0.14	0/528	0.31	0/703
49	BO	0.15	0/984	0.35	0/1323
50	BP	0.16	0/1132	0.35	0/1504
51	BQ	0.17	0/1130	0.42	0/1507
52	BR	0.18	0/1193	0.35	0/1593
53	BS	0.19	0/828	0.38	0/1091
54	BT	0.16	0/742	0.36	0/996
55	BU	0.16	0/903	0.41	0/1216
56	BV	0.15	0/910	0.29	0/1216
57	BW	0.16	0/895	0.37	0/1198
58	BX	0.18	0/916	0.38	0/1221
59	BY	0.17	0/1009	0.37	0/1332
60	BZ	0.17	0/843	0.43	0/1115
61	Ba	0.17	0/720	0.37	0/952
62	Bb	0.24	0/574	0.44	0/760
63	Bc	0.16	0/454	0.32	0/599
64	Bd	0.15	0/425	0.37	0/561
65	Be	0.19	0/240	0.46	0/305
66	Bf	0.16	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	0.19	0/1888	0.40	0/2516
70	CB	0.20	0/1898	0.43	0/2553
71	CC	0.16	0/1537	0.39	0/2065
72	CD	0.15	0/1728	0.36	0/2306
73	CE	0.19	0/1372	0.46	0/1836
74	CF	0.16	0/1707	0.39	0/2286

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	CG	0.21	0/1165	0.44	0/1558
76	CH	0.16	0/1746	0.37	0/2338
77	CI	0.16	2/83322 (0.0%)	0.28	0/129924
78	CJ	0.14	0/2858	0.27	0/4455
79	CK	0.17	0/3679	0.29	0/5732
All	All	0.17	5/221479 (0.0%)	0.33	0/325095

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	AL	0	1
10	AN	0	1
28	AZ	0	1
35	BA	0	1
62	Bb	0	1
65	Be	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	1140	A2M	O3'-P	5.19	1.61	1.56
77	CI	3444	A2M	O3'-P	5.11	1.61	1.56
3	AC	669	A2M	O3'-P	5.10	1.61	1.56
13	AT	283	PRO	CA-C	-5.07	1.49	1.51
3	AC	27	A2M	O3'-P	5.06	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	AL	18	ARG	Sidechain
10	AN	99	LEU	Peptide
28	AZ	66	ARG	Sidechain
35	BA	163	ARG	Sidechain
62	Bb	17	ARG	Sidechain
65	Be	23	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	506	536	536	18	0
2	AB	455	447	446	13	0
3	AC	36183	18258	18278	265	0
4	AE	1756	1851	1851	28	0
5	AH	1080	1135	1135	25	0
6	AJ	1495	1548	1549	34	0
7	AK	819	842	842	15	0
8	AL	1006	1047	1047	15	0
9	AM	1143	1213	1213	20	0
10	AN	1190	1249	1249	26	0
11	AO	1104	1139	1139	13	0
12	AP	807	874	874	12	0
13	AT	2436	2393	2393	53	0
14	AX	668	690	690	4	0
15	Ac	598	656	656	15	0
16	Af	505	506	505	6	0
17	AD	1738	1806	1809	31	0
18	AF	2076	2177	2177	23	0
19	AG	1199	1269	1269	8	0
20	AI	1694	1696	1696	18	0
21	AQ	638	635	635	8	0
22	AR	1098	1168	1167	9	0
23	AS	811	864	863	12	0
24	AU	1725	1815	1815	33	0
25	AV	1840	1989	1989	30	0
26	AW	1238	1339	1339	25	0
27	AY	1208	1294	1294	8	0
28	AZ	1002	1021	1021	22	0
29	Aa	1034	1080	1080	20	0
30	Ab	998	1060	1065	38	0
31	Ad	652	676	676	11	0
32	Ae	93	101	101	2	0
33	Ag	1477	1567	1567	25	0
34	Ah	1686	1772	1772	26	0
35	BA	1921	2022	2022	23	0
36	BB	3197	3343	3342	39	0
37	BC	2928	3110	3110	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	2385	2409	2409	22	0
39	BE	1766	1902	1902	21	0
40	BF	1640	1790	1790	20	0
41	BG	1242	1274	1274	13	0
42	BH	1511	1637	1636	17	0
43	BI	1542	1698	1698	10	0
44	BJ	1450	1488	1488	18	0
45	BK	1299	1370	1368	10	0
46	BL	825	850	850	21	0
47	BM	969	1031	1031	8	0
48	BN	515	530	530	4	0
49	BO	967	1040	1040	8	0
50	BP	1115	1205	1205	12	0
51	BQ	1107	1182	1182	10	0
52	BR	1164	1213	1213	10	0
53	BS	813	884	884	7	0
54	BT	732	769	769	6	0
55	BU	888	929	929	9	0
56	BV	895	971	971	7	0
57	BW	876	912	912	10	0
58	BX	906	997	997	10	0
59	BY	1001	1138	1138	4	0
60	BZ	832	917	917	8	0
61	Ba	705	737	737	4	0
62	Bb	568	635	635	7	0
63	Bc	444	483	483	1	0
64	Bd	430	465	465	1	0
65	Be	239	289	289	3	0
66	Bf	842	911	912	3	0
67	Bg	694	738	738	12	0
68	Bh	1001	1067	1066	4	0
69	CA	1851	1988	1988	23	0
70	CB	1863	2003	2003	23	0
71	CC	1519	1603	1603	20	0
72	CD	1690	1745	1745	11	0
73	CE	1349	1383	1383	32	0
74	CF	1676	1777	1777	16	0
75	CG	1143	1217	1217	12	0
76	CH	1701	1749	1749	10	0
77	CI	76342	38567	38467	506	0
78	CJ	2558	1295	1296	9	0
79	CK	3315	1682	1685	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	154658	154583	1812	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 (1812) 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	1.52
5:AH:17:ILE:HD12	5:AH:58:MET:HE3	1.33	1.10
33:Ag:60:ILE:HD11	33:Ag:92:VAL:HG12	1.32	1.04
10:AN:118:ARG:HE	10:AN:123:LEU:HD21	1.28	0.96
77:CI:4274:U:O2'	77:CI:4275:OMU:H6	1.71	0.91
4:AE:48:ILE:HD11	4:AE:86:LEU:HD11	1.54	0.90
77:CI:2542:B9H:C4	77:CI:2542:B9H:C2	2.53	0.85
4:AE:106:ARG:HG3	4:AE:175:VAL:HG22	1.57	0.85
25:AV:35:GLU:OE2	25:AV:49:VAL:HG12	1.77	0.84
29:Aa:47:ILE:HD11	29:Aa:63:VAL:HG11	1.59	0.84
73:CE:95:ARG:HH11	73:CE:175:LEU:HD11	1.44	0.82
37:BC:134:PRO:HA	37:BC:150:LEU:HD11	1.63	0.80
46:BL:56:LEU:HD12	46:BL:61:VAL:HG23	1.63	0.80
37:BC:230:LEU:HD21	37:BC:235:LEU:HD23	1.65	0.79
34:Ah:158:ILE:HG21	34:Ah:162:LEU:HD23	1.64	0.79
13:AT:164:ILE:HD11	13:AT:221:LEU:HD23	1.63	0.79
11:AO:8:ASP:OD1	11:AO:9:VAL:HG13	1.85	0.77
5:AH:17:ILE:HD11	5:AH:54:VAL:HG13	1.67	0.77
43:BI:95:TRP:CH2	43:BI:99:MET:HE3	2.19	0.77
77:CI:1129:C:H2'	77:CI:1130:G:C8	2.20	0.76
76:CH:3:ALA:O	76:CH:7:ILE:HD12	1.85	0.76
4:AE:123:LEU:HD11	4:AE:152:PHE:HB3	1.69	0.75
13:AT:39:THR:HG22	13:AT:60:ARG:HD2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AM:116:ASP:OD2	9:AM:118:THR:HG22	1.87	0.75
9:AM:102:GLU:OE2	13:AT:58:ALA:HB2	1.87	0.74
52:BR:103:VAL:HG12	52:BR:108:TYR:HB2	1.69	0.74
75:CG:56:GLN:CD	77:CI:4517:OMG:C5	2.60	0.74
23:AS:47:ALA:O	23:AS:50:VAL:HG12	1.89	0.73
59:BY:121:VAL:O	74:CF:150:LEU:HD11	1.89	0.72
33:Ag:60:ILE:CD1	33:Ag:92:VAL:HG12	2.16	0.72
77:CI:4225:G:H2'	77:CI:4226:A2M:H8	1.70	0.72
35:BA:180:LEU:HD11	67:Bg:26:VAL:HG11	1.72	0.72
36:BB:57:VAL:HG22	36:BB:367:PHE:HB3	1.72	0.72
15:Ac:92:LEU:HD11	15:Ac:109:TYR:CE1	2.24	0.71
15:Ac:69:THR:OG1	15:Ac:72:VAL:HG23	1.90	0.71
3:AC:1126:C:OP1	5:AH:129:LYS:HD3	1.91	0.71
73:CE:102:THR:HG21	77:CI:3916:C:O2'	1.91	0.71
10:AN:118:ARG:NE	10:AN:123:LEU:HD21	2.04	0.71
77:CI:4070:1MA:N6	77:CI:4082:G:HO2'	1.87	0.71
62:Bb:8:ILE:HD13	62:Bb:56:LEU:HD11	1.73	0.71
13:AT:195:LEU:HD22	13:AT:209:SER:OG	1.91	0.71
37:BC:230:LEU:CD2	37:BC:235:LEU:HD23	2.21	0.71
74:CF:58:ILE:HG23	74:CF:70:VAL:HG11	1.72	0.70
1:AA:11:LEU:HD12	6:AJ:33:ILE:HD11	1.71	0.70
77:CI:3312:A:C2	77:CI:3351:A:H4'	2.27	0.70
3:AC:439:G:N2	3:AC:456:A:N1	2.39	0.70
73:CE:78:LYS:O	73:CE:82:ILE:HD12	1.92	0.70
43:BI:28:GLU:OE1	43:BI:49:LEU:HD22	1.92	0.69
8:AL:20:VAL:HG11	8:AL:28:MET:CE	2.23	0.69
70:CB:137[A]:ARG:HD2	70:CB:146:LEU:HD11	1.75	0.69
33:Ag:76:GLN:O	33:Ag:80:VAL:HG23	1.92	0.69
6:AJ:49:LEU:HD12	9:AM:50:LYS:HG3	1.74	0.69
2:AB:46:TYR:O	2:AB:50:ILE:HD12	1.93	0.69
77:CI:3377:A2M:H2	77:CI:3593:G:O4'	1.93	0.68
30:Ab:37:LYS:HD2	30:Ab:57:VAL:HG23	1.75	0.68
26:AW:63:LEU:HD11	26:AW:69:ARG:NH1	2.08	0.68
77:CI:3381:G:H2'	77:CI:3382:A2M:H8	1.74	0.68
17:AD:103:MET:SD	17:AD:188:LEU:HD21	2.33	0.68
33:Ag:134:VAL:HG12	33:Ag:136:PRO:O	1.94	0.68
75:CG:136:LEU:O	75:CG:136:LEU:HD23	1.93	0.68
71:CC:103:VAL:HG11	71:CC:144:LEU:HD21	1.75	0.67
1:AA:56:LEU:HD21	6:AJ:140:ASP:OD2	1.94	0.67
25:AV:1:MET:SD	25:AV:24:LEU:HD13	2.34	0.67
57:BW:106:TYR:HB2	57:BW:107:PRO:HD3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BK:119:ALA:HB1	45:BK:124:THR:O	1.94	0.67
6:AJ:178:ILE:HG22	6:AJ:182:LYS:NZ	2.10	0.67
25:AV:2:LYS:HD3	25:AV:15:LEU:HD21	1.77	0.66
30:Ab:44:LEU:HD21	30:Ab:75:ILE:HD11	1.77	0.66
33:Ag:69:LEU:HD21	33:Ag:132:ASP:OD1	1.95	0.66
69:CA:147:LEU:HD22	69:CA:152:ILE:HD11	1.77	0.66
49:BO:40:ILE:HG23	70:CB:50:ASP:OD2	1.95	0.66
42:BH:39:THR:HG22	42:BH:41:SER:H	1.60	0.66
5:AH:17:ILE:HD12	5:AH:58:MET:CE	2.19	0.66
13:AT:241:PHE:HE1	13:AT:248:LEU:HD13	1.59	0.66
25:AV:7:PHE:CE2	25:AV:9:ALA:HB3	2.29	0.66
36:BB:223:THR:HG22	36:BB:338:VAL:HG23	1.77	0.66
46:BL:101:ARG:NH1	46:BL:103:VAL:HG21	2.11	0.66
71:CC:167:VAL:CG2	71:CC:172:ILE:HG22	2.26	0.66
77:CI:4551:G:H2'	77:CI:4552:C:C6	2.31	0.66
7:AK:21:MET:HE2	7:AK:45:VAL:HG11	1.76	0.66
75:CG:56:GLN:NE2	77:CI:4517:OMG:C4	2.62	0.65
4:AE:113:LEU:HD23	4:AE:118:ALA:HB2	1.78	0.65
56:BV:24:GLN:OE1	77:CI:1129:C:H5'	1.97	0.65
37:BC:8:ILE:HD11	37:BC:24:LEU:HB2	1.77	0.65
4:AE:99:ILE:HD12	4:AE:173:ARG:NH2	2.12	0.65
26:AW:87:LEU:HD13	26:AW:100:LEU:HD21	1.77	0.65
33:Ag:50:GLU:OE1	33:Ag:60:ILE:HG22	1.97	0.65
5:AH:17:ILE:CD1	5:AH:58:MET:HE3	2.21	0.65
40:BF:15:LEU:HD11	40:BF:129:LEU:CD1	2.27	0.64
11:AO:60:THR:HG23	11:AO:75:MET:HE2	1.79	0.64
49:BO:71:LEU:HD11	49:BO:101:ASP:OD2	1.98	0.64
33:Ag:43:LEU:HD22	33:Ag:72:PHE:CE1	2.33	0.64
3:AC:1588:G:C6	11:AO:78:ILE:HD11	2.32	0.64
10:AN:15:VAL:HG22	10:AN:20:ILE:HD13	1.79	0.64
4:AE:200:PRO:O	4:AE:201:LYS:HG2	1.98	0.64
44:BJ:80:ILE:HD13	44:BJ:129:VAL:HG13	1.79	0.64
76:CH:200:LEU:HD22	76:CH:204:ARG:HH12	1.61	0.64
9:AM:63:PHE:HE1	9:AM:92:LEU:HD22	1.62	0.63
10:AN:20:ILE:CG2	10:AN:29:ALA:HB1	2.28	0.63
48:BN:47:ARG:NH1	48:BN:54:LEU:HD21	2.13	0.63
8:AL:20:VAL:HG11	8:AL:28:MET:HE3	1.80	0.63
15:Ac:113:THR:O	15:Ac:113:THR:HG22	1.98	0.63
70:CB:162:ASP:HB2	70:CB:163:PRO:HD3	1.81	0.63
6:AJ:25:THR:HG21	6:AJ:46:ALA:HB2	1.81	0.63
36:BB:56:ILE:HD12	36:BB:365:LEU:HD22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BB:160:ILE:HD11	36:BB:190:VAL:HG13	1.80	0.63
4:AE:48:ILE:HD11	4:AE:86:LEU:CD1	2.28	0.63
39:BE:211:ILE:O	39:BE:211:ILE:HG22	1.97	0.63
49:BO:89:LYS:HG2	49:BO:95:THR:HG23	1.78	0.63
73:CE:164:ARG:O	73:CE:168:GLN:OE1	2.17	0.63
13:AT:173:LEU:HD23	13:AT:175:LYS:HE3	1.80	0.63
30:Ab:117:VAL:HG23	30:Ab:121:ALA:HB2	1.80	0.63
78:CJ:28:C:H1'	78:CJ:54:A:H61	1.64	0.63
13:AT:191:HIS:CD2	13:AT:195:LEU:HD21	2.34	0.63
54:BT:34:THR:HG23	54:BT:95:ALA:HB2	1.80	0.63
20:AI:77:ILE:HD12	20:AI:122:LEU:HD11	1.82	0.62
35:BA:231:ALA:HB1	77:CI:3326:C:H5'	1.80	0.62
10:AN:20:ILE:HG23	10:AN:29:ALA:HB1	1.82	0.62
77:CI:661:C:H2'	77:CI:662:C:C6	2.35	0.62
3:AC:1553:G:H3'	3:AC:1554:C:H5''	1.82	0.62
43:BI:129:GLY:O	43:BI:130:ASN:OD1	2.17	0.62
13:AT:39:THR:HG22	13:AT:60:ARG:CD	2.30	0.62
17:AD:71:LEU:HD13	17:AD:84:PHE:CE2	2.34	0.62
29:Aa:38:LEU:HD23	29:Aa:41:MET:CE	2.30	0.62
77:CI:2542:B9H:C4	77:CI:2542:B9H:C31	2.75	0.62
13:AT:241:PHE:CE1	13:AT:248:LEU:HD13	2.35	0.61
37:BC:134:PRO:CA	37:BC:150:LEU:HD11	2.28	0.61
64:Bd:80:PRO:O	64:Bd:84:GLN:OE1	2.17	0.61
77:CI:1129:C:H42	77:CI:1138:A:P	2.23	0.61
77:CI:4274:U:HO2'	77:CI:4275:OMU:H6	1.65	0.61
43:BI:95:TRP:CZ2	43:BI:99:MET:HE3	2.35	0.61
28:AZ:53:ILE:HG23	28:AZ:88:LEU:HD23	1.82	0.61
20:AI:84:GLN:O	20:AI:88:LEU:HD23	2.00	0.61
24:AU:272:HIS:O	24:AU:276:THR:HG23	2.01	0.61
20:AI:5:LEU:HD21	21:AQ:41:ARG:HD3	1.81	0.61
30:Ab:94:HIS:HE1	30:Ab:96:LEU:HD12	1.66	0.61
60:BZ:73:ILE:O	60:BZ:77:VAL:HG22	2.00	0.61
34:Ah:119:LEU:HD12	34:Ah:120:PRO:HD2	1.83	0.61
39:BE:187:LEU:HD12	39:BE:191:ARG:HA	1.82	0.61
48:BN:47:ARG:CZ	48:BN:54:LEU:HD21	2.30	0.61
69:CA:184:ILE:O	69:CA:185:ASN:OD1	2.19	0.61
21:AQ:9:VAL:HG11	24:AU:177:PRO:HD3	1.81	0.61
25:AV:124:LEU:HD12	25:AV:125:THR:OG1	2.01	0.61
3:AC:1417:C:HO2'	11:AO:4:VAL:N	1.98	0.61
36:BB:86:VAL:HG13	36:BB:162:ILE:HG23	1.82	0.61
77:CI:2112:U:C5'	79:CK:14:OMU:HM21	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AU:166:ARG:HB2	24:AU:248:TYR:CD1	2.36	0.60
74:CF:125:ILE:HG22	74:CF:143:GLU:OE2	2.01	0.60
24:AU:166:ARG:HB2	24:AU:248:TYR:CE1	2.36	0.60
51:BQ:87:VAL:HG11	51:BQ:89:ILE:HD12	1.82	0.60
1:AA:48:GLY:O	1:AA:50:VAL:HG23	2.01	0.60
40:BF:36:VAL:HG12	40:BF:105:LEU:HD11	1.81	0.60
10:AN:33:ILE:HG22	10:AN:35:GLY:H	1.67	0.60
24:AU:164:PRO:HB2	24:AU:248:TYR:HE2	1.64	0.60
29:Aa:36:ARG:HD2	29:Aa:110:ILE:HD12	1.82	0.60
41:BG:85:LYS:O	41:BG:89:GLU:OE1	2.19	0.60
9:AM:62:ARG:NH1	9:AM:108:ILE:HG22	2.16	0.60
22:AR:85:VAL:HG23	22:AR:85:VAL:O	2.01	0.60
6:AJ:138:ALA:HB2	6:AJ:203:ASN:OD1	2.02	0.60
37:BC:144:ILE:HG21	37:BC:150:LEU:CD2	2.32	0.60
29:Aa:47:ILE:HD11	29:Aa:63:VAL:CG1	2.31	0.59
37:BC:10:VAL:HG22	37:BC:153:VAL:HG11	1.84	0.59
39:BE:104:VAL:HG11	39:BE:113:ARG:NH1	2.17	0.59
58:BX:93:ARG:O	58:BX:97:ILE:HD12	2.02	0.59
77:CI:1122:C:H2'	77:CI:1123:C:C6	2.37	0.59
24:AU:209:VAL:HB	24:AU:210:PRO:HD3	1.84	0.59
73:CE:95:ARG:NH1	73:CE:175:LEU:HD11	2.14	0.59
77:CI:3312:A:N1	77:CI:3351:A:H4'	2.18	0.59
3:AC:64:A:H2	3:AC:83:A:H62	1.49	0.59
3:AC:637:C:C4	3:AC:638:U:C4	2.90	0.59
30:Ab:6:THR:CG2	30:Ab:28:LEU:HD22	2.32	0.59
77:CI:1153:U:H2'	77:CI:1154:C:C6	2.37	0.59
34:Ah:43:ILE:HD11	34:Ah:60:LEU:HD21	1.84	0.59
42:BH:3:VAL:HG12	69:CA:120:ILE:HD13	1.85	0.59
3:AC:1589:A:H2'	3:AC:1590:A:C8	2.38	0.59
9:AM:6:PRO:C	9:AM:7:LEU:HD23	2.28	0.59
9:AM:31:LEU:HD21	9:AM:33:LYS:HG2	1.84	0.59
13:AT:275:ILE:O	13:AT:277:THR:HG23	2.03	0.58
67:Bg:42:CYS:HB3	67:Bg:60:CYS:SG	2.42	0.58
77:CI:472:C:H2'	77:CI:473:C:C6	2.38	0.58
20:AI:42:LYS:HE2	20:AI:48:ILE:HD11	1.84	0.58
39:BE:162:THR:HG22	57:BW:106:TYR:CE1	2.37	0.58
72:CD:193:ASP:O	72:CD:193:ASP:OD1	2.21	0.58
74:CF:23:ASP:OD2	76:CH:197:THR:HG21	2.03	0.58
74:CF:58:ILE:HG23	74:CF:70:VAL:CG1	2.33	0.58
10:AN:72:GLN:NE2	10:AN:99:LEU:HD12	2.18	0.58
62:Bb:13:LEU:HD23	62:Bb:16:ARG:NH2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:CF:46:ILE:HD11	74:CF:51:ALA:HA	1.85	0.58
3:AC:120:U:H1'	18:AF:33:THR:HG23	1.84	0.58
3:AC:439:G:N2	3:AC:456:A:C2	2.71	0.58
3:AC:1228:G:C2	3:AC:1229:A:C8	2.91	0.58
2:AB:14:PHE:HA	3:AC:1557:A:C2	2.38	0.58
9:AM:100:VAL:HG12	9:AM:101:ASP:H	1.67	0.58
26:AW:84:ILE:HD11	26:AW:148:ILE:HG21	1.85	0.58
7:AK:47:LYS:O	7:AK:50:GLN:HG2	2.04	0.58
30:Ab:35:VAL:HG23	30:Ab:40:ILE:HD11	1.84	0.58
3:AC:368:U:H4'	3:AC:372:A:C8	2.39	0.57
13:AT:134:THR:HG22	13:AT:134:THR:O	2.03	0.57
27:AY:40:LEU:HB3	27:AY:45:LEU:HD12	1.85	0.57
77:CI:938:U:H2'	77:CI:939:C:C6	2.39	0.57
77:CI:454:U:H2'	77:CI:455:C:C6	2.38	0.57
77:CI:1685:OMG:O2'	77:CI:1686:C:P	2.62	0.57
45:BK:104:SER:O	45:BK:107:LYS:HG2	2.03	0.57
6:AJ:68:ILE:CD1	6:AJ:151:ILE:HD11	2.34	0.57
33:Ag:26:ALA:O	33:Ag:30:LEU:HD23	2.05	0.57
6:AJ:68:ILE:HD11	6:AJ:151:ILE:HD11	1.85	0.57
37:BC:153:VAL:HG22	37:BC:257:PHE:CE2	2.40	0.57
72:CD:48:LEU:HB2	72:CD:142:LEU:HD23	1.85	0.57
3:AC:982:A:H2'	3:AC:983:G:C8	2.40	0.57
7:AK:95:ARG:O	7:AK:96:ARG:HG3	2.04	0.57
32:Ae:85:LYS:O	32:Ae:89:GLN:OE1	2.21	0.57
35:BA:219:ILE:HG22	35:BA:221:LYS:O	2.05	0.57
77:CI:2447:U:C2	77:CI:2448:U:C5	2.91	0.57
39:BE:112:THR:O	39:BE:113:ARG:HD2	2.03	0.56
46:BL:56:LEU:HD12	46:BL:61:VAL:CG2	2.33	0.56
55:BU:25:TYR:CE1	55:BU:88:LEU:HD12	2.39	0.56
1:AA:50:VAL:HG13	1:AA:54:ASP:OD2	2.05	0.56
3:AC:1201:A:OP2	23:AS:2:THR:HG21	2.04	0.56
77:CI:1874:C:C2	77:CI:1875:C:C5	2.93	0.56
3:AC:102:A:H4'	3:AC:104:A:C8	2.40	0.56
15:Ac:92:LEU:HD11	15:Ac:109:TYR:HE1	1.69	0.56
67:Bg:16:THR:HG22	77:CI:2632:G:C8	2.41	0.56
4:AE:172:VAL:HG22	4:AE:185:LYS:HG3	1.87	0.56
10:AN:15:VAL:HB	10:AN:68:ILE:HD11	1.87	0.56
25:AV:98:ARG:HE	25:AV:106:LEU:HD21	1.70	0.56
27:AY:89:TYR:CE1	27:AY:150:VAL:HG23	2.39	0.56
14:AX:64:LEU:HD11	16:Af:106:TYR:CD2	2.39	0.56
3:AC:963:A:H4'	28:AZ:66:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AH:79:GLU:CD	5:AH:80:ARG:H	2.12	0.56
26:AW:84:ILE:HD11	26:AW:148:ILE:CG2	2.36	0.56
75:CG:56:GLN:HB3	77:CI:4517:OMG:C8	2.41	0.56
77:CI:2234:C:C5	77:CI:2235:G:C8	2.94	0.56
31:Ad:67:THR:HG21	31:Ad:72:ARG:NH1	2.21	0.56
36:BB:57:VAL:HG12	36:BB:73:VAL:HG22	1.87	0.56
18:AF:173:ILE:HD11	18:AF:230:LYS:HA	1.88	0.56
30:Ab:56:PHE:CE1	30:Ab:94:HIS:CD2	2.93	0.56
36:BB:108:GLU:OE2	36:BB:138:GLN:NE2	2.39	0.56
46:BL:63:ILE:HG23	46:BL:70:ILE:HG23	1.88	0.56
59:BY:86:LYS:HD2	59:BY:92:ARG:NH1	2.21	0.56
77:CI:233:U:H1'	77:CI:234:G:C8	2.41	0.56
3:AC:1293:C:C2	3:AC:1294:A:C8	2.94	0.56
4:AE:7:LYS:HE2	12:AP:25:THR:HG21	1.88	0.56
39:BE:78:ARG:O	53:BS:116:LEU:HD22	2.06	0.56
56:BV:66:THR:O	56:BV:66:THR:HG22	2.05	0.56
59:BY:37:THR:O	59:BY:37:THR:HG22	2.04	0.56
3:AC:963:A:H5''	28:AZ:66:ARG:HD3	1.87	0.55
30:Ab:44:LEU:HD23	30:Ab:55:ILE:HG21	1.88	0.55
33:Ag:43:LEU:HD22	33:Ag:72:PHE:CD1	2.41	0.55
42:BH:42:THR:HA	42:BH:45:GLN:OE1	2.05	0.55
1:AA:45:ASN:O	6:AJ:139:VAL:HG13	2.06	0.55
3:AC:1317:C:C2	3:AC:1318:C:C5	2.94	0.55
12:AP:97:ILE:O	12:AP:97:ILE:HG22	2.06	0.55
24:AU:267:GLN:O	24:AU:270:THR:HG23	2.06	0.55
44:BJ:80:ILE:CD1	44:BJ:129:VAL:HG13	2.37	0.55
13:AT:18:VAL:HG21	13:AT:307:VAL:HG22	1.89	0.55
30:Ab:104:ARG:HE	30:Ab:108:LYS:HE2	1.72	0.55
46:BL:47:ILE:HG21	46:BL:56:LEU:HD13	1.86	0.55
77:CI:4282:U:C2	77:CI:4283:PSU:C6	2.95	0.55
3:AC:65:C:C2	25:AV:133:LEU:HD11	2.41	0.55
6:AJ:153:LEU:HD22	6:AJ:192:LYS:HG3	1.88	0.55
26:AW:63:LEU:HD11	26:AW:69:ARG:HH12	1.71	0.55
77:CI:2415:A:C2	77:CI:2432:A:C8	2.94	0.55
3:AC:1204:G:H2'	3:AC:1205:A:C8	2.42	0.55
26:AW:84:ILE:HG23	26:AW:86:VAL:HG13	1.89	0.55
77:CI:739:A:H62	77:CI:827:G:H21	1.53	0.55
13:AT:54:ILE:HG23	13:AT:55:PRO:HD2	1.89	0.55
47:BM:91:LYS:O	47:BM:92:ASP:CG	2.50	0.55
57:BW:105:LEU:O	57:BW:105:LEU:HD23	2.06	0.55
4:AE:113:LEU:HD11	4:AE:117:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Ab:94:HIS:CE1	30:Ab:96:LEU:HD12	2.42	0.55
34:Ah:101:ILE:HD12	34:Ah:190:LEU:HD11	1.89	0.55
77:CI:4290:A:H3'	77:CI:4291:PSU:H4'	1.89	0.55
24:AU:266:TYR:O	24:AU:270:THR:HG22	2.07	0.55
37:BC:345:ARG:O	37:BC:349:LEU:HD13	2.06	0.55
38:BD:62:CYS:HB3	38:BD:105:LEU:HD22	1.88	0.55
3:AC:322:C:C2	3:AC:323:C:C5	2.95	0.54
29:Aa:42:MET:HE2	29:Aa:49:GLU:HA	1.89	0.54
43:BI:99:MET:HE1	43:BI:127:VAL:O	2.07	0.54
77:CI:3748:G:C2	77:CI:3749:C:C5	2.96	0.54
71:CC:120:GLU:HG2	77:CI:4266:A:H2	1.72	0.54
73:CE:12:MET:CE	78:CJ:51:G:H21	2.21	0.54
5:AH:87:GLU:HG2	5:AH:88:VAL:HG23	1.88	0.54
77:CI:472:C:C2	77:CI:473:C:C5	2.95	0.54
77:CI:3566:G:N3	77:CI:3568:OMC:C4	2.76	0.54
4:AE:198:ILE:O	4:AE:198:ILE:HG22	2.08	0.54
13:AT:256:ILE:HD12	13:AT:289:LEU:HD21	1.89	0.54
25:AV:197:GLN:O	25:AV:200:LYS:HG2	2.08	0.54
40:BF:15:LEU:HD11	40:BF:129:LEU:HD11	1.88	0.54
77:CI:3568:OMC:C5	77:CI:3569:C:C5	2.95	0.54
3:AC:218:C:C2	3:AC:219:A:C8	2.96	0.54
70:CB:209:SER:HA	70:CB:212:LYS:HG3	1.90	0.54
73:CE:39:VAL:HA	73:CE:123:ILE:HD11	1.90	0.54
4:AE:99:ILE:HD12	4:AE:173:ARG:HH22	1.71	0.54
73:CE:50:PHE:HD1	73:CE:70:VAL:HG12	1.73	0.54
77:CI:939:C:H2'	77:CI:940:C:C6	2.42	0.54
77:CI:4552:C:C4	77:CI:4553:C:C5	2.95	0.54
51:BQ:135:ARG:NE	77:CI:3776:C:O2'	2.41	0.54
77:CI:1141:C:H2'	77:CI:1142:G:C8	2.43	0.54
7:AK:80:ARG:NH2	7:AK:90:VAL:HG12	2.21	0.54
40:BF:105:LEU:HD13	40:BF:109:PRO:HD3	1.89	0.54
42:BH:158:THR:HG22	42:BH:159:PRO:HD2	1.90	0.54
54:BT:38:ILE:HD11	54:BT:46:VAL:HG21	1.90	0.54
77:CI:1039:C:N4	77:CI:1040:C:H41	2.06	0.54
3:AC:96:C:H2'	3:AC:97:U:C6	2.43	0.54
13:AT:309:VAL:HG13	13:AT:309:VAL:O	2.08	0.54
24:AU:210:PRO:HD3	24:AU:236:PHE:HE2	1.72	0.54
35:BA:137:ILE:HD11	35:BA:149:LYS:HB3	1.88	0.54
77:CI:3415:A:H61	77:CI:3427:U:H3	1.54	0.54
3:AC:1278:C:H2'	3:AC:1279:A:H8	1.71	0.54
77:CI:1128:C:O2'	77:CI:1129:C:C6	2.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:1661:C:H4'	3:AC:1664:A:H62	1.73	0.53
27:AY:11:LEU:O	27:AY:11:LEU:HD23	2.08	0.53
29:Aa:42:MET:HE3	29:Aa:50:PHE:CD1	2.43	0.53
3:AC:458:C:C2	3:AC:459:A:C8	2.96	0.53
5:AH:40:ILE:O	5:AH:40:ILE:HG13	2.08	0.53
77:CI:2388:U:C2	77:CI:2389:U:C5	2.96	0.53
3:AC:573:U:H5'	30:Ab:60:PHE:O	2.08	0.53
17:AD:103:MET:HG2	17:AD:215:VAL:HB	1.91	0.53
25:AV:208:GLU:O	25:AV:211:LYS:HG2	2.08	0.53
30:Ab:117:VAL:HG23	30:Ab:121:ALA:CB	2.38	0.53
61:Ba:39:TYR:HB3	61:Ba:40:PRO:HD3	1.90	0.53
3:AC:818:G:N2	3:AC:819:A:H62	2.06	0.53
9:AM:63:PHE:CE1	9:AM:92:LEU:HD22	2.44	0.53
18:AF:184:THR:C	18:AF:189:LEU:HD13	2.34	0.53
25:AV:41:LEU:HD12	25:AV:41:LEU:O	2.09	0.53
45:BK:26:PRO:O	45:BK:29:THR:HG22	2.07	0.53
77:CI:2383:C:C2	77:CI:2384:U:C6	2.97	0.53
77:CI:4150:G:C2	77:CI:4151:A:N7	2.77	0.53
8:AL:107:ILE:O	8:AL:111:MET:HE3	2.08	0.53
46:BL:76:VAL:HB	46:BL:77:PRO:HD2	1.91	0.53
2:AB:36:LEU:HD23	4:AE:16:ILE:HD11	1.90	0.53
3:AC:572:U:OP1	30:Ab:37:LYS:HG3	2.09	0.53
5:AH:103:LYS:HE2	5:AH:117:LEU:HD12	1.89	0.53
17:AD:44:ILE:HD11	17:AD:86:LEU:HD12	1.90	0.53
23:AS:44:ILE:HG12	23:AS:67:LEU:CD1	2.38	0.53
24:AU:69:LEU:O	24:AU:72:ASP:OD1	2.27	0.53
77:CI:1121:A:H2'	77:CI:1122:C:H6	1.73	0.53
77:CI:1128:C:O2'	77:CI:1129:C:P	2.66	0.53
3:AC:1229:A:H2'	3:AC:1230:G:C8	2.44	0.53
6:AJ:32:ASP:OD2	6:AJ:35:LEU:HD13	2.09	0.53
46:BL:42:PHE:CZ	46:BL:46:ARG:HD3	2.43	0.53
67:Bg:89:LEU:O	67:Bg:92:GLN:O	2.25	0.53
17:AD:66:VAL:HG13	17:AD:101:HIS:NE2	2.23	0.53
18:AF:59:ASP:O	18:AF:62:LYS:HG2	2.09	0.53
77:CI:4192:C:H2'	77:CI:4193:G:H8	1.74	0.53
17:AD:144:LYS:HD2	17:AD:208:HIS:ND1	2.24	0.53
23:AS:45:VAL:HG11	23:AS:64:LEU:HD13	1.91	0.53
69:CA:52:VAL:HG11	77:CI:1085:C:O2	2.09	0.53
70:CB:58:PRO:HG2	70:CB:61:ILE:HD12	1.91	0.53
71:CC:118:LEU:HD11	71:CC:167:VAL:HG12	1.90	0.53
77:CI:1140:A2M:H2'	77:CI:1141:C:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:2240:A:H61	77:CI:2248:C:H42	1.55	0.53
20:AI:13:GLU:O	20:AI:17:LYS:HG3	2.10	0.52
37:BC:339:THR:O	37:BC:343:GLN:HG2	2.09	0.52
40:BF:61:ARG:HD2	40:BF:66:PRO:HB3	1.92	0.52
3:AC:1165:G:O2'	3:AC:1166:G:H5'	2.09	0.52
73:CE:175:LEU:C	73:CE:175:LEU:HD12	2.34	0.52
3:AC:116:OMU:O5'	3:AC:116:OMU:H6	2.10	0.52
10:AN:98:VAL:HG11	10:AN:106:LYS:HD3	1.91	0.52
50:BP:74:TYR:HE2	50:BP:77:LYS:HG3	1.74	0.52
77:CI:1131:U:C6	77:CI:1131:U:OP1	2.62	0.52
77:CI:2234:C:C6	77:CI:2235:G:C8	2.97	0.52
77:CI:3395:A:H2'	77:CI:3396:A:C8	2.44	0.52
77:CI:3915:U:H2'	77:CI:3916:C:C6	2.45	0.52
3:AC:929:G:H2'	3:AC:930:G:C8	2.44	0.52
38:BD:4:VAL:HG11	77:CI:3902:G:H5'	1.92	0.52
77:CI:1437:G:H21	77:CI:1455:A:H1'	1.75	0.52
77:CI:3444:A2M:H2	77:CI:4206:U:O2	2.09	0.52
3:AC:126:G:C8	25:AV:199:THR:HG21	2.45	0.52
36:BB:60:VAL:HG21	36:BB:67:VAL:HG13	1.90	0.52
75:CG:91:TRP:HE1	77:CI:4517:OMG:C3'	2.21	0.52
76:CH:49:ARG:HG2	77:CI:113:A:H4'	1.91	0.52
77:CI:1146:C:H2'	77:CI:1147:A:H8	1.73	0.52
3:AC:912:C:O2'	3:AC:913:C:H5'	2.09	0.52
3:AC:1019:U:C2	3:AC:1020:C:C5	2.97	0.52
77:CI:3893:G:H2'	77:CI:3894:A:H8	1.74	0.52
18:AF:87:MET:HE3	18:AF:123:LEU:HB2	1.91	0.52
30:Ab:44:LEU:HD23	30:Ab:55:ILE:CG2	2.39	0.52
33:Ag:43:LEU:HB3	33:Ag:72:PHE:HE1	1.74	0.52
38:BD:246:ALA:HA	38:BD:249:GLU:HG2	1.92	0.52
58:BX:92:LYS:O	58:BX:96:LEU:HD13	2.09	0.52
3:AC:1316:U:C2	3:AC:1317:C:C6	2.98	0.52
75:CG:38:VAL:HG21	75:CG:50:MET:SD	2.49	0.52
3:AC:219:A:C5	3:AC:220:U:C5	2.98	0.52
37:BC:144:ILE:HG21	37:BC:150:LEU:HD23	1.92	0.52
42:BH:176:ARG:O	52:BR:56:VAL:HG21	2.10	0.52
46:BL:17:GLN:HG3	46:BL:18:VAL:H	1.75	0.52
73:CE:108:GLY:O	73:CE:109:ILE:HD13	2.08	0.52
77:CI:4552:C:C2	77:CI:4553:C:C6	2.98	0.52
69:CA:81:LYS:O	69:CA:84:ARG:HG2	2.09	0.52
77:CI:4056:G:H2'	77:CI:4057:C:H6	1.75	0.52
7:AK:50:GLN:O	7:AK:53:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:CC:45:LEU:CD2	71:CC:57:VAL:HG22	2.41	0.51
78:CJ:111:C:H2'	78:CJ:112:U:O4'	2.10	0.51
17:AD:46:LYS:HE3	28:AZ:21:VAL:HG12	1.92	0.51
30:Ab:9:THR:OG1	30:Ab:23:MET:HB2	2.09	0.51
77:CI:717:A:H2'	77:CI:718:C:C6	2.45	0.51
77:CI:2221:C:H2'	77:CI:2222:G:O4'	2.11	0.51
10:AN:78:LYS:O	10:AN:78:LYS:HG2	2.10	0.51
4:AE:7:LYS:O	4:AE:10:LYS:HG2	2.11	0.51
37:BC:211:TYR:CE2	37:BC:214:ASP:OD1	2.63	0.51
73:CE:31:ASP:O	73:CE:35:ARG:HG3	2.10	0.51
3:AC:1828:U:C2	3:AC:1829:C:C5	2.98	0.51
19:AG:77:VAL:HG22	19:AG:86:ILE:HD12	1.93	0.51
22:AR:28:LYS:HE2	22:AR:32:LEU:HD22	1.92	0.51
74:CF:64:VAL:HA	74:CF:67:HIS:ND1	2.25	0.51
77:CI:2446:C:H2'	77:CI:2447:U:H6	1.75	0.51
1:AA:57:THR:O	1:AA:57:THR:HG23	2.10	0.51
3:AC:1843:4AC:O5'	3:AC:1843:4AC:H6	2.09	0.51
69:CA:57:LYS:O	69:CA:61:LEU:HG	2.10	0.51
73:CE:102:THR:HG22	73:CE:102:THR:O	2.10	0.51
3:AC:1124:C:C2	3:AC:1125:C:C6	2.99	0.51
3:AC:1537:G:H2'	3:AC:1538:A:H8	1.75	0.51
3:AC:1680:A:H2'	6:AJ:60:ARG:HD2	1.91	0.51
36:BB:223:THR:HG22	36:BB:338:VAL:CG2	2.41	0.51
36:BB:268:ARG:HH21	77:CI:3554:G:N2	2.09	0.51
77:CI:4308:C:C2	77:CI:4309:C:C5	2.99	0.51
3:AC:854:C:C2	3:AC:855:A:C8	2.99	0.51
12:AP:46:LYS:O	12:AP:46:LYS:HG3	2.10	0.51
13:AT:189:ILE:HG13	13:AT:189:ILE:O	2.11	0.51
13:AT:234:ASP:CG	13:AT:235:ILE:H	2.18	0.51
40:BF:105:LEU:HD13	40:BF:109:PRO:CD	2.41	0.51
79:CK:14:OMU:HM22	79:CK:15:G:O4'	2.11	0.51
1:AA:44:ARG:CD	1:AA:58:LEU:HD11	2.41	0.51
3:AC:120:U:C2	3:AC:121:U:C5	2.99	0.51
14:AX:64:LEU:HD11	16:Af:106:TYR:CG	2.46	0.51
17:AD:97:LEU:HD13	17:AD:229:MET:HE1	1.93	0.51
24:AU:210:PRO:HD3	24:AU:236:PHE:CE2	2.46	0.51
77:CI:1682:G:H8	77:CI:1683:C:H2'	1.75	0.51
77:CI:2540:C:C2	77:CI:2541:C:C5	2.99	0.51
77:CI:3912:A:O2'	77:CI:3913:C:C6	2.57	0.51
77:CI:4192:C:H2'	77:CI:4193:G:C8	2.46	0.51
77:CI:4346:A:N1	77:CI:4355:A:C8	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:352:G:C2	3:AC:353:U:C6	2.99	0.51
3:AC:442:C:H2'	3:AC:443:C:C6	2.46	0.51
3:AC:513:A:C2	3:AC:514:G:C8	2.99	0.51
12:AP:68:THR:HG23	12:AP:70:CYS:O	2.11	0.51
2:AB:13:LYS:HG3	2:AB:14:PHE:CE2	2.46	0.50
3:AC:858:U:H2'	3:AC:859:A:C8	2.45	0.50
3:AC:1680:A:P	6:AJ:60:ARG:HE	2.34	0.50
13:AT:18:VAL:HG21	13:AT:307:VAL:CG2	2.41	0.50
13:AT:42:MET:HE2	13:AT:57:ARG:HG2	1.93	0.50
17:AD:103:MET:SD	17:AD:188:LEU:HD11	2.51	0.50
25:AV:200:LYS:O	25:AV:203:LYS:HG2	2.11	0.50
34:Ah:29:LEU:C	34:Ah:29:LEU:HD12	2.36	0.50
77:CI:2501:A:H2'	77:CI:2502:A:C8	2.46	0.50
1:AA:37:ASP:OD1	1:AA:37:ASP:N	2.41	0.50
43:BI:28:GLU:OE1	43:BI:49:LEU:CD2	2.57	0.50
58:BX:43:LYS:HE2	58:BX:52:ARG:CZ	2.41	0.50
72:CD:30:LYS:HG2	72:CD:66:GLU:OE1	2.12	0.50
77:CI:938:U:H2'	77:CI:939:C:H6	1.74	0.50
3:AC:1537:G:H2'	3:AC:1538:A:C8	2.46	0.50
39:BE:100:VAL:HG22	39:BE:117:LEU:HD21	1.93	0.50
41:BG:4:TYR:CE1	41:BG:18:ARG:HD2	2.47	0.50
67:Bg:16:THR:HG22	77:CI:2632:G:N7	2.26	0.50
77:CI:1040:C:C2	77:CI:1041:G:C8	2.99	0.50
77:CI:2168:A:H2'	77:CI:2169:U:C6	2.47	0.50
77:CI:2255:C:C2	77:CI:2256:U:C6	2.99	0.50
3:AC:1061:A:H1'	3:AC:1063:A:N7	2.25	0.50
13:AT:107:ASP:HB2	13:AT:125:ARG:HB3	1.93	0.50
25:AV:41:LEU:HD12	25:AV:45:TRP:CD1	2.46	0.50
28:AZ:137:SER:O	28:AZ:138:ASP:OD1	2.29	0.50
37:BC:10:VAL:HG13	37:BC:153:VAL:HG12	1.93	0.50
39:BE:203:ILE:HD11	57:BW:105:LEU:HD21	1.93	0.50
77:CI:1836:G:H2'	77:CI:1837:C:C6	2.47	0.50
77:CI:3893:G:H2'	77:CI:3894:A:C8	2.47	0.50
3:AC:457:C:N3	3:AC:458:C:C5	2.80	0.50
3:AC:811:A:H3'	3:AC:812:A:C5'	2.42	0.50
5:AH:20:TYR:CD2	5:AH:38:ILE:HD12	2.47	0.50
19:AG:12:LYS:HA	19:AG:56:ILE:HD13	1.93	0.50
36:BB:217:ILE:HD12	36:BB:347:LEU:HB3	1.93	0.50
5:AH:119:VAL:HG13	5:AH:119:VAL:O	2.12	0.50
7:AK:21:MET:HE2	7:AK:45:VAL:CG1	2.40	0.50
8:AL:97:TYR:CZ	8:AL:99:GLY:O	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Ag:153:LEU:HD11	33:Ag:186:ASN:OD1	2.12	0.50
57:BW:24:HIS:HA	57:BW:91:ASN:OD1	2.12	0.50
71:CC:18:ILE:HG12	71:CC:27:VAL:HG22	1.93	0.50
77:CI:174:C:N3	77:CI:175:C:C5	2.80	0.50
77:CI:241:G:C5	77:CI:242:U:C5	3.00	0.50
77:CI:1131:U:O4'	77:CI:1471:G:OP2	2.30	0.50
77:CI:3377:A2M:H2'	77:CI:3378:A:C8	2.47	0.50
77:CI:3775:G:O3'	77:CI:3776:C:O4'	2.30	0.50
77:CI:4061:U:C2	77:CI:4062:G:C8	2.99	0.50
47:BM:69:LYS:HG3	47:BM:71:GLU:OE2	2.11	0.50
77:CI:1121:A:H2'	77:CI:1122:C:C6	2.45	0.50
77:CI:3376:A:H2'	77:CI:3377:A2M:C8	2.42	0.50
77:CI:4099:C:C2	77:CI:4100:U:C5	2.99	0.50
19:AG:124:ASP:OD2	19:AG:145:VAL:HG13	2.12	0.50
25:AV:147:LEU:HD22	25:AV:151:ASP:OD2	2.12	0.50
33:Ag:69:LEU:HD11	33:Ag:132:ASP:OD1	2.11	0.50
36:BB:86:VAL:HG13	36:BB:162:ILE:CG2	2.41	0.50
42:BH:41:SER:O	42:BH:45:GLN:OE1	2.30	0.50
66:Bf:9:ARG:HD3	77:CI:3945:U:OP1	2.12	0.50
77:CI:1132:C:OP1	77:CI:1132:C:H4'	2.12	0.50
79:CK:83:C:H4'	79:CK:84:A:OP2	2.11	0.50
3:AC:1438:C:O2'	3:AC:1439:A:P	2.70	0.50
26:AW:74:GLY:O	26:AW:78:LEU:HD13	2.11	0.50
42:BH:125:GLN:O	42:BH:129:GLU:HG3	2.11	0.50
70:CB:164:ILE:CG2	76:CH:22:LEU:HD11	2.42	0.50
3:AC:1713:A:H2'	3:AC:1714:C:C6	2.47	0.49
20:AI:97:THR:HG23	20:AI:97:THR:O	2.12	0.49
23:AS:49:ALA:O	23:AS:53:ILE:HD12	2.11	0.49
24:AU:202:THR:HG23	26:AW:58:ARG:HH22	1.77	0.49
44:BJ:69:GLU:HA	44:BJ:69:GLU:OE2	2.12	0.49
13:AT:104:HIS:NE2	13:AT:122:SER:OG	2.45	0.49
24:AU:166:ARG:HB3	24:AU:247:THR:HB	1.94	0.49
77:CI:1446:G:H5'	77:CI:1447:A:OP1	2.13	0.49
3:AC:1688:C:C2	3:AC:1689:C:C5	3.00	0.49
3:AC:1794:A:C2	3:AC:1795:C:C5	2.99	0.49
7:AK:48:ALA:O	7:AK:52:LEU:HD13	2.13	0.49
13:AT:64:HIS:CG	13:AT:65:PHE:H	2.30	0.49
26:AW:87:LEU:CD1	26:AW:100:LEU:HD21	2.42	0.49
69:CA:147:LEU:HD22	69:CA:152:ILE:CD1	2.42	0.49
10:AN:15:VAL:CG2	10:AN:20:ILE:HD13	2.42	0.49
42:BH:4:ASP:HB2	69:CA:120:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BL:27:HIS:HB2	46:BL:28:PRO:HD3	1.94	0.49
67:Bg:61:MET:HE3	77:CI:2408:G:H22	1.77	0.49
1:AA:11:LEU:CD1	6:AJ:33:ILE:HD11	2.42	0.49
2:AB:24:CYS:SG	2:AB:39:CYS:HB3	2.52	0.49
3:AC:1309:U:HO2'	3:AC:1310:C:H6	1.53	0.49
33:Ag:158:LEU:HD12	33:Ag:189:PHE:CE2	2.48	0.49
40:BF:199:ASN:HB3	75:CG:104:MET:HE2	1.94	0.49
70:CB:42:GLY:O	70:CB:43:GLN:HG2	2.11	0.49
71:CC:91:LYS:HG2	71:CC:145:ILE:CD1	2.42	0.49
73:CE:26:VAL:CG2	73:CE:33:LEU:HD23	2.41	0.49
73:CE:50:PHE:CD1	73:CE:70:VAL:HG12	2.46	0.49
74:CF:55:ILE:HD11	74:CF:154:VAL:HG11	1.93	0.49
77:CI:433:A:C2	77:CI:3526:A2M:H4'	2.48	0.49
3:AC:68:A:N6	3:AC:82:G:C2	2.81	0.49
18:AF:139:LEU:HD12	18:AF:139:LEU:C	2.37	0.49
26:AW:130:ILE:HG21	26:AW:145:PRO:HA	1.94	0.49
77:CI:424:U:H2'	77:CI:425:U:H6	1.78	0.49
77:CI:473:C:C2	77:CI:474:C:C5	3.01	0.49
77:CI:1323:G:H2'	77:CI:1324:C:C6	2.48	0.49
77:CI:2141:U:C2	77:CI:2142:U:C5	3.01	0.49
77:CI:2446:C:C2	77:CI:2447:U:C6	3.01	0.49
77:CI:4114:U:H2'	77:CI:4115:U:C6	2.48	0.49
3:AC:1538:A:O2'	3:AC:1605:G:H4'	2.13	0.49
8:AL:20:VAL:HG13	8:AL:24:GLN:HG3	1.95	0.49
28:AZ:34:PHE:CD1	28:AZ:98:ARG:NH1	2.80	0.49
41:BG:94:MET:HE1	41:BG:146:ILE:HB	1.95	0.49
51:BQ:135:ARG:NH1	77:CI:2509:G:C5'	2.76	0.49
60:BZ:3:LEU:CD2	74:CF:172:GLU:OE2	2.60	0.49
69:CA:154:MET:HA	69:CA:157:ILE:HD12	1.95	0.49
77:CI:4651:U:H2'	77:CI:4652:C:C6	2.48	0.49
3:AC:220:U:C2	3:AC:221:U:C5	3.01	0.49
18:AF:139:LEU:HD21	18:AF:169:ILE:HD11	1.95	0.49
26:AW:67:ASP:O	26:AW:71:LEU:HD23	2.13	0.49
52:BR:140:VAL:HG12	52:BR:140:VAL:O	2.11	0.49
71:CC:21:LYS:HG3	71:CC:21:LYS:O	2.13	0.49
77:CI:50:C:C2	77:CI:51:A:C8	3.00	0.49
77:CI:201:C:C2	77:CI:202:C:C5	3.01	0.49
77:CI:392:U:C2	77:CI:393:U:C5	3.01	0.49
3:AC:1273:C:O2'	3:AC:1274:C:H6	1.95	0.49
3:AC:1825:A:H2'	77:CI:3419:A:H61	1.78	0.49
10:AN:26:ILE:HG23	10:AN:45:LEU:CD2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Af:118:ARG:HE	16:Af:119:ARG:H	1.61	0.49
24:AU:102:LEU:HD22	24:AU:130:ILE:HG12	1.95	0.49
60:BZ:93:VAL:HG12	60:BZ:97:MET:HE2	1.93	0.49
66:Bf:33:LEU:HD23	66:Bf:33:LEU:O	2.12	0.49
1:AA:59:LEU:HD23	6:AJ:123:GLU:OE1	2.13	0.48
3:AC:128:U:O4'	3:AC:217:G:C8	2.66	0.48
3:AC:637:C:H2'	3:AC:638:U:O4'	2.13	0.48
5:AH:114:LEU:O	5:AH:117:LEU:HD22	2.13	0.48
13:AT:191:HIS:NE2	13:AT:195:LEU:HD21	2.28	0.48
36:BB:337:VAL:HG11	36:BB:345:LEU:HD13	1.94	0.48
73:CE:39:VAL:HG22	73:CE:123:ILE:HD11	1.94	0.48
77:CI:1122:C:C2	77:CI:1123:C:C5	3.01	0.48
8:AL:83:MET:HB3	8:AL:116:LEU:HD12	1.94	0.48
17:AD:143:THR:HB	17:AD:205:TYR:CE2	2.48	0.48
18:AF:87:MET:SD	18:AF:100:ARG:HD3	2.53	0.48
28:AZ:20:GLN:O	28:AZ:20:GLN:HG2	2.13	0.48
30:Ab:118:ARG:HG3	30:Ab:119:GLY:H	1.78	0.48
37:BC:230:LEU:HD21	37:BC:235:LEU:HA	1.95	0.48
40:BF:194:GLU:O	40:BF:198:THR:HG23	2.12	0.48
77:CI:2167:C:H2'	77:CI:2168:A:H8	1.78	0.48
77:CI:4048:G:O4'	77:CI:4102:5MC:HM53	2.13	0.48
3:AC:1446:U:O2'	3:AC:1447:A:H8	1.95	0.48
9:AM:55:VAL:HG22	9:AM:63:PHE:CE2	2.48	0.48
27:AY:45:LEU:HD13	27:AY:53:ILE:HD12	1.95	0.48
30:Ab:20:ARG:HA	30:Ab:75:ILE:O	2.13	0.48
44:BJ:106:VAL:HG13	44:BJ:126:ILE:CD1	2.43	0.48
77:CI:162:A:H2'	77:CI:163:A:C8	2.48	0.48
77:CI:2112:U:H5'	79:CK:14:OMU:HM21	1.94	0.48
77:CI:3532:G:H2'	77:CI:3533:G:C8	2.49	0.48
77:CI:4502:G:H2'	77:CI:4503:G:O4'	2.12	0.48
3:AC:289:G:H1	3:AC:296:C:H42	1.61	0.48
3:AC:1271:G:C2	3:AC:1272:C:C5	3.01	0.48
3:AC:1588:G:C6	11:AO:67:ARG:HD2	2.48	0.48
7:AK:5:LYS:O	7:AK:9:ILE:HG12	2.14	0.48
25:AV:25:ARG:HA	25:AV:28:TYR:HD2	1.78	0.48
38:BD:104:LEU:HD13	38:BD:247:ILE:HG23	1.95	0.48
77:CI:1660:A:C2	77:CI:1661:C:C5	3.01	0.48
77:CI:2541:C:C5	77:CI:2542:B9H:N4	2.81	0.48
77:CI:3749:C:H2'	77:CI:3750:G:O4'	2.13	0.48
20:AI:134:LEU:HD22	20:AI:144:THR:HG21	1.94	0.48
23:AS:58:VAL:HG13	28:AZ:125:LYS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ah:46:VAL:HG21	34:Ah:56:ARG:HE	1.78	0.48
34:Ah:53:LYS:NZ	34:Ah:55:TYR:CE2	2.81	0.48
34:Ah:103:LEU:HD23	34:Ah:172:LEU:HD23	1.95	0.48
50:BP:47:MET:HE1	50:BP:118:ILE:HD12	1.96	0.48
56:BV:129:LEU:HD23	56:BV:129:LEU:H	1.79	0.48
77:CI:3376:A:H2'	77:CI:3377:A2M:H8	1.95	0.48
77:CI:4615:A:H2'	77:CI:4616:A:C8	2.48	0.48
3:AC:85:A:H5''	30:Ab:118:ARG:HE	1.77	0.48
3:AC:805:U:H2'	3:AC:806:U:C6	2.49	0.48
3:AC:997:A:H2'	3:AC:998:A:C8	2.48	0.48
3:AC:1149:A:H4'	3:AC:1150:A:O4'	2.14	0.48
23:AS:44:ILE:HG12	23:AS:67:LEU:HD11	1.95	0.48
24:AU:66:LEU:HD21	24:AU:86:LEU:CD1	2.43	0.48
60:BZ:63:VAL:HG23	60:BZ:65:LYS:HG3	1.96	0.48
77:CI:37:U:H2'	77:CI:38:A:O4'	2.13	0.48
77:CI:1875:C:C2	77:CI:1876:C:C5	3.02	0.48
77:CI:3352:U:C2	77:CI:3353:U:C6	3.01	0.48
30:Ab:110:ARG:O	30:Ab:114:MET:HG2	2.13	0.48
34:Ah:67:TRP:O	34:Ah:191:GLU:OE1	2.31	0.48
34:Ah:158:ILE:CG2	34:Ah:162:LEU:HD23	2.40	0.48
35:BA:102:LEU:HB2	35:BA:107:MET:HE2	1.96	0.48
50:BP:115:ARG:HA	50:BP:118:ILE:HG12	1.96	0.48
3:AC:572:U:O2'	30:Ab:60:PHE:O	2.24	0.48
3:AC:1316:U:C4	3:AC:1317:C:C5	3.02	0.48
3:AC:1825:A:N1	3:AC:1827:G:N7	2.61	0.48
9:AM:50:LYS:HA	9:AM:53:GLU:HG3	1.95	0.48
17:AD:52:THR:HG22	17:AD:58:ALA:H	1.78	0.48
70:CB:93:THR:O	70:CB:97:LYS:HG2	2.13	0.48
3:AC:823:PSU:C4	3:AC:828:A:C6	2.99	0.48
3:AC:1799:C:H2'	3:AC:1800:G:O4'	2.14	0.48
5:AH:66:VAL:O	5:AH:68:GLY:N	2.47	0.48
8:AL:60:LEU:HD23	8:AL:76:VAL:HG21	1.96	0.48
9:AM:100:VAL:HG12	9:AM:101:ASP:N	2.28	0.48
11:AO:99:VAL:O	11:AO:103:VAL:HG23	2.13	0.48
29:Aa:32:LYS:O	29:Aa:35:VAL:HG22	2.14	0.48
31:Ad:48:SER:O	31:Ad:49:HIS:HB2	2.14	0.48
35:BA:196:TRP:HB3	35:BA:197:PRO:HD3	1.94	0.48
45:BK:115:LYS:CE	45:BK:126:VAL:HG21	2.44	0.48
47:BM:13:LYS:HD2	47:BM:128:LEU:HD11	1.94	0.48
77:CI:2449:G:H2'	77:CI:2450:G:N2	2.28	0.48
77:CI:4108:C:C2	77:CI:4184:G:C2	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:4610:C:H2'	77:CI:4611:G:C8	2.48	0.48
3:AC:29:G:H2'	3:AC:30:C:C6	2.49	0.48
3:AC:115:U:H2'	3:AC:116:OMU:C6	2.43	0.48
36:BB:303:ALA:HB2	36:BB:314:ILE:HD13	1.95	0.48
46:BL:85:TYR:CD2	77:CI:2388:U:C5	3.02	0.48
46:BL:91:LEU:HD12	46:BL:96:LEU:HB3	1.96	0.48
6:AJ:136:ARG:HB3	6:AJ:203:ASN:HD22	1.79	0.47
44:BJ:154:LEU:HD13	44:BJ:157:ARG:CZ	2.43	0.47
48:BN:46:PRO:HA	48:BN:49:ILE:HD13	1.95	0.47
71:CC:71:ARG:HG2	77:CI:4346:A:H4'	1.94	0.47
77:CI:174:C:C2	77:CI:175:C:C6	3.02	0.47
77:CI:204:U:H2'	77:CI:205:C:H6	1.78	0.47
77:CI:3566:G:C2	77:CI:3568:OMC:C4	2.87	0.47
3:AC:906:C:H2'	3:AC:907:U:C6	2.49	0.47
3:AC:943:G:N2	28:AZ:138:ASP:OD2	2.47	0.47
10:AN:51:ASP:OD1	10:AN:54:LYS:HD2	2.14	0.47
35:BA:112:ILE:HG23	35:BA:133:TYR:CD1	2.49	0.47
70:CB:137[A]:ARG:HG2	70:CB:142:THR:HG21	1.96	0.47
77:CI:1128:C:H41	77:CI:1138:A:C5'	2.27	0.47
77:CI:3913:C:N3	77:CI:3914:C:C5	2.82	0.47
77:CI:4246:U:H2'	77:CI:4247:C:C6	2.49	0.47
79:CK:19:C:H2'	79:CK:20:A:C8	2.50	0.47
20:AI:205:ARG:HB2	20:AI:210:ILE:HD11	1.97	0.47
36:BB:219:VAL:HG11	36:BB:337:VAL:CG1	2.44	0.47
37:BC:350:ARG:O	37:BC:354:LEU:HD23	2.14	0.47
70:CB:217:LYS:O	70:CB:220:GLU:HG3	2.14	0.47
77:CI:424:U:H2'	77:CI:425:U:C6	2.50	0.47
77:CI:4266:A:C2	77:CI:4267:C:C5	3.02	0.47
3:AC:12:U:H2'	3:AC:13:C:C6	2.50	0.47
3:AC:496:U:H2'	3:AC:497:C:O4'	2.14	0.47
14:AX:52:LEU:HD21	14:AX:65:VAL:CG1	2.44	0.47
17:AD:57:ILE:HD12	70:CB:260:GLU:OE2	2.14	0.47
33:Ag:29:GLU:HG2	33:Ag:29:GLU:O	2.14	0.47
36:BB:67:VAL:O	36:BB:67:VAL:HG22	2.15	0.47
36:BB:104:THR:HG22	77:CI:4379:A:O2'	2.15	0.47
39:BE:214:VAL:HG13	39:BE:264:GLN:CD	2.39	0.47
77:CI:240:G:H2'	77:CI:241:G:O4'	2.14	0.47
77:CI:1475:C:H2'	77:CI:1476:C:H6	1.80	0.47
77:CI:2048:C:H2'	77:CI:2049:U:C6	2.49	0.47
77:CI:4428:C:C2	77:CI:4429:C:C5	3.03	0.47
1:AA:24:GLN:HB2	1:AA:26:GLN:NE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AJ:135:ARG:HH22	28:AZ:66:ARG:HD2	1.79	0.47
7:AK:86:PRO:HB2	7:AK:88:GLU:OE1	2.15	0.47
8:AL:20:VAL:HG12	8:AL:25:LEU:HG	1.96	0.47
49:BO:76:ILE:HA	49:BO:101:ASP:OD1	2.14	0.47
77:CI:1281:C:H2'	77:CI:1282:C:H6	1.78	0.47
18:AF:59:ASP:OD1	18:AF:62:LYS:HE3	2.15	0.47
18:AF:64:ILE:HG21	30:Ab:17:LEU:HD23	1.96	0.47
22:AR:105:PHE:HD1	22:AR:121:LYS:HB3	1.78	0.47
26:AW:80:ARG:O	26:AW:83:ARG:HG2	2.14	0.47
52:BR:34:ASN:O	77:CI:94:A:H5''	2.14	0.47
77:CI:660:C:C2	77:CI:661:C:C5	3.02	0.47
77:CI:3259:G:H2'	77:CI:3260:C:H6	1.79	0.47
77:CI:3935:A:N3	77:CI:3935:A:H2'	2.30	0.47
3:AC:561:A:N6	3:AC:589:G:O6	2.48	0.47
3:AC:953:G:H2'	3:AC:954:C:C6	2.50	0.47
3:AC:959:G:H2'	3:AC:960:G:C8	2.49	0.47
3:AC:1375:C:H2'	3:AC:1376:G:O4'	2.15	0.47
3:AC:1406:A:H2'	3:AC:1407:G:O4'	2.15	0.47
6:AJ:25:THR:HG21	6:AJ:46:ALA:CB	2.45	0.47
10:AN:101:ASN:ND2	73:CE:121:PRO:HD3	2.29	0.47
13:AT:14:HIS:NE2	13:AT:35:SER:HB2	2.30	0.47
13:AT:62:HIS:HD2	13:AT:82:SER:HB2	1.80	0.47
17:AD:165:ARG:HG2	17:AD:169:MET:HE1	1.95	0.47
33:Ag:8:ILE:HG22	33:Ag:8:ILE:O	2.15	0.47
38:BD:50:ARG:NH1	38:BD:52:ILE:HG13	2.29	0.47
46:BL:87:THR:O	46:BL:91:LEU:HD23	2.14	0.47
62:Bb:2:PRO:HB2	77:CI:2448:U:O2	2.15	0.47
62:Bb:47:ILE:HD11	62:Bb:56:LEU:HD22	1.97	0.47
77:CI:220:C:O2	77:CI:220:C:H2'	2.15	0.47
77:CI:660:C:C2	77:CI:661:C:C6	3.02	0.47
77:CI:1606:A:O4'	77:CI:1608:G:C8	2.68	0.47
77:CI:2542:B9H:O2'	77:CI:2543:A:OP2	2.33	0.47
77:CI:3526:A2M:HM'2	77:CI:3526:A2M:H1'	1.80	0.47
77:CI:3913:C:C2	77:CI:3914:C:C5	3.03	0.47
3:AC:164:A:H2'	3:AC:165:G:C8	2.50	0.47
3:AC:1026:U:H2'	3:AC:1027:C:O4'	2.14	0.47
13:AT:64:HIS:ND1	13:AT:83:TRP:HB2	2.30	0.47
26:AW:88:ASP:O	26:AW:92:MET:HE3	2.15	0.47
36:BB:248:LEU:O	36:BB:248:LEU:HD23	2.15	0.47
37:BC:105:THR:HG22	37:BC:109:ARG:NH2	2.30	0.47
77:CI:272:U:H2'	77:CI:273:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:4193:G:H2'	77:CI:4194:U:C6	2.49	0.47
3:AC:1395:G:H2'	3:AC:1396:C:O2	2.15	0.47
3:AC:1706:C:H2'	3:AC:1707:G:C8	2.50	0.47
10:AN:67:VAL:HG12	10:AN:71:MET:HE2	1.97	0.47
18:AF:43:PRO:HD2	18:AF:46:ILE:HD12	1.97	0.47
29:Aa:42:MET:HE3	29:Aa:50:PHE:CE1	2.50	0.47
34:Ah:130:THR:O	34:Ah:134:GLU:OE1	2.33	0.47
58:BX:93:ARG:O	58:BX:97:ILE:CD1	2.63	0.47
77:CI:1475:C:H2'	77:CI:1476:C:C6	2.50	0.47
77:CI:4552:C:N3	77:CI:4553:C:C6	2.83	0.47
77:CI:4615:A:H2'	77:CI:4616:A:H8	1.80	0.47
77:CI:4618:C:C2	77:CI:4619:A:C8	3.03	0.47
78:CJ:17:C:H2'	78:CJ:18:C:C6	2.50	0.47
3:AC:107:A:H2'	3:AC:108:G:C8	2.50	0.47
3:AC:638:U:N3	3:AC:639:C:C5	2.83	0.47
24:AU:166:ARG:CB	24:AU:248:TYR:CE1	2.98	0.47
26:AW:38:ARG:HE	26:AW:39:ASN:ND2	2.13	0.47
46:BL:63:ILE:HA	46:BL:71:THR:O	2.14	0.47
73:CE:94:LEU:HD12	73:CE:166:PHE:CZ	2.50	0.47
77:CI:129:C:H2'	77:CI:130:G:H8	1.79	0.47
77:CI:472:C:H2'	77:CI:473:C:H6	1.79	0.47
77:CI:2300:G:N7	79:CK:126:C:N4	2.63	0.47
77:CI:3948:PSU:N3	77:CI:3949:C:C5	2.83	0.47
3:AC:987:G:C8	28:AZ:137:SER:O	2.68	0.46
24:AU:130:ILE:HD13	24:AU:159:LYS:HG2	1.96	0.46
38:BD:236:MET:O	38:BD:239:MET:HG2	2.14	0.46
50:BP:49:ILE:HD13	50:BP:80:ILE:HD13	1.96	0.46
50:BP:74:TYR:OH	79:CK:75:G:OP2	2.33	0.46
56:BV:84:GLU:O	56:BV:87:VAL:HG22	2.16	0.46
77:CI:1129:C:O2'	77:CI:2104:G:N2	2.48	0.46
77:CI:1281:C:C2	77:CI:1282:C:C5	3.03	0.46
17:AD:46:LYS:CE	28:AZ:21:VAL:HG12	2.45	0.46
29:Aa:38:LEU:HD23	29:Aa:41:MET:HE3	1.96	0.46
35:BA:135:THR:HB	35:BA:149:LYS:HG2	1.98	0.46
77:CI:236:G:C2'	77:CI:237:B9B:OP1	2.63	0.46
79:CK:92:U:H2'	79:CK:93:C:O4'	2.15	0.46
3:AC:1390:C:C2	3:AC:1391:U:C5	3.04	0.46
3:AC:1629:C:H2'	3:AC:1630:C:C6	2.51	0.46
11:AO:18:LEU:HD13	11:AO:134:ILE:HD12	1.97	0.46
26:AW:81:LEU:HD12	26:AW:97:ILE:HD12	1.98	0.46
57:BW:4:ARG:NH2	57:BW:8:LYS:HG3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:CC:47:LEU:C	71:CC:48:LEU:HD22	2.40	0.46
73:CE:33:LEU:HD11	73:CE:67:LYS:O	2.15	0.46
77:CI:100:C:C2	77:CI:101:A:C8	3.03	0.46
77:CI:947:G:C2	77:CI:1038:G:N1	2.83	0.46
3:AC:1274:C:H1'	3:AC:1276:G:OP1	2.16	0.46
6:AJ:49:LEU:HD11	9:AM:49:TYR:HB3	1.97	0.46
10:AN:4:VAL:C	10:AN:5:ILE:HG13	2.40	0.46
15:Ac:50:PHE:HZ	15:Ac:87:ALA:HB2	1.81	0.46
35:BA:207:VAL:HG13	35:BA:208:GLU:OE1	2.15	0.46
40:BF:147:TRP:CZ2	40:BF:149:TYR:O	2.69	0.46
46:BL:23:LEU:HD23	46:BL:110:TYR:HB2	1.98	0.46
77:CI:1350:A:H2'	77:CI:1351:U:C6	2.50	0.46
3:AC:830:C:OP1	18:AF:21:ASP:OD1	2.34	0.46
3:AC:943:G:N2	28:AZ:138:ASP:HB2	2.31	0.46
3:AC:986:G:C1'	28:AZ:138:ASP:OD2	2.64	0.46
3:AC:1008:C:H2'	3:AC:1009:A:C8	2.51	0.46
3:AC:1403:A:N1	3:AC:1406:A:C2	2.83	0.46
3:AC:1598:C:H4'	3:AC:1604:G:O6	2.15	0.46
9:AM:48:GLN:HE22	9:AM:52:LEU:HD11	1.80	0.46
12:AP:66:ARG:HG3	12:AP:68:THR:HG22	1.96	0.46
13:AT:229:THR:C	13:AT:230:LEU:HD12	2.40	0.46
17:AD:87:ILE:HB	17:AD:101:HIS:CD2	2.50	0.46
33:Ag:36:LEU:HA	33:Ag:39:GLN:OE1	2.15	0.46
33:Ag:63:PHE:CZ	33:Ag:95:ILE:HD11	2.51	0.46
55:BU:26:THR:HG21	77:CI:4645:G:OP1	2.15	0.46
73:CE:57:VAL:HG11	73:CE:60:PHE:CD2	2.50	0.46
77:CI:1700:C:H5''	77:CI:1873:A:OP1	2.15	0.46
77:CI:2432:A:OP1	77:CI:2432:A:O4'	2.34	0.46
77:CI:3570:C:C2	77:CI:3571:U:C5	3.04	0.46
77:CI:3918:C:H2'	77:CI:3919:G:O4'	2.16	0.46
3:AC:1396:C:C2	3:AC:1475:A:C2	3.04	0.46
13:AT:221:LEU:HD12	13:AT:221:LEU:N	2.31	0.46
25:AV:21:GLU:O	25:AV:25:ARG:HG2	2.15	0.46
35:BA:124:GLY:O	35:BA:125:LYS:HB2	2.15	0.46
60:BZ:33:LEU:HD13	60:BZ:41:ARG:NH2	2.31	0.46
60:BZ:34:THR:HG21	77:CI:276:C:H5'	1.98	0.46
77:CI:162:A:H2'	77:CI:163:A:H8	1.80	0.46
1:AA:17:VAL:HG23	1:AA:17:VAL:O	2.14	0.46
1:AA:60:GLU:HG2	6:AJ:204:ARG:HD3	1.98	0.46
3:AC:494:A:C2	3:AC:495:C:C6	3.04	0.46
3:AC:1534:A:C2	3:AC:1537:G:N3	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:1541:G:OP2	11:AO:43:LYS:CE	2.64	0.46
3:AC:1554:C:OP1	3:AC:1554:C:H3'	2.15	0.46
11:AO:39:LEU:HD11	11:AO:52:TRP:CD2	2.51	0.46
17:AD:126:ASP:OD1	17:AD:136:ARG:HD3	2.16	0.46
24:AU:272:HIS:CE1	24:AU:276:THR:CG2	2.98	0.46
36:BB:36:ASP:HB3	36:BB:39:LYS:HE2	1.96	0.46
36:BB:194:LEU:O	36:BB:198:ARG:HG3	2.15	0.46
41:BG:33:ALA:HA	41:BG:36:ILE:HG22	1.97	0.46
51:BQ:87:VAL:CG1	51:BQ:89:ILE:HD12	2.45	0.46
72:CD:200:ILE:HG13	72:CD:200:ILE:O	2.16	0.46
76:CH:126:THR:HG23	76:CH:127:TYR:CD2	2.51	0.46
77:CI:1609:C:H2'	77:CI:1610:C:H6	1.80	0.46
77:CI:1682:G:OP2	77:CI:1683:C:H3'	2.15	0.46
77:CI:3315:A:H2'	77:CI:3316:U:H6	1.80	0.46
79:CK:141:C:H2'	79:CK:142:U:C6	2.51	0.46
3:AC:593:C:H3'	3:AC:594:C:H5''	1.97	0.46
3:AC:875:G:H2'	3:AC:876:A:H8	1.81	0.46
3:AC:1628:C:H2'	3:AC:1629:C:H6	1.81	0.46
10:AN:85:ASN:H	10:AN:97:GLN:HG2	1.80	0.46
30:Ab:58:PHE:CE1	30:Ab:90:ARG:NH1	2.84	0.46
51:BQ:54:THR:H	51:BQ:57:MET:HE3	1.80	0.46
51:BQ:100:VAL:HG13	51:BQ:106:LEU:C	2.40	0.46
77:CI:1614:C:C2	77:CI:1615:U:C5	3.04	0.46
77:CI:3343:G:H2'	77:CI:3344:C:C6	2.51	0.46
77:CI:3512:U:C2	77:CI:3513:C:C5	3.03	0.46
77:CI:3950:U:H2'	77:CI:3951:U:H5'	1.97	0.46
3:AC:164:A:H2'	3:AC:165:G:H8	1.81	0.46
3:AC:349:A:H2'	3:AC:350:A:C8	2.51	0.46
3:AC:1533:C:H5'	3:AC:1605:G:H21	1.80	0.46
3:AC:1857:C:H2'	3:AC:1858:G:C8	2.51	0.46
5:AH:91:LEU:HD21	20:AI:17:LYS:HB3	1.96	0.46
15:Ac:79:ILE:HD11	15:Ac:83:LEU:CD2	2.46	0.46
35:BA:245:ARG:NH1	77:CI:3315:A:H5''	2.31	0.46
47:BM:121:VAL:HG21	47:BM:136:ALA:HB2	1.98	0.46
50:BP:50:ARG:NH1	50:BP:110:LYS:HD3	2.31	0.46
73:CE:141:ILE:HA	73:CE:144:LYS:HE3	1.97	0.46
77:CI:1361:G:O2'	77:CI:2568:A:H8	1.99	0.46
77:CI:3723:U:H2'	77:CI:3724:U:C6	2.50	0.46
77:CI:3867:A:H4'	77:CI:3868:A:N3	2.31	0.46
79:CK:5:U:C2	79:CK:6:C:C5	3.04	0.46
3:AC:963:A:H4'	28:AZ:66:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:1715:U:H2'	3:AC:1716:A:C8	2.51	0.46
18:AF:136:ILE:O	18:AF:136:ILE:HG13	2.16	0.46
22:AR:87:ASN:OD1	22:AR:134:TYR:CE1	2.69	0.46
30:Ab:51:THR:HG22	30:Ab:53:ASP:H	1.81	0.46
38:BD:41:LYS:HE2	38:BD:41:LYS:HA	1.98	0.46
77:CI:25:A:C8	77:CI:341:G:C8	3.04	0.46
77:CI:1523:G:H2'	77:CI:1524:C:H6	1.81	0.46
77:CI:2611:G:C2'	77:CI:2612:C:OP2	2.64	0.46
77:CI:3398:C:C2	77:CI:3399:G:C8	3.04	0.46
3:AC:1626:U:N3	3:AC:1627:C:C5	2.84	0.45
6:AJ:200:ALA:O	6:AJ:203:ASN:OD1	2.34	0.45
8:AL:85:ILE:HA	8:AL:89:MET:HE2	1.98	0.45
10:AN:83:PHE:CD1	10:AN:83:PHE:O	2.69	0.45
23:AS:45:VAL:HG21	23:AS:53:ILE:HD13	1.97	0.45
24:AU:202:THR:HG23	26:AW:58:ARG:NH2	2.31	0.45
43:BI:28:GLU:OE1	43:BI:49:LEU:HD13	2.17	0.45
55:BU:32:ARG:HB3	55:BU:48:GLU:HG3	1.98	0.45
61:Ba:36:LYS:HE2	77:CI:372:A:OP1	2.16	0.45
67:Bg:17:ARG:O	67:Bg:18:TYR:CD1	2.69	0.45
69:CA:221:LYS:O	69:CA:222:ARG:HB2	2.17	0.45
77:CI:3571:U:O2'	77:CI:3572:G:H5'	2.16	0.45
1:AA:31:ARG:HE	1:AA:43:ILE:HD11	1.80	0.45
2:AB:13:LYS:HG3	2:AB:14:PHE:CD2	2.51	0.45
3:AC:350:A:H2'	3:AC:351:C:C6	2.51	0.45
3:AC:1546:A:H2'	3:AC:1547:G:C8	2.51	0.45
3:AC:1798:U:H2'	3:AC:1799:C:C6	2.50	0.45
3:AC:1827:G:C5	3:AC:1828:U:C5	3.04	0.45
10:AN:26:ILE:HG23	10:AN:45:LEU:HD21	1.97	0.45
13:AT:83:TRP:HA	13:AT:107:ASP:HA	1.98	0.45
13:AT:201:SER:OG	13:AT:202:PRO:HD2	2.15	0.45
37:BC:209:ILE:HB	37:BC:229:LEU:HD13	1.97	0.45
77:CI:7:C:H2'	77:CI:8:U:C6	2.51	0.45
77:CI:353:A:C4	77:CI:379:G:N7	2.84	0.45
77:CI:390:C:C2	77:CI:391:U:C5	3.04	0.45
77:CI:716:G:H2'	77:CI:717:A:H8	1.81	0.45
77:CI:1129:C:N4	77:CI:1138:A:P	2.89	0.45
77:CI:3352:U:C4	77:CI:3353:U:C5	3.04	0.45
2:AB:14:PHE:CZ	3:AC:1618:G:H4'	2.51	0.45
5:AH:30:THR:O	5:AH:34:VAL:HG23	2.17	0.45
9:AM:44:PRO:HB2	9:AM:81:ILE:HD11	1.98	0.45
74:CF:60:ARG:HD2	74:CF:67:HIS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:424:U:C2	77:CI:425:U:C5	3.04	0.45
77:CI:1128:C:H41	77:CI:1138:A:H5''	1.81	0.45
3:AC:637:C:H2'	3:AC:638:U:C6	2.51	0.45
17:AD:71:LEU:HD13	17:AD:84:PHE:CD2	2.52	0.45
37:BC:163:LYS:O	37:BC:166:GLU:HG2	2.17	0.45
39:BE:158:LEU:HB3	39:BE:202:VAL:CG1	2.47	0.45
57:BW:4:ARG:O	77:CI:4593:G:O6	2.34	0.45
70:CB:207:VAL:CG1	70:CB:211:ASP:OD1	2.65	0.45
77:CI:1317:G:H2'	77:CI:1318:C:C6	2.51	0.45
77:CI:1483:G:OP1	77:CI:1484:U:C5	2.70	0.45
77:CI:2559:U:H2'	77:CI:2560:OMC:H6	1.81	0.45
2:AB:56:ASP:C	2:AB:56:ASP:OD1	2.59	0.45
3:AC:350:A:H2'	3:AC:351:C:H6	1.82	0.45
3:AC:1349:G:C8	3:AC:1350:G:C8	3.05	0.45
17:AD:108:ASP:HA	17:AD:111:CYS:SG	2.57	0.45
18:AF:53:LYS:HG3	18:AF:53:LYS:O	2.16	0.45
19:AG:120:VAL:HG13	19:AG:124:ASP:OD2	2.17	0.45
34:Ah:107:THR:OG1	34:Ah:108:PRO:HD3	2.16	0.45
35:BA:101:VAL:HG22	35:BA:165:VAL:HG22	1.98	0.45
40:BF:105:LEU:C	40:BF:105:LEU:HD12	2.42	0.45
55:BU:65:ASP:OD2	55:BU:67:ARG:HB2	2.17	0.45
69:CA:204:PHE:CD1	69:CA:222:ARG:HG2	2.51	0.45
77:CI:423:G:H2'	77:CI:424:U:C6	2.51	0.45
77:CI:2241:U:N3	77:CI:2242:G:N7	2.65	0.45
77:CI:2415:A:C2	77:CI:2432:A:N9	2.85	0.45
79:CK:127:U:H5'	79:CK:128:C:OP1	2.15	0.45
3:AC:1124:C:C4	3:AC:1125:C:C5	3.04	0.45
3:AC:1541:G:OP2	11:AO:43:LYS:HE3	2.16	0.45
5:AH:89:SER:HB3	20:AI:198:MET:HE3	1.98	0.45
8:AL:82:ASP:OD1	8:AL:82:ASP:C	2.59	0.45
21:AQ:59:ILE:HD13	21:AQ:62:MET:HE3	1.98	0.45
29:Aa:104:LEU:HD23	29:Aa:125:ILE:HA	1.98	0.45
34:Ah:103:LEU:HD13	34:Ah:170:LYS:HD3	1.99	0.45
74:CF:33:ILE:HG22	74:CF:37:LYS:HE2	1.99	0.45
77:CI:1430:G:H1'	77:CI:2269:A:N6	2.31	0.45
77:CI:1697:G:H2'	77:CI:1698:A:O4'	2.17	0.45
77:CI:2600:A:O2'	77:CI:4286:G:H4'	2.16	0.45
77:CI:4307:G:H2'	77:CI:4308:C:H6	1.81	0.45
3:AC:1829:C:H2'	3:AC:1830:G:O4'	2.16	0.45
8:AL:110:GLU:HB2	10:AN:117:ILE:CG2	2.46	0.45
13:AT:17:TRP:CE2	13:AT:303:THR:HG23	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AT:25:PRO:HA	13:AT:293:ALA:HB1	1.99	0.45
18:AF:11:ARG:HD3	18:AF:28:ALA:HB2	1.98	0.45
37:BC:150:LEU:HB2	37:BC:151:PRO:HD3	1.97	0.45
40:BF:185:VAL:O	40:BF:189:ILE:HG12	2.17	0.45
41:BG:29:THR:HG21	41:BG:146:ILE:HD11	1.99	0.45
61:Ba:83:THR:HG23	61:Ba:84:PRO:HD2	1.99	0.45
65:Be:22:GLN:O	65:Be:25:LYS:HG2	2.17	0.45
69:CA:215:GLU:OE2	69:CA:221:LYS:O	2.34	0.45
77:CI:1685:OMG:O6	77:CI:1698:A:N3	2.50	0.45
3:AC:1737:G:H2'	3:AC:1738:G:C8	2.52	0.45
5:AH:29:HIS:O	5:AH:32:LYS:HG2	2.16	0.45
18:AF:95:THR:HG22	18:AF:95:THR:O	2.16	0.45
22:AR:52:LEU:HD11	22:AR:73:GLN:HB2	1.97	0.45
26:AW:44:TRP:O	26:AW:47:LYS:HG2	2.16	0.45
34:Ah:110:ARG:O	34:Ah:114:GLU:HG3	2.17	0.45
35:BA:36:GLU:OE2	35:BA:163:ARG:HD2	2.17	0.45
36:BB:101:THR:HG21	77:CI:4378:A:N3	2.31	0.45
53:BS:100:PRO:HA	53:BS:107:ARG:HH22	1.82	0.45
53:BS:111:ALA:O	53:BS:115:ARG:HG2	2.17	0.45
71:CC:63:ASN:OD1	71:CC:66:GLU:HG2	2.17	0.45
74:CF:50:PRO:O	74:CF:51:ALA:HB3	2.16	0.45
75:CG:13:ALA:HB1	75:CG:55:MET:HB2	1.99	0.45
77:CI:2501:A:H2'	77:CI:2502:A:H8	1.82	0.45
3:AC:17:C:H2'	3:AC:18:C:C6	2.51	0.45
3:AC:954:C:H2'	3:AC:955:U:O4'	2.17	0.45
13:AT:73:SER:O	13:AT:74:ASP:HB2	2.16	0.45
37:BC:252:TRP:CG	37:BC:257:PHE:CE1	3.05	0.45
39:BE:78:ARG:NH1	77:CI:881:U:C5	2.84	0.45
44:BJ:99:ASP:OD1	44:BJ:100:LEU:N	2.50	0.45
73:CE:32:ARG:HG3	73:CE:126:TYR:OH	2.16	0.45
77:CI:153:G:H2'	77:CI:154:G:H8	1.82	0.45
77:CI:1159:G:H2'	77:CI:1160:C:C6	2.51	0.45
77:CI:1170:U:H2'	77:CI:1171:C:C6	2.52	0.45
77:CI:1360:A:C2	77:CI:2569:A:H8	2.35	0.45
77:CI:1873:A:C4	77:CI:1874:C:C5	3.05	0.45
77:CI:2655:C:H2'	77:CI:2656:U:C6	2.52	0.45
77:CI:3260:C:C2	77:CI:3261:C:C6	3.05	0.45
77:CI:4308:C:H2'	77:CI:4309:C:H6	1.82	0.45
4:AE:65:ARG:O	4:AE:69:LEU:HD13	2.17	0.45
4:AE:72:VAL:HG11	7:AK:70:TYR:CE1	2.52	0.45
11:AO:42:HIS:NE2	11:AO:43:LYS:NZ	2.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AX:51:VAL:O	14:AX:108:CYS:HA	2.17	0.45
20:AI:110:ASN:O	20:AI:113:GLN:OE1	2.35	0.45
36:BB:293:ILE:HD11	36:BB:298:LEU:HD13	1.99	0.45
47:BM:85:ARG:HD3	77:CI:2603:G:OP1	2.17	0.45
70:CB:231:ASP:O	70:CB:235:ARG:HG3	2.17	0.45
77:CI:1390:G:O2'	77:CI:1425:G:H4'	2.17	0.45
77:CI:1687:G:O2'	77:CI:1709:A:N6	2.50	0.45
77:CI:2167:C:H2'	77:CI:2168:A:C8	2.52	0.45
77:CI:2240:A:N6	77:CI:2248:C:H42	2.15	0.45
77:CI:3929:A:H2'	77:CI:3930:G:C8	2.52	0.45
77:CI:3999:U:H2'	77:CI:4000:C:C6	2.51	0.45
77:CI:4113:C:H2'	77:CI:4114:U:C6	2.52	0.45
77:CI:4552:C:O2	77:CI:4552:C:H2'	2.17	0.45
3:AC:120:U:O2	3:AC:120:U:H2'	2.16	0.44
3:AC:508:G:OP2	30:Ab:104:ARG:NH2	2.50	0.44
13:AT:59:LEU:HD23	13:AT:90:TRP:CD2	2.52	0.44
19:AG:55:TYR:CD2	19:AG:115:PRO:HG2	2.51	0.44
20:AI:147:LEU:HD11	20:AI:163:CYS:SG	2.56	0.44
24:AU:102:LEU:HD23	24:AU:131:GLY:C	2.42	0.44
28:AZ:77:ALA:O	28:AZ:81:VAL:HG23	2.17	0.44
31:Ad:8:LEU:HD23	31:Ad:8:LEU:H	1.82	0.44
44:BJ:15:ARG:HB3	44:BJ:27:LEU:HD23	1.99	0.44
77:CI:1660:A:N3	77:CI:1661:C:C5	2.84	0.44
77:CI:1708:U:H2'	77:CI:1709:A:H8	1.82	0.44
77:CI:2112:U:H5''	79:CK:14:OMU:HM21	1.98	0.44
77:CI:3888:A:C4	77:CI:3890:G:N7	2.85	0.44
79:CK:4:C:H2'	79:CK:5:U:H6	1.81	0.44
3:AC:1048:C:H2'	3:AC:1049:G:O4'	2.17	0.44
6:AJ:76:MET:HB2	6:AJ:89:THR:HG21	1.99	0.44
7:AK:80:ARG:HH21	7:AK:90:VAL:HG12	1.80	0.44
13:AT:261:LEU:N	13:AT:261:LEU:HD12	2.32	0.44
16:Af:121:CYS:SG	16:Af:146:LEU:HD23	2.57	0.44
25:AV:112:VAL:O	25:AV:112:VAL:HG13	2.17	0.44
26:AW:81:LEU:CD1	26:AW:97:ILE:HD12	2.47	0.44
36:BB:82:PRO:HG3	36:BB:171:LEU:HD21	1.99	0.44
38:BD:4:VAL:HG11	77:CI:3902:G:C5'	2.47	0.44
50:BP:28:LYS:HE3	77:CI:241:G:P	2.58	0.44
71:CC:167:VAL:HG23	71:CC:172:ILE:HG22	1.97	0.44
77:CI:718:C:C2	77:CI:719:C:C5	3.05	0.44
77:CI:745:G:C2	77:CI:746:G:N7	2.85	0.44
77:CI:1129:C:H2'	77:CI:1130:G:H8	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:2446:C:H2'	77:CI:2447:U:C6	2.52	0.44
77:CI:4284:U:C2	77:CI:4285:G:C8	3.05	0.44
3:AC:1628:C:C2	3:AC:1629:C:C5	3.06	0.44
13:AT:14:HIS:HE2	13:AT:35:SER:HB2	1.81	0.44
17:AD:124:HIS:HA	17:AD:137:LEU:O	2.17	0.44
21:AQ:51:LYS:HE3	21:AQ:76:ASP:OD2	2.17	0.44
25:AV:29:GLU:O	25:AV:29:GLU:CD	2.60	0.44
25:AV:198:ARG:O	25:AV:201:LYS:HG2	2.17	0.44
30:Ab:104:ARG:HE	30:Ab:108:LYS:CE	2.30	0.44
35:BA:68:ARG:HD2	35:BA:70:LYS:HD3	2.00	0.44
44:BJ:39:VAL:O	44:BJ:43:ARG:HG2	2.18	0.44
45:BK:115:LYS:HE2	45:BK:126:VAL:HG21	2.00	0.44
46:BL:72:VAL:O	46:BL:72:VAL:HG12	2.17	0.44
77:CI:423:G:H2'	77:CI:424:U:H6	1.82	0.44
77:CI:2107:C:O2	77:CI:2107:C:H2'	2.17	0.44
77:CI:3958:C:O2'	77:CI:3961:OMU:H5	2.17	0.44
77:CI:4427:C:O2	77:CI:4427:C:H2'	2.16	0.44
3:AC:570:A:H2'	3:AC:571:C:O4'	2.17	0.44
3:AC:1850:G:C4	77:CI:3426:C:OP1	2.71	0.44
4:AE:106:ARG:CG	4:AE:175:VAL:HG22	2.40	0.44
6:AJ:98:GLU:OE1	15:Ac:101:SER:OG	2.35	0.44
35:BA:117:GLU:CD	35:BA:122:ASP:O	2.60	0.44
49:BO:93:ASN:HB2	49:BO:95:THR:HG22	1.99	0.44
50:BP:49:ILE:HD11	50:BP:70:VAL:HG21	1.99	0.44
69:CA:242:MET:HB3	69:CA:254:ASP:OD2	2.16	0.44
71:CC:113:GLU:HG2	71:CC:125:ARG:HG2	1.99	0.44
77:CI:1534:C:O2'	77:CI:1535:G:H5'	2.17	0.44
77:CI:4191:OMC:HM22	77:CI:4192:C:O4'	2.17	0.44
77:CI:4322:C:H2'	77:CI:4323:U:O4'	2.18	0.44
77:CI:4428:C:H2'	77:CI:4429:C:H6	1.82	0.44
3:AC:219:A:C6	3:AC:220:U:C5	3.06	0.44
3:AC:1229:A:H2'	3:AC:1230:G:H8	1.82	0.44
3:AC:1688:C:H2'	3:AC:1689:C:H6	1.82	0.44
10:AN:18:THR:O	10:AN:20:ILE:HD12	2.17	0.44
13:AT:304:ASP:O	13:AT:304:ASP:OD1	2.35	0.44
50:BP:50:ARG:HG2	50:BP:51:LYS:N	2.32	0.44
61:Ba:86:PRO:O	61:Ba:87:LYS:C	2.60	0.44
73:CE:151:ILE:HD11	73:CE:156:ARG:HG3	2.00	0.44
73:CE:175:LEU:HB2	73:CE:176:PRO:HD2	1.98	0.44
77:CI:241:G:C4	77:CI:242:U:C6	3.06	0.44
77:CI:1659:C:H2'	77:CI:1660:A:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:946:U:H2'	3:AC:947:U:C6	2.53	0.44
38:BD:36:LEU:HG	38:BD:50:ARG:HD3	2.00	0.44
73:CE:26:VAL:HG22	73:CE:33:LEU:HD23	2.00	0.44
77:CI:78:U:N3	77:CI:79:C:C5	2.86	0.44
77:CI:286:U:H2'	77:CI:287:U:C6	2.52	0.44
77:CI:1044:G:C2	77:CI:1045:G:C8	3.05	0.44
77:CI:2477:G:H2'	77:CI:2478:G:C8	2.53	0.44
3:AC:1238:C:H2'	3:AC:1239:U:O4'	2.18	0.44
3:AC:1280:C:C2	3:AC:1281:G:C8	3.05	0.44
13:AT:14:HIS:CE1	13:AT:35:SER:HB2	2.52	0.44
30:Ab:102:THR:HG22	30:Ab:103:SER:N	2.32	0.44
47:BM:91:LYS:O	47:BM:92:ASP:OD1	2.36	0.44
52:BR:24:LYS:HD2	52:BR:26:ARG:HH21	1.82	0.44
3:AC:295:U:H3'	3:AC:296:C:C5'	2.47	0.44
3:AC:1037:A:C5	3:AC:1038:G:C8	3.06	0.44
16:Af:101:ALA:O	16:Af:102:VAL:HG13	2.17	0.44
24:AU:166:ARG:HG3	24:AU:248:TYR:HE1	1.81	0.44
26:AW:119:LEU:H	26:AW:119:LEU:HD12	1.83	0.44
34:Ah:103:LEU:CD2	34:Ah:172:LEU:HD23	2.47	0.44
36:BB:220:ILE:HD11	36:BB:348:ARG:CD	2.48	0.44
51:BQ:42:LEU:HD21	51:BQ:96:VAL:CG1	2.47	0.44
77:CI:1146:C:H2'	77:CI:1147:A:C8	2.51	0.44
77:CI:4249:U:C2	77:CI:4250:G:C8	3.06	0.44
3:AC:636:G:C6	3:AC:637:C:C4	3.06	0.44
3:AC:1534:A:H2	3:AC:1537:G:N3	2.16	0.44
3:AC:1843:4AC:O7	3:AC:1843:4AC:H5	2.18	0.44
19:AG:16:ILE:O	19:AG:16:ILE:HG13	2.17	0.44
28:AZ:34:PHE:HB3	28:AZ:41:PHE:HB2	1.99	0.44
39:BE:106:GLY:HA3	39:BE:109:ASN:OD1	2.18	0.44
39:BE:110:GLY:N	39:BE:113:ARG:HH12	2.16	0.44
39:BE:112:THR:C	39:BE:113:ARG:HD2	2.43	0.44
42:BH:178:ARG:HA	42:BH:184:ARG:O	2.18	0.44
56:BV:90:MET:HA	56:BV:90:MET:HE3	1.99	0.44
3:AC:321:G:H2'	3:AC:322:C:H6	1.82	0.43
3:AC:438:G:C6	3:AC:439:G:C6	3.06	0.43
3:AC:571:C:C4	3:AC:572:U:C4	3.06	0.43
3:AC:1658:G:O2'	3:AC:1659:G:H5'	2.18	0.43
5:AH:77:GLU:O	5:AH:82:ASP:HB2	2.18	0.43
8:AL:64:LYS:NZ	8:AL:89:MET:HA	2.33	0.43
10:AN:36:VAL:HG13	10:AN:40:TYR:HD2	1.83	0.43
17:AD:97:LEU:CD1	17:AD:229:MET:HE1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AU:191:VAL:HG11	24:AU:236:PHE:HA	2.00	0.43
35:BA:180:LEU:CD1	67:Bg:26:VAL:HG11	2.46	0.43
44:BJ:165:PRO:O	44:BJ:166:ARG:HB3	2.17	0.43
62:Bb:64:LEU:HD23	62:Bb:64:LEU:H	1.82	0.43
77:CI:163:A:H2'	77:CI:164:G:H8	1.83	0.43
77:CI:373:OMG:HM21	77:CI:1458:C:O3'	2.18	0.43
77:CI:1672:C:H2'	77:CI:1673:A2M:H8	2.00	0.43
77:CI:1713:C:O2'	77:CI:1720:U:H5''	2.18	0.43
77:CI:1873:A:C2	77:CI:1874:C:C6	3.06	0.43
77:CI:3259:G:H2'	77:CI:3260:C:C6	2.53	0.43
77:CI:3289:A:C2	77:CI:3290:U:C5	3.06	0.43
77:CI:4190:A:H2'	77:CI:4191:OMC:H6	1.83	0.43
1:AA:11:LEU:HB2	1:AA:35:MET:HE2	1.99	0.43
2:AB:14:PHE:HA	3:AC:1557:A:N1	2.34	0.43
3:AC:848:A:N7	3:AC:849:U:C2	2.86	0.43
38:BD:33:ARG:O	38:BD:37:VAL:HG22	2.18	0.43
38:BD:79:TYR:O	38:BD:82:GLU:HG2	2.18	0.43
38:BD:90:VAL:HG12	38:BD:91:GLY:N	2.33	0.43
40:BF:101:ARG:O	40:BF:101:ARG:HG2	2.17	0.43
77:CI:660:C:H2'	77:CI:661:C:H6	1.82	0.43
77:CI:1332:C:C2	77:CI:1333:C:C5	3.05	0.43
77:CI:1361:G:O2'	77:CI:2568:A:C8	2.71	0.43
77:CI:4365:C:H2'	77:CI:4366:C:C6	2.53	0.43
77:CI:4575:C:C2	77:CI:4576:C:C5	3.06	0.43
79:CK:5:U:H2'	79:CK:6:C:H6	1.83	0.43
3:AC:1114:A:H2'	3:AC:1115:U:C6	2.54	0.43
3:AC:1629:C:H2'	3:AC:1630:C:H6	1.83	0.43
5:AH:34:VAL:O	5:AH:38:ILE:HG12	2.18	0.43
13:AT:35:SER:HB3	13:AT:37:ASP:OD1	2.18	0.43
15:Ac:73:VAL:CG2	15:Ac:84:ALA:HB1	2.48	0.43
25:AV:52:ILE:HG23	25:AV:109:LEU:HD11	2.00	0.43
31:Ad:8:LEU:HG	31:Ad:9:HIS:ND1	2.33	0.43
38:BD:7:VAL:HG13	38:BD:8:LYS:N	2.33	0.43
41:BG:14:SER:OG	41:BG:151:THR:HG22	2.18	0.43
70:CB:67:ARG:HG3	76:CH:29:GLN:HE21	1.82	0.43
70:CB:146:LEU:HA	70:CB:149:ASN:OD1	2.19	0.43
70:CB:159:HIS:CE1	70:CB:185:LYS:HD3	2.53	0.43
71:CC:76:HIS:O	71:CC:80:MET:HG3	2.17	0.43
71:CC:128:MET:SD	71:CC:157:SER:HB3	2.58	0.43
73:CE:68:ILE:HG13	73:CE:69:ALA:N	2.33	0.43
77:CI:669:G:O6	77:CI:670:G:C6	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:756:U:C2	77:CI:757:G:C8	3.07	0.43
77:CI:1122:C:H2'	77:CI:1123:C:H6	1.81	0.43
77:CI:1527:U:H2'	77:CI:1528:U:H6	1.82	0.43
77:CI:2032:A:H2'	77:CI:2033:C:O4'	2.19	0.43
77:CI:4067:C:C2	77:CI:4068:C:C5	3.06	0.43
77:CI:4364:U:C2	77:CI:4365:C:C6	3.05	0.43
3:AC:119:U:C4	3:AC:120:U:C5	3.06	0.43
12:AP:20:ILE:HD11	12:AP:91:LEU:HB2	1.99	0.43
15:Ac:113:THR:O	15:Ac:113:THR:CG2	2.66	0.43
28:AZ:78:ALA:HB3	28:AZ:118:ALA:HB3	2.00	0.43
30:Ab:18:LEU:HD13	30:Ab:20:ARG:CZ	2.49	0.43
34:Ah:93:THR:O	34:Ah:93:THR:HG22	2.17	0.43
42:BH:20:SER:OG	42:BH:25:LEU:HD23	2.18	0.43
44:BJ:90:THR:HG23	45:BK:156:TYR:CD1	2.54	0.43
55:BU:27:ILE:CD1	55:BU:86:VAL:HG22	2.47	0.43
77:CI:140:G:H2'	77:CI:141:C:O4'	2.18	0.43
77:CI:1274:C:H2'	77:CI:1275:A:H8	1.83	0.43
77:CI:1291:C:O2	77:CI:1291:C:H2'	2.18	0.43
77:CI:4193:G:H2'	77:CI:4194:U:H6	1.83	0.43
3:AC:457:C:C2	3:AC:458:C:C5	3.06	0.43
21:AQ:80:SER:O	21:AQ:83:PHE:HB2	2.19	0.43
29:Aa:76:SER:HB2	29:Aa:77:PRO:HD3	2.00	0.43
33:Ag:72:PHE:O	33:Ag:76:GLN:HG3	2.17	0.43
37:BC:292:ILE:O	37:BC:298:ILE:HD12	2.18	0.43
37:BC:319:LEU:HD13	69:CA:174:GLU:OE1	2.19	0.43
38:BD:65:ALA:HB2	38:BD:74:ILE:HD13	2.00	0.43
44:BJ:30:MET:HB2	44:BJ:32:ILE:HD11	2.00	0.43
59:BY:64:THR:O	59:BY:67:GLU:HG2	2.18	0.43
70:CB:158:ALA:HB2	70:CB:190:LEU:HD12	2.00	0.43
77:CI:220:C:C2	77:CI:221:C:C5	3.07	0.43
77:CI:307:A:H3'	77:CI:308:G:H21	1.83	0.43
77:CI:1351:U:C2	77:CI:1352:G:C8	3.07	0.43
77:CI:1354:U:H3	77:CI:1431:G:H1	1.67	0.43
77:CI:1873:A:N3	77:CI:1874:C:C6	2.86	0.43
77:CI:2046:C:C2	77:CI:2047:G:C8	3.06	0.43
77:CI:3928:A:H2'	77:CI:3929:A:C8	2.53	0.43
77:CI:3946:G:H5''	77:CI:3948:PSU:C6	2.53	0.43
77:CI:4392:G:H2'	77:CI:4393:C:C6	2.54	0.43
77:CI:4640:G:H2'	77:CI:4641:G:C8	2.53	0.43
1:AA:11:LEU:HB2	1:AA:35:MET:CE	2.49	0.43
3:AC:329:U:O2'	3:AC:330:G:P	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:394:U:HO2'	3:AC:395:G:H8	1.64	0.43
3:AC:838:A:H61	30:Ab:9:THR:CG2	2.31	0.43
3:AC:849:U:H2'	3:AC:850:A:H8	1.83	0.43
3:AC:943:G:H2'	3:AC:944:U:C6	2.52	0.43
24:AU:200:ARG:HA	24:AU:221:ASP:OD2	2.19	0.43
30:Ab:44:LEU:HA	30:Ab:47:MET:HG2	2.01	0.43
34:Ah:76:THR:HG22	34:Ah:108:PRO:HG2	2.00	0.43
34:Ah:158:ILE:HG22	34:Ah:159:SER:H	1.82	0.43
46:BL:102:VAL:HG22	46:BL:112:LEU:CD2	2.48	0.43
47:BM:16:ILE:HD12	47:BM:88:TYR:CD2	2.53	0.43
50:BP:50:ARG:HH21	79:CK:83:C:N4	2.16	0.43
55:BU:22:THR:HB	55:BU:122:VAL:CG2	2.48	0.43
69:CA:247:THR:HG22	69:CA:248:HIS:N	2.33	0.43
70:CB:58:PRO:CG	70:CB:61:ILE:HD12	2.48	0.43
75:CG:96:ASP:O	75:CG:99:GLU:HG3	2.18	0.43
77:CI:220:C:N3	77:CI:221:C:C5	2.87	0.43
77:CI:300:A:H2'	77:CI:301:G:H8	1.83	0.43
77:CI:1169:G:H2'	77:CI:1170:U:C6	2.53	0.43
77:CI:2296:C:C2	77:CI:2297:G:C8	3.06	0.43
77:CI:3747:G:C8	77:CI:3748:G:C8	3.06	0.43
77:CI:4005:C:C2	77:CI:4006:U:C5	3.06	0.43
77:CI:4056:G:O2'	77:CI:4057:C:P	2.77	0.43
3:AC:430:C:C2	3:AC:431:C:C5	3.06	0.43
3:AC:1752:C:O2	3:AC:1785:G:O6	2.36	0.43
4:AE:74:GLN:NE2	4:AE:75:LYS:HG3	2.33	0.43
6:AJ:48:TYR:HB3	9:AM:49:TYR:CE2	2.53	0.43
15:Ac:97:ILE:CG2	15:Ac:109:TYR:HB3	2.49	0.43
18:AF:149:TYR:N	18:AF:150:PRO:HD3	2.34	0.43
20:AI:54:THR:HG22	20:AI:162:PRO:O	2.18	0.43
22:AR:94:ILE:HG12	22:AR:125:VAL:HG21	2.01	0.43
30:Ab:35:VAL:HG23	30:Ab:40:ILE:CD1	2.48	0.43
31:Ad:47:PHE:CE2	31:Ad:48:SER:O	2.71	0.43
35:BA:101:VAL:C	35:BA:102:LEU:HD12	2.43	0.43
35:BA:247:ARG:N	35:BA:247:ARG:HD2	2.34	0.43
36:BB:19:ARG:NH1	36:BB:235:TRP:CZ3	2.86	0.43
36:BB:280:ILE:HD13	77:CI:4332:U:C4	2.54	0.43
39:BE:182:LEU:HD23	39:BE:182:LEU:C	2.44	0.43
49:BO:89:LYS:HE3	49:BO:137:TYR:CE1	2.54	0.43
63:Bc:29:MET:HA	63:Bc:29:MET:HE3	1.99	0.43
77:CI:1006:G:H2'	77:CI:1007:A:O4'	2.19	0.43
77:CI:2383:C:N3	77:CI:2384:U:C5	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:3747:G:N7	77:CI:3748:G:C8	2.87	0.43
77:CI:4346:A:N6	77:CI:4347:A:C2	2.87	0.43
4:AE:137:VAL:HG22	4:AE:151:LYS:HG3	2.00	0.43
5:AH:13:ALA:O	5:AH:17:ILE:HG12	2.18	0.43
6:AJ:76:MET:HB2	6:AJ:89:THR:CG2	2.49	0.43
7:AK:34:GLU:O	7:AK:34:GLU:HG2	2.19	0.43
8:AL:53:GLN:HG3	8:AL:83:MET:SD	2.58	0.43
25:AV:98:ARG:NE	25:AV:106:LEU:HD21	2.32	0.43
40:BF:48:TYR:CE1	40:BF:52:LEU:HD11	2.54	0.43
41:BG:36:ILE:HD11	41:BG:44:ALA:CB	2.49	0.43
45:BK:141:VAL:HG13	45:BK:141:VAL:O	2.19	0.43
46:BL:82:TYR:CD1	77:CI:2387:U:H2'	2.54	0.43
71:CC:41:ILE:HG22	71:CC:43:VAL:HG13	2.00	0.43
74:CF:136:LYS:HG3	74:CF:136:LYS:O	2.18	0.43
77:CI:1403:C:H5''	77:CI:1404:U:O5'	2.19	0.43
77:CI:2294:U:H2'	77:CI:2295:C:C6	2.54	0.43
77:CI:3969:C:C2	77:CI:3970:A:C8	3.06	0.43
78:CJ:24:C:H2'	78:CJ:25:G:O4'	2.19	0.43
9:AM:52:LEU:O	9:AM:56:LEU:HD23	2.19	0.43
25:AV:35:GLU:OE1	25:AV:51:ARG:HG2	2.18	0.43
34:Ah:103:LEU:HD13	34:Ah:170:LYS:CD	2.49	0.43
40:BF:48:TYR:HE1	40:BF:52:LEU:HD11	1.83	0.43
49:BO:129:ARG:CG	49:BO:130:PRO:HD2	2.49	0.43
54:BT:57:LYS:O	54:BT:61:GLU:HG3	2.18	0.43
67:Bg:52:VAL:O	67:Bg:52:VAL:HG13	2.19	0.43
77:CI:205:C:O2	77:CI:209:U:O4	2.37	0.43
77:CI:1287:C:H2'	77:CI:1288:G:O4'	2.19	0.43
77:CI:1881:G:H2'	77:CI:1882:U:C6	2.53	0.43
77:CI:4070:1MA:H2'	77:CI:4071:G:O4'	2.19	0.43
77:CI:4652:C:H2'	77:CI:4653:G:O4'	2.19	0.43
77:CI:4654:U:H4'	77:CI:4655:A:H5'	2.00	0.43
2:AB:13:LYS:O	2:AB:14:PHE:CG	2.72	0.43
3:AC:1200:A:H5''	23:AS:2:THR:HG22	2.01	0.43
3:AC:1379:A:H4'	3:AC:1380:A:O5'	2.19	0.43
3:AC:1855:U:H2'	3:AC:1856:G:H8	1.84	0.43
10:AN:41:ALA:O	10:AN:45:LEU:HD13	2.18	0.43
10:AN:84:LEU:HD22	10:AN:97:GLN:HG3	2.00	0.43
13:AT:234:ASP:CG	13:AT:235:ILE:N	2.77	0.43
17:AD:188:LEU:HD23	17:AD:188:LEU:O	2.19	0.43
20:AI:11:LYS:O	20:AI:15:VAL:HG23	2.18	0.43
35:BA:11:GLY:HA3	77:CI:3326:C:O2'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BD:50:ARG:NH1	38:BD:147:ASP:OD1	2.51	0.43
41:BG:126:ARG:HB2	41:BG:140:MET:HE1	2.01	0.43
62:Bb:17:ARG:NH2	62:Bb:38:CYS:SG	2.92	0.43
77:CI:25:A:H2'	77:CI:26:C:H6	1.83	0.43
77:CI:723:U:H2'	77:CI:724:C:C6	2.53	0.43
77:CI:1578:A:H2'	77:CI:1579:C:H6	1.84	0.43
77:CI:2295:C:H2'	77:CI:2296:C:C6	2.54	0.43
77:CI:2446:C:C2	77:CI:2447:U:C5	3.07	0.43
3:AC:153:G:H22	3:AC:165:G:H1	1.66	0.42
5:AH:66:VAL:O	5:AH:66:VAL:HG23	2.18	0.42
13:AT:260:ASP:OD1	13:AT:262:GLU:OE1	2.37	0.42
15:Ac:88:LEU:HB3	15:Ac:109:TYR:CE2	2.54	0.42
18:AF:139:LEU:HD11	18:AF:147:ILE:HD12	2.01	0.42
25:AV:121:ILE:HD12	25:AV:124:LEU:HD21	2.01	0.42
35:BA:108:PRO:HD3	67:Bg:90:LYS:HE3	2.01	0.42
38:BD:268:ARG:HH11	77:CI:1007:A:H4'	1.84	0.42
58:BX:92:LYS:O	58:BX:96:LEU:CD1	2.67	0.42
73:CE:46:GLN:HG3	78:CJ:39:C:O2'	2.19	0.42
77:CI:1537:U:C6	77:CI:3869:A:O4'	2.71	0.42
79:CK:71:A:C2	79:CK:88:A:C1'	3.01	0.42
3:AC:94:G:O2'	3:AC:509:A:O2'	2.36	0.42
3:AC:512:U:H2'	3:AC:513:A:C8	2.53	0.42
3:AC:986:G:H1'	28:AZ:138:ASP:OD2	2.18	0.42
3:AC:1273:C:O2'	3:AC:1274:C:C6	2.69	0.42
3:AC:1445:U:C2'	3:AC:1446:U:H5'	2.49	0.42
3:AC:1538:A:C5	3:AC:1539:C:C5	3.08	0.42
3:AC:1822:U:C2	3:AC:1823:A:C8	3.06	0.42
8:AL:107:ILE:O	8:AL:108:LYS:HB2	2.18	0.42
12:AP:56:MET:HG3	12:AP:86:LYS:HE3	2.01	0.42
17:AD:91:VAL:HG22	17:AD:96:CYS:SG	2.59	0.42
21:AQ:23:ILE:HD11	24:AU:251:LEU:HA	2.00	0.42
38:BD:41:LYS:HD2	45:BK:93:ILE:HD13	2.01	0.42
53:BS:36:ASP:OD1	53:BS:36:ASP:C	2.61	0.42
70:CB:165:GLU:OE2	76:CH:22:LEU:HD13	2.19	0.42
77:CI:199:G:O3'	77:CI:200:U:H4'	2.19	0.42
77:CI:2168:A:H2'	77:CI:2169:U:H6	1.83	0.42
3:AC:828:A:C6	3:AC:829:G:C5	3.07	0.42
3:AC:1626:U:C2	3:AC:1627:C:C6	3.06	0.42
5:AH:99:ASP:O	5:AH:102:THR:HG22	2.19	0.42
6:AJ:78:MET:O	6:AJ:79:HIS:HB2	2.19	0.42
6:AJ:99:ILE:HG23	15:Ac:67:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Aa:53:ILE:CD1	29:Aa:62:VAL:HG23	2.50	0.42
35:BA:69:PHE:O	35:BA:70:LYS:HG3	2.19	0.42
35:BA:137:ILE:CD1	35:BA:155:LYS:HD2	2.48	0.42
38:BD:83:LEU:N	38:BD:84:PRO:HD2	2.34	0.42
41:BG:132:ALA:O	77:CI:1413:A:OP2	2.37	0.42
67:Bg:17:ARG:O	77:CI:3294:A:N1	2.52	0.42
69:CA:174:GLU:HB3	69:CA:270:ASN:ND2	2.34	0.42
75:CG:100:ARG:HA	75:CG:103:LYS:HG2	2.01	0.42
77:CI:944:G:H1	77:CI:1040:C:H42	1.68	0.42
77:CI:2175:C:C2	77:CI:2176:A:C8	3.07	0.42
77:CI:2571:A:H2'	77:CI:2572:G:C8	2.54	0.42
77:CI:2615:G:H2'	77:CI:2616:C:H6	1.84	0.42
77:CI:3530:A:H2'	77:CI:3531:A:C8	2.54	0.42
77:CI:4079:A:N7	77:CI:4130:G:C6	2.87	0.42
77:CI:4599:G:C2	77:CI:4600:U:C5	3.08	0.42
3:AC:1186:C:C2	3:AC:1187:U:C6	3.08	0.42
3:AC:1709:C:H2'	3:AC:1710:G:H5''	2.01	0.42
3:AC:1822:U:H2'	3:AC:1823:A:C8	2.55	0.42
3:AC:1850:G:N3	77:CI:3426:C:OP1	2.53	0.42
4:AE:38:GLU:OE1	4:AE:40:ARG:HG3	2.19	0.42
9:AM:31:LEU:CD2	9:AM:33:LYS:HG2	2.49	0.42
15:Ac:79:ILE:HD11	15:Ac:83:LEU:HD23	2.02	0.42
18:AF:38:LEU:C	18:AF:38:LEU:HD23	2.44	0.42
18:AF:173:ILE:O	18:AF:173:ILE:HG23	2.18	0.42
22:AR:73:GLN:NE2	22:AR:78:GLY:HA2	2.34	0.42
25:AV:116:LYS:NZ	25:AV:119:LYS:O	2.52	0.42
27:AY:115:LEU:O	27:AY:119:GLU:HG3	2.18	0.42
32:Ae:87:ARG:O	32:Ae:90:THR:HG22	2.18	0.42
34:Ah:130:THR:OG1	34:Ah:131:PRO:HD3	2.18	0.42
37:BC:301:ALA:HB1	42:BH:132:LYS:HD3	2.01	0.42
49:BO:129:ARG:HG2	49:BO:130:PRO:HD2	2.02	0.42
58:BX:93:ARG:HG2	58:BX:97:ILE:HD13	2.00	0.42
60:BZ:45:ARG:CZ	60:BZ:49:GLY:O	2.68	0.42
69:CA:109:PRO:HG3	69:CA:166:TYR:CE2	2.54	0.42
69:CA:258:ARG:HG3	69:CA:258:ARG:O	2.20	0.42
77:CI:112:C:C2	77:CI:113:A:C8	3.07	0.42
77:CI:672:G:H2'	77:CI:672:G:N3	2.35	0.42
77:CI:2411:C:C2	77:CI:2412:U:C5	3.07	0.42
77:CI:3380:U:H2'	77:CI:3381:G:H8	1.85	0.42
3:AC:16:G:H2'	3:AC:17:C:C6	2.54	0.42
3:AC:1752:C:O2'	3:AC:1753:C:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AQ:21:ASN:O	21:AQ:21:ASN:OD1	2.37	0.42
29:Aa:28:ARG:HB3	29:Aa:29:PRO:HD3	2.00	0.42
30:Ab:18:LEU:HD13	30:Ab:20:ARG:NH2	2.34	0.42
36:BB:219:VAL:HG11	36:BB:337:VAL:HG13	2.01	0.42
69:CA:169:LEU:O	69:CA:172:VAL:HG12	2.19	0.42
70:CB:162:ASP:HB2	70:CB:163:PRO:CD	2.49	0.42
72:CD:31:ILE:HG22	72:CD:62:SER:HB2	2.02	0.42
75:CG:91:TRP:HE1	77:CI:4517:OMG:H3'	1.83	0.42
77:CI:78:U:C2	77:CI:79:C:C6	3.07	0.42
77:CI:1695:C:H1'	77:CI:1739:C:O2	2.19	0.42
77:CI:3569:C:C2	77:CI:3570:C:C5	3.08	0.42
77:CI:4428:C:N3	77:CI:4429:C:C5	2.88	0.42
3:AC:345:U:H2'	3:AC:346:U:C6	2.54	0.42
3:AC:818:G:H22	3:AC:819:A:H62	1.68	0.42
3:AC:1569:C:H2'	3:AC:1570:A:C8	2.55	0.42
13:AT:57:ARG:HB2	13:AT:94:THR:HG23	2.01	0.42
24:AU:233:LEU:HD23	24:AU:233:LEU:C	2.44	0.42
29:Aa:112:ASP:OD1	29:Aa:115:GLU:HB3	2.19	0.42
30:Ab:91:LEU:HA	30:Ab:94:HIS:NE2	2.34	0.42
34:Ah:161:LEU:H	34:Ah:161:LEU:HD12	1.84	0.42
36:BB:29:VAL:HG11	36:BB:32:PHE:CZ	2.55	0.42
36:BB:189:THR:O	36:BB:193:LYS:HG3	2.20	0.42
56:BV:119:ALA:HB3	68:Bh:119:ARG:HH12	1.85	0.42
62:Bb:5:ILE:HD11	62:Bb:43:TYR:HB3	2.00	0.42
70:CB:185:LYS:HG3	70:CB:185:LYS:O	2.20	0.42
73:CE:120:ASP:HB3	73:CE:123:ILE:HG22	2.01	0.42
77:CI:851:C:O2'	77:CI:852:G:H5'	2.19	0.42
77:CI:1541:G:H5''	78:CJ:102:U:H1'	2.01	0.42
2:AB:21:CYS:HB3	2:AB:24:CYS:SG	2.60	0.42
4:AE:212:GLU:OE1	4:AE:212:GLU:HA	2.18	0.42
13:AT:304:ASP:OD1	13:AT:304:ASP:C	2.63	0.42
20:AI:205:ARG:HH11	20:AI:205:ARG:HG3	1.85	0.42
43:BI:4:LEU:HD11	43:BI:29:THR:HG23	2.01	0.42
43:BI:135:LYS:O	43:BI:139:MET:HG3	2.20	0.42
47:BM:15:ARG:HB2	77:CI:4273:G:H5'	2.01	0.42
70:CB:146:LEU:O	70:CB:149:ASN:OD1	2.37	0.42
72:CD:75:TYR:O	72:CD:78:LYS:HG2	2.20	0.42
74:CF:127:PHE:CD1	74:CF:143:GLU:OE2	2.73	0.42
77:CI:2616:C:O2	77:CI:2616:C:H2'	2.20	0.42
1:AA:12:ALA:HB1	1:AA:32:VAL:HB	2.02	0.42
3:AC:120:U:C2	3:AC:121:U:C6	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:609:C:N3	3:AC:610:U:C4	2.88	0.42
3:AC:1231:C:C2	3:AC:1232:C:C5	3.08	0.42
17:AD:44:ILE:CD1	17:AD:86:LEU:HD12	2.49	0.42
24:AU:81:ILE:HG23	24:AU:86:LEU:HB2	2.01	0.42
29:Aa:26:LEU:HD11	29:Aa:60:LYS:CD	2.49	0.42
30:Ab:20:ARG:HD2	30:Ab:74:MET:SD	2.59	0.42
34:Ah:158:ILE:HG22	34:Ah:159:SER:N	2.35	0.42
36:BB:293:ILE:CD1	36:BB:298:LEU:HD13	2.50	0.42
37:BC:11:TYR:CZ	37:BC:148:PRO:HB2	2.55	0.42
37:BC:33:ARG:HG3	37:BC:122:TYR:OH	2.20	0.42
38:BD:15:ARG:HD2	77:CI:1545:A:O4'	2.19	0.42
40:BF:110:PRO:O	40:BF:113:ASP:OD1	2.38	0.42
52:BR:32:ARG:CD	77:CI:37:U:H5''	2.49	0.42
53:BS:26:SER:HG	77:CI:1607:A:H2	1.65	0.42
74:CF:91:ALA:HB1	74:CF:96:ILE:HB	2.01	0.42
77:CI:928:G:H1	77:CI:1064:G:N2	2.18	0.42
77:CI:1128:C:O2'	77:CI:1129:C:O5'	2.37	0.42
77:CI:1273:C:C2	77:CI:1274:C:C5	3.08	0.42
77:CI:1327:U:H2'	77:CI:1328:A:C8	2.55	0.42
77:CI:1529:U:H2'	77:CI:1530:U:C6	2.55	0.42
77:CI:1613:G:H2'	77:CI:1614:C:H6	1.84	0.42
77:CI:1648:G:H2'	77:CI:1649:C:C6	2.54	0.42
77:CI:2383:C:C4	77:CI:2384:U:C5	3.08	0.42
77:CI:2389:U:H2'	77:CI:2390:C:H6	1.84	0.42
77:CI:2573:C:C2	77:CI:2574:C:C5	3.07	0.42
77:CI:4057:C:C4	77:CI:4058:PSU:C2	3.08	0.42
77:CI:4552:C:N3	77:CI:4553:C:C5	2.88	0.42
3:AC:71:G:H2'	3:AC:72:C:O4'	2.19	0.42
3:AC:1317:C:H2'	3:AC:1318:C:H6	1.84	0.42
13:AT:32:LEU:HD13	13:AT:71:ILE:HD11	2.01	0.42
22:AR:47:ALA:O	22:AR:102:VAL:HG22	2.19	0.42
25:AV:146:ASN:ND2	25:AV:146:ASN:O	2.53	0.42
39:BE:173:LEU:HD12	39:BE:182:LEU:CD2	2.50	0.42
40:BF:30:GLY:HA2	40:BF:101:ARG:NH1	2.34	0.42
44:BJ:82:LEU:C	44:BJ:82:LEU:HD12	2.45	0.42
44:BJ:149:LYS:HE3	77:CI:805:C:H5'	2.00	0.42
54:BT:28:VAL:HG21	54:BT:37:MET:HG3	2.01	0.42
68:Bh:116:ALA:O	68:Bh:119:ARG:HG2	2.19	0.42
77:CI:479:G:H2'	77:CI:480:C:H6	1.84	0.42
77:CI:2573:C:H2'	77:CI:2574:C:H6	1.85	0.42
77:CI:3782:G:H2'	77:CI:3783:C:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:3936:A:H5''	77:CI:3938:G:O6	2.19	0.42
2:AB:24:CYS:SG	2:AB:26:ASN:HB3	2.60	0.42
3:AC:641:A:H2'	3:AC:642:A:C8	2.54	0.42
3:AC:654:A:H2'	3:AC:655:A:O4'	2.20	0.42
3:AC:819:A:C4	3:AC:820:G:C8	3.08	0.42
3:AC:1729:U:H2'	3:AC:1730:U:O4'	2.20	0.42
5:AH:75:GLU:O	5:AH:79:GLU:HB2	2.20	0.42
13:AT:207:CYS:SG	13:AT:219:TRP:HB2	2.60	0.42
18:AF:87:MET:HG2	18:AF:123:LEU:O	2.19	0.42
25:AV:50:VAL:HG12	25:AV:113:ILE:HA	2.01	0.42
46:BL:80:LYS:HG2	46:BL:110:TYR:CE2	2.55	0.42
69:CA:170:LYS:O	69:CA:174:GLU:HG2	2.19	0.42
71:CC:36:ARG:HD3	71:CC:38:PHE:CZ	2.55	0.42
77:CI:174:C:C2	77:CI:175:C:C5	3.07	0.42
77:CI:321:U:H2'	77:CI:322:C:C6	2.55	0.42
77:CI:1114:G:H2'	77:CI:1115:C:C5	2.54	0.42
77:CI:1274:C:H2'	77:CI:1275:A:C8	2.55	0.42
77:CI:3351:A:C4	77:CI:3352:U:C6	3.07	0.42
77:CI:3361:A:C6	77:CI:3362:G:C8	3.08	0.42
77:CI:3589:U:C2	77:CI:3590:C:C5	3.07	0.42
77:CI:3780:A:N3	77:CI:3781:A:C8	2.88	0.42
77:CI:4517:OMG:O4'	77:CI:4517:OMG:OP2	2.38	0.42
77:CI:4599:G:C2	77:CI:4600:U:C6	3.07	0.42
79:CK:128:C:H2'	79:CK:129:C:C6	2.54	0.42
3:AC:4:C:C2	3:AC:5:U:C5	3.08	0.41
3:AC:10:G:H21	24:AU:114:LYS:HA	1.86	0.41
3:AC:369:U:H2'	3:AC:370:C:H2'	2.02	0.41
3:AC:417:U:H2'	3:AC:418:C:O4'	2.20	0.41
4:AE:27:ARG:NH1	7:AK:62:PHE:O	2.53	0.41
18:AF:124:CYS:HB3	18:AF:141:THR:HB	2.02	0.41
23:AS:37:LYS:HD3	23:AS:70:LYS:HE2	2.02	0.41
31:Ad:57:VAL:O	31:Ad:57:VAL:HG12	2.18	0.41
33:Ag:60:ILE:O	33:Ag:60:ILE:HG13	2.20	0.41
40:BF:110:PRO:N	40:BF:111:PRO:CD	2.83	0.41
56:BV:26:ASP:OD2	77:CI:436:C:H4'	2.20	0.41
69:CA:124:SER:O	69:CA:128:ARG:HG3	2.20	0.41
71:CC:10:VAL:CG2	71:CC:55:LEU:HB3	2.49	0.41
73:CE:41:GLU:OE1	73:CE:47:THR:HA	2.20	0.41
76:CH:145:ASN:O	76:CH:149:GLN:HG3	2.20	0.41
77:CI:2256:U:N3	77:CI:2257:C:C5	2.88	0.41
77:CI:4280:C:O2'	77:CI:4281:A:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:CK:5:U:N3	79:CK:6:C:C5	2.88	0.41
3:AC:1304:C:C2	3:AC:1305:U:C6	3.08	0.41
6:AJ:173:LEU:O	6:AJ:177:LEU:HG	2.20	0.41
12:AP:106:ILE:HD12	12:AP:110:VAL:HG11	2.01	0.41
26:AW:82:VAL:HG22	26:AW:92:MET:HE1	2.02	0.41
34:Ah:119:LEU:HD22	34:Ah:153:LYS:HD3	2.01	0.41
39:BE:153:THR:OG1	39:BE:154:PRO:HD2	2.20	0.41
42:BH:158:THR:CG2	42:BH:159:PRO:HD2	2.49	0.41
44:BJ:85:ASP:OD2	44:BJ:90:THR:HB	2.20	0.41
54:BT:58:SER:HB3	58:BX:96:LEU:HD23	2.01	0.41
77:CI:1269:B8Q:N4	77:CI:1270:G:N7	2.68	0.41
77:CI:1524:C:O2'	77:CI:1525:A:H5'	2.20	0.41
77:CI:1659:C:C2	77:CI:1680:G:N2	2.88	0.41
77:CI:1746:A:N6	77:CI:1841:G:N2	2.67	0.41
77:CI:3349:U:H2'	77:CI:3350:G:O4'	2.20	0.41
77:CI:3529:C:H2'	77:CI:3530:A:H8	1.85	0.41
77:CI:3588:G:H2'	77:CI:3589:U:H6	1.85	0.41
77:CI:4364:U:O2	77:CI:4364:U:H2'	2.20	0.41
78:CJ:16:A:H2'	78:CJ:17:C:O4'	2.19	0.41
79:CK:4:C:C2	79:CK:5:U:C5	3.08	0.41
79:CK:141:C:C2	79:CK:142:U:C5	3.08	0.41
3:AC:945:A:H2'	3:AC:946:U:H6	1.85	0.41
3:AC:1047:U:H2'	3:AC:1048:C:C6	2.54	0.41
3:AC:1343:U:H1'	3:AC:1344:U:H5	1.84	0.41
3:AC:1539:C:C2	3:AC:1540:U:C5	3.07	0.41
17:AD:72:ALA:HB3	28:AZ:128:ARG:NH2	2.35	0.41
20:AI:34:MET:HE3	20:AI:34:MET:HB3	1.99	0.41
24:AU:69:LEU:HD21	24:AU:273:LEU:HD21	2.02	0.41
24:AU:269:PHE:O	24:AU:273:LEU:HG	2.20	0.41
36:BB:378:ARG:HD3	48:BN:11:TYR:CD2	2.54	0.41
37:BC:159:GLU:O	37:BC:214:ASP:O	2.37	0.41
50:BP:110:LYS:O	50:BP:115:ARG:HD3	2.20	0.41
57:BW:104:MET:O	57:BW:105:LEU:HB3	2.20	0.41
66:Bf:63:THR:HG21	66:Bf:89:LYS:HG2	2.03	0.41
75:CG:46:ARG:HD2	77:CI:834:U:H6	1.85	0.41
77:CI:3452:U:C2	77:CI:3453:C:C5	3.08	0.41
77:CI:4219:A:H2'	77:CI:4220:C:C6	2.55	0.41
77:CI:4533:C:O2	77:CI:4533:C:H2'	2.20	0.41
3:AC:322:C:O2	3:AC:323:C:C6	2.73	0.41
3:AC:836:C:H42	30:Ab:10:ARG:NH2	2.18	0.41
3:AC:838:A:H61	30:Ab:9:THR:HG22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:1047:U:O2'	3:AC:1048:C:OP1	2.36	0.41
3:AC:1630:C:H2'	3:AC:1631:A:O4'	2.20	0.41
3:AC:1846:A:H2'	3:AC:1847:G:C8	2.56	0.41
7:AK:15:LEU:HD22	7:AK:49:MET:HE1	2.02	0.41
12:AP:20:ILE:HG12	12:AP:91:LEU:O	2.21	0.41
12:AP:54:VAL:HG12	12:AP:56:MET:HE2	2.01	0.41
13:AT:21:ILE:HD13	13:AT:299:PHE:HB3	2.02	0.41
13:AT:60:ARG:O	13:AT:61:GLY:C	2.63	0.41
17:AD:85:LYS:HB3	17:AD:101:HIS:NE2	2.35	0.41
17:AD:142:PHE:HD1	17:AD:209:ASP:HB2	1.85	0.41
27:AY:57:SER:O	27:AY:58:HIS:HB2	2.20	0.41
27:AY:150:VAL:HG22	27:AY:151:ALA:N	2.34	0.41
33:Ag:169:LYS:O	33:Ag:172:THR:HG22	2.19	0.41
37:BC:122:TYR:CD1	37:BC:280:PRO:HG3	2.55	0.41
42:BH:158:THR:HG22	42:BH:159:PRO:CD	2.50	0.41
43:BI:105:LEU:HD22	43:BI:135:LYS:HG3	2.03	0.41
51:BQ:100:VAL:O	51:BQ:100:VAL:HG12	2.20	0.41
77:CI:420:A:C8	77:CI:421:C:C5	3.08	0.41
77:CI:2239:G:N3	77:CI:2252:G:C2	2.89	0.41
77:CI:2611:G:O2'	77:CI:2612:C:P	2.79	0.41
2:AB:22:ARG:NH1	4:AE:16:ILE:HG21	2.36	0.41
3:AC:116:OMU:HM23	3:AC:116:OMU:H1'	1.94	0.41
3:AC:126:G:OP1	25:AV:198:ARG:HD2	2.21	0.41
6:AJ:110:GLN:O	6:AJ:113:VAL:HG22	2.21	0.41
15:Ac:58:LEU:HD23	15:Ac:62:VAL:HG21	2.02	0.41
17:AD:85:LYS:HB3	17:AD:101:HIS:CE1	2.55	0.41
19:AG:82:MET:HE3	19:AG:85:THR:HG22	2.02	0.41
24:AU:183:LYS:HA	24:AU:195:LEU:O	2.21	0.41
36:BB:56:ILE:HD12	36:BB:365:LEU:CD2	2.49	0.41
36:BB:285:TYR:CD1	36:BB:363:ILE:CD1	3.03	0.41
40:BF:34:VAL:HG22	40:BF:103:LYS:CG	2.50	0.41
42:BH:154:LYS:HE2	42:BH:158:THR:HG21	2.02	0.41
46:BL:42:PHE:CE1	46:BL:93:LYS:HE3	2.56	0.41
52:BR:24:LYS:HZ1	77:CI:1132:C:P	2.43	0.41
72:CD:54:SER:HB3	72:CD:135:ILE:HD11	2.01	0.41
77:CI:718:C:H2'	77:CI:719:C:H6	1.86	0.41
77:CI:763:G:H2'	77:CI:764:G:C8	2.56	0.41
77:CI:942:A:C4	77:CI:943:C:C5	3.08	0.41
77:CI:943:C:C2	77:CI:944:G:C8	3.09	0.41
77:CI:1280:C:C2	77:CI:1281:C:C5	3.08	0.41
77:CI:1546:U:C4	77:CI:1547:G:N7	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:2132:A:H2'	77:CI:2133:C:C6	2.55	0.41
77:CI:3943:C:H2'	77:CI:3944:U:O4'	2.21	0.41
1:AA:14:VAL:HG13	1:AA:30:VAL:HB	2.03	0.41
3:AC:430:C:H2'	3:AC:431:C:H6	1.86	0.41
3:AC:638:U:C2	3:AC:639:C:C5	3.08	0.41
3:AC:1350:G:H2'	3:AC:1351:U:C6	2.55	0.41
3:AC:1687:G:H2'	3:AC:1688:C:H6	1.86	0.41
4:AE:167:TYR:OH	4:AE:202:LYS:O	2.37	0.41
6:AJ:200:ALA:HA	6:AJ:203:ASN:OD1	2.21	0.41
12:AP:19:ARG:HB3	12:AP:117:ALA:HB3	2.02	0.41
13:AT:208:ALA:HB1	13:AT:239:LEU:HD21	2.02	0.41
22:AR:22:TRP:HE3	22:AR:28:LYS:HD2	1.86	0.41
23:AS:41:ILE:HA	23:AS:67:LEU:O	2.21	0.41
33:Ag:38:ALA:HA	33:Ag:41:ARG:HG3	2.01	0.41
39:BE:211:ILE:O	39:BE:211:ILE:CG2	2.66	0.41
55:BU:64:ILE:HG23	55:BU:68:LEU:HD23	2.02	0.41
65:Be:23:ARG:HH22	77:CI:3441:5MC:P	2.44	0.41
68:Bh:26:SER:OG	68:Bh:28:GLU:OE1	2.34	0.41
70:CB:98:LEU:HD12	70:CB:98:LEU:HA	1.97	0.41
73:CE:136:ARG:HE	73:CE:157:ILE:CD1	2.33	0.41
77:CI:391:U:C2	77:CI:392:U:C6	3.08	0.41
77:CI:478:G:H2'	77:CI:479:G:H8	1.86	0.41
77:CI:660:C:N3	77:CI:661:C:C5	2.88	0.41
77:CI:1198:C:C2	77:CI:1199:G:C8	3.09	0.41
77:CI:1685:OMG:O2'	77:CI:1686:C:OP2	2.38	0.41
77:CI:2118:U:H2'	77:CI:2119:A2M:H8	2.02	0.41
77:CI:3847:A:H2'	77:CI:3848:C:H6	1.85	0.41
79:CK:108:A:C2	79:CK:112:G:C6	3.08	0.41
3:AC:75:G:H3'	3:AC:76:U:H5''	2.02	0.41
3:AC:562:A:N6	3:AC:588:A:C8	2.89	0.41
3:AC:582:U:H1'	30:Ab:62:THR:HG21	2.02	0.41
3:AC:1273:C:O2'	3:AC:1274:C:P	2.78	0.41
3:AC:1538:A:H2'	3:AC:1539:C:H6	1.85	0.41
3:AC:1673:U:C2	3:AC:1674:U:C5	3.09	0.41
4:AE:106:ARG:NH2	4:AE:107:TYR:CE2	2.88	0.41
4:AE:200:PRO:O	4:AE:201:LYS:CG	2.68	0.41
6:AJ:136:ARG:CB	6:AJ:203:ASN:HD22	2.34	0.41
15:Ac:99:LEU:HA	15:Ac:109:TYR:HD1	1.86	0.41
36:BB:16:PHE:O	36:BB:19:ARG:HG3	2.21	0.41
39:BE:76:TYR:CD1	39:BE:77:LYS:HG3	2.56	0.41
52:BR:93:ASN:OD1	52:BR:93:ASN:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BS:61:ASN:OD1	77:CI:1631:G:H1'	2.20	0.41
57:BW:104:MET:HE2	77:CI:4592:C:OP1	2.21	0.41
73:CE:78:LYS:HA	73:CE:81:GLU:HG2	2.03	0.41
77:CI:386:A:H3'	77:CI:387:G:H5''	2.02	0.41
77:CI:390:C:H2'	77:CI:391:U:H6	1.85	0.41
77:CI:2277:G:H3'	77:CI:2278:G7M:H8	2.02	0.41
77:CI:3381:G:H2'	77:CI:3382:A2M:C8	2.47	0.41
77:CI:3742:G:H2'	77:CI:3743:G:O4'	2.21	0.41
77:CI:3915:U:H2'	77:CI:3916:C:H6	1.84	0.41
77:CI:4265:A:C4	77:CI:4266:A:C8	3.08	0.41
78:CJ:3:C:H2'	78:CJ:4:U:H6	1.86	0.41
3:AC:1074:U:C2	3:AC:1075:C:C5	3.09	0.41
3:AC:1396:C:O2	3:AC:1396:C:O4'	2.38	0.41
6:AJ:139:VAL:HG12	6:AJ:140:ASP:N	2.35	0.41
9:AM:45:ARG:HA	9:AM:48:GLN:HB2	2.03	0.41
11:AO:4:VAL:HB	11:AO:8:ASP:OD2	2.21	0.41
11:AO:104:LEU:HD13	11:AO:121:ARG:HD2	2.03	0.41
13:AT:230:LEU:HD12	13:AT:230:LEU:N	2.35	0.41
19:AG:33:LEU:HG	19:AG:33:LEU:O	2.21	0.41
23:AS:58:VAL:CG1	28:AZ:125:LYS:HB3	2.51	0.41
26:AW:106:LEU:O	26:AW:112:THR:HG21	2.20	0.41
27:AY:22:VAL:HG13	27:AY:26:LEU:HD23	2.02	0.41
45:BK:35:LYS:NZ	77:CI:1626:G:H5''	2.36	0.41
51:BQ:42:LEU:HD21	51:BQ:96:VAL:HG12	2.01	0.41
58:BX:48:VAL:HG23	58:BX:49:CYS:N	2.35	0.41
72:CD:188:LYS:O	72:CD:200:ILE:HD11	2.21	0.41
73:CE:26:VAL:O	73:CE:26:VAL:HG23	2.21	0.41
77:CI:1483:G:O2'	77:CI:1655:G:H4'	2.21	0.41
77:CI:2176:A:H5'	77:CI:2177:G:H5''	2.03	0.41
77:CI:3412:G:C8	77:CI:3435:G:C8	3.08	0.41
77:CI:4501:G:H2'	77:CI:4502:G:O4'	2.20	0.41
79:CK:141:C:H2'	79:CK:142:U:H6	1.86	0.41
3:AC:171:A:OP1	3:AC:171:A:H4'	2.20	0.41
3:AC:675:C:H2'	3:AC:676:U:C6	2.55	0.41
3:AC:1130:G:H3'	3:AC:1131:G:H21	1.85	0.41
3:AC:1222:G:H2'	3:AC:1223:G:C8	2.56	0.41
3:AC:1351:U:O2'	20:AI:112:ILE:HD13	2.20	0.41
3:AC:1563:C:H2'	3:AC:1564:G:H8	1.85	0.41
3:AC:1684:C:N3	3:AC:1685:C:C5	2.88	0.41
3:AC:1737:G:H2'	3:AC:1738:G:H8	1.85	0.41
16:Af:125:GLU:HG3	16:Af:125:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AD:71:LEU:HD13	17:AD:84:PHE:HE2	1.83	0.41
25:AV:38:ALA:HB2	25:AV:50:VAL:HG22	2.03	0.41
26:AW:138:ARG:O	26:AW:139:LYS:HB2	2.21	0.41
31:Ad:45:THR:O	31:Ad:45:THR:HG23	2.19	0.41
33:Ag:159:ASP:O	33:Ag:160:LYS:HB3	2.19	0.41
34:Ah:93:THR:O	34:Ah:93:THR:CG2	2.69	0.41
36:BB:247:GLY:HA2	77:CI:2594:G:H5'	2.03	0.41
38:BD:91:GLY:O	38:BD:94:ASN:ND2	2.54	0.41
39:BE:64:TYR:HB2	39:BE:69:MET:SD	2.61	0.41
44:BJ:48:VAL:HG11	44:BJ:54:MET:SD	2.61	0.41
44:BJ:175:PHE:O	44:BJ:176:PHE:HB2	2.21	0.41
57:BW:4:ARG:HD2	77:CI:4409:G:OP1	2.21	0.41
60:BZ:45:ARG:NH2	60:BZ:49:GLY:O	2.54	0.41
68:Bh:108:MET:HE2	77:CI:2019:A:H5''	2.03	0.41
69:CA:215:GLU:O	69:CA:218:THR:O	2.38	0.41
73:CE:78:LYS:O	73:CE:81:GLU:HG2	2.21	0.41
77:CI:108:A:H4'	77:CI:109:G:OP1	2.21	0.41
77:CI:935:C:C5	77:CI:1053:G:N2	2.89	0.41
77:CI:1106:C:H2'	77:CI:1107:G:O4'	2.20	0.41
77:CI:1128:C:O2	77:CI:3524:A:C4	2.74	0.41
77:CI:1528:U:H2'	77:CI:1529:U:H6	1.85	0.41
77:CI:1686:C:C6	77:CI:1687:G:C8	3.08	0.41
77:CI:2410:C:C2	77:CI:2411:C:C5	3.09	0.41
77:CI:2620:A:H2'	77:CI:2621:U:H6	1.86	0.41
77:CI:3264:C:H2'	77:CI:3265:U:O4'	2.21	0.41
77:CI:3361:A:C5	77:CI:3362:G:C8	3.09	0.41
77:CI:3364:G:H2'	77:CI:3365:C:H6	1.86	0.41
77:CI:3504:A:H2'	77:CI:3505:C:H6	1.86	0.41
77:CI:3933:C:O2'	77:CI:3936:A:C8	2.72	0.41
77:CI:4342:A:C2	77:CI:4343:C:C6	3.09	0.41
77:CI:4386:G:H2'	77:CI:4386:G:N3	2.35	0.41
77:CI:4391:C:H2'	77:CI:4392:G:C8	2.56	0.41
79:CK:82:A:OP2	79:CK:82:A:H4'	2.21	0.41
3:AC:302:A:C2	34:Ah:73:THR:HG21	2.56	0.41
3:AC:527:A:H61	3:AC:560:G:H22	1.69	0.41
3:AC:571:C:O2'	30:Ab:34:THR:HB	2.21	0.41
3:AC:1234:G:C6	3:AC:1527:G:C6	3.09	0.41
3:AC:1688:C:N3	3:AC:1689:C:C5	2.89	0.41
4:AE:106:ARG:HD3	4:AE:174:HIS:O	2.21	0.41
10:AN:99:LEU:O	10:AN:100:ALA:C	2.63	0.41
13:AT:201:SER:HB2	13:AT:206:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AF:170:THR:O	18:AF:170:THR:HG22	2.20	0.41
24:AU:174:ILE:HD12	24:AU:174:ILE:HA	1.98	0.41
33:Ag:126:HIS:CD2	33:Ag:181:THR:HB	2.56	0.41
36:BB:228:TYR:CE2	77:CI:2592:A:H1'	2.56	0.41
38:BD:180:PHE:HB2	38:BD:190:PHE:CE1	2.56	0.41
39:BE:173:LEU:HD11	39:BE:184:THR:CG2	2.50	0.41
42:BH:75:ARG:NH1	42:BH:137:VAL:HG13	2.36	0.41
46:BL:108:GLU:OE1	46:BL:108:GLU:O	2.39	0.41
51:BQ:135:ARG:NH1	77:CI:2509:G:H5'	2.36	0.41
77:CI:1370:C:H2'	77:CI:1371:A:O4'	2.21	0.41
77:CI:1881:G:H2'	77:CI:1882:U:H6	1.86	0.41
77:CI:2173:A:C4	77:CI:2174:A:C8	3.09	0.41
77:CI:2500:A:H2'	77:CI:2501:A:C8	2.56	0.41
77:CI:3293:G:N2	77:CI:3295:C:H5''	2.36	0.41
77:CI:3323:G:H2'	77:CI:3324:G:H8	1.86	0.41
3:AC:828:A:C4	3:AC:829:G:C8	3.09	0.40
3:AC:985:C:O2	28:AZ:138:ASP:CB	2.69	0.40
5:AH:11:LYS:O	5:AH:14:ARG:HG2	2.20	0.40
7:AK:15:LEU:HD21	7:AK:71:LEU:HD13	2.03	0.40
13:AT:68:ASP:OD1	13:AT:68:ASP:O	2.39	0.40
13:AT:244:ASN:OD1	13:AT:245:ARG:N	2.54	0.40
20:AI:147:LEU:CD1	20:AI:163:CYS:SG	3.09	0.40
41:BG:5:SER:HA	79:CK:11:C:O2'	2.20	0.40
44:BJ:52:LYS:O	44:BJ:53:LYS:C	2.64	0.40
45:BK:38:ASP:OD2	45:BK:38:ASP:C	2.63	0.40
46:BL:60:VAL:HG13	46:BL:75:GLU:OE2	2.20	0.40
55:BU:87:ARG:HH12	55:BU:122:VAL:HG11	1.87	0.40
71:CC:126:VAL:HG11	71:CC:161:ILE:HG12	2.04	0.40
72:CD:150:GLU:O	72:CD:154:ARG:HG3	2.21	0.40
77:CI:842:U:C2	77:CI:843:C:C5	3.09	0.40
77:CI:1131:U:O4'	77:CI:1131:U:P	2.79	0.40
77:CI:2655:C:H2'	77:CI:2656:U:H6	1.85	0.40
77:CI:3452:U:N3	77:CI:3453:C:C5	2.89	0.40
77:CI:3723:U:H2'	77:CI:3724:U:H6	1.85	0.40
79:CK:140:C:H2'	79:CK:141:C:C6	2.57	0.40
3:AC:502:C:O2	3:AC:502:C:H2'	2.20	0.40
3:AC:571:C:H2'	3:AC:572:U:O4'	2.21	0.40
3:AC:1554:C:OP1	3:AC:1555:C:OP2	2.40	0.40
3:AC:1725:A:C2	3:AC:1812:C:O2	2.75	0.40
13:AT:168:CYS:HB3	13:AT:198:VAL:HG21	2.02	0.40
17:AD:86:LEU:HB3	17:AD:98:THR:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AQ:30:ALA:O	21:AQ:60:ARG:HD3	2.21	0.40
25:AV:16:ILE:O	25:AV:16:ILE:HG13	2.21	0.40
29:Aa:105:THR:O	29:Aa:105:THR:HG23	2.21	0.40
42:BH:39:THR:HG23	42:BH:132:LYS:NZ	2.36	0.40
55:BU:38:PHE:CE2	55:BU:78:ARG:NH2	2.89	0.40
58:BX:2:VAL:HG12	58:BX:3:GLN:N	2.36	0.40
76:CH:203:TYR:C	76:CH:204:ARG:HD3	2.46	0.40
77:CI:119:G:H4'	77:CI:120:A:OP2	2.22	0.40
77:CI:435:A:N6	77:CI:1126:A:C2	2.89	0.40
77:CI:472:C:O2	77:CI:473:C:C5	2.74	0.40
77:CI:802:C:C4	77:CI:803:C:C5	3.09	0.40
77:CI:1120:C:H2'	77:CI:1121:A:H8	1.86	0.40
77:CI:1140:A2M:HM'3	77:CI:1140:A2M:H1'	1.94	0.40
77:CI:1257:G:N1	77:CI:1258:U:C4	2.89	0.40
77:CI:1484:U:O2	77:CI:1484:U:H2'	2.21	0.40
77:CI:3367:C:H2'	77:CI:3368:U:C1'	2.50	0.40
77:CI:3576:A:H2'	77:CI:3577:G:H8	1.86	0.40
3:AC:42:A:C8	3:AC:427:A:C2	3.09	0.40
3:AC:59:U:H5''	3:AC:504:C:N4	2.37	0.40
3:AC:186:C:H2'	3:AC:187:G:H8	1.87	0.40
3:AC:495:C:C2	3:AC:496:U:C5	3.10	0.40
3:AC:596:U:H2'	3:AC:597:U:C6	2.56	0.40
3:AC:1159:G:H5''	29:Aa:76:SER:OG	2.20	0.40
6:AJ:139:VAL:CG1	6:AJ:140:ASP:N	2.84	0.40
8:AL:41:GLN:OE1	8:AL:41:GLN:N	2.54	0.40
17:AD:21:VAL:O	17:AD:21:VAL:HG12	2.19	0.40
24:AU:211:LYS:O	24:AU:215:MET:HG3	2.22	0.40
29:Aa:35:VAL:O	29:Aa:39:THR:HG23	2.21	0.40
31:Ad:15:GLU:OE2	31:Ad:23:ARG:HD3	2.22	0.40
31:Ad:21:LYS:O	31:Ad:22:LYS:HB2	2.22	0.40
33:Ag:137:SER:HB3	33:Ag:162:GLN:HB2	2.04	0.40
34:Ah:43:ILE:HD13	34:Ah:57:ALA:HA	2.04	0.40
36:BB:258:HIS:HB3	36:BB:259:PRO:HD3	2.04	0.40
41:BG:36:ILE:HD11	41:BG:44:ALA:HA	2.04	0.40
42:BH:177:ALA:O	42:BH:178:ARG:C	2.64	0.40
77:CI:163:A:H2'	77:CI:164:G:C8	2.56	0.40
77:CI:716:G:H2'	77:CI:717:A:C8	2.55	0.40
77:CI:1260:C:N3	77:CI:1261:G:N7	2.70	0.40
77:CI:1581:U:H2'	77:CI:1582:A:C8	2.57	0.40
77:CI:2295:C:H2'	77:CI:2296:C:H6	1.85	0.40
77:CI:2396:G:H2'	77:CI:2397:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:CI:2447:U:O2	77:CI:2448:U:C5	2.74	0.40
77:CI:3391:A:H2'	77:CI:3392:A:C8	2.56	0.40
77:CI:4237:C:H2'	77:CI:4238:C:O4'	2.22	0.40
77:CI:4378:A:H2'	77:CI:4379:A:C8	2.56	0.40
77:CI:4517:OMG:O3'	77:CI:4517:OMG:HM22	2.22	0.40
79:CK:62:A:H4'	79:CK:63:U:O5'	2.22	0.40
79:CK:89:U:H2'	79:CK:90:C:C6	2.56	0.40
3:AC:528:C:H41	3:AC:559:G:H1	1.70	0.40
3:AC:817:A:H2'	3:AC:818:G:O4'	2.22	0.40
3:AC:1345:A:H4'	3:AC:1346:G:OP1	2.21	0.40
3:AC:1521:G:H5''	3:AC:1522:C:OP2	2.20	0.40
3:AC:1538:A:C4	3:AC:1539:C:C6	3.10	0.40
4:AE:69:LEU:HA	4:AE:72:VAL:HG22	2.02	0.40
6:AJ:48:TYR:HD1	9:AM:49:TYR:CZ	2.38	0.40
17:AD:137:LEU:HG	17:AD:215:VAL:HG22	2.04	0.40
26:AW:57:ALA:O	26:AW:61:LEU:HD23	2.21	0.40
26:AW:60:LEU:HD22	26:AW:70:ARG:HA	2.03	0.40
29:Aa:26:LEU:HD11	29:Aa:60:LYS:HD3	2.02	0.40
29:Aa:80:ASP:OD1	29:Aa:80:ASP:O	2.40	0.40
31:Ad:32:PHE:CE2	31:Ad:47:PHE:HB2	2.56	0.40
36:BB:245:HIS:O	36:BB:246:ARG:HG2	2.20	0.40
38:BD:237:GLU:O	38:BD:241:LYS:HG2	2.22	0.40
41:BG:36:ILE:HD11	41:BG:44:ALA:HB1	2.03	0.40
44:BJ:165:PRO:C	44:BJ:167:PHE:H	2.28	0.40
50:BP:50:ARG:HE	79:CK:71:A:H2'	1.86	0.40
52:BR:21:ARG:HB3	77:CI:1132:C:OP2	2.21	0.40
52:BR:110:LYS:HE2	77:CI:1210:G:N7	2.36	0.40
53:BS:45:PHE:O	53:BS:48:LYS:HG2	2.22	0.40
54:BT:15:ASN:O	54:BT:19:GLN:HG3	2.21	0.40
71:CC:54:ARG:HH11	71:CC:54:ARG:HG3	1.86	0.40
72:CD:100:ASN:O	72:CD:101:LYS:C	2.65	0.40
77:CI:1144:A:C8	77:CI:3523:C:C4	3.10	0.40
77:CI:1386:G:C6	77:CI:1387:B9B:N1	2.90	0.40
77:CI:1403:C:H3'	77:CI:1404:U:H4'	2.03	0.40
77:CI:2097:A:O2'	77:CI:2098:G:H5'	2.21	0.40
77:CI:2166:C:O2	77:CI:2166:C:H2'	2.21	0.40
77:CI:2254:C:N4	77:CI:2255:C:H41	2.20	0.40
77:CI:2331:U:O2	77:CI:2345:C:C4	2.74	0.40
77:CI:2614:A:H2'	77:CI:2615:G:O4'	2.21	0.40
77:CI:3889:A:N7	77:CI:3926:A:C2	2.90	0.40
3:AC:657:G:H5'	3:AC:663:G:N2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:825:C:H1'	26:AW:144:ILE:HG21	2.03	0.40
3:AC:1018:U:H2'	3:AC:1019:U:H6	1.86	0.40
3:AC:1840:U:H2'	3:AC:1841:U:C6	2.56	0.40
5:AH:36:GLU:HB3	5:AH:47:ARG:HD2	2.01	0.40
10:AN:40:TYR:CE2	10:AN:44:VAL:HG21	2.56	0.40
12:AP:110:VAL:O	12:AP:110:VAL:HG13	2.20	0.40
24:AU:66:LEU:HD21	24:AU:86:LEU:HD12	2.03	0.40
25:AV:24:LEU:O	25:AV:28:TYR:CD2	2.74	0.40
30:Ab:44:LEU:HD11	30:Ab:48:TYR:CE2	2.57	0.40
31:Ad:19:HIS:O	31:Ad:21:LYS:O	2.39	0.40
33:Ag:98:ARG:HG2	33:Ag:125:VAL:HG13	2.03	0.40
35:BA:54:ARG:HD2	35:BA:56:ALA:O	2.22	0.40
36:BB:303:ALA:HB2	36:BB:314:ILE:CD1	2.52	0.40
40:BF:81:TRP:CZ2	40:BF:99:LEU:HD21	2.56	0.40
40:BF:141:LEU:O	40:BF:145:VAL:HG22	2.21	0.40
41:BG:104:LEU:HD23	41:BG:104:LEU:C	2.47	0.40
58:BX:90:ARG:NH2	77:CI:3776:C:OP1	2.55	0.40
65:Be:16:LYS:HG2	65:Be:20:MET:HE2	2.03	0.40
67:Bg:7:LYS:NZ	77:CI:2631:C:H2'	2.37	0.40
69:CA:112:ALA:HB3	69:CA:145:VAL:CG2	2.51	0.40
72:CD:156:LYS:HD2	72:CD:165:ILE:HD11	2.04	0.40
74:CF:55:ILE:CD1	74:CF:154:VAL:HG11	2.51	0.40
77:CI:873:C:O2	77:CI:873:C:H2'	2.21	0.40
77:CI:1288:G:N2	77:CI:1303:G:C5	2.90	0.40
77:CI:3311:A:H2'	77:CI:3312:A:C8	2.57	0.40
77:CI:3332:C:C4'	77:CI:3333:G:OP2	2.70	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	22
6	AJ	187/204 (92%)	180 (96%)	6 (3%)	1 (0%)	24	34
7	AK	95/165 (58%)	94 (99%)	1 (1%)	0	100	100
8	AL	121/145 (83%)	118 (98%)	3 (2%)	0	100	100
9	AM	142/146 (97%)	137 (96%)	5 (4%)	0	100	100
10	AN	142/152 (93%)	139 (98%)	3 (2%)	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%)	298 (96%)	13 (4%)	0	100	100
14	AX	83/132 (63%)	78 (94%)	5 (6%)	0	100	100
15	Ac	73/125 (58%)	72 (99%)	1 (1%)	0	100	100
16	Af	60/156 (38%)	57 (95%)	3 (5%)	0	100	100
17	AD	212/264 (80%)	207 (98%)	5 (2%)	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%)	209 (99%)	3 (1%)	0	100	100
21	AQ	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
22	AR	139/143 (97%)	134 (96%)	5 (4%)	0	100	100
23	AS	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
24	AU	220/293 (75%)	215 (98%)	5 (2%)	0	100	100
25	AV	225/249 (90%)	216 (96%)	9 (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%)	130 (98%)	2 (2%)	0	100	100
29	Aa	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
30	Ab	119/133 (90%)	114 (96%)	4 (3%)	1 (1%)	16	22
31	Ad	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
32	Ae	11/133 (8%)	10 (91%)	1 (9%)	0	100	100
33	Ag	179/194 (92%)	170 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Ah	204/208 (98%)	198 (97%)	6 (3%)	0	100	100
35	BA	249/257 (97%)	241 (97%)	8 (3%)	0	100	100
36	BB	394/403 (98%)	388 (98%)	6 (2%)	0	100	100
37	BC	364/419 (87%)	357 (98%)	7 (2%)	0	100	100
38	BD	291/297 (98%)	287 (99%)	4 (1%)	0	100	100
39	BE	212/296 (72%)	205 (97%)	6 (3%)	1 (0%)	24	34
40	BF	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
41	BG	151/184 (82%)	147 (97%)	3 (2%)	1 (1%)	18	25
42	BH	184/188 (98%)	180 (98%)	4 (2%)	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%)	157 (100%)	0	0	100	100
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%)	113 (97%)	3 (3%)	0	100	100
50	BP	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
51	BQ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
52	BR	145/148 (98%)	138 (95%)	7 (5%)	0	100	100
53	BS	95/160 (59%)	93 (98%)	2 (2%)	0	100	100
54	BT	92/115 (80%)	90 (98%)	2 (2%)	0	100	100
55	BU	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
56	BV	106/135 (78%)	106 (100%)	0	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%)	84 (100%)	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	Be	23/25 (92%)	23 (100%)	0	0	100	100
66	Bf	101/106 (95%)	96 (95%)	5 (5%)	0	100	100
67	Bg	87/92 (95%)	85 (98%)	2 (2%)	0	100	100
68	Bh	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
69	CA	221/270 (82%)	214 (97%)	7 (3%)	0	100	100
70	CB	227/266 (85%)	221 (97%)	6 (3%)	0	100	100
71	CC	188/192 (98%)	186 (99%)	2 (1%)	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%)	195 (95%)	10 (5%)	0	100	100
75	CG	137/217 (63%)	136 (99%)	1 (1%)	0	100	100
76	CH	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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 (94) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	37	ASN
4	AE	4	GLN
4	AE	165	ASN
4	AE	207	HIS
5	AH	48	ASN
6	AJ	31	ASN
6	AJ	114	ASN
6	AJ	186	ASN
7	AK	42	ASN
7	AK	50	GLN
9	AM	48	GLN
9	AM	77	HIS
10	AN	73	ASN
11	AO	142	ASN
13	AT	119	GLN
13	AT	181	ASN
13	AT	191	HIS
16	Af	151	ASN
17	AD	186	ASN
18	AF	67	GLN
18	AF	201	HIS

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Mol	Chain	Res	Type
19	AG	19	ASN
23	AS	72	HIS
25	AV	202	ASN
27	AY	62	GLN
29	Aa	56	HIS
29	Aa	70	ASN
29	Aa	92	ASN
31	Ad	51	GLN
33	Ag	126	HIS
33	Ag	157	HIS
33	Ag	168	HIS
34	Ah	138	ASN
34	Ah	167	GLN
35	BA	217	GLN
36	BB	11	HIS
36	BB	25	HIS
36	BB	145	GLN
36	BB	179	HIS
36	BB	204	GLN
36	BB	213	GLN
36	BB	258	HIS
37	BC	286	ASN
37	BC	329	ASN
38	BD	291	GLN
39	BE	165	HIS
39	BE	199	GLN
40	BF	50	ASN
40	BF	150	GLN
41	BG	56	GLN
42	BH	21	GLN
43	BI	27	ASN
45	BK	3	ASN
46	BL	38	ASN
47	BM	77	HIS
49	BO	69	ASN
50	BP	20	ASN
52	BR	17	HIS
52	BR	19	HIS
52	BR	60	HIS
52	BR	85	GLN
53	BS	6	ASN
53	BS	12	GLN

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Mol	Chain	Res	Type
53	BS	17	HIS
53	BS	50	ASN
53	BS	114	GLN
54	BT	72	HIS
55	BU	118	GLN
56	BV	117	GLN
57	BW	56	ASN
58	BX	73	HIS
58	BX	100	GLN
59	BY	98	HIS
60	BZ	15	HIS
61	Ba	76	HIS
63	Bc	17	GLN
67	Bg	34	HIS
67	Bg	56	HIS
68	Bh	36	ASN
69	CA	80	HIS
69	CA	261	GLN
70	CB	112	GLN
70	CB	208	ASN
71	CC	98	HIS
71	CC	188	GLN
72	CD	73	ASN
72	CD	144	ASN
72	CD	166	HIS
74	CF	149	GLN
75	CG	34	ASN
75	CG	66	HIS
76	CH	29	GLN
76	CH	37	HIS
76	CH	117	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	AC	1686/1871 (90%)	318 (18%)	3 (0%)
77	CI	3541/4731 (74%)	660 (18%)	17 (0%)
78	CJ	119/121 (98%)	9 (7%)	0
79	CK	155/156 (99%)	27 (17%)	2 (1%)
All	All	5501/6879 (79%)	1014 (18%)	22 (0%)

All (1014) 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
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

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Mol	Chain	Res	Type
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	486	A
3	AC	488	U
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
3	AC	894	U
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

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Mol	Chain	Res	Type
3	AC	934	G
3	AC	935	G
3	AC	956	A
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	1088	A
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
3	AC	1257	G
3	AC	1258	G
3	AC	1260	A
3	AC	1274	C
3	AC	1275	G

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Mol	Chain	Res	Type
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	1347	U
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	1450	G
3	AC	1455	A
3	AC	1463	U
3	AC	1464	U
3	AC	1491	G
3	AC	1498	G
3	AC	1499	A
3	AC	1509	A

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Mol	Chain	Res	Type
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	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
3	AC	1774	C
3	AC	1775	C
3	AC	1779	C
3	AC	1783	G

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Mol	Chain	Res	Type
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	1827	G
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
77	CI	127	G
77	CI	133	C
77	CI	134	G

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Mol	Chain	Res	Type
77	CI	136	C
77	CI	137	G
77	CI	139	G
77	CI	144	G
77	CI	159	C
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
77	CI	383	A
77	CI	387	G
77	CI	401	G
77	CI	407	A

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Mol	Chain	Res	Type
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
77	CI	692	A
77	CI	702	U
77	CI	703	G
77	CI	710	C

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Mol	Chain	Res	Type
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
77	CI	1013	C
77	CI	1015	C
77	CI	1019	G
77	CI	1031	U

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Mol	Chain	Res	Type
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	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
77	CI	1194	G
77	CI	1195	U
77	CI	1201	A
77	CI	1208	G
77	CI	1211	A

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Mol	Chain	Res	Type
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	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
77	CI	1454	G
77	CI	1455	A
77	CI	1458	C
77	CI	1464	G
77	CI	1466	A
77	CI	1467	G

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Mol	Chain	Res	Type
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	1592	U
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
77	CI	1689	G
77	CI	1693	A
77	CI	1698	A
77	CI	1700	C

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Mol	Chain	Res	Type
77	CI	1701	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	2023	U
77	CI	2035	A
77	CI	2036	G
77	CI	2045	C
77	CI	2056	A
77	CI	2057	G
77	CI	2069	A
77	CI	2070	G
77	CI	2078	G

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Mol	Chain	Res	Type
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	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	2278	G7M
77	CI	2285	A
77	CI	2302	G
77	CI	2315	G
77	CI	2329	A
77	CI	2332	G
77	CI	2342	G
77	CI	2343	A
77	CI	2345	C

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Mol	Chain	Res	Type
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	2510	G
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
77	CI	2553	C
77	CI	2554	A
77	CI	2570	C
77	CI	2582	U
77	CI	2583	G

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Mol	Chain	Res	Type
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	2662	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
77	CI	3376	A
77	CI	3404	U
77	CI	3409	G
77	CI	3415	A

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Mol	Chain	Res	Type
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	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
77	CI	3566	G
77	CI	3567	A
77	CI	3574	U
77	CI	3585	C
77	CI	3597	G

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Mol	Chain	Res	Type
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	3783	C
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
77	CI	3904	G
77	CI	3906	A
77	CI	3909	G
77	CI	3912	A

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Mol	Chain	Res	Type
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	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	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
77	CI	4167	U
77	CI	4168	A
77	CI	4174	C
77	CI	4179	G
77	CI	4183	G

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Mol	Chain	Res	Type
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	4313	G
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
77	CI	4420	G
77	CI	4426	U
77	CI	4427	C
77	CI	4436	U

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Mol	Chain	Res	Type
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	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	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	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
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

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Mol	Chain	Res	Type
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	97	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
79	CK	110	U
79	CK	111	U
79	CK	114	G
79	CK	121	G
79	CK	122	G
79	CK	123	U

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Mol	Chain	Res	Type
79	CK	124	U
79	CK	125	C
79	CK	126	C
79	CK	127	U
79	CK	128	C

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	AC	1047	U
3	AC	1438	C
3	AC	1826	A
77	CI	143	U
77	CI	1403	C
77	CI	1446	G
77	CI	1465	U
77	CI	1482	A
77	CI	1683	C
77	CI	1685	OMG
77	CI	2171	U
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
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	2MG	CI	877	77	23,26,27	0.49	0	32,38,41	0.51	0
77	5MC	CI	3441	77	18,22,23	0.61	0	26,32,35	0.49	0
77	OMC	CI	3360	77	19,22,23	0.55	0	26,31,34	0.60	0
77	B9B	CI	1387	77	25,28,29	1.76	7 (28%)	35,40,43	3.01	11 (31%)
77	A2M	CI	3444	77	22,25,26	3.33	10 (45%)	31,36,39	2.64	13 (41%)
77	OMC	CI	2121	77	19,22,23	0.60	0	26,31,34	1.35	4 (15%)
79	OMU	CK	14	79	19,22,23	3.58	8 (42%)	26,31,34	1.70	5 (19%)
77	OMG	CI	373	77	23,26,27	0.53	0	33,38,41	0.56	0
77	A2M	CI	1673	77	22,25,26	3.44	10 (45%)	31,36,39	2.65	12 (38%)
77	B9H	CI	2542	77	20,25,26	4.78	4 (20%)	22,35,38	1.55	4 (18%)
77	B8T	CI	4138	77	19,22,23	3.24	8 (42%)	26,31,34	0.80	1 (3%)
77	B8Q	CI	1269	77	17,22,23	4.66	5 (29%)	22,32,35	2.05	6 (27%)
3	4AC	AC	1843	3	21,24,25	3.74	10 (47%)	29,34,37	0.94	3 (10%)
3	PSU	AC	823	3	18,21,22	1.02	1 (5%)	22,30,33	1.84	5 (22%)
77	PSU	CI	4283	77	18,21,22	0.98	1 (5%)	22,30,33	1.74	4 (18%)
77	OMU	CI	3961	77	19,22,23	3.53	8 (42%)	26,31,34	1.68	5 (19%)
77	OMG	CI	4278	77	23,26,27	0.49	0	33,38,41	0.51	0
77	PSU	CI	2264	77	18,21,22	1.04	1 (5%)	22,30,33	1.91	5 (22%)
77	PSU	CI	4105	77	18,21,22	1.08	1 (5%)	22,30,33	1.79	4 (18%)
77	1MA	CI	4070	77	21,25,26	0.49	0	31,37,40	0.78	1 (3%)
77	OMG	CI	1852	77	23,26,27	0.54	0	33,38,41	0.45	0
3	A2M	AC	166	3	22,25,26	3.42	9 (40%)	31,36,39	2.64	12 (38%)
77	P7G	CI	3539	77	24,28,29	5.20	9 (37%)	27,41,44	1.75	3 (11%)
77	OMG	CI	1685	77	23,26,27	0.56	0	33,38,41	0.56	0
77	A2M	CI	2119	77	22,25,26	3.43	10 (45%)	31,36,39	2.57	11 (35%)
77	A2M	CI	1337	77	22,25,26	3.41	10 (45%)	31,36,39	2.70	11 (35%)
77	A2M	CI	4226	77	22,25,26	3.42	9 (40%)	31,36,39	2.57	10 (32%)
77	2MG	CI	4519	77	23,26,27	0.49	0	32,38,41	0.56	0
77	5MC	CI	3990	77	18,22,23	0.56	0	26,32,35	0.55	0
3	PSU	AC	1244	3	18,21,22	1.08	1 (5%)	22,30,33	1.80	4 (18%)
3	OMG	AC	645	3	23,26,27	0.50	0	33,38,41	0.46	0
77	A2M	CI	2157	77	22,25,26	3.38	9 (40%)	31,36,39	2.62	11 (35%)
77	6MZ	CI	3875	77	22,25,26	3.79	9 (40%)	30,36,39	2.36	11 (36%)
64	MLZ	Bd	98	64	8,9,10	0.79	0	4,9,11	0.65	0
77	A2M	CI	3526	77	22,25,26	3.41	10 (45%)	31,36,39	2.66	12 (38%)
77	MHG	CI	4026	77	29,32,33	5.62	11 (37%)	34,46,49	2.49	12 (35%)

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	2.55	10 (28%)
77	A2M	CI	398	77	22,25,26	3.41	10 (45%)	31,36,39	2.64	12 (38%)
77	E7G	CI	1599	77	24,27,28	5.58	10 (41%)	30,40,43	2.25	9 (30%)
77	A2M	CI	1140	77	22,25,26	3.38	9 (40%)	31,36,39	2.63	10 (32%)
3	B8N	AC	1249	3	24,29,30	3.29	6 (25%)	29,42,45	1.86	5 (17%)
77	PSU	CI	1490	77	18,21,22	1.09	1 (5%)	22,30,33	1.81	4 (18%)
3	OMC	AC	518	3	19,22,23	0.53	0	26,31,34	0.59	0
3	PSU	AC	824	3	18,21,22	1.13	1 (5%)	22,30,33	1.78	4 (18%)
77	OMG	CI	2529	77	23,26,27	0.54	0	33,38,41	0.49	0
77	OMC	CI	2178	77	19,22,23	0.55	0	26,31,34	0.54	0
3	A2M	AC	27	3	22,25,26	3.39	9 (40%)	31,36,39	2.66	13 (41%)
77	I4U	CI	1472	77	21,24,25	3.53	9 (42%)	27,34,37	1.05	1 (3%)
77	PSU	CI	1496	77	18,21,22	1.08	1 (5%)	22,30,33	1.81	4 (18%)
77	PSU	CI	4155	77	18,21,22	1.07	1 (5%)	22,30,33	1.85	4 (18%)
77	OMU	CI	4275	77	19,22,23	3.47	8 (42%)	26,31,34	1.60	5 (19%)
77	OMG	CI	2120	77	23,26,27	0.51	0	33,38,41	0.47	0
77	OMC	CI	3528	77	19,22,23	0.54	0	26,31,34	0.65	0
77	PSU	CI	3374	77	18,21,22	1.08	1 (5%)	22,30,33	1.89	4 (18%)
77	OMC	CI	3568	77	19,22,23	0.55	0	26,31,34	0.89	2 (7%)
77	B9B	CI	237	77	25,28,29	1.75	6 (24%)	35,40,43	2.84	11 (31%)
3	A2M	AC	669	3	22,25,26	3.36	9 (40%)	31,36,39	2.54	10 (32%)
77	A2M	CI	3377	77	22,25,26	3.41	9 (40%)	31,36,39	2.60	13 (41%)
77	PSU	CI	4291	77	18,21,22	1.06	1 (5%)	22,30,33	1.84	6 (27%)
77	PSU	CI	1395	77	18,21,22	1.12	1 (5%)	22,30,33	1.70	4 (18%)
3	A2M	AC	1032	3	22,25,26	3.43	9 (40%)	31,36,39	2.64	12 (38%)
77	OMG	CI	4149	77	23,26,27	0.51	0	33,38,41	0.49	0
77	OMC	CI	2560	77	19,22,23	0.53	0	26,31,34	0.60	0
77	P7G	CI	1711	77,78	24,28,29	5.01	9 (37%)	27,41,44	1.05	1 (3%)
77	PSU	CI	4097	77	18,21,22	1.06	1 (5%)	22,30,33	1.77	5 (22%)
77	E7G	CI	2053	77	24,27,28	5.61	11 (45%)	30,40,43	2.20	9 (30%)
77	A2M	CI	3382	77	22,25,26	3.41	9 (40%)	31,36,39	2.59	11 (35%)
77	I4U	CI	3849	77	21,24,25	3.54	9 (42%)	27,34,37	0.97	1 (3%)
77	PSU	CI	4058	77	18,21,22	1.04	1 (5%)	22,30,33	1.88	4 (18%)
77	PSU	CI	3948	77	18,21,22	1.07	1 (5%)	22,30,33	1.83	5 (22%)
77	UR3	CI	1668	77	19,22,23	2.99	8 (42%)	26,32,35	1.32	2 (7%)
77	PSU	CI	4186	77	18,21,22	1.08	1 (5%)	22,30,33	1.82	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
77	OMG	CI	4292	77	23,26,27	0.51	0	33,38,41	0.43	0
77	PSU	CI	3388	77	18,21,22	1.13	1 (5%)	22,30,33	1.86	5 (22%)
77	G7M	CI	4205	77	23,26,27	2.96	9 (39%)	35,39,42	2.47	10 (28%)
37	MLZ	BC	333	37	8,9,10	0.81	0	4,9,11	0.69	0
77	UR3	CI	4252	77	19,22,23	3.04	8 (42%)	26,32,35	1.36	3 (11%)
77	OMG	CI	1335	77	23,26,27	0.53	0	33,38,41	0.52	0
3	OMU	AC	116	3	19,22,23	3.55	8 (42%)	26,31,34	1.62	5 (19%)
77	A2M	CI	1347	77	22,25,26	3.43	9 (40%)	31,36,39	2.59	10 (32%)
77	5MC	CI	4102	77	18,22,23	0.55	0	26,32,35	0.68	0
3	UR3	AC	1831	3	19,22,23	3.03	8 (42%)	26,32,35	1.37	3 (11%)
77	OMG	CI	1438	77	23,26,27	0.50	0	33,38,41	0.50	0
3	OMG	AC	684	3	23,26,27	0.50	0	33,38,41	0.55	0
3	PSU	AC	1082	3	18,21,22	1.05	1 (5%)	22,30,33	1.87	5 (22%)
77	A2M	CI	3484	77	22,25,26	3.40	9 (40%)	31,36,39	2.65	12 (38%)
77	OMG	CI	4517	77	23,26,27	0.47	0	33,38,41	0.94	1 (3%)
77	2MG	CI	1330	77	23,26,27	0.47	0	32,38,41	0.56	0
77	OMG	CI	3451	77	23,26,27	0.51	0	33,38,41	0.43	0
77	OMG	CI	2180	77	23,26,27	0.51	0	33,38,41	0.43	0
77	G7M	CI	1418	77	23,26,27	2.95	9 (39%)	35,39,42	2.48	10 (28%)
77	OMC	CI	2617	77	19,22,23	0.52	0	26,31,34	0.73	1 (3%)
77	OMC	CI	3546	77	19,22,23	0.62	0	26,31,34	0.80	1 (3%)
77	OMG	CI	4025	77	23,26,27	0.52	0	33,38,41	0.56	0
77	OMC	CI	4191	77	19,22,23	0.56	0	26,31,34	0.67	0
77	OMG	CI	3851	77	23,26,27	0.51	0	33,38,41	0.44	0
77	B8W	CI	3840	77	23,26,27	1.87	4 (17%)	33,38,41	2.53	14 (42%)
77	PSU	CI	3423	77	18,21,22	1.04	1 (5%)	22,30,33	1.71	4 (18%)
3	PSU	AC	613	3	18,21,22	1.01	1 (5%)	22,30,33	1.93	5 (22%)
77	E6G	CI	4010	77	24,27,28	2.12	5 (20%)	34,39,42	5.87	16 (47%)

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	2MG	CI	877	77	-	2/9/27/28	0/3/3/3
77	5MC	CI	3441	77	-	0/7/25/26	0/2/2/2
77	OMC	CI	3360	77	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	B9B	CI	1387	77	-	2/11/29/30	0/3/3/3
77	A2M	CI	3444	77	-	1/9/27/28	0/3/3/3
77	OMC	CI	2121	77	-	2/9/27/28	0/2/2/2
79	OMU	CK	14	79	-	4/9/27/28	0/2/2/2
77	OMG	CI	373	77	-	0/9/27/28	0/3/3/3
77	A2M	CI	1673	77	-	2/9/27/28	0/3/3/3
77	B9H	CI	2542	77	-	2/12/47/48	0/2/2/2
77	B8T	CI	4138	77	-	0/7/27/28	0/2/2/2
77	B8Q	CI	1269	77	-	0/7/42/43	0/2/2/2
3	4AC	AC	1843	3	-	0/11/29/30	0/2/2/2
3	PSU	AC	823	3	-	3/7/25/26	0/2/2/2
77	PSU	CI	4283	77	-	0/7/25/26	0/2/2/2
77	OMU	CI	3961	77	-	3/9/27/28	0/2/2/2
77	OMG	CI	4278	77	-	0/9/27/28	0/3/3/3
77	PSU	CI	2264	77	-	0/7/25/26	0/2/2/2
77	PSU	CI	4105	77	-	5/7/25/26	0/2/2/2
77	1MA	CI	4070	77	-	0/7/25/26	0/3/3/3
77	OMG	CI	1852	77	-	0/9/27/28	0/3/3/3
3	A2M	AC	166	3	-	0/9/27/28	0/3/3/3
77	P7G	CI	3539	77	-	1/10/40/41	0/3/3/3
77	OMG	CI	1685	77	-	2/9/27/28	0/3/3/3
77	A2M	CI	2119	77	-	0/9/27/28	0/3/3/3
77	A2M	CI	1337	77	-	1/9/27/28	0/3/3/3
77	A2M	CI	4226	77	-	0/9/27/28	0/3/3/3
77	2MG	CI	4519	77	-	2/9/27/28	0/3/3/3
77	5MC	CI	3990	77	-	0/7/25/26	0/2/2/2
3	PSU	AC	1244	3	-	3/7/25/26	0/2/2/2
3	OMG	AC	645	3	-	1/9/27/28	0/3/3/3
77	A2M	CI	2157	77	-	0/9/27/28	0/3/3/3
77	6MZ	CI	3875	77	-	0/9/27/28	0/3/3/3
64	MLZ	Bd	98	64	-	1/7/8/10	-
77	A2M	CI	3526	77	-	3/9/27/28	0/3/3/3
77	MHG	CI	4026	77	-	5/16/46/47	0/3/3/3
77	G7M	CI	2278	77	-	2/7/25/26	0/3/3/3
77	A2M	CI	398	77	-	1/9/27/28	0/3/3/3
77	E7G	CI	1599	77	-	2/9/39/40	0/3/3/3
77	A2M	CI	1140	77	-	3/9/27/28	0/3/3/3
3	B8N	AC	1249	3	-	6/16/34/35	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	PSU	CI	1490	77	-	1/7/25/26	0/2/2/2
3	OMC	AC	518	3	-	0/9/27/28	0/2/2/2
3	PSU	AC	824	3	-	0/7/25/26	0/2/2/2
77	OMG	CI	2529	77	-	2/9/27/28	0/3/3/3
77	OMC	CI	2178	77	-	1/9/27/28	0/2/2/2
3	A2M	AC	27	3	-	1/9/27/28	0/3/3/3
77	I4U	CI	1472	77	-	0/9/29/30	0/2/2/2
77	PSU	CI	1496	77	-	0/7/25/26	0/2/2/2
77	PSU	CI	4155	77	-	1/7/25/26	0/2/2/2
77	OMU	CI	4275	77	-	0/9/27/28	0/2/2/2
77	OMG	CI	2120	77	-	2/9/27/28	0/3/3/3
77	OMC	CI	3528	77	-	2/9/27/28	0/2/2/2
77	PSU	CI	3374	77	-	2/7/25/26	0/2/2/2
77	OMC	CI	3568	77	-	0/9/27/28	0/2/2/2
77	B9B	CI	237	77	-	6/11/29/30	0/3/3/3
3	A2M	AC	669	3	-	4/9/27/28	0/3/3/3
77	A2M	CI	3377	77	-	2/9/27/28	0/3/3/3
77	PSU	CI	4291	77	-	5/7/25/26	0/2/2/2
77	PSU	CI	1395	77	-	0/7/25/26	0/2/2/2
3	A2M	AC	1032	3	-	0/9/27/28	0/3/3/3
77	OMG	CI	4149	77	-	2/9/27/28	0/3/3/3
77	OMC	CI	2560	77	-	1/9/27/28	0/2/2/2
77	P7G	CI	1711	77,78	-	0/10/40/41	0/3/3/3
77	PSU	CI	4097	77	-	1/7/25/26	0/2/2/2
77	E7G	CI	2053	77	-	0/9/39/40	0/3/3/3
77	A2M	CI	3382	77	-	0/9/27/28	0/3/3/3
77	I4U	CI	3849	77	-	2/9/29/30	0/2/2/2
77	PSU	CI	4058	77	-	0/7/25/26	0/2/2/2
77	PSU	CI	3948	77	-	2/7/25/26	0/2/2/2
77	UR3	CI	1668	77	-	0/7/25/26	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	PSU	CI	3388	77	-	2/7/25/26	0/2/2/2
77	G7M	CI	4205	77	-	2/7/25/26	0/3/3/3
37	MLZ	BC	333	37	-	1/7/8/10	-
77	UR3	CI	4252	77	-	0/7/25/26	0/2/2/2
77	OMG	CI	1335	77	-	0/9/27/28	0/3/3/3
3	OMU	AC	116	3	-	0/9/27/28	0/2/2/2
77	A2M	CI	1347	77	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	5MC	CI	4102	77	-	6/7/25/26	0/2/2/2
3	UR3	AC	1831	3	-	0/7/25/26	0/2/2/2
77	OMG	CI	1438	77	-	2/9/27/28	0/3/3/3
3	OMG	AC	684	3	-	1/9/27/28	0/3/3/3
3	PSU	AC	1082	3	-	0/7/25/26	0/2/2/2
77	A2M	CI	3484	77	-	1/9/27/28	0/3/3/3
77	OMG	CI	4517	77	-	4/9/27/28	0/3/3/3
77	2MG	CI	1330	77	-	0/9/27/28	0/3/3/3
77	OMG	CI	3451	77	-	0/9/27/28	0/3/3/3
77	OMG	CI	2180	77	-	0/9/27/28	0/3/3/3
77	G7M	CI	1418	77	-	2/7/25/26	0/3/3/3
77	OMC	CI	2617	77	-	0/9/27/28	0/2/2/2
77	OMC	CI	3546	77	-	3/9/27/28	0/2/2/2
77	OMG	CI	4025	77	-	2/9/27/28	0/3/3/3
77	OMC	CI	4191	77	-	0/9/27/28	0/2/2/2
77	OMG	CI	3851	77	-	0/9/27/28	0/3/3/3
77	B8W	CI	3840	77	-	2/9/27/28	0/3/3/3
77	PSU	CI	3423	77	-	1/7/25/26	0/2/2/2
3	PSU	AC	613	3	-	2/7/25/26	0/2/2/2
77	E6G	CI	4010	77	-	3/10/28/29	0/3/3/3

All (394) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	2053	E7G	C8-N9	22.79	1.58	1.46
77	CI	1599	E7G	C8-N9	22.67	1.58	1.46
77	CI	4026	MHG	C8-N9	19.84	1.57	1.46
77	CI	3539	P7G	C8-N9	18.27	1.56	1.46
77	CI	1711	P7G	C8-N9	17.30	1.55	1.46
77	CI	2542	B9H	C4-N3	14.20	1.70	1.48
77	CI	3875	6MZ	C6-N6	11.57	1.46	1.34
77	CI	4026	MHG	C8-N7	11.53	1.56	1.45
77	CI	1269	B8Q	C4-N3	11.36	1.66	1.48
77	CI	2542	B9H	C6-C5	11.23	1.58	1.33
77	CI	4026	MHG	C2-N3	10.98	1.52	1.31
77	CI	1472	I4U	C4-N3	10.84	1.45	1.31
77	CI	1269	B8Q	C6-C5	10.71	1.57	1.33
77	CI	3849	I4U	C4-N3	10.59	1.45	1.31
77	CI	3539	P7G	C8-N7	10.57	1.55	1.45
77	CI	1711	P7G	C8-N7	10.13	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	2053	E7G	C5-N7	9.52	1.46	1.35
77	CI	1599	E7G	C5-N7	9.43	1.46	1.35
77	CI	1269	B8Q	C2-N1	9.36	1.52	1.38
3	AC	1249	B8N	C4-N3	-9.12	1.23	1.40
77	CI	4026	MHG	C2-N2	8.97	1.53	1.33
3	AC	166	A2M	O4'-C1'	8.72	1.62	1.42
77	CI	1347	A2M	C2'-C1'	-8.70	1.30	1.53
77	CI	2119	A2M	C2'-C1'	-8.68	1.30	1.53
3	AC	1032	A2M	C2'-C1'	-8.66	1.30	1.53
3	AC	1032	A2M	O4'-C1'	8.62	1.62	1.42
77	CI	1140	A2M	C2'-C1'	-8.61	1.30	1.53
79	CK	14	OMU	C2-N3	8.60	1.53	1.38
77	CI	1673	A2M	C2'-C1'	-8.58	1.31	1.53
3	AC	166	A2M	C2'-C1'	-8.57	1.31	1.53
77	CI	1337	A2M	O4'-C1'	8.55	1.62	1.42
77	CI	3382	A2M	O4'-C1'	8.54	1.62	1.42
77	CI	4226	A2M	C2'-C1'	-8.54	1.31	1.53
77	CI	3377	A2M	O4'-C1'	8.54	1.62	1.42
77	CI	3484	A2M	C2'-C1'	-8.53	1.31	1.53
77	CI	4226	A2M	O4'-C1'	8.52	1.62	1.42
77	CI	398	A2M	O4'-C1'	8.51	1.62	1.42
77	CI	2119	A2M	O4'-C1'	8.50	1.62	1.42
77	CI	398	A2M	C2'-C1'	-8.49	1.31	1.53
3	AC	116	OMU	C2-N3	8.49	1.53	1.38
3	AC	27	A2M	O4'-C1'	8.49	1.62	1.42
77	CI	3444	A2M	C2'-C1'	-8.48	1.31	1.53
77	CI	3377	A2M	C2'-C1'	-8.48	1.31	1.53
77	CI	3382	A2M	C2'-C1'	-8.48	1.31	1.53
77	CI	1347	A2M	O4'-C1'	8.47	1.62	1.42
77	CI	1337	A2M	C2'-C1'	-8.47	1.31	1.53
77	CI	1673	A2M	O4'-C1'	8.47	1.62	1.42
77	CI	2157	A2M	C2'-C1'	-8.43	1.31	1.53
3	AC	27	A2M	C2'-C1'	-8.40	1.31	1.53
77	CI	3526	A2M	O4'-C1'	8.40	1.61	1.42
77	CI	2157	A2M	O4'-C1'	8.39	1.61	1.42
77	CI	3484	A2M	O4'-C1'	8.37	1.61	1.42
77	CI	3526	A2M	C2'-C1'	-8.35	1.31	1.53
3	AC	669	A2M	O4'-C1'	8.34	1.61	1.42
77	CI	3961	OMU	C2-N3	8.30	1.52	1.38
77	CI	1140	A2M	O4'-C1'	8.24	1.61	1.42
77	CI	2542	B9H	C2-N3	-8.23	1.27	1.37
77	CI	4275	OMU	C2-N3	8.21	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	3875	6MZ	O4'-C1'	8.11	1.61	1.42
77	CI	3444	A2M	O4'-C1'	8.08	1.61	1.42
77	CI	4026	MHG	C2-N1	8.02	1.49	1.36
3	AC	669	A2M	C2'-C1'	-7.99	1.32	1.53
3	AC	1843	4AC	C4-N3	7.82	1.46	1.32
79	CK	14	OMU	C2-N1	7.77	1.50	1.38
77	CI	3961	OMU	C2-N1	7.73	1.50	1.38
3	AC	116	OMU	C2-N1	7.72	1.50	1.38
3	AC	1843	4AC	C6-C5	7.70	1.53	1.35
77	CI	4275	OMU	C2-N1	7.64	1.50	1.38
3	AC	1249	B8N	C6-N1	7.46	1.55	1.36
77	CI	3539	P7G	C2-N1	7.39	1.51	1.33
77	CI	1711	P7G	C2-N1	7.37	1.51	1.33
77	CI	2542	B9H	C2-N1	7.33	1.49	1.38
3	AC	1831	UR3	C2-N1	7.30	1.49	1.38
3	AC	1249	B8N	C6-C5	7.21	1.45	1.34
77	CI	4252	UR3	C2-N1	7.19	1.48	1.38
77	CI	2278	G7M	C4-N3	7.06	1.51	1.34
77	CI	4138	B8T	C4-N3	7.06	1.45	1.32
77	CI	1668	UR3	C2-N1	7.04	1.48	1.38
77	CI	1418	G7M	C4-N3	7.03	1.51	1.34
77	CI	4205	G7M	C4-N3	7.03	1.51	1.34
77	CI	1711	P7G	C5-C4	6.95	1.51	1.37
77	CI	3539	P7G	C5-C4	6.89	1.51	1.37
3	AC	1843	4AC	C2-N3	6.88	1.50	1.36
3	AC	669	A2M	O4'-C4'	-6.70	1.30	1.45
77	CI	4252	UR3	C6-C5	6.70	1.50	1.35
77	CI	1668	UR3	C6-C5	6.67	1.50	1.35
3	AC	1831	UR3	C6-C5	6.63	1.50	1.35
77	CI	4205	G7M	C2-N2	6.57	1.49	1.34
77	CI	4010	E6G	O6-C6	6.55	1.45	1.35
77	CI	2278	G7M	C2-N2	6.51	1.49	1.34
77	CI	1418	G7M	C2-N2	6.51	1.49	1.34
77	CI	3526	A2M	O4'-C4'	-6.44	1.30	1.45
77	CI	2119	A2M	O4'-C4'	-6.42	1.30	1.45
77	CI	1347	A2M	O4'-C4'	-6.40	1.30	1.45
77	CI	398	A2M	O4'-C4'	-6.37	1.30	1.45
77	CI	3484	A2M	O4'-C4'	-6.36	1.30	1.45
77	CI	1673	A2M	O4'-C4'	-6.35	1.30	1.45
77	CI	1337	A2M	O4'-C4'	-6.35	1.30	1.45
77	CI	1140	A2M	O4'-C4'	-6.35	1.30	1.45
3	AC	1249	B8N	C2-N1	6.34	1.58	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	3382	A2M	O4'-C4'	-6.32	1.30	1.45
77	CI	4226	A2M	O4'-C4'	-6.31	1.30	1.45
3	AC	27	A2M	O4'-C4'	-6.31	1.30	1.45
77	CI	3444	A2M	O4'-C4'	-6.30	1.30	1.45
3	AC	1032	A2M	O4'-C4'	-6.29	1.30	1.45
77	CI	2157	A2M	O4'-C4'	-6.29	1.30	1.45
77	CI	4138	B8T	C2-N3	6.27	1.49	1.36
77	CI	3849	I4U	C6-C5	6.24	1.49	1.35
77	CI	3377	A2M	O4'-C4'	-6.20	1.31	1.45
3	AC	166	A2M	O4'-C4'	-6.14	1.31	1.45
77	CI	3961	OMU	C6-C5	6.12	1.49	1.35
3	AC	116	OMU	C6-C5	6.09	1.49	1.35
77	CI	4138	B8T	C6-C5	6.07	1.49	1.35
77	CI	1418	G7M	C2-N3	6.05	1.47	1.33
77	CI	1599	E7G	C2-N3	6.05	1.47	1.33
77	CI	3849	I4U	C2-N3	6.02	1.48	1.36
77	CI	4275	OMU	C6-C5	6.02	1.49	1.35
77	CI	1472	I4U	C2-N3	6.02	1.48	1.36
77	CI	3875	6MZ	O4'-C4'	-6.01	1.31	1.45
77	CI	4026	MHG	C4-N3	6.01	1.48	1.34
77	CI	1472	I4U	C6-C5	6.00	1.49	1.35
79	CK	14	OMU	C6-C5	5.99	1.49	1.35
77	CI	4010	E6G	C2-N2	5.97	1.45	1.33
77	CI	4205	G7M	C2-N3	5.96	1.47	1.33
77	CI	2278	G7M	C2-N3	5.90	1.47	1.33
77	CI	2053	E7G	C2-N3	5.88	1.47	1.33
77	CI	3539	P7G	C4-N3	5.85	1.47	1.37
77	CI	4252	UR3	C2-N3	5.84	1.50	1.39
77	CI	237	B9B	C2-N2	5.76	1.45	1.33
77	CI	1711	P7G	C4-N3	5.71	1.47	1.37
77	CI	1387	B9B	C2-N2	5.70	1.45	1.33
3	AC	1831	UR3	C2-N3	5.69	1.50	1.39
77	CI	1668	UR3	C2-N3	5.61	1.49	1.39
77	CI	3875	6MZ	C2'-C1'	-5.53	1.35	1.53
77	CI	3840	B8W	C2-N2	5.45	1.44	1.33
77	CI	1599	E7G	C4-N3	5.37	1.47	1.34
77	CI	1269	B8Q	C2-N3	-5.30	1.26	1.35
77	CI	2053	E7G	C4-N3	5.28	1.46	1.34
77	CI	4026	MHG	C6-N1	5.22	1.48	1.38
3	AC	1843	4AC	C7-N4	5.13	1.46	1.37
77	CI	3840	B8W	O6-C6	5.03	1.43	1.35
77	CI	3539	P7G	C2-N3	4.92	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AC	1843	4AC	C4-N4	4.87	1.46	1.39
77	CI	1711	P7G	C2-N3	4.82	1.49	1.37
77	CI	2053	E7G	C2-N2	4.74	1.45	1.34
77	CI	3849	I4U	C5-C4	4.74	1.49	1.43
77	CI	2278	G7M	O6-C6	-4.73	1.14	1.23
77	CI	1418	G7M	O6-C6	-4.71	1.14	1.23
3	AC	1843	4AC	C2-N1	4.71	1.50	1.40
77	CI	1599	E7G	C2-N2	4.71	1.45	1.34
77	CI	4138	B8T	C4-N4	4.69	1.45	1.35
77	CI	1472	I4U	C5-C4	4.66	1.49	1.43
77	CI	4205	G7M	O6-C6	-4.64	1.14	1.23
77	CI	3526	A2M	C6-N6	4.50	1.45	1.34
3	AC	166	A2M	C6-N6	4.50	1.45	1.34
77	CI	398	A2M	C6-N6	4.49	1.45	1.34
77	CI	3377	A2M	C6-N6	4.49	1.45	1.34
3	AC	27	A2M	C6-N6	4.49	1.45	1.34
77	CI	4226	A2M	C6-N6	4.49	1.45	1.34
77	CI	1337	A2M	C6-N6	4.48	1.45	1.34
77	CI	3382	A2M	C6-N6	4.47	1.45	1.34
77	CI	2157	A2M	C6-N6	4.46	1.45	1.34
77	CI	3484	A2M	C6-N6	4.45	1.45	1.34
77	CI	1140	A2M	C6-N6	4.45	1.45	1.34
3	AC	669	A2M	C6-N6	4.45	1.45	1.34
77	CI	4026	MHG	C5-C4	4.43	1.52	1.38
77	CI	2119	A2M	C6-N6	4.42	1.45	1.34
77	CI	1347	A2M	C6-N6	4.42	1.45	1.34
79	CK	14	OMU	C4-N3	4.42	1.46	1.38
3	AC	1032	A2M	C6-N6	4.41	1.45	1.34
77	CI	1673	A2M	C6-N6	4.40	1.45	1.34
77	CI	3444	A2M	C6-N6	4.31	1.44	1.34
3	AC	1843	4AC	C5-C4	4.28	1.49	1.40
3	AC	116	OMU	C4-N3	4.21	1.46	1.38
77	CI	2053	E7G	C2-N1	4.21	1.48	1.37
77	CI	3539	P7G	C6-N1	4.15	1.45	1.38
77	CI	1711	P7G	C6-N1	4.13	1.45	1.38
77	CI	1472	I4U	C2-N1	4.12	1.48	1.40
77	CI	1599	E7G	C2-N1	4.12	1.47	1.37
77	CI	4138	B8T	C2-N1	4.11	1.48	1.40
77	CI	3849	I4U	C2-N1	4.10	1.48	1.40
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	3539	P7G	C2-N2	4.06	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	4275	OMU	C4-N3	3.97	1.45	1.38
77	CI	4205	G7M	C5-C6	3.92	1.54	1.43
3	AC	1843	4AC	O2-C2	-3.91	1.16	1.23
77	CI	4138	B8T	C5-C4	3.89	1.49	1.40
77	CI	1418	G7M	C5-C6	3.89	1.54	1.43
77	CI	4252	UR3	C6-N1	3.87	1.47	1.38
77	CI	2278	G7M	C5-C6	3.87	1.54	1.43
79	CK	14	OMU	C6-N1	3.84	1.47	1.38
77	CI	1668	UR3	C6-N1	3.81	1.47	1.38
3	AC	1831	UR3	C6-N1	3.81	1.47	1.38
77	CI	3961	OMU	C6-N1	3.77	1.47	1.38
77	CI	3961	OMU	C5-C4	3.71	1.51	1.43
3	AC	116	OMU	C5-C4	3.70	1.51	1.43
3	AC	116	OMU	C6-N1	3.69	1.46	1.38
3	AC	824	PSU	C6-C5	3.69	1.39	1.35
77	CI	1395	PSU	C6-C5	3.64	1.39	1.35
77	CI	237	B9B	O6-C6	3.60	1.40	1.35
77	CI	1490	PSU	C6-C5	3.59	1.39	1.35
77	CI	1599	E7G	C6-N1	3.55	1.45	1.38
79	CK	14	OMU	C5-C4	3.54	1.51	1.43
77	CI	4275	OMU	O4-C4	-3.52	1.17	1.24
77	CI	2053	E7G	C6-N1	3.52	1.45	1.38
77	CI	3388	PSU	C6-C5	3.51	1.39	1.35
77	CI	1496	PSU	C6-C5	3.51	1.39	1.35
77	CI	4275	OMU	C5-C4	3.50	1.51	1.43
77	CI	4275	OMU	C6-N1	3.50	1.46	1.38
77	CI	4275	OMU	O2-C2	-3.50	1.16	1.23
77	CI	3374	PSU	C6-C5	3.50	1.39	1.35
77	CI	4105	PSU	C6-C5	3.49	1.39	1.35
77	CI	3961	OMU	O4-C4	-3.49	1.17	1.24
77	CI	4186	PSU	C6-C5	3.49	1.39	1.35
79	CK	14	OMU	O4-C4	-3.47	1.17	1.24
77	CI	4026	MHG	C5-C6	3.47	1.52	1.43
77	CI	4026	MHG	O6-C6	-3.47	1.17	1.23
77	CI	3961	OMU	O2-C2	-3.46	1.16	1.23
3	AC	116	OMU	O2-C2	-3.46	1.16	1.23
3	AC	1843	4AC	C6-N1	3.45	1.46	1.38
77	CI	4097	PSU	C6-C5	3.45	1.39	1.35
77	CI	4291	PSU	C6-C5	3.44	1.39	1.35
77	CI	1387	B9B	O6-C6	3.42	1.40	1.35
3	AC	1244	PSU	C6-C5	3.42	1.39	1.35
79	CK	14	OMU	O2-C2	-3.42	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AC	116	OMU	O4-C4	-3.39	1.17	1.24
77	CI	4155	PSU	C6-C5	3.39	1.39	1.35
77	CI	3423	PSU	C6-C5	3.37	1.39	1.35
77	CI	1418	G7M	C5-N7	-3.31	1.35	1.39
77	CI	4058	PSU	C6-C5	3.29	1.39	1.35
77	CI	2264	PSU	C6-C5	3.29	1.39	1.35
77	CI	1673	A2M	O3'-C3'	-3.26	1.35	1.43
3	AC	823	PSU	C6-C5	3.25	1.39	1.35
77	CI	3849	I4U	C6-N1	3.22	1.45	1.38
77	CI	4252	UR3	C4-N3	3.20	1.48	1.40
3	AC	1082	PSU	C6-C5	3.19	1.39	1.35
77	CI	4205	G7M	C5-N7	-3.18	1.35	1.39
77	CI	1599	E7G	C5-C6	3.16	1.51	1.43
77	CI	3948	PSU	C6-C5	3.16	1.39	1.35
77	CI	2053	E7G	C5-C6	3.15	1.51	1.43
77	CI	4138	B8T	C6-N1	3.15	1.45	1.38
77	CI	3526	A2M	O3'-C3'	-3.14	1.35	1.43
3	AC	27	A2M	O2'-C2'	3.13	1.50	1.42
3	AC	1831	UR3	C4-N3	3.12	1.47	1.40
77	CI	1472	I4U	C6-N1	3.09	1.45	1.38
77	CI	1337	A2M	O3'-C3'	-3.08	1.35	1.43
77	CI	1668	UR3	C4-N3	3.07	1.47	1.40
77	CI	3526	A2M	O2'-C2'	3.07	1.50	1.42
77	CI	2278	G7M	C5-N7	-3.06	1.35	1.39
3	AC	1032	A2M	O3'-C3'	-3.05	1.35	1.43
3	AC	613	PSU	C6-C5	3.05	1.38	1.35
77	CI	398	A2M	O3'-C3'	-3.05	1.35	1.43
3	AC	166	A2M	O3'-C3'	-3.05	1.35	1.43
77	CI	3377	A2M	O2'-C2'	3.05	1.50	1.42
77	CI	4026	MHG	C72-C71	3.03	1.59	1.52
77	CI	3444	A2M	C5-C4	-3.03	1.33	1.39
77	CI	1472	I4U	O4-C41	-3.02	1.40	1.47
77	CI	1140	A2M	O2'-C2'	3.01	1.50	1.42
77	CI	1673	A2M	C5-C4	-3.01	1.33	1.39
77	CI	1387	B9B	C5-C4	-3.01	1.33	1.39
77	CI	3875	6MZ	O3'-C3'	-3.00	1.35	1.43
3	AC	166	A2M	O2'-C2'	2.98	1.50	1.42
77	CI	2157	A2M	O2'-C2'	2.98	1.50	1.42
77	CI	3484	A2M	O3'-C3'	-2.97	1.36	1.43
77	CI	1347	A2M	C5-C4	-2.96	1.33	1.39
77	CI	3382	A2M	O2'-C2'	2.95	1.50	1.42
77	CI	1347	A2M	O3'-C3'	-2.95	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	3849	I4U	O4-C41	-2.94	1.40	1.47
3	AC	1032	A2M	O2'-C2'	2.93	1.50	1.42
77	CI	3484	A2M	O2'-C2'	2.93	1.50	1.42
3	AC	27	A2M	O3'-C3'	-2.93	1.36	1.43
77	CI	398	A2M	O2'-C2'	2.93	1.50	1.42
77	CI	4283	PSU	C6-C5	2.92	1.38	1.35
77	CI	2157	A2M	O3'-C3'	-2.91	1.36	1.43
77	CI	4226	A2M	C5-C4	-2.91	1.33	1.39
3	AC	669	A2M	O2'-C2'	2.91	1.50	1.42
77	CI	3382	A2M	O3'-C3'	-2.91	1.36	1.43
77	CI	2119	A2M	O2'-C2'	2.90	1.50	1.42
77	CI	3377	A2M	O3'-C3'	-2.88	1.36	1.43
77	CI	4205	G7M	C6-N1	2.87	1.44	1.38
77	CI	4226	A2M	O2'-C2'	2.87	1.50	1.42
77	CI	2119	A2M	O3'-C3'	-2.87	1.36	1.43
3	AC	669	A2M	O3'-C3'	-2.87	1.36	1.43
77	CI	2157	A2M	C5-C4	-2.86	1.33	1.39
77	CI	2278	G7M	C6-N1	2.86	1.44	1.38
3	AC	669	A2M	C5-C4	-2.85	1.33	1.39
77	CI	3484	A2M	C5-C4	-2.84	1.33	1.39
77	CI	4226	A2M	O3'-C3'	-2.84	1.36	1.43
77	CI	237	B9B	C5-C4	-2.84	1.33	1.39
77	CI	1337	A2M	C5-C4	-2.83	1.33	1.39
77	CI	2119	A2M	C5-C4	-2.82	1.33	1.39
77	CI	1673	A2M	O2'-C2'	2.82	1.49	1.42
77	CI	1337	A2M	O2'-C2'	2.82	1.49	1.42
77	CI	1418	G7M	C6-N1	2.80	1.44	1.38
77	CI	398	A2M	C5-C4	-2.78	1.33	1.39
77	CI	4138	B8T	O2-C2	-2.77	1.18	1.23
77	CI	3377	A2M	C5-N7	-2.77	1.33	1.39
77	CI	3526	A2M	C5-C4	-2.75	1.33	1.39
77	CI	3377	A2M	C5-C4	-2.75	1.33	1.39
77	CI	1347	A2M	O2'-C2'	2.74	1.49	1.42
77	CI	3382	A2M	C5-N7	-2.74	1.33	1.39
3	AC	1032	A2M	C5-C4	-2.74	1.33	1.39
77	CI	1140	A2M	C5-C4	-2.73	1.33	1.39
3	AC	27	A2M	C5-C4	-2.73	1.33	1.39
77	CI	1472	I4U	O2-C2	-2.73	1.18	1.23
77	CI	3849	I4U	O2-C2	-2.73	1.18	1.23
77	CI	1668	UR3	O2-C2	-2.72	1.17	1.22
77	CI	3444	A2M	O2'-C2'	2.71	1.49	1.42
3	AC	1831	UR3	O2-C2	-2.71	1.17	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CI	3382	A2M	C5-C4	-2.70	1.34	1.39
3	AC	166	A2M	C5-C4	-2.70	1.34	1.39
77	CI	1140	A2M	C5-N7	-2.68	1.34	1.39
3	AC	1831	UR3	O4-C4	-2.68	1.17	1.23
77	CI	4252	UR3	O2-C2	-2.68	1.17	1.22
77	CI	1668	UR3	O4-C4	-2.66	1.17	1.23
77	CI	2119	A2M	C5-N7	-2.65	1.34	1.39
77	CI	2157	A2M	C5-N7	-2.65	1.34	1.39
77	CI	1140	A2M	O3'-C3'	-2.64	1.36	1.43
77	CI	4226	A2M	C5-N7	-2.63	1.34	1.39
77	CI	1673	A2M	C5-N7	-2.62	1.34	1.39
77	CI	1337	A2M	C5-N7	-2.61	1.34	1.39
77	CI	3484	A2M	C5-N7	-2.61	1.34	1.39
3	AC	669	A2M	C5-N7	-2.60	1.34	1.39
3	AC	27	A2M	C5-N7	-2.59	1.34	1.39
77	CI	3875	6MZ	C5-C4	-2.58	1.34	1.39
77	CI	2053	E7G	O6-C6	-2.57	1.18	1.23
3	AC	1843	4AC	O7-C7	-2.56	1.17	1.23
3	AC	166	A2M	C5-N7	-2.56	1.34	1.39
77	CI	4205	G7M	C2-N1	2.56	1.44	1.37
3	AC	1032	A2M	C5-N7	-2.55	1.34	1.39
77	CI	3444	A2M	C5-N7	-2.54	1.34	1.39
77	CI	1347	A2M	C5-N7	-2.54	1.34	1.39
77	CI	3444	A2M	O3'-C3'	-2.54	1.37	1.43
77	CI	1599	E7G	O6-C6	-2.54	1.18	1.23
77	CI	398	A2M	C5-N7	-2.53	1.34	1.39
77	CI	3840	B8W	C5-N7	-2.52	1.34	1.39
77	CI	3526	A2M	C5-N7	-2.52	1.34	1.39
77	CI	3849	I4U	O4-C4	2.51	1.40	1.35
77	CI	1418	G7M	C2-N1	2.50	1.43	1.37
77	CI	2278	G7M	C2-N1	2.50	1.43	1.37
77	CI	3875	6MZ	C5-N7	-2.50	1.34	1.39
77	CI	1673	A2M	O5'-C5'	-2.50	1.38	1.44
77	CI	4252	UR3	O4-C4	-2.49	1.18	1.23
77	CI	3840	B8W	C5-C4	-2.49	1.34	1.39
77	CI	2053	E7G	C5-C4	2.47	1.46	1.38
77	CI	1599	E7G	C5-C4	2.45	1.46	1.38
77	CI	4205	G7M	CN7-N7	2.41	1.51	1.46
77	CI	4010	E6G	C8-N7	2.41	1.36	1.31
77	CI	1387	B9B	C8-N9	-2.40	1.33	1.37
77	CI	3875	6MZ	O2'-C2'	2.38	1.48	1.43
77	CI	237	B9B	C8-N9	-2.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AC	1249	B8N	O4-C4	-2.34	1.18	1.23
77	CI	4226	A2M	C8-N9	-2.31	1.33	1.37
77	CI	2278	G7M	CN7-N7	2.30	1.50	1.46
77	CI	3377	A2M	C8-N9	-2.29	1.33	1.37
77	CI	1418	G7M	CN7-N7	2.29	1.50	1.46
77	CI	2053	E7G	C4-N9	-2.28	1.35	1.37
77	CI	4010	E6G	C2-N1	2.26	1.39	1.35
77	CI	3382	A2M	C8-N9	-2.25	1.33	1.37
77	CI	1472	I4U	O4-C4	2.24	1.39	1.35
77	CI	3539	P7G	O6-C6	-2.23	1.20	1.23
77	CI	1711	P7G	O6-C6	-2.23	1.20	1.23
3	AC	1032	A2M	C8-N9	-2.21	1.33	1.37
77	CI	4010	E6G	C5-N7	-2.20	1.34	1.39
77	CI	3484	A2M	C8-N9	-2.19	1.33	1.37
77	CI	1387	B9B	C5-N7	-2.19	1.34	1.39
77	CI	3526	A2M	C8-N9	-2.18	1.33	1.37
77	CI	1387	B9B	C5-C6	-2.18	1.37	1.41
77	CI	4252	UR3	C5-C4	2.16	1.49	1.43
77	CI	1269	B8Q	O2-C2	-2.15	1.18	1.22
77	CI	237	B9B	C5-N7	-2.15	1.35	1.39
77	CI	1347	A2M	C8-N9	-2.14	1.33	1.37
77	CI	1387	B9B	C4-N9	-2.13	1.32	1.37
77	CI	2119	A2M	C8-N9	-2.13	1.33	1.37
77	CI	3875	6MZ	C8-N9	-2.12	1.33	1.37
77	CI	3526	A2M	O5'-C5'	-2.12	1.39	1.44
3	AC	1831	UR3	C5-C4	2.12	1.49	1.43
3	AC	669	A2M	O5'-C5'	-2.12	1.39	1.44
77	CI	1337	A2M	C8-N9	-2.11	1.33	1.37
77	CI	1673	A2M	C8-N9	-2.10	1.33	1.37
77	CI	2157	A2M	C8-N9	-2.10	1.33	1.37
77	CI	1668	UR3	C5-C4	2.08	1.49	1.43
77	CI	3444	A2M	O5'-C5'	-2.07	1.39	1.44
3	AC	1249	B8N	C31-N3	2.06	1.52	1.47
77	CI	1337	A2M	O5'-C5'	-2.05	1.39	1.44
77	CI	398	A2M	O5'-C5'	-2.05	1.39	1.44
3	AC	27	A2M	C8-N9	-2.05	1.33	1.37
77	CI	1140	A2M	C8-N9	-2.04	1.33	1.37
77	CI	398	A2M	C8-N9	-2.02	1.33	1.37
77	CI	2119	A2M	O5'-C5'	-2.01	1.39	1.44
77	CI	237	B9B	C5-C6	-2.01	1.37	1.41
77	CI	3444	A2M	C8-N9	-2.01	1.33	1.37
3	AC	166	A2M	C8-N9	-2.00	1.33	1.37

All (471) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	4010	E6G	O6-C6-C5	21.32	143.56	116.57
77	CI	4010	E6G	O6-C6-N1	-17.99	94.94	120.00
77	CI	4010	E6G	C1'-N9-C8	-9.88	104.83	127.14
77	CI	4010	E6G	C4-N9-C1'	8.61	147.11	126.59
77	CI	4010	E6G	N2-C2-N3	8.41	130.33	117.25
77	CI	1387	B9B	O6-C6-N1	7.98	131.11	120.00
77	CI	3539	P7G	C4-C5-N7	7.66	110.71	106.67
77	CI	1387	B9B	O6-C6-C5	-7.21	107.44	116.57
77	CI	4026	MHG	C4-C5-N7	6.92	111.06	104.91
77	CI	237	B9B	O6-C6-N1	6.82	129.49	120.00
77	CI	1387	B9B	N9-C8-N7	-6.61	104.87	113.91
77	CI	4026	MHG	C2-N3-C4	6.57	120.19	112.04
77	CI	237	B9B	N9-C8-N7	-6.46	105.08	113.91
77	CI	2278	G7M	C1'-N9-C4	-6.40	107.49	126.50
77	CI	1337	A2M	N6-C6-N1	-6.35	104.45	118.35
77	CI	3444	A2M	N6-C6-N1	-6.30	104.55	118.35
77	CI	1140	A2M	N6-C6-N1	-6.30	104.56	118.35
77	CI	3840	B8W	C5-C4-N3	-6.29	120.12	127.19
77	CI	1347	A2M	N6-C6-N1	-6.26	104.64	118.35
77	CI	1673	A2M	N6-C6-N1	-6.21	104.76	118.35
77	CI	3484	A2M	N6-C6-N1	-6.21	104.76	118.35
77	CI	1387	B9B	C4-N9-C8	6.15	112.39	105.73
77	CI	3526	A2M	N6-C6-N1	-6.14	104.89	118.35
3	AC	27	A2M	N6-C6-N1	-6.13	104.92	118.35
77	CI	2119	A2M	N6-C6-N1	-6.12	104.94	118.35
77	CI	3377	A2M	N6-C6-N1	-6.10	104.98	118.35
3	AC	1032	A2M	N6-C6-N1	-6.10	104.99	118.35
77	CI	1418	G7M	CN7-N7-C5	6.10	134.35	126.77
3	AC	166	A2M	N6-C6-N1	-6.10	105.00	118.35
77	CI	2278	G7M	CN7-N7-C5	6.09	134.33	126.77
77	CI	398	A2M	N6-C6-N1	-6.06	105.07	118.35
77	CI	237	B9B	C5-C4-N3	-6.01	120.43	127.19
77	CI	4226	A2M	N6-C6-N1	-6.00	105.22	118.35
77	CI	1269	B8Q	N3-C2-N1	6.00	124.18	117.13
3	AC	669	A2M	N6-C6-N1	-6.00	105.22	118.35
77	CI	2157	A2M	N6-C6-N1	-5.99	105.23	118.35
77	CI	237	B9B	O6-C6-C5	-5.94	109.04	116.57
77	CI	3382	A2M	N6-C6-N1	-5.92	105.38	118.35
3	AC	1249	B8N	C5-C4-N3	5.91	127.11	116.17
77	CI	3840	B8W	N2-C2-N3	5.88	126.40	117.25
77	CI	237	B9B	C4-N9-C8	5.88	112.10	105.73
77	CI	4205	G7M	C1'-N9-C4	-5.87	109.05	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	2053	E7G	C4-C5-N7	5.85	110.11	104.91
77	CI	3382	A2M	C5-C4-N3	-5.83	119.14	126.75
77	CI	4010	E6G	C5-C4-N3	-5.83	120.64	127.19
77	CI	1599	E7G	C4-C5-N7	5.79	110.06	104.91
77	CI	4205	G7M	CN7-N7-C5	5.69	133.84	126.77
77	CI	1387	B9B	C5-C4-N3	-5.69	120.79	127.19
77	CI	1673	A2M	N3-C2-N1	-5.63	119.79	128.60
77	CI	1418	G7M	C1'-N9-C4	-5.58	109.94	126.50
3	AC	166	A2M	C5-C4-N3	-5.56	119.50	126.75
77	CI	2119	A2M	N3-C2-N1	-5.51	119.98	128.60
77	CI	3377	A2M	C5-C4-N3	-5.49	119.59	126.75
77	CI	3840	B8W	O6-C6-N1	5.49	126.58	119.01
77	CI	398	A2M	C5-C4-N3	-5.49	119.59	126.75
3	AC	669	A2M	N3-C2-N1	-5.49	120.02	128.60
77	CI	3444	A2M	N3-C2-N1	-5.48	120.03	128.60
3	AC	1032	A2M	C5-C4-N3	-5.48	119.60	126.75
77	CI	1140	A2M	C5-C6-N6	5.47	135.34	123.43
77	CI	1337	A2M	C5-C6-N6	5.46	135.31	123.43
77	CI	398	A2M	N3-C2-N1	-5.44	120.09	128.60
3	AC	1032	A2M	N3-C2-N1	-5.43	120.11	128.60
77	CI	1140	A2M	N3-C2-N1	-5.42	120.12	128.60
77	CI	1347	A2M	N3-C2-N1	-5.42	120.12	128.60
77	CI	4226	A2M	N3-C2-N1	-5.42	120.13	128.60
77	CI	1337	A2M	N3-C2-N1	-5.41	120.14	128.60
3	AC	27	A2M	N3-C2-N1	-5.39	120.17	128.60
77	CI	1347	A2M	C5-C6-N6	5.39	135.16	123.43
77	CI	2157	A2M	N3-C2-N1	-5.38	120.19	128.60
77	CI	1337	A2M	C5-C4-N3	-5.38	119.73	126.75
77	CI	237	B9B	N3-C4-N9	5.37	134.45	126.99
77	CI	3484	A2M	C5-C4-N3	-5.37	119.74	126.75
3	AC	166	A2M	N3-C2-N1	-5.36	120.21	128.60
77	CI	3484	A2M	C5-C6-N6	5.35	135.08	123.43
77	CI	1140	A2M	C5-C4-N3	-5.35	119.77	126.75
77	CI	3377	A2M	C5-C6-N6	5.35	135.07	123.43
3	AC	27	A2M	C5-C4-N3	-5.35	119.78	126.75
77	CI	3484	A2M	N3-C2-N1	-5.34	120.24	128.60
77	CI	1673	A2M	C5-C6-N6	5.33	135.04	123.43
77	CI	3875	6MZ	N1-C2-N3	-5.33	120.27	128.60
77	CI	4010	E6G	N2-C2-N1	-5.32	108.97	117.25
3	AC	27	A2M	C5-C6-N6	5.32	135.01	123.43
77	CI	3382	A2M	N3-C2-N1	-5.31	120.29	128.60
77	CI	3875	6MZ	C5-C4-N3	-5.29	119.84	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	3444	A2M	C5-C6-N6	5.29	134.95	123.43
3	AC	669	A2M	C5-C4-N3	-5.29	119.84	126.75
77	CI	2119	A2M	C5-C6-N6	5.25	134.85	123.43
77	CI	3526	A2M	C5-C6-N6	5.24	134.83	123.43
77	CI	3526	A2M	N3-C2-N1	-5.21	120.44	128.60
3	AC	1032	A2M	C5-C6-N6	5.21	134.78	123.43
77	CI	2278	G7M	C1'-N9-C8	5.21	144.33	126.74
77	CI	2157	A2M	C5-C6-N6	5.21	134.76	123.43
3	AC	166	A2M	C5-C6-N6	5.20	134.74	123.43
77	CI	398	A2M	C5-C6-N6	5.18	134.71	123.43
77	CI	2157	A2M	C5-C4-N3	-5.18	119.99	126.75
77	CI	4226	A2M	C5-C6-N6	5.17	134.68	123.43
77	CI	3444	A2M	C5-C4-N3	-5.16	120.02	126.75
77	CI	1387	B9B	N3-C4-N9	5.15	134.14	126.99
77	CI	4226	A2M	C5-C4-N3	-5.15	120.04	126.75
77	CI	3526	A2M	C5-C4-N3	-5.14	120.04	126.75
77	CI	2119	A2M	C5-C4-N3	-5.14	120.05	126.75
3	AC	669	A2M	C5-C6-N6	5.13	134.60	123.43
77	CI	3961	OMU	C4-N3-C2	-5.13	119.81	126.58
77	CI	1347	A2M	C5-C4-N3	-5.12	120.06	126.75
77	CI	1599	E7G	C5-C6-N1	5.09	119.95	110.99
77	CI	3377	A2M	N3-C2-N1	-5.07	120.67	128.60
77	CI	3382	A2M	C5-C6-N6	5.06	134.43	123.43
77	CI	4026	MHG	C5-C6-N1	5.01	119.81	110.99
77	CI	2264	PSU	C4-N3-C2	-5.00	119.14	126.34
3	AC	1831	UR3	C4-N3-C2	-4.94	119.91	124.56
77	CI	3374	PSU	N1-C2-N3	4.94	120.72	115.13
77	CI	2542	B9H	C31-N3-C2	4.92	123.36	117.21
77	CI	1673	A2M	C5-C4-N3	-4.91	120.34	126.75
77	CI	4252	UR3	C4-N3-C2	-4.91	119.94	124.56
3	AC	613	PSU	N1-C2-N3	4.91	120.69	115.13
77	CI	2053	E7G	C5-C6-N1	4.88	119.59	110.99
77	CI	4058	PSU	N1-C2-N3	4.87	120.64	115.13
77	CI	2264	PSU	N1-C2-N3	4.86	120.64	115.13
77	CI	3388	PSU	C4-N3-C2	-4.84	119.36	126.34
77	CI	4205	G7M	C1'-N9-C8	4.84	143.07	126.74
77	CI	1668	UR3	C4-N3-C2	-4.84	120.01	124.56
3	AC	613	PSU	C4-N3-C2	-4.84	119.37	126.34
77	CI	1496	PSU	N1-C2-N3	4.83	120.60	115.13
77	CI	4058	PSU	C4-N3-C2	-4.82	119.40	126.34
77	CI	3374	PSU	C4-N3-C2	-4.82	119.40	126.34
77	CI	4105	PSU	C4-N3-C2	-4.77	119.47	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	116	OMU	C4-N3-C2	-4.75	120.31	126.58
77	CI	3388	PSU	N1-C2-N3	4.75	120.52	115.13
77	CI	4155	PSU	C4-N3-C2	-4.75	119.50	126.34
77	CI	4291	PSU	C4-N3-C2	-4.73	119.53	126.34
77	CI	3948	PSU	N1-C2-N3	4.72	120.48	115.13
3	AC	1082	PSU	N1-C2-N3	4.71	120.47	115.13
77	CI	4026	MHG	C5-C4-N3	-4.70	119.17	128.13
77	CI	1418	G7M	C5-C4-N3	-4.67	119.19	128.15
77	CI	4291	PSU	N1-C2-N3	4.67	120.42	115.13
77	CI	3423	PSU	C4-N3-C2	-4.67	119.61	126.34
77	CI	4186	PSU	C4-N3-C2	-4.67	119.61	126.34
3	AC	1082	PSU	C4-N3-C2	-4.65	119.64	126.34
77	CI	4205	G7M	C5-C4-N3	-4.65	119.24	128.15
77	CI	2278	G7M	CN7-N7-C8	-4.64	117.68	124.84
77	CI	4155	PSU	N1-C2-N3	4.63	120.37	115.13
77	CI	4105	PSU	N1-C2-N3	4.62	120.37	115.13
77	CI	4186	PSU	N1-C2-N3	4.62	120.37	115.13
77	CI	4097	PSU	C4-N3-C2	-4.61	119.69	126.34
77	CI	1490	PSU	C4-N3-C2	-4.61	119.70	126.34
3	AC	823	PSU	C4-N3-C2	-4.60	119.71	126.34
3	AC	1244	PSU	C4-N3-C2	-4.59	119.72	126.34
77	CI	3526	A2M	N9-C8-N7	-4.59	107.64	113.91
77	CI	4283	PSU	C4-N3-C2	-4.57	119.75	126.34
77	CI	1490	PSU	N1-C2-N3	4.57	120.30	115.13
77	CI	1599	E7G	C2-N3-C4	4.56	120.43	112.30
77	CI	4097	PSU	N1-C2-N3	4.56	120.30	115.13
3	AC	1244	PSU	N1-C2-N3	4.56	120.30	115.13
77	CI	4205	G7M	C2-N3-C4	4.56	120.43	112.30
77	CI	1418	G7M	C1'-N9-C8	4.56	142.14	126.74
3	AC	824	PSU	C4-N3-C2	-4.56	119.77	126.34
77	CI	3948	PSU	C4-N3-C2	-4.56	119.77	126.34
77	CI	1673	A2M	N9-C8-N7	-4.55	107.69	113.91
77	CI	4010	E6G	N9-C8-N7	-4.55	107.69	113.91
3	AC	824	PSU	N1-C2-N3	4.55	120.28	115.13
79	CK	14	OMU	C4-N3-C2	-4.54	120.59	126.58
77	CI	1418	G7M	CN7-N7-C8	-4.53	117.84	124.84
77	CI	1496	PSU	C4-N3-C2	-4.52	119.83	126.34
77	CI	1347	A2M	N9-C8-N7	-4.51	107.74	113.91
77	CI	2278	G7M	C5-C4-N3	-4.49	119.53	128.15
77	CI	3875	6MZ	C4-C5-C6	4.48	120.28	116.81
77	CI	1395	PSU	C4-N3-C2	-4.48	119.88	126.34
77	CI	2278	G7M	C2-N3-C4	4.47	120.26	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	823	PSU	N1-C2-N3	4.46	120.18	115.13
77	CI	4275	OMU	C4-N3-C2	-4.46	120.70	126.58
77	CI	3840	B8W	N9-C8-N7	-4.45	107.83	113.91
77	CI	2053	E7G	C2-N3-C4	4.44	120.21	112.30
77	CI	1395	PSU	N1-C2-N3	4.44	120.16	115.13
77	CI	4283	PSU	N1-C2-N3	4.41	120.13	115.13
77	CI	1418	G7M	C2-N3-C4	4.39	120.13	112.30
77	CI	2157	A2M	N9-C8-N7	-4.37	107.93	113.91
77	CI	1269	B8Q	C31-N3-C4	4.33	120.77	114.25
77	CI	3444	A2M	N9-C8-N7	-4.31	108.02	113.91
77	CI	3423	PSU	N1-C2-N3	4.29	119.99	115.13
77	CI	2119	A2M	N9-C8-N7	-4.28	108.06	113.91
77	CI	3484	A2M	N9-C8-N7	-4.28	108.06	113.91
3	AC	27	A2M	N9-C8-N7	-4.27	108.07	113.91
77	CI	4205	G7M	CN7-N7-C8	-4.25	118.28	124.84
77	CI	1599	E7G	C5-C4-N3	-4.24	120.06	128.13
77	CI	1337	A2M	N9-C8-N7	-4.23	108.13	113.91
3	AC	166	A2M	N9-C8-N7	-4.19	108.19	113.91
77	CI	398	A2M	N9-C8-N7	-4.15	108.23	113.91
77	CI	3875	6MZ	N9-C8-N7	-4.13	108.26	113.91
3	AC	1249	B8N	C4-N3-C2	-4.13	120.24	125.46
3	AC	1032	A2M	N9-C8-N7	-4.09	108.32	113.91
3	AC	669	A2M	N9-C8-N7	-4.08	108.34	113.91
77	CI	4205	G7M	C5-C6-N1	4.06	120.26	111.79
77	CI	2278	G7M	C5-C6-N1	4.03	120.20	111.79
77	CI	1418	G7M	C5-C6-N1	4.01	120.16	111.79
77	CI	4226	A2M	N9-C8-N7	-3.98	108.47	113.91
77	CI	1140	A2M	N9-C8-N7	-3.98	108.47	113.91
77	CI	2053	E7G	C5-C4-N3	-3.98	120.55	128.13
77	CI	3961	OMU	N3-C2-N1	3.87	120.03	114.89
77	CI	237	B9B	C5-N7-C8	3.76	108.86	103.51
77	CI	4026	MHG	N9-C4-N3	3.74	131.06	125.47
77	CI	4010	E6G	C61-O6-C6	-3.74	113.95	117.59
77	CI	1418	G7M	N9-C4-N3	3.73	133.44	125.94
77	CI	1387	B9B	C4-N9-C1'	-3.71	117.75	126.59
77	CI	1472	I4U	C5-C4-N3	-3.71	119.27	124.91
3	AC	116	OMU	N3-C2-N1	3.70	119.81	114.89
77	CI	3382	A2M	C2-N3-C4	3.68	120.45	111.75
77	CI	1387	B9B	C5-N7-C8	3.68	108.73	103.51
77	CI	3377	A2M	N9-C8-N7	-3.65	108.92	113.91
77	CI	4026	MHG	C2-N1-C6	-3.63	120.30	124.48
77	CI	4205	G7M	O6-C6-C5	-3.62	119.89	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	1032	A2M	C2-N3-C4	3.62	120.31	111.75
77	CI	2278	G7M	O6-C6-C5	-3.62	119.90	128.06
77	CI	398	A2M	C2-N3-C4	3.60	120.27	111.75
77	CI	3382	A2M	N3-C4-N9	3.60	133.02	127.08
77	CI	4205	G7M	N9-C4-N3	3.60	133.16	125.94
3	AC	166	A2M	C2-N3-C4	3.59	120.24	111.75
77	CI	3382	A2M	N9-C8-N7	-3.59	109.01	113.91
77	CI	1140	A2M	C2-N3-C4	3.58	120.21	111.75
77	CI	1337	A2M	C2-N3-C4	3.58	120.21	111.75
3	AC	1032	A2M	N3-C4-N9	3.58	132.98	127.08
77	CI	3444	A2M	C2-N3-C4	3.57	120.19	111.75
3	AC	669	A2M	C2-N3-C4	3.55	120.13	111.75
77	CI	2119	A2M	C2-N3-C4	3.54	120.12	111.75
77	CI	3484	A2M	C2-N3-C4	3.54	120.11	111.75
77	CI	3840	B8W	N3-C4-N9	3.53	131.89	126.99
3	AC	27	A2M	C2-N3-C4	3.53	120.08	111.75
77	CI	1418	G7M	O6-C6-C5	-3.52	120.11	128.06
77	CI	1347	A2M	C2-N3-C4	3.52	120.07	111.75
3	AC	166	A2M	N3-C4-N9	3.51	132.86	127.08
77	CI	1673	A2M	C2-N3-C4	3.50	120.02	111.75
77	CI	4275	OMU	N3-C2-N1	3.49	119.53	114.89
77	CI	2157	A2M	C2-N3-C4	3.49	120.00	111.75
77	CI	2278	G7M	N9-C4-N3	3.48	132.93	125.94
77	CI	3526	A2M	C2-N3-C4	3.47	119.95	111.75
77	CI	4226	A2M	C2-N3-C4	3.47	119.95	111.75
77	CI	3875	6MZ	C2-N3-C4	3.43	119.86	111.75
77	CI	3849	I4U	C5-C4-N3	-3.43	119.70	124.91
77	CI	3377	A2M	C2-N3-C4	3.41	119.82	111.75
79	CK	14	OMU	C1'-N1-C2	3.41	123.74	117.57
77	CI	1269	B8Q	O2-C2-N3	-3.37	118.00	122.95
77	CI	2121	OMC	C1'-N1-C2	3.36	125.91	118.42
3	AC	823	PSU	O2-C2-N1	-3.34	119.11	122.79
77	CI	1711	P7G	C4-C5-N7	3.32	108.42	106.67
77	CI	398	A2M	N3-C4-N9	3.32	132.56	127.08
77	CI	3526	A2M	C5-N7-C8	3.32	108.22	103.51
77	CI	3875	6MZ	N3-C4-N9	3.32	132.55	127.08
77	CI	1673	A2M	C5-N7-C8	3.31	108.22	103.51
77	CI	237	B9B	N3-C2-N1	-3.31	120.23	125.42
77	CI	2157	A2M	C2'-C1'-N9	-3.30	107.98	113.53
77	CI	4226	A2M	C2'-C1'-N9	-3.29	107.98	113.53
77	CI	3484	A2M	N3-C4-N9	3.27	132.48	127.08
77	CI	3840	B8W	C5-N7-C8	3.26	108.14	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	1140	A2M	N3-C4-N9	3.26	132.45	127.08
3	AC	27	A2M	N3-C4-N9	3.26	132.45	127.08
77	CI	1673	A2M	C2'-C1'-N9	-3.26	108.05	113.53
77	CI	3961	OMU	C5-C4-N3	3.25	119.70	114.84
77	CI	3840	B8W	N1-C2-N3	-3.25	120.33	125.42
77	CI	1337	A2M	N3-C4-N9	3.23	132.40	127.08
79	CK	14	OMU	C5-C4-N3	3.23	119.67	114.84
77	CI	2157	A2M	N3-C4-N9	3.23	132.40	127.08
77	CI	1347	A2M	C5-N7-C8	3.21	108.07	103.51
77	CI	1387	B9B	N3-C2-N1	-3.20	120.39	125.42
77	CI	2157	A2M	C5-N7-C8	3.19	108.05	103.51
3	AC	27	A2M	C5-N7-C8	3.18	108.03	103.51
77	CI	3377	A2M	N3-C4-N9	3.16	132.29	127.08
77	CI	1337	A2M	C5-N7-C8	3.16	108.00	103.51
77	CI	1418	G7M	C2-N1-C6	-3.16	119.33	125.10
77	CI	2119	A2M	C5-N7-C8	3.15	107.98	103.51
79	CK	14	OMU	O4-C4-C5	-3.15	119.62	125.16
77	CI	4205	G7M	C2-N1-C6	-3.15	119.36	125.10
3	AC	166	A2M	C2'-C1'-N9	-3.14	108.24	113.53
77	CI	3484	A2M	C5-N7-C8	3.11	107.93	103.51
77	CI	3526	A2M	N3-C4-N9	3.11	132.21	127.08
3	AC	669	A2M	N3-C4-N9	3.11	132.20	127.08
79	CK	14	OMU	N3-C2-N1	3.10	119.00	114.89
77	CI	3875	6MZ	C5-N7-C8	3.09	107.91	103.51
77	CI	398	A2M	C5-N7-C8	3.08	107.89	103.51
77	CI	4010	E6G	C5-N7-C8	3.08	107.89	103.51
77	CI	4226	A2M	N3-C4-N9	3.07	132.15	127.08
77	CI	2119	A2M	N3-C4-N9	3.07	132.14	127.08
3	AC	166	A2M	C5-N7-C8	3.07	107.87	103.51
77	CI	3444	A2M	C5-N7-C8	3.07	107.86	103.51
77	CI	1347	A2M	N3-C4-N9	3.06	132.12	127.08
3	AC	116	OMU	C5-C4-N3	3.05	119.41	114.84
77	CI	1599	E7G	O6-C6-C5	-3.05	120.06	127.54
3	AC	1082	PSU	O2-C2-N1	-3.04	119.45	122.79
77	CI	4275	OMU	C5-C4-N3	3.04	119.38	114.84
77	CI	3484	A2M	C2'-C1'-N9	-3.03	108.42	113.53
77	CI	2278	G7M	C2-N1-C6	-3.02	119.58	125.10
77	CI	1269	B8Q	C1'-N1-C2	3.02	122.08	116.99
77	CI	4010	E6G	N3-C2-N1	-3.01	120.70	125.42
77	CI	2053	E7G	C5-C4-N9	3.01	110.25	106.35
77	CI	3444	A2M	N3-C4-N9	3.00	132.03	127.08
3	AC	669	A2M	C5-N7-C8	2.99	107.76	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	613	PSU	O2-C2-N1	-2.99	119.50	122.79
3	AC	1249	B8N	N3-C2-N1	2.98	120.97	116.76
77	CI	3377	A2M	C2'-C1'-N9	-2.98	108.51	113.53
3	AC	1032	A2M	C5-N7-C8	2.97	107.73	103.51
77	CI	1599	E7G	N9-C4-N3	2.96	129.89	125.47
77	CI	1140	A2M	C5-N7-C8	2.95	107.70	103.51
77	CI	4517	OMG	C2'-C1'-N9	2.94	119.93	114.22
77	CI	3388	PSU	O2-C2-N1	-2.93	119.56	122.79
77	CI	2264	PSU	O2-C2-N1	-2.92	119.58	122.79
77	CI	1490	PSU	O2-C2-N1	-2.91	119.58	122.79
77	CI	4226	A2M	C5-N7-C8	2.90	107.63	103.51
77	CI	2053	E7G	O6-C6-C5	-2.90	120.43	127.54
77	CI	2121	OMC	C1'-N1-C6	-2.89	114.53	120.84
77	CI	4026	MHG	O6-C6-C5	-2.88	120.47	127.54
77	CI	3377	A2M	C5-N7-C8	2.88	107.60	103.51
77	CI	1337	A2M	C2'-C1'-N9	-2.86	108.72	113.53
77	CI	1599	E7G	C5-C4-N9	2.86	110.06	106.35
3	AC	1249	B8N	O4-C4-N3	-2.85	115.13	119.98
77	CI	4283	PSU	O2-C2-N1	-2.85	119.66	122.79
77	CI	1673	A2M	N3-C4-N9	2.84	131.77	127.08
77	CI	3875	6MZ	C3'-C2'-C1'	2.82	106.79	101.43
77	CI	1599	E7G	C2-N1-C6	-2.82	119.95	125.10
3	AC	1244	PSU	O2-C2-N1	-2.82	119.69	122.79
77	CI	4155	PSU	O2-C2-N1	-2.81	119.70	122.79
77	CI	3374	PSU	O2-C2-N1	-2.80	119.70	122.79
77	CI	2121	OMC	O2-C2-N1	2.79	124.66	118.89
77	CI	4058	PSU	O2-C2-N1	-2.79	119.72	122.79
77	CI	4010	E6G	N3-C4-N9	2.79	130.87	126.99
77	CI	3840	B8W	C5-C6-N1	-2.78	119.60	123.46
77	CI	4275	OMU	O4-C4-C5	-2.77	120.28	125.16
77	CI	3382	A2M	C5-N7-C8	2.77	107.44	103.51
77	CI	3961	OMU	O4-C4-C5	-2.76	120.31	125.16
77	CI	237	B9B	N2-C2-N3	2.73	121.49	117.25
77	CI	3444	A2M	C4'-O4'-C1'	-2.72	103.47	109.47
77	CI	4186	PSU	O2-C2-N1	-2.72	119.80	122.79
3	AC	27	A2M	C2'-C1'-N9	-2.71	108.97	113.53
77	CI	237	B9B	C4-N9-C1'	-2.70	120.16	126.59
77	CI	1269	B8Q	C31-N3-C2	2.69	121.70	117.79
3	AC	116	OMU	O4-C4-C5	-2.68	120.45	125.16
3	AC	1032	A2M	C2'-C1'-N9	-2.67	109.04	113.53
77	CI	4026	MHG	C5-C4-N9	2.64	109.77	106.35
3	AC	613	PSU	C6-N1-C2	-2.59	120.04	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	3526	A2M	C4-N9-C8	2.59	108.53	105.73
77	CI	1496	PSU	O2-C2-N1	-2.58	119.95	122.79
77	CI	4105	PSU	O2-C2-N1	-2.58	119.95	122.79
77	CI	2053	E7G	C2-N1-C6	-2.57	120.40	125.10
77	CI	2542	B9H	O2-C2-N3	-2.57	118.81	122.07
77	CI	3875	6MZ	C9-N6-C6	-2.57	120.66	122.87
77	CI	3948	PSU	C6-N1-C2	-2.57	120.05	122.68
77	CI	3840	B8W	C2-N1-C6	2.57	120.00	115.93
77	CI	3948	PSU	O2-C2-N1	-2.56	119.97	122.79
77	CI	3840	B8W	N2-C2-N1	-2.56	113.27	117.25
3	AC	1249	B8N	C31-N3-C4	2.56	121.08	117.31
77	CI	1599	E7G	C8-N7-C71	2.55	126.58	120.50
77	CI	1496	PSU	C6-N1-C2	-2.55	120.08	122.68
77	CI	4155	PSU	C6-C5-C4	2.54	119.97	118.20
77	CI	3374	PSU	C6-N1-C2	-2.53	120.10	122.68
77	CI	3840	B8W	O6-C6-C5	-2.51	113.82	116.97
3	AC	27	A2M	O2'-C2'-C1'	2.50	113.95	109.08
77	CI	4283	PSU	C6-N1-C2	-2.50	120.13	122.68
3	AC	1082	PSU	C6-N1-C2	-2.50	120.13	122.68
77	CI	2053	E7G	N9-C4-N3	2.50	129.20	125.47
77	CI	2121	OMC	C4-N3-C2	2.49	124.28	120.25
77	CI	3526	A2M	C4'-O4'-C1'	-2.49	103.97	109.47
77	CI	3444	A2M	O4'-C1'-N9	2.49	112.97	108.06
77	CI	4070	1MA	N1-C6-N6	2.49	126.10	119.77
77	CI	2542	B9H	O2-C2-N1	-2.49	116.90	122.72
77	CI	3423	PSU	O2-C2-N1	-2.48	120.06	122.79
77	CI	4138	B8T	C6-C5-C4	2.47	119.98	116.96
77	CI	4026	MHG	C21-N2-C2	-2.47	118.42	123.86
3	AC	824	PSU	O2-C2-N1	-2.46	120.08	122.79
77	CI	4186	PSU	C6-C5-C4	2.45	119.91	118.20
77	CI	2053	E7G	C8-N7-C71	2.45	126.33	120.50
77	CI	3377	A2M	C3'-C2'-C1'	2.44	107.48	102.89
77	CI	4291	PSU	O2-C2-N1	-2.44	120.11	122.79
77	CI	1395	PSU	O2-C2-N1	-2.43	120.11	122.79
3	AC	1831	UR3	C6-N1-C2	-2.43	119.61	121.79
77	CI	398	A2M	C2'-C1'-N9	-2.42	109.46	113.53
77	CI	4097	PSU	O2-C2-N1	-2.42	120.13	122.79
77	CI	3382	A2M	C3'-C2'-C1'	2.40	107.39	102.89
77	CI	1347	A2M	C4-N9-C8	2.40	108.32	105.73
3	AC	1032	A2M	C1'-N9-C8	-2.39	121.74	127.14
77	CI	3382	A2M	C6-C5-C4	2.37	120.37	117.18
77	CI	1673	A2M	C5'-C4'-C3'	-2.37	106.29	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	3539	P7G	C5-C4-N3	-2.37	119.82	124.00
3	AC	824	PSU	C6-N1-C2	-2.37	120.26	122.68
77	CI	2542	B9H	C2'-C1'-N1	-2.35	109.65	114.22
77	CI	4058	PSU	C6-N1-C2	-2.35	120.28	122.68
77	CI	3377	A2M	C6-C5-C4	2.35	120.34	117.18
77	CI	4026	MHG	N1-C2-N3	-2.35	120.32	123.95
77	CI	4105	PSU	C6-C5-C4	2.33	119.83	118.20
77	CI	4010	E6G	C5-C4-N9	2.33	108.49	105.78
77	CI	1673	A2M	C4-N9-C8	2.32	108.24	105.73
77	CI	1140	A2M	C3'-C2'-C1'	2.31	107.24	102.89
77	CI	2157	A2M	C4-N9-C8	2.30	108.22	105.73
3	AC	823	PSU	C6-C5-C4	2.29	119.80	118.20
3	AC	1244	PSU	C6-N1-C2	-2.29	120.34	122.68
77	CI	1395	PSU	C6-N1-C2	-2.29	120.35	122.68
77	CI	2264	PSU	C6-C5-C4	2.28	119.80	118.20
3	AC	1843	4AC	C6-C5-C4	2.28	119.75	116.96
77	CI	3526	A2M	C4-C5-N7	-2.27	107.85	110.62
77	CI	4097	PSU	C6-N1-C2	-2.27	120.36	122.68
77	CI	4252	UR3	C1'-N1-C2	2.27	120.82	116.99
3	AC	1082	PSU	O4'-C1'-C2'	2.26	108.33	105.14
77	CI	3840	B8W	C4-C5-N7	-2.25	107.87	110.62
77	CI	3840	B8W	C4-N9-C8	2.25	108.17	105.73
77	CI	4252	UR3	C6-N1-C2	-2.25	119.78	121.79
3	AC	1032	A2M	C4-N9-C8	2.23	108.15	105.73
77	CI	237	B9B	C2-N3-C4	2.23	120.06	113.89
77	CI	4291	PSU	C6-C5-C4	2.21	119.75	118.20
77	CI	4010	E6G	C4-C5-N7	-2.21	107.93	110.62
77	CI	3484	A2M	C4-N9-C8	2.20	108.11	105.73
77	CI	3948	PSU	C6-C5-C4	2.20	119.73	118.20
3	AC	669	A2M	C3'-C2'-C1'	2.19	107.02	102.89
77	CI	1673	A2M	C4-C5-N7	-2.18	107.96	110.62
77	CI	4026	MHG	C72-C71-N7	-2.18	110.26	112.41
77	CI	3388	PSU	C6-C5-C4	2.18	119.72	118.20
77	CI	1668	UR3	C6-N1-C2	-2.17	119.84	121.79
77	CI	1140	A2M	C2'-C1'-N9	-2.17	109.88	113.53
3	AC	613	PSU	C6-C5-C4	2.16	119.71	118.20
77	CI	1387	B9B	N2-C2-N3	2.16	120.61	117.25
77	CI	3840	B8W	C2-N3-C4	2.16	119.86	113.89
77	CI	3382	A2M	C2'-C1'-N9	-2.16	109.90	113.53
77	CI	3568	OMC	C1'-N1-C2	2.15	123.23	118.42
77	CI	4010	E6G	C2-N3-C4	2.14	119.82	113.89
77	CI	3875	6MZ	C4-N9-C8	2.14	108.05	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	3526	A2M	C2'-C1'-N9	-2.14	109.93	113.53
3	AC	166	A2M	C6-C5-C4	2.14	120.06	117.18
3	AC	27	A2M	C4-N9-C8	2.14	108.05	105.73
3	AC	1843	4AC	CM7-C7-N4	2.14	118.99	115.29
77	CI	2119	A2M	C2'-C1'-N9	-2.13	109.94	113.53
3	AC	1831	UR3	C1'-N1-C2	2.13	120.58	116.99
77	CI	2119	A2M	C4-N9-C8	2.13	108.04	105.73
77	CI	3388	PSU	C6-N1-C2	-2.13	120.51	122.68
3	AC	116	OMU	O2-C2-N1	-2.12	119.96	122.79
3	AC	166	A2M	C4-N9-C8	2.12	108.03	105.73
77	CI	2617	OMC	C1'-N1-C2	2.12	123.15	118.42
77	CI	1347	A2M	C4-C5-N7	-2.12	108.04	110.62
77	CI	1387	B9B	C2-N3-C4	2.11	119.73	113.89
77	CI	398	A2M	C6-C5-C4	2.11	120.02	117.18
77	CI	3444	A2M	C4-N9-C8	2.10	108.00	105.73
3	AC	27	A2M	C6-C5-C4	2.09	120.00	117.18
77	CI	1269	B8Q	O2-C2-N1	-2.09	117.82	122.72
77	CI	4010	E6G	C4-N9-C8	2.09	107.99	105.73
77	CI	2264	PSU	C6-N1-C2	-2.09	120.55	122.68
77	CI	3377	A2M	C4-C5-N7	-2.09	108.08	110.62
77	CI	1337	A2M	C4-C5-N7	-2.08	108.08	110.62
77	CI	3539	P7G	O6-C6-C5	-2.08	119.75	125.59
3	AC	1032	A2M	C6-C5-C4	2.08	119.98	117.18
3	AC	27	A2M	C4-C5-N7	-2.08	108.09	110.62
77	CI	3423	PSU	C6-N1-C2	-2.07	120.56	122.68
77	CI	4291	PSU	C6-N1-C2	-2.07	120.56	122.68
77	CI	3484	A2M	C4-C5-N7	-2.07	108.10	110.62
3	AC	1843	4AC	N4-C4-N3	2.06	117.31	113.85
77	CI	1490	PSU	C6-N1-C2	-2.06	120.58	122.68
77	CI	2119	A2M	C4-C5-N7	-2.06	108.11	110.62
77	CI	4186	PSU	C6-N1-C2	-2.06	120.58	122.68
77	CI	3546	OMC	C4-N3-C2	2.06	123.58	120.25
77	CI	3484	A2M	C6-C5-C4	2.06	119.95	117.18
77	CI	4026	MHG	C6-C5-N7	-2.05	128.17	131.67
77	CI	3444	A2M	O4'-C1'-C2'	-2.05	102.98	106.57
77	CI	398	A2M	C3'-C2'-C1'	2.05	106.73	102.89
3	AC	166	A2M	C1'-N9-C8	-2.04	122.52	127.14
77	CI	2157	A2M	C1'-N9-C8	-2.04	122.53	127.14
3	AC	823	PSU	C6-N1-C2	-2.03	120.61	122.68
77	CI	398	A2M	C4-C5-N7	-2.03	108.15	110.62
77	CI	1337	A2M	C4-N9-C8	2.03	107.93	105.73
77	CI	4275	OMU	C2'-C1'-N1	-2.02	110.30	114.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	CI	3961	OMU	O2-C2-N1	-2.01	120.11	122.79
77	CI	3377	A2M	C5-C4-N9	2.01	108.12	105.78
3	AC	669	A2M	C6-C5-C4	2.01	119.88	117.18
77	CI	3568	OMC	C4-N3-C2	2.01	123.50	120.25
77	CI	3444	A2M	C4-C5-N7	-2.01	108.18	110.62
77	CI	4097	PSU	O4'-C1'-C2'	2.00	107.97	105.14
77	CI	4226	A2M	C6-C5-C4	2.00	119.88	117.18
77	CI	3875	6MZ	C4-C5-N7	-2.00	108.18	110.62
77	CI	4291	PSU	O4'-C1'-C2'	2.00	107.97	105.14

There are no chirality outliers.

All (139) 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	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'
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

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Mol	Chain	Res	Type	Atoms
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'-C4'-C5'-O5'
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-C4
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	237	B9B	C4'-C5'-O5'-P
77	CI	237	B9B	C3'-C4'-C5'-O5'
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'
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	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'

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Mol	Chain	Res	Type	Atoms
64	Bd	98	MLZ	CD-CE-NZ-CM
77	CI	3360	OMC	C2'-C1'-N1-C2
77	CI	1673	A2M	C3'-C4'-C5'-O5'
77	CI	2278	G7M	O4'-C4'-C5'-O5'
77	CI	3546	OMC	O4'-C4'-C5'-O5'
77	CI	3961	OMU	O4'-C4'-C5'-O5'
77	CI	4517	OMG	O4'-C4'-C5'-O5'
77	CI	3377	A2M	C3'-C2'-O2'-CM'
77	CI	3849	I4U	C3'-C4'-C5'-O5'
77	CI	3948	PSU	C3'-C4'-C5'-O5'
77	CI	237	B9B	O4'-C4'-C5'-O5'
77	CI	2278	G7M	C3'-C4'-C5'-O5'
77	CI	4102	5MC	C3'-C4'-C5'-O5'
77	CI	237	B9B	O6-C61-C62-C63
77	CI	1599	E7G	O4'-C4'-C5'-O5'
77	CI	2178	OMC	O4'-C4'-C5'-O5'
77	CI	1140	A2M	C1'-C2'-O2'-CM'
77	CI	4026	MHG	C71-C72-C73-C74
77	CI	3360	OMC	O4'-C1'-N1-C6
77	CI	4102	5MC	O4'-C1'-N1-C6
3	AC	645	OMG	C4'-C5'-O5'-P
77	CI	877	2MG	C3'-C4'-C5'-O5'
77	CI	3388	PSU	C3'-C4'-C5'-O5'
77	CI	3849	I4U	O4'-C4'-C5'-O5'
77	CI	4205	G7M	C3'-C4'-C5'-O5'
77	CI	3539	P7G	C72-C71-N7-C8
79	CK	14	OMU	C3'-C2'-O2'-CM2
77	CI	1140	A2M	C4'-C5'-O5'-P
37	BC	333	MLZ	N-CA-CB-CG
77	CI	1140	A2M	C3'-C4'-C5'-O5'
77	CI	4292	OMG	C3'-C4'-C5'-O5'
79	CK	14	OMU	C3'-C4'-C5'-O5'
77	CI	398	A2M	C4'-C5'-O5'-P
77	CI	3360	OMC	O4'-C1'-N1-C2
77	CI	3546	OMC	C4'-C5'-O5'-P
77	CI	3961	OMU	C4'-C5'-O5'-P
77	CI	4155	PSU	C4'-C5'-O5'-P
77	CI	1418	G7M	C4'-C5'-O5'-P
77	CI	1418	G7M	C3'-C4'-C5'-O5'
77	CI	4102	5MC	O4'-C1'-N1-C2
3	AC	1249	B8N	C32-C33-C34-O36
3	AC	1244	PSU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
77	CI	1337	A2M	O4'-C1'-N9-C8
77	CI	1387	B9B	C62-C61-O6-C6
77	CI	4105	PSU	O4'-C1'-C5-C4
77	CI	4186	PSU	O4'-C1'-C5-C4
77	CI	4026	MHG	C2'-C1'-N9-C4
77	CI	4149	OMG	C3'-C2'-O2'-CM2
77	CI	877	2MG	C4'-C5'-O5'-P
77	CI	2542	B9H	C32-C31-N3-C4
77	CI	4291	PSU	C4'-C5'-O5'-P
77	CI	1673	A2M	O4'-C4'-C5'-O5'
77	CI	3388	PSU	O4'-C4'-C5'-O5'
77	CI	4205	G7M	O4'-C4'-C5'-O5'
77	CI	3423	PSU	O4'-C4'-C5'-O5'
3	AC	684	OMG	O4'-C4'-C5'-O5'
77	CI	4149	OMG	C1'-C2'-O2'-CM2
3	AC	1249	B8N	C32-C33-C34-O35
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	1599	E7G	C3'-C4'-C5'-O5'
77	CI	3444	A2M	O4'-C4'-C5'-O5'
77	CI	4026	MHG	O4'-C4'-C5'-O5'
77	CI	4097	PSU	O4'-C4'-C5'-O5'
77	CI	1387	B9B	C2'-C1'-N9-C8
3	AC	669	A2M	C2'-C1'-N9-C8
77	CI	2560	OMC	C2'-C1'-N1-C2

There are no ring outliers.

32 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	CI	3441	5MC	1	0
77	CI	1387	B9B	1	0
77	CI	3444	A2M	1	0
79	CK	14	OMU	4	0
77	CI	373	OMG	1	0
77	CI	1673	A2M	1	0
77	CI	2542	B9H	5	0
77	CI	1269	B8Q	1	0
3	AC	1843	4AC	2	0
3	AC	823	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	CI	4283	PSU	1	0
77	CI	3961	OMU	1	0
77	CI	4070	1MA	2	0
77	CI	1685	OMG	3	0
77	CI	2119	A2M	1	0
77	CI	4226	A2M	1	0
77	CI	3526	A2M	2	0
77	CI	2278	G7M	1	0
77	CI	1140	A2M	2	0
77	CI	4275	OMU	2	0
77	CI	3568	OMC	3	0
77	CI	237	B9B	1	0
77	CI	3377	A2M	4	0
77	CI	4291	PSU	1	0
77	CI	2560	OMC	1	0
77	CI	3382	A2M	2	0
77	CI	4058	PSU	1	0
77	CI	3948	PSU	2	0
3	AC	116	OMU	3	0
77	CI	4102	5MC	1	0
77	CI	4517	OMG	7	0
77	CI	4191	OMC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

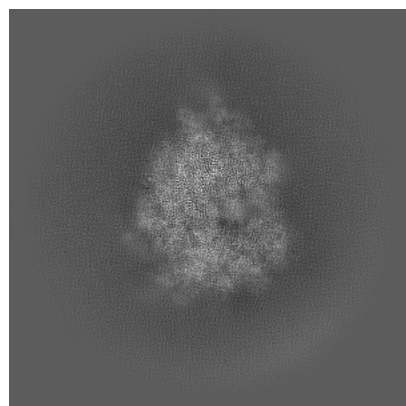
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-58361. These allow visual inspection of the internal detail of the map and identification of artifacts.

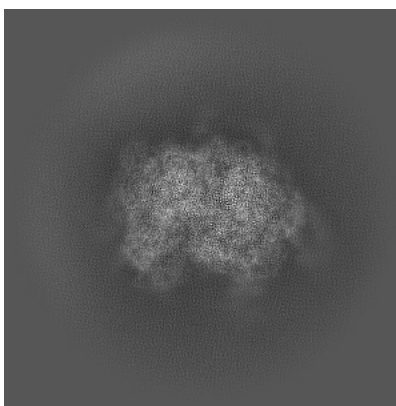
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

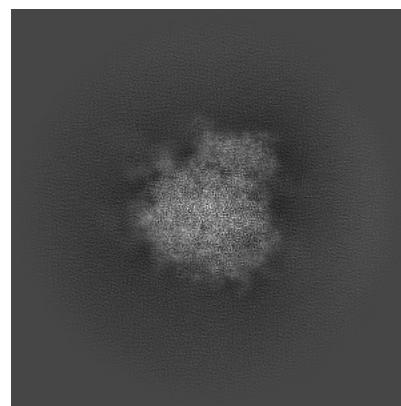
6.1.1 Primary map



X

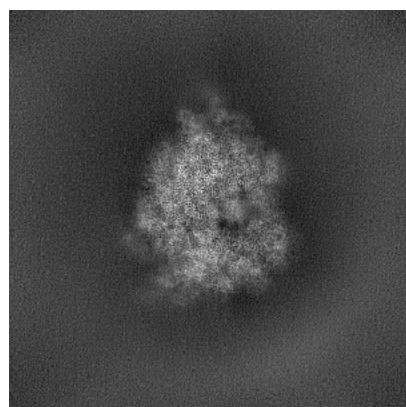


Y

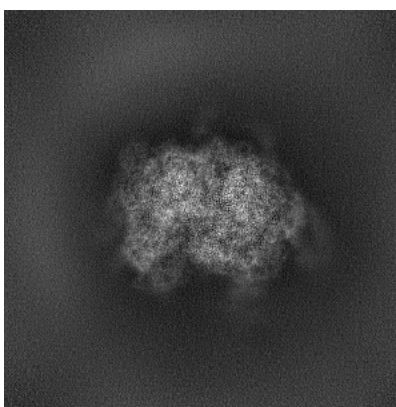


Z

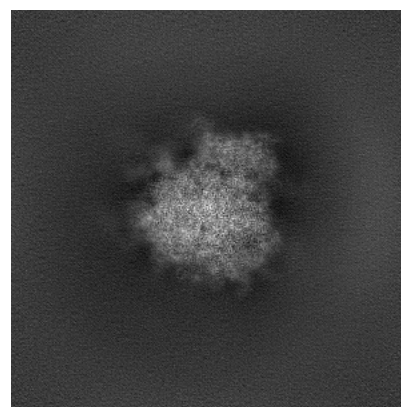
6.1.2 Raw map



X



Y

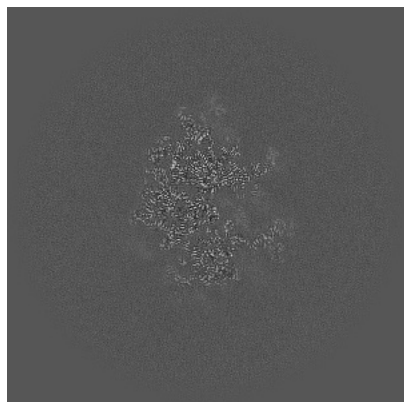


Z

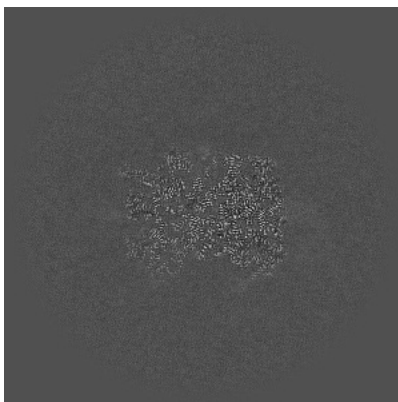
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

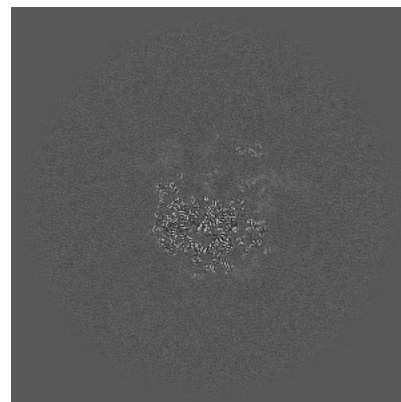
6.2.1 Primary map



X Index: 256

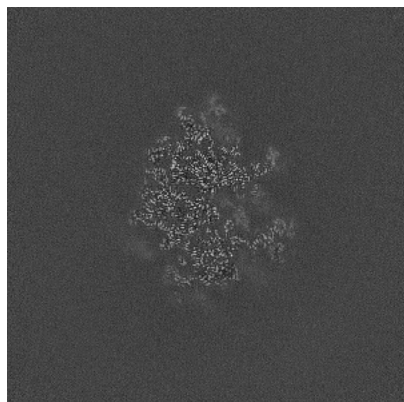


Y Index: 256

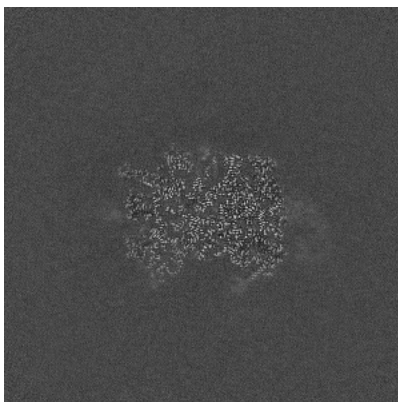


Z Index: 256

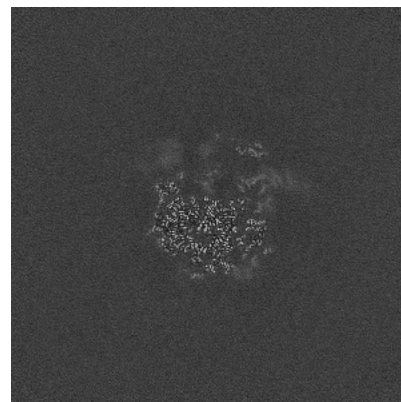
6.2.2 Raw map



X Index: 256



Y Index: 256

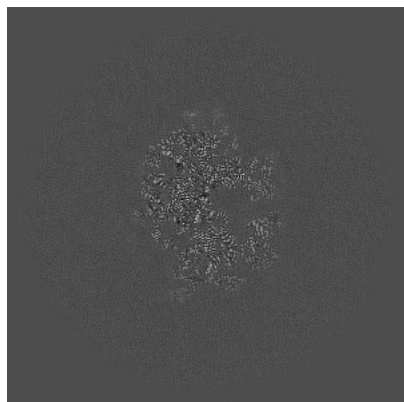


Z Index: 256

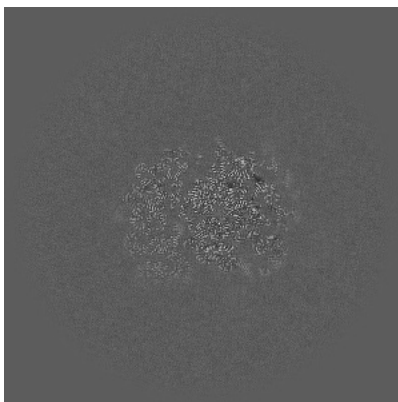
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

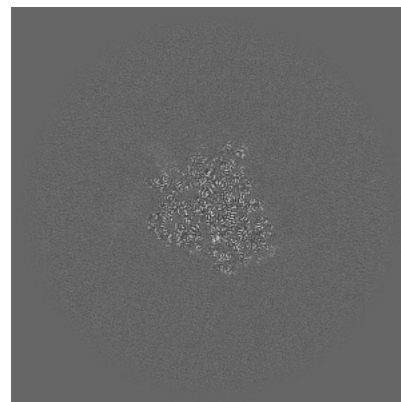
6.3.1 Primary map



X Index: 272

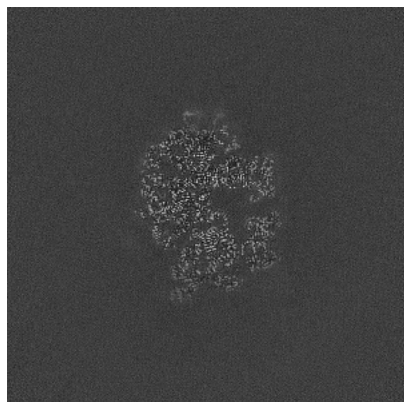


Y Index: 243

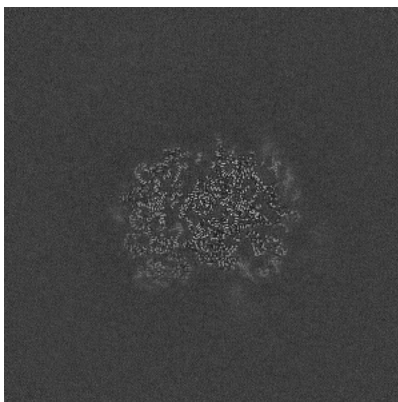


Z Index: 289

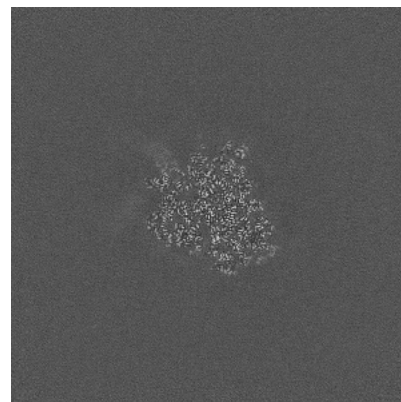
6.3.2 Raw map



X Index: 273



Y Index: 242

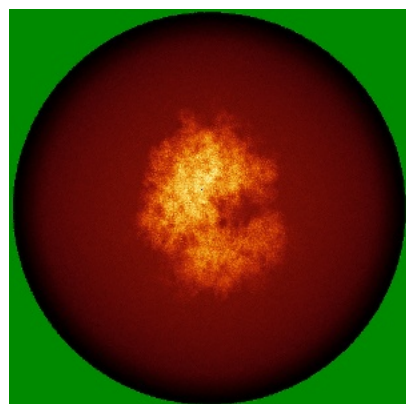


Z Index: 289

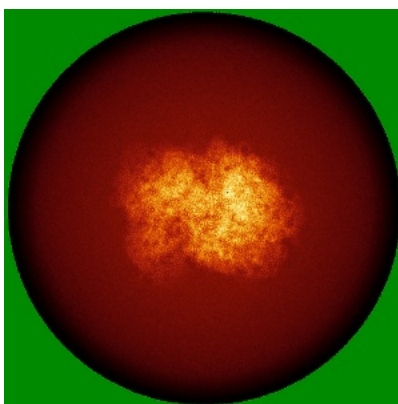
The images above show the largest variance slices of the map in three orthogonal directions.

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

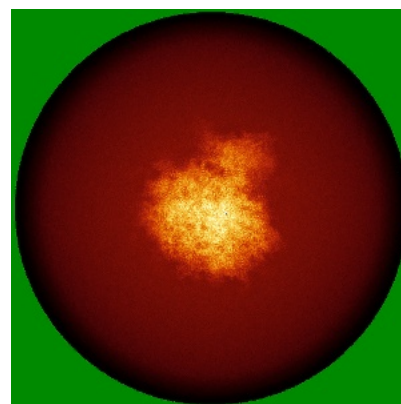
6.4.1 Primary map



X

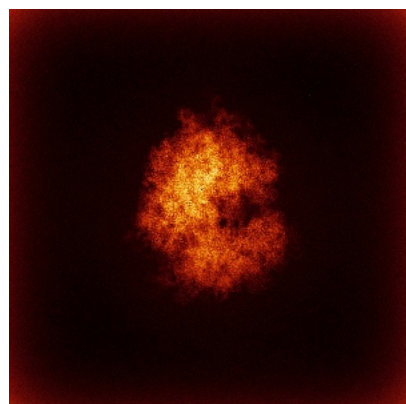


Y

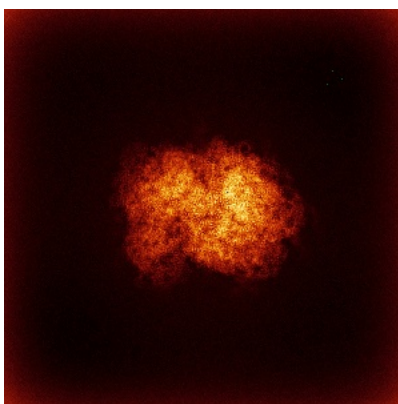


Z

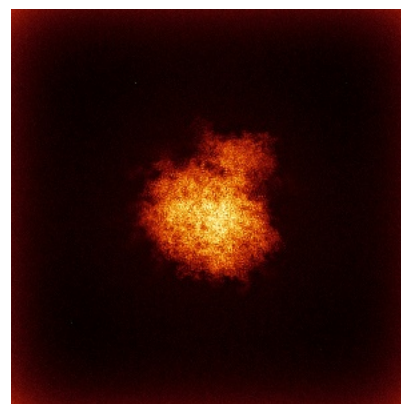
6.4.2 Raw map



X



Y

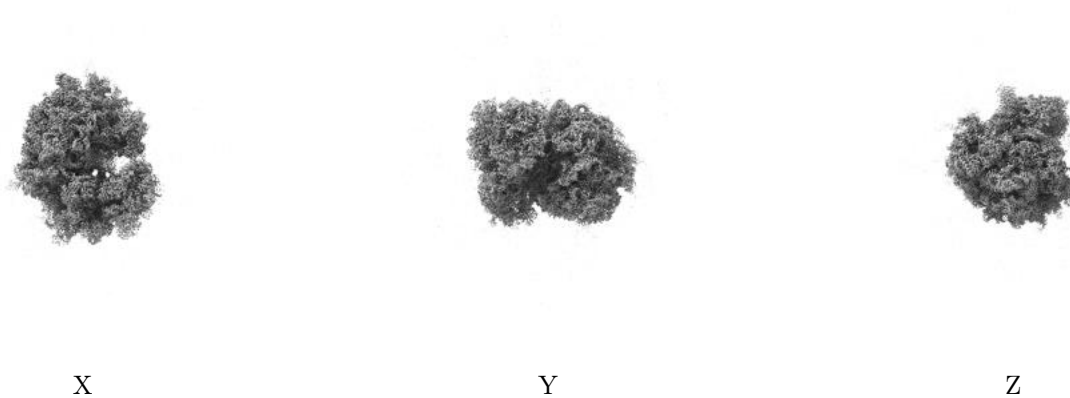


Z

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.

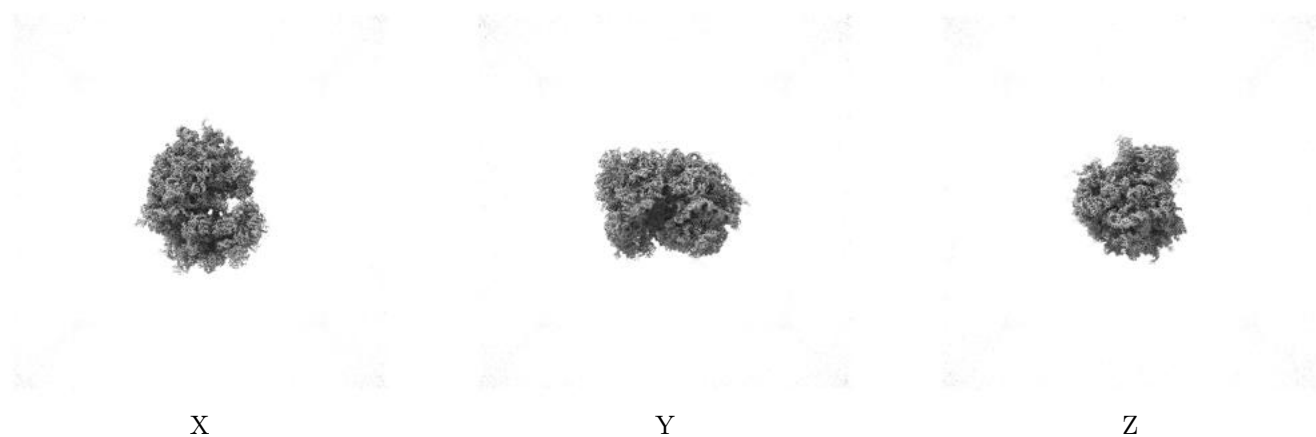
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

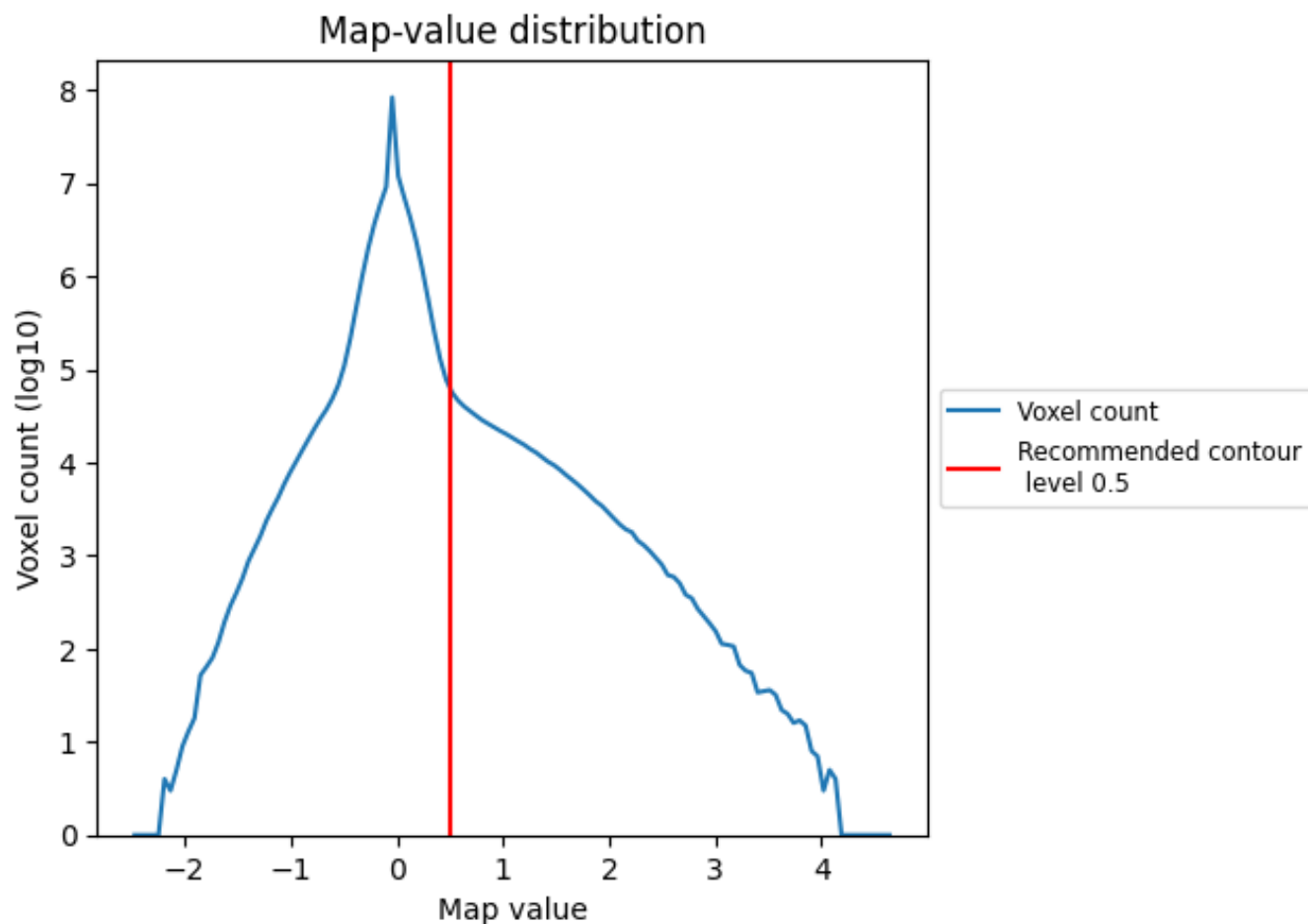
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

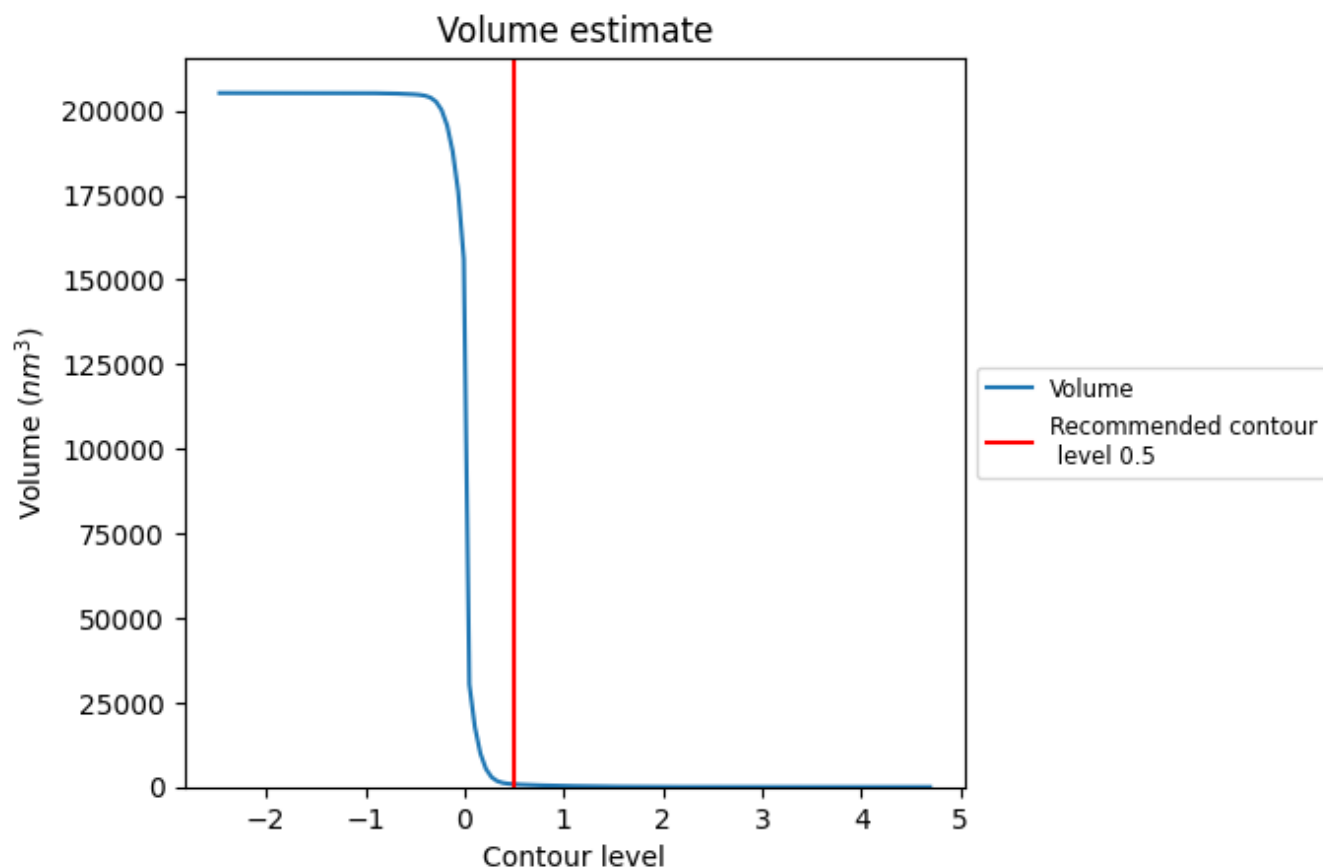
This section contains the results of statistical analysis of the map.

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.

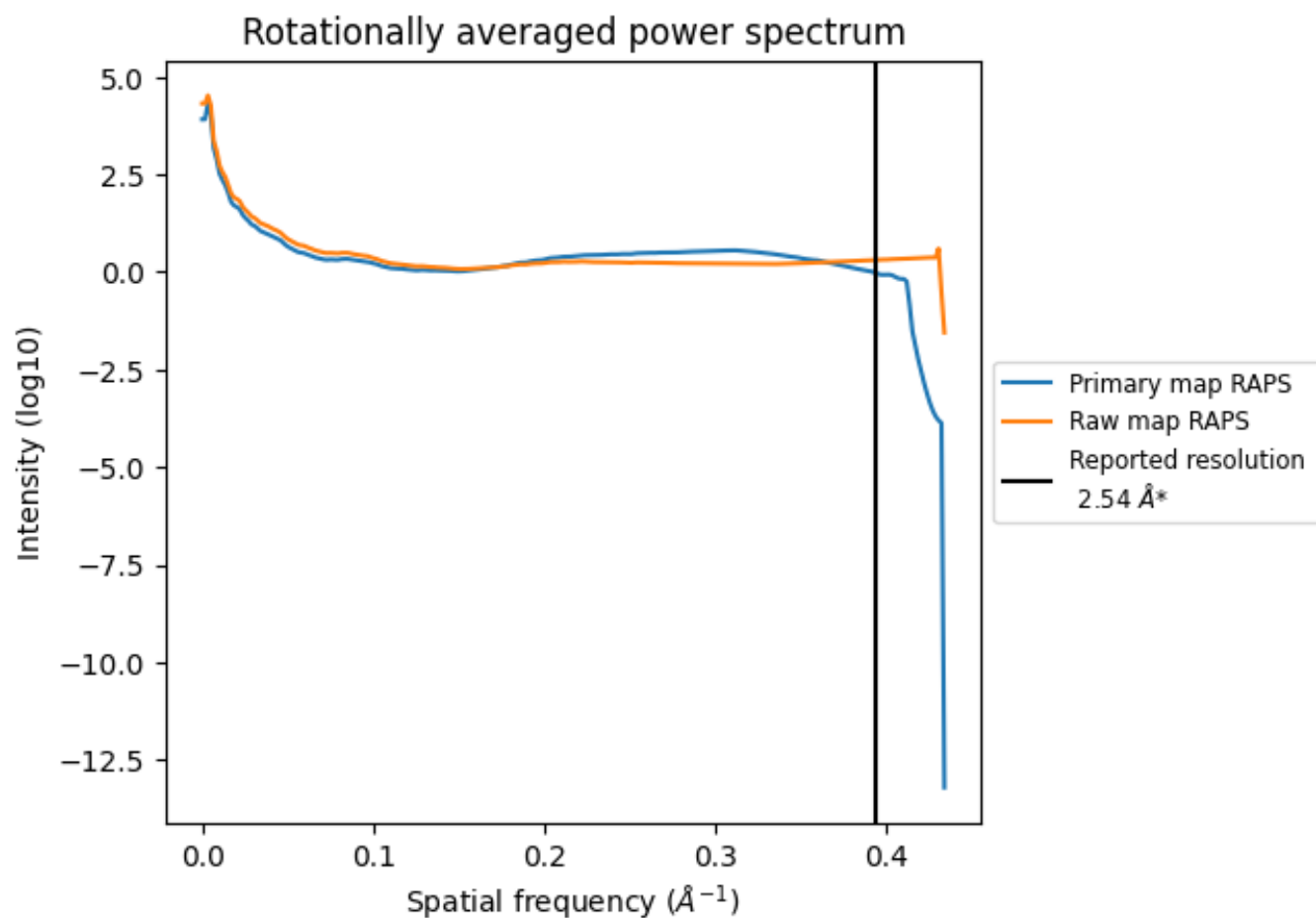
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 811 nm^3 ; this corresponds to an approximate mass of 732 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 ⓘ

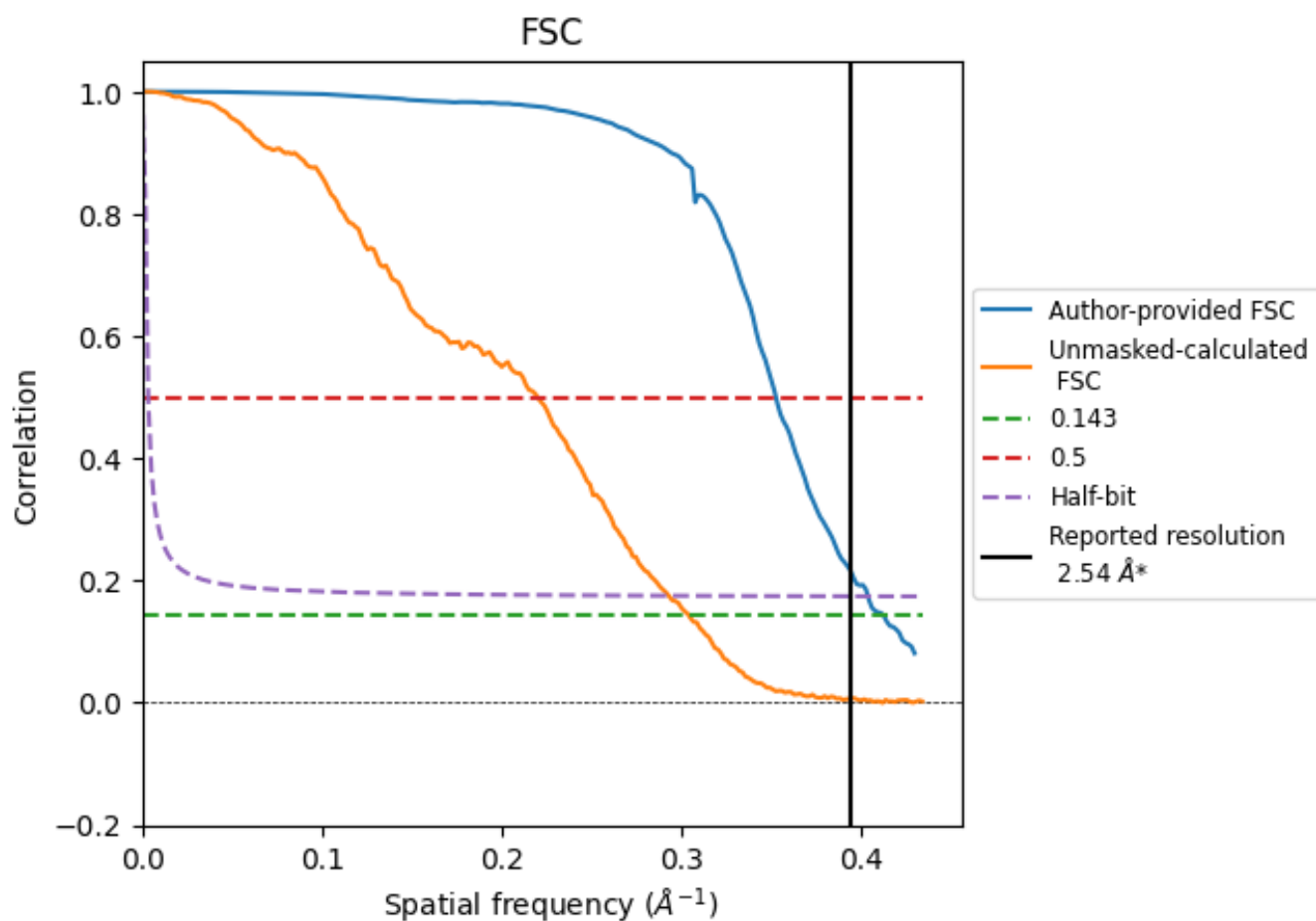


*Reported resolution corresponds to spatial frequency of 0.394 Å⁻¹

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 0.394 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

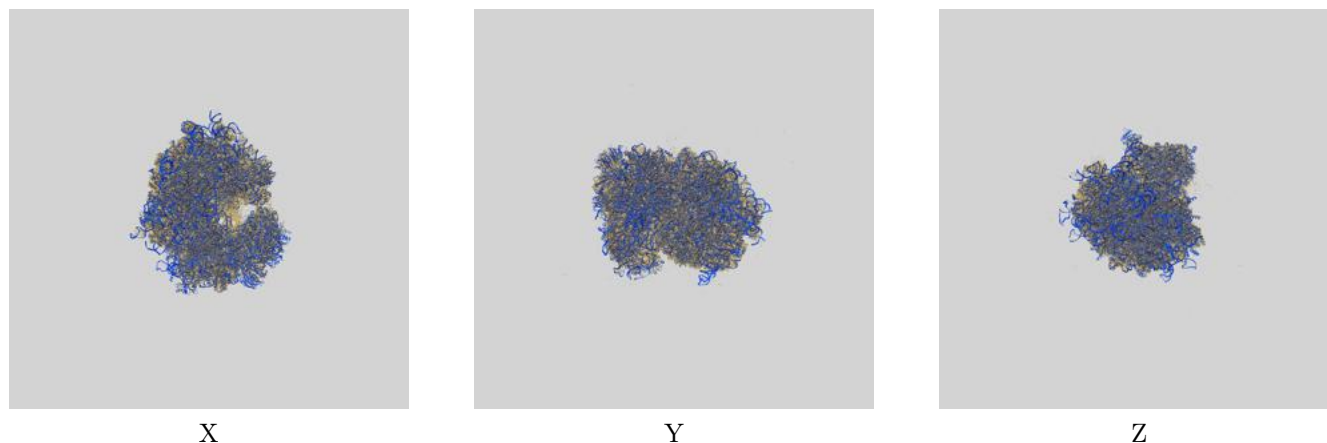
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.43	2.84	2.48
Unmasked-calculated*	3.29	4.55	3.41

*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 3.29 differs from the reported value 2.54 by more than 10 %

9 Map-model fit [i](#)

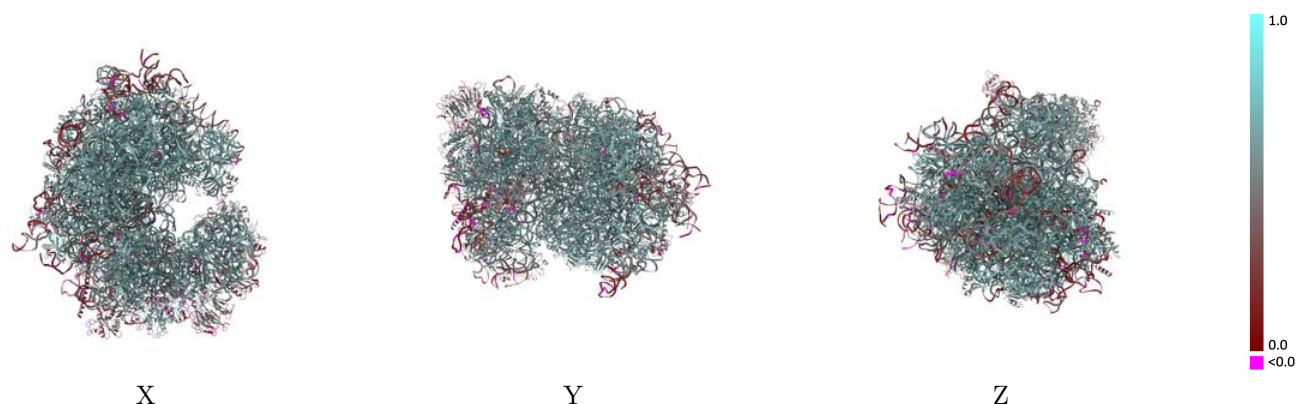
This section contains information regarding the fit between EMDB map EMD-58361 and PDB model 31FX. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



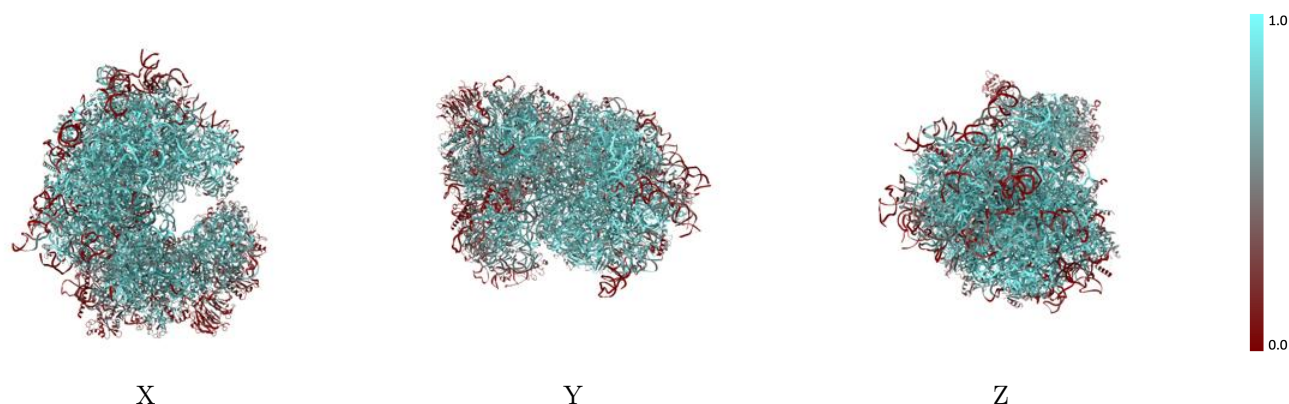
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



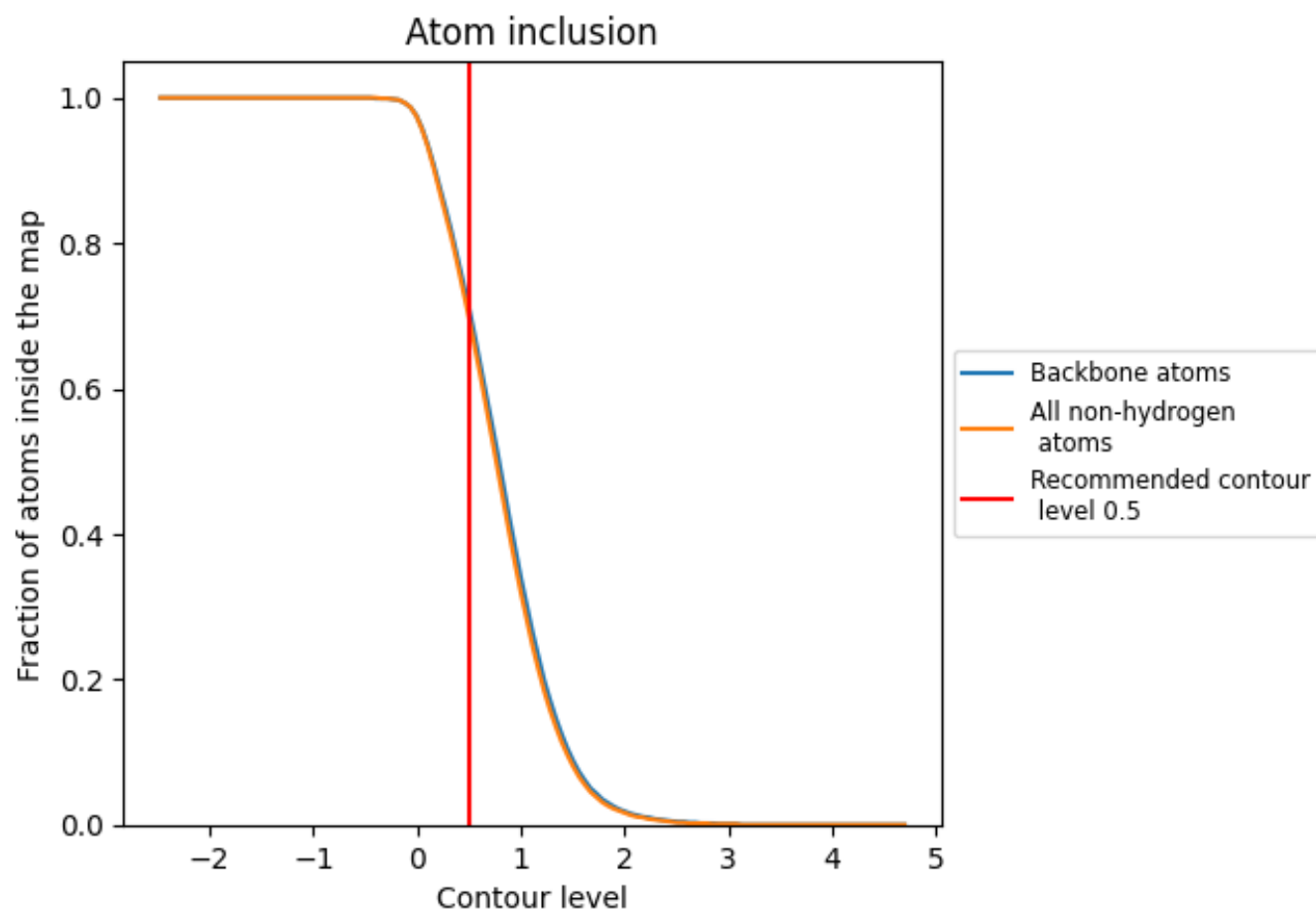
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 70% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.5550
AA	 0.3720	 0.4070
AB	 0.7330	 0.5800
AC	 0.7150	 0.5400
AD	 0.6620	 0.5810
AE	 0.4730	 0.4960
AF	 0.4780	 0.4640
AG	 0.5890	 0.5280
AH	 0.3690	 0.4350
AI	 0.6360	 0.5630
AJ	 0.5640	 0.5270
AK	 0.4380	 0.5070
AL	 0.5520	 0.5140
AM	 0.5720	 0.5370
AN	 0.5600	 0.5130
AO	 0.6170	 0.5720
AP	 0.4150	 0.4770
AQ	 0.6010	 0.5560
AR	 0.6980	 0.5620
AS	 0.7270	 0.5900
AT	 0.1950	 0.3650
AU	 0.7040	 0.5960
AV	 0.3410	 0.4210
AW	 0.2660	 0.2320
AX	 0.0530	 0.2260
AY	 0.6550	 0.5860
AZ	 0.6950	 0.5620
Aa	 0.7650	 0.6040
Ab	 0.4200	 0.4550
Ac	 0.4360	 0.4580
Ad	 0.4630	 0.4740
Ae	 0.3710	 0.2570
Af	 0.0510	 0.1790
Ag	 0.3200	 0.4100
Ah	 0.4470	 0.4420



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Chain	Atom inclusion	Q-score
BA	 0.8630	 0.6350
BB	 0.8060	 0.6110
BC	 0.8110	 0.6060
BD	 0.7060	 0.5850
BE	 0.6640	 0.5660
BF	 0.8160	 0.6230
BG	 0.8290	 0.6260
BH	 0.8650	 0.6440
BI	 0.6690	 0.5390
BJ	 0.8350	 0.6220
BK	 0.7440	 0.5930
BL	 0.4490	 0.4780
BM	 0.8300	 0.6350
BN	 0.7980	 0.6430
BO	 0.7570	 0.6040
BP	 0.7830	 0.6180
BQ	 0.7100	 0.5950
BR	 0.8770	 0.6390
BS	 0.6340	 0.5580
BT	 0.7120	 0.5780
BU	 0.7340	 0.5890
BV	 0.8300	 0.6340
BW	 0.8620	 0.6320
BX	 0.7650	 0.6010
BY	 0.7560	 0.6090
BZ	 0.6880	 0.5910
Ba	 0.8560	 0.6330
Bb	 0.5410	 0.5360
Bc	 0.8010	 0.6300
Bd	 0.7700	 0.6240
Be	 0.7060	 0.6190
Bf	 0.7610	 0.6040
Bg	 0.8160	 0.6260
Bh	 0.8370	 0.6220
CA	 0.8200	 0.6160
CB	 0.6700	 0.5640
CC	 0.7210	 0.6020
CD	 0.7510	 0.5980
CE	 0.6300	 0.5360
CF	 0.7190	 0.5710
CG	 0.7320	 0.5840
CH	 0.9020	 0.6570

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Chain	Atom inclusion	Q-score
CI	 0.7580	 0.5600
CJ	 0.9120	 0.6340
CK	 0.8250	 0.5880