



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 06:05 am BST

PDB ID : 9HMW / pdb_00009hmw
EMDB ID : EMD-52299
Title : Structure of the Arabidopsis thaliana 80S ribosome OVAC mutant in complex with P- and E-site tRNAs and mRNA
Authors : Faille, A.; Warren, A.J.
Deposited on : 2024-12-09
Resolution : 2.25 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.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

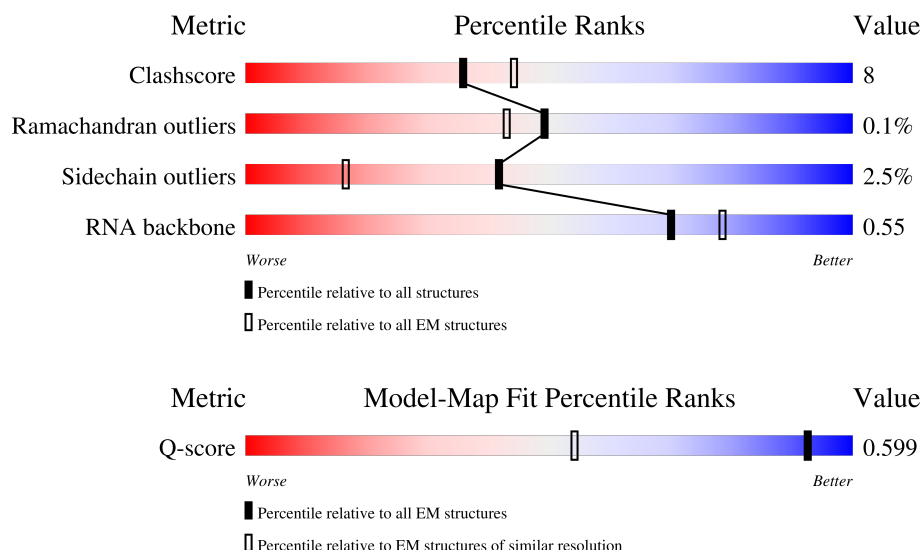
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.25 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	3458 (1.75 - 2.75)

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	3	164	8% 60% 33% 5%
2	A	3385	8% 60% 28% 5% 7%
3	W2	76	58% 51% 45%

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Mol	Chain	Length	Quality of chain
3	i2	76	
4	C3	121	
5	BC	25	
6	BM	176	
7	BO	146	
8	AR	83	
9	AU	119	
10	Ma	131	
11	Ia	194	
12	AE	130	
13	AX	112	
14	AP	135	
15	Ja	262	
16	Ea	204	
17	AL	217	
18	Va	142	
19	Ka	133	
20	AW	112	
21	BD	105	
22	BS	389	
23	AM	164	
24	AC	284	
25	BI	140	
26	AH	134	
27	BT	406	

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Mol	Chain	Length	Quality of chain
28	AV	133	
29	AD	207	
30	AJ	187	
31	BQ	258	
32	BH	206	
33	Da	151	
34	BK	301	
35	AT	112	
36	Pa	62	
37	BP	123	
38	BN	154	
39	BG	256	
40	Fa	120	
41	Ha	146	
42	BU	182	
43	BR	247	
44	Xa	160	
45	BV	262	
46	BJ	221	
47	AO	164	
48	BW	82	
49	AK	214	
50	Na	86	
51	AB	197	
52	BF	233	

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Mol	Chain	Length	Quality of chain
53	AA	250	
54	AG	206	
55	Ga	128	
56	BA	51	
57	AF	146	
58	Wa	152	
59	Ta	249	
60	AZ	69	
61	BE	92	
62	Za	298	
63	AQ	143	
64	Oa	64	
65	Ua	150	
66	Ya	150	
67	BB	141	
68	AN	124	
69	Ra	190	
70	BL	143	
71	La	108	
72	Aa	222	
73	AY	95	
74	Ca	56	
75	h1	1805	
76	B1	12	
77	Ba	122	

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Mol	Chain	Length	Quality of chain
78	AI	177	
79	L3	23	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
82	TER	A	3401	-	-	X	-

2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 209233 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called Ribosomal RNA 5.8S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	162	Total	C	N	O	P	0	0
			3453	1544	617	1130	162		

- Molecule 2 is a RNA chain called Ribosomal RNA 25S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3149	Total	C	N	O	P	1	0
			67524	30161	12266	21947	3150		

- Molecule 3 is a RNA chain called Transfer RNA Phe (GAA).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	i2	76	Total	C	N	O	P	0	0
			1630	726	298	530	76		
3	W2	76	Total	C	N	O	P	0	0
			1629	726	298	529	76		

- Molecule 4 is a RNA chain called Ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C3	119	Total	C	N	O	P	0	0
			2536	1132	454	831	119		

- Molecule 5 is a protein called Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BC	25	Total	C	N	O	S	0	0
			237	145	62	27	3		

- Molecule 6 is a protein called Large ribosomal subunit protein uL22z.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BM	155	Total	C	N	O	S	0	0
			1246	774	247	221	4		

- Molecule 7 is a protein called Large ribosomal subunit protein uL24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BO	125	Total	C	N	O	S	0	0
			1030	637	211	179	3		

- Molecule 8 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AR	51	Total	C	N	O	S	0	0
			425	258	100	66	1		

- Molecule 9 is a protein called Large ribosomal subunit protein eL31y.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AU	109	Total	C	N	O	S	0	0
			888	558	168	160	2		

- Molecule 10 is a protein called Small ribosomal subunit protein eS26y.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Ma	98	Total	C	N	O	S	0	0
			789	485	166	132	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6z/uL6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ia	190	Total	C	N	O	S	0	0
			1512	961	270	275	6		

- Molecule 12 is a protein called Small ribosomal subunit protein uS8z/uS8w.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AE	129	Total	C	N	O	S	0	0
			1033	660	188	180	5		

- Molecule 13 is a protein called Large ribosomal subunit protein eL36y.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AX	97	Total	C	N	O	S	0	0
			786	492	166	126	2		

- Molecule 14 is a protein called Large ribosomal subunit protein eL27x.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AP	134	Total	C	N	O	S	0	0
			1092	706	200	183	3		

- Molecule 15 is a protein called Small ribosomal subunit protein eS4x.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ja	258	Total	C	N	O	S	0	0
			2074	1325	386	357	6		

- Molecule 16 is a protein called Large ribosomal subunit protein eL15z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ea	203	Total	C	N	O	S	1	0
			1713	1070	361	279	3		

- Molecule 17 is a protein called Ribosomal protein L18ae/LX family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AL	175	Total	C	N	O	S	0	0
			1485	960	273	244	8		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12y.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Va	139	Total	C	N	O	S	0	0
			1082	689	207	183	3		

- Molecule 19 is a protein called Small ribosomal subunit protein eS24y.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ka	120	Total	C	N	O	S	0	0
			986	627	191	165	3		

- Molecule 20 is a protein called Large ribosomal subunit protein eL33y.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AW	111	Total	C	N	O	S	0	0
			901	568	174	155	4		

- Molecule 21 is a protein called Large ribosomal subunit protein eL42z/eL42y.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BD	97	Total	C	N	O	S	0	0
			792	497	158	132	5		

- Molecule 22 is a protein called Large ribosomal subunit protein uL3z.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BS	386	Total	C	N	O	S	0	0
			3111	1981	581	532	17		

- Molecule 23 is a protein called Large ribosomal subunit protein eL21z/eL21y.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AM	163	Total	C	N	O	S	0	0
			1307	827	254	222	4		

- Molecule 24 is a protein called Small ribosomal subunit protein uS5y/uS5u/uS5v.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AC	215	Total	C	N	O	S	0	0
			1672	1075	300	290	7		

- Molecule 25 is a protein called Large ribosomal subunit protein uL14x/uL14z/uL14y.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BI	131	Total	C	N	O	S	0	0
			986	624	183	171	8		

- Molecule 26 is a protein called Large ribosomal subunit protein eL14y.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AH	128	Total	C	N	O	S	0	0
			1042	665	194	179	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4z.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BT	393	Total	C	N	O	S	0	0
			3056	1934	573	535	14		

- Molecule 28 is a protein called Large ribosomal subunit protein eL32z.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AV	126	Total	C	N	O	S	0	0
			1028	649	204	171	4		

- Molecule 29 is a protein called Small ribosomal subunit protein uS7y.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AD	184	Total	C	N	O	S	0	0
			1454	912	275	261	6		

- Molecule 30 is a protein called Large ribosomal subunit protein eL18x.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AJ	186	Total	C	N	O	S	0	0
			1468	932	283	249	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL2z.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BQ	245	Total	C	N	O	S	1	0
			1881	1179	379	316	7		

- Molecule 32 is a protein called Large ribosomal subunit protein uL13y.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BH	205	Total	C	N	O	S	0	0
			1636	1038	314	273	11		

- Molecule 33 is a protein called Small ribosomal subunit protein uS15y.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Da	149	Total	C	N	O	S	0	0
			1190	759	223	206	2		

- Molecule 34 is a protein called Large ribosomal subunit protein uL18z.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BK	281	Total	C	N	O	S	0	0
			2277	1441	418	414	4		

- Molecule 35 is a protein called Large ribosomal subunit protein eL30y.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AT	94	Total	C	N	O	S	0	0
			720	457	127	131	5		

- Molecule 36 is a protein called Small ribosomal subunit protein eS30z/eS30y/eS30x.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Pa	49	Total	C	N	O	0	0
			389	236	92	61		

- Molecule 37 is a protein called Large ribosomal subunit protein uL29x.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BP	120	Total	C	N	O	S	0	0
			975	617	191	166	1		

- Molecule 38 is a protein called Large ribosomal subunit protein uL23y.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	117	Total	C	N	O	S	0	0
			955	615	170	168	2		

- Molecule 39 is a protein called Large ribosomal subunit protein eL8y.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BG	234	Total	C	N	O	S	0	0
			1874	1207	339	323	5		

- Molecule 40 is a protein called Large ribosomal subunit protein eL34z.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Fa	111	Total	C	N	O	S	0	0
			896	560	187	148	1		

- Molecule 41 is a protein called Large ribosomal subunit protein uL15x.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ha	145	Total	C	N	O	S	0	0
			1156	744	225	184	3		

- Molecule 42 is a protein called Large ribosomal subunit protein uL5z.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BU	169	Total	C	N	O	S	0	0
			1366	863	254	242	7		

- Molecule 43 is a protein called Ribosomal protein L30/L7 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BR	232	Total	C	N	O	S	0	0
			1898	1221	348	325	4		

- Molecule 44 is a protein called Small ribosomal subunit protein uS17z.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Xa	146	Total	C	N	O	S	0	0
			1163	742	224	192	5		

- Molecule 45 is a protein called Small ribosomal subunit protein eS1y.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BV	212	Total	C	N	O	S	0	0
			1718	1087	313	310	8		

- Molecule 46 is a protein called Large ribosomal subunit protein uL16y.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BJ	207	Total	C	N	O	S	0	0
			1653	1047	327	268	11		

- Molecule 47 is a protein called Large ribosomal subunit protein eL24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AO	62	Total	C	N	O	S	0	0
			528	343	100	81	4		

- Molecule 48 is a protein called Small ribosomal subunit protein eS21y.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	73	Total	C	N	O	S	0	0
			568	355	104	107	2		

- Molecule 49 is a protein called Large ribosomal subunit protein eL19x.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AK	178	Total	C	N	O	S	0	0
			1480	920	308	241	11		

- Molecule 50 is a protein called Small ribosomal subunit protein eS27y.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Na	83	Total	C	N	O	S	0	0
			647	405	118	117	7		

- Molecule 51 is a protein called Small ribosomal subunit protein uS4y.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AB	180	Total	C	N	O	S	0	0
			1514	953	303	254	4		

- Molecule 52 is a protein called Large ribosomal subunit protein eL6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BF	190	Total	C	N	O	S	0	0
			1491	966	273	250	2		

- Molecule 53 is a protein called Small ribosomal subunit protein uS3z.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AA	208	Total	C	N	O	S	0	0
			1625	1031	296	290	8		

- Molecule 54 is a protein called Large ribosomal subunit protein eL13z.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AG	203	Total	C	N	O	S	0	0
			1648	1041	326	277	4		

- Molecule 55 is a protein called Ubiquitin-ribosomal protein eL40z fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Ga	52	Total	C	N	O	S	0	0
			433	271	89	66	7		

- Molecule 56 is a protein called Large ribosomal subunit protein eL39z/eL39x.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BA	50	Total	C	N	O	S	0	0
			444	282	97	63	2		

- Molecule 57 is a protein called Small ribosomal subunit protein uS9z.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AF	138	Total	C	N	O	S	0	0
			1113	708	213	187	5		

- Molecule 58 is a protein called Small ribosomal subunit protein uS13z/uS13y/uS13x.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Wa	139	Total	C	N	O	S	0	0
			1136	709	224	198	5		

- Molecule 59 is a protein called Small ribosomal subunit protein eS6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ta	225	Total	C	N	O	S	0	0
			1795	1123	354	310	8		

- Molecule 60 is a protein called Large ribosomal subunit protein eL38z/eL38y.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AZ	68	Total	C	N	O	S	0	0
			562	359	103	98	2		

- Molecule 61 is a protein called Large ribosomal subunit protein eL43y.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BE	90	Total	C	N	O	S	0	0
			702	441	135	120	6		

- Molecule 62 is a protein called Small ribosomal subunit protein uS2z.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Za	198	Total	C	N	O	S	0	0
			1575	1000	283	279	13		

- Molecule 63 is a protein called Large ribosomal subunit protein eL28z.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AQ	136	Total	C	N	O	S	0	0
			1056	667	197	190	2		

- Molecule 64 is a protein called Small ribosomal subunit protein eS28x.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Oa	59	Total	C	N	O	S	0	0
			471	289	96	84	2		

- Molecule 65 is a protein called Small ribosomal subunit protein uS11y.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ua	127	Total	C	N	O	S	0	0
			962	591	189	177	5		

- Molecule 66 is a protein called Small ribosomal subunit protein uS19y.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ya	129	Total	C	N	O	S	0	0
			1024	657	190	172	5		

- Molecule 67 is a protein called Small ribosomal subunit protein eS17w.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BB	119	Total	C	N	O	S	0	0
			955	597	175	178	5		

- Molecule 68 is a protein called Large ribosomal subunit protein eL22z.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AN	99	Total	C	N	O	S	0	0
			808	517	143	146	2		

- Molecule 69 is a protein called Small ribosomal subunit protein eS7x.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ra	184	Total	C	N	O	S	0	0
			1506	955	275	270	6		

- Molecule 70 is a protein called Small ribosomal subunit protein eS19x.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BL	136	Total	C	N	O	S	0	0
			1064	673	202	186	3		

- Molecule 71 is a protein called Small ribosomal subunit protein eS25w.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	La	71	Total	C	N	O	S	0	0
			562	354	105	99	4		

- Molecule 72 is a protein called Small ribosomal subunit protein eS8z.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aa	185	Total	C	N	O	S	0	0
			1494	928	296	266	4		

- Molecule 73 is a protein called Large ribosomal subunit protein eL37z.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AY	87	Total	C	N	O	S	0	0
			705	429	157	113	6		

- Molecule 74 is a protein called Small ribosomal subunit protein uS14z/uS14y/uS14x.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ca	55	Total	C	N	O	S	0	0
			440	273	91	71	5		

- Molecule 75 is a RNA chain called Ribosomal RNA 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	h1	1612	Total	C	N	O	P	0	0
			34449	15422	6154	11261	1612		

- Molecule 76 is a RNA chain called Messenger RNA (poly-U).

Mol	Chain	Residues	Atoms					AltConf	Trace
76	B1	12	Total	C	N	O	P	0	0
			240	108	24	96	12		

- Molecule 77 is a protein called Small ribosomal subunit protein uS10y.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ba	101	Total	C	N	O	S	0	0
			799	505	149	142	3		

- Molecule 78 is a protein called Small ribosomal subunit protein eS10z.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AI	92	Total	C	N	O	S	0	0
			779	514	127	133	5		

- Molecule 79 is a protein called Nascent polypeptide (poly-A).

Mol	Chain	Residues	Atoms				AltConf	Trace
79	L3	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	3	5	Total	Mg	0
			5	5	
80	A	197	Total	Mg	0
			197	197	
80	i2	1	Total	Mg	0
			1	1	
80	C3	4	Total	Mg	0
			4	4	
80	BM	1	Total	Mg	0
			1	1	
80	Ja	1	Total	Mg	0
			1	1	
80	BS	4	Total	Mg	0
			4	4	
80	AM	1	Total	Mg	0
			1	1	
80	AC	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
80	BI	1	Total 1	Mg 1	0
80	BR	1	Total 1	Mg 1	0
80	BV	1	Total 1	Mg 1	0
80	AG	1	Total 1	Mg 1	0
80	Ta	1	Total 1	Mg 1	0
80	AY	2	Total 2	Mg 2	0
80	h1	77	Total 77	Mg 77	0

- Molecule 81 is POTASSIUM ION (CCD ID: K) (formula: K).

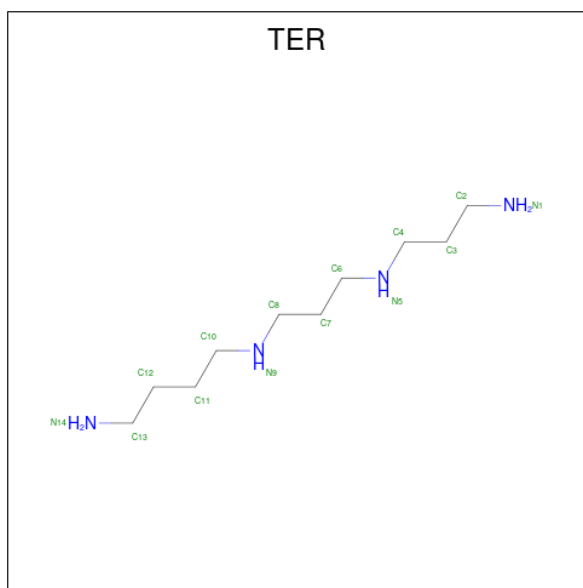
Mol	Chain	Residues	Atoms		AltConf
81	3	4	Total 4	K 4	0
81	A	125	Total 125	K 125	0
81	C3	1	Total 1	K 1	0
81	BM	2	Total 2	K 2	0
81	AR	1	Total 1	K 1	0
81	Ea	1	Total 1	K 1	0
81	Va	2	Total 2	K 2	0
81	BD	1	Total 1	K 1	0
81	BS	2	Total 2	K 2	0
81	AV	1	Total 1	K 1	0
81	AJ	1	Total 1	K 1	0
81	BQ	2	Total 2	K 2	0

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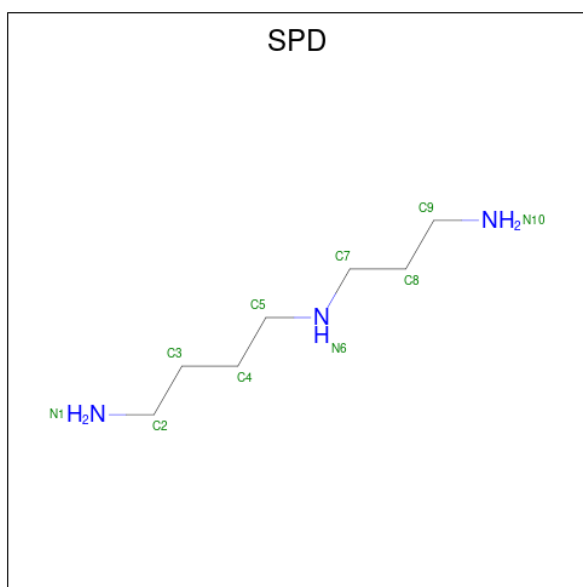
Mol	Chain	Residues	Atoms		AltConf
81	Fa	1	Total	K	0
			1	1	
81	BJ	1	Total	K	0
			1	1	
81	AG	1	Total	K	0
			1	1	
81	Wa	1	Total	K	0
			1	1	
81	Ua	1	Total	K	0
			1	1	
81	Ca	1	Total	K	0
			1	1	
81	h1	40	Total	K	0
			40	40	

- Molecule 82 is N-(3-AMINO-PROPYL)-N-(5-AMINOPROPYL)-1,4-DIAMINOBUTANE (CCD ID: TER) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



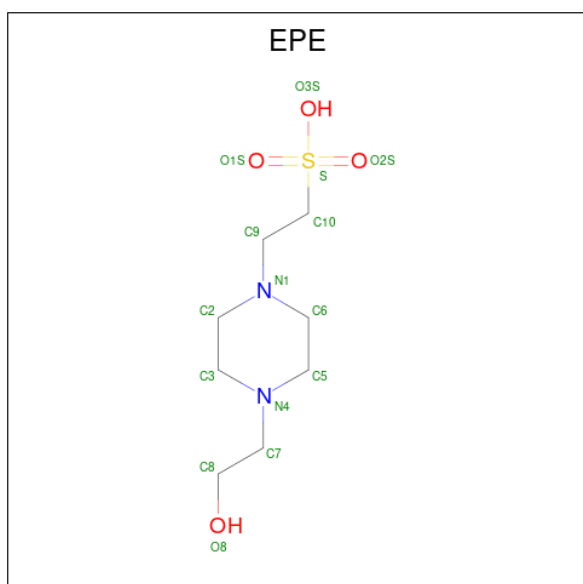
Mol	Chain	Residues	Atoms			AltConf
82	A	1	Total	C	N	0
			14	10	4	

- Molecule 83 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
83	A	1	Total	C	N	0
			10	7	3	
83	A	1	Total	C	N	0
			10	7	3	
83	A	1	Total	C	N	0
			10	7	3	
83	A	1	Total	C	N	0
			10	7	3	

- Molecule 84 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					AltConf
84	A	1	Total	C	N	O	S	0
			15	8	2	4	1	

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

Mol	Chain	Residues	Atoms		AltConf
85	Ma	1	Total	Zn	0
			1	1	
85	BD	1	Total	Zn	0
			1	1	
85	Ga	1	Total	Zn	0
			1	1	
85	BE	1	Total	Zn	0
			1	1	
85	AY	1	Total	Zn	0
			1	1	
85	Ca	1	Total	Zn	0
			1	1	

- Molecule 86 is water.

Mol	Chain	Residues	Atoms		AltConf
86	3	328	Total	O	0
			328	328	
86	A	7443	Total	O	0
			7443	7443	
86	i2	10	Total	O	0
			10	10	
86	C3	180	Total	O	0
			180	180	
86	BC	13	Total	O	0
			13	13	
86	BM	74	Total	O	0
			74	74	
86	BO	34	Total	O	0
			34	34	
86	AR	43	Total	O	0
			43	43	
86	AU	27	Total	O	0
			27	27	
86	Ma	32	Total	O	0
			32	32	
86	Ia	28	Total	O	0
			28	28	

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Mol	Chain	Residues	Atoms		AltConf
86	AE	15	Total 15	O 15	0
86	AX	30	Total 30	O 30	0
86	AP	20	Total 20	O 20	0
86	Ja	20	Total 20	O 20	0
86	Ea	137	Total 137	O 137	0
86	AL	71	Total 71	O 71	0
86	Va	33	Total 33	O 33	0
86	AW	65	Total 65	O 65	0
86	BD	74	Total 74	O 74	0
86	BS	173	Total 173	O 173	0
86	AM	86	Total 86	O 86	0
86	AC	21	Total 21	O 21	0
86	BI	40	Total 40	O 40	0
86	AH	21	Total 21	O 21	0
86	BT	146	Total 146	O 146	0
86	AV	72	Total 72	O 72	0
86	AD	5	Total 5	O 5	0
86	AJ	119	Total 119	O 119	0
86	BQ	132	Total 132	O 132	0
86	BH	84	Total 84	O 84	0
86	Da	26	Total 26	O 26	0

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Mol	Chain	Residues	Atoms		AltConf
86	BK	69	Total 69	O 69	0
86	AT	13	Total 13	O 13	0
86	Pa	2	Total 2	O 2	0
86	BP	22	Total 22	O 22	0
86	BN	33	Total 33	O 33	0
86	BG	39	Total 39	O 39	0
86	Fa	64	Total 64	O 64	0
86	Ha	93	Total 93	O 93	0
86	BU	8	Total 8	O 8	0
86	BR	79	Total 79	O 79	0
86	Xa	16	Total 16	O 16	0
86	BV	16	Total 16	O 16	0
86	BJ	39	Total 39	O 39	0
86	AO	23	Total 23	O 23	0
86	BW	2	Total 2	O 2	0
86	AK	47	Total 47	O 47	0
86	Na	5	Total 5	O 5	0
86	AB	7	Total 7	O 7	0
86	BF	18	Total 18	O 18	0
86	AA	2	Total 2	O 2	0
86	AG	87	Total 87	O 87	0

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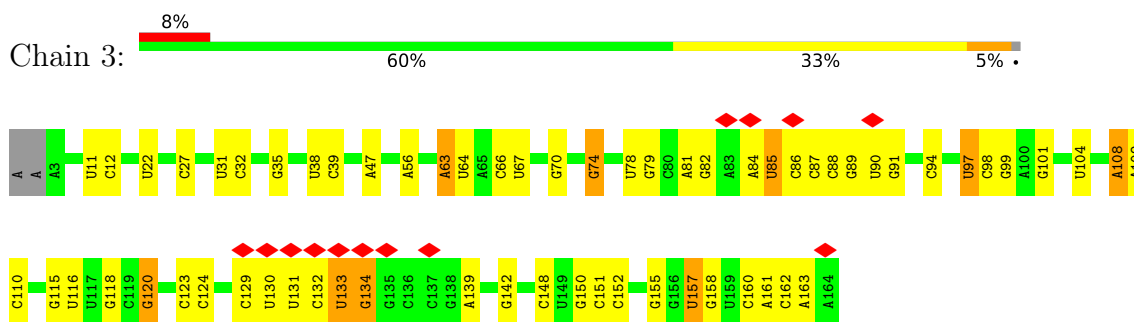
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Mol	Chain	Residues	Atoms		AltConf
86	Ga	21	Total 21	O 21	0
86	BA	27	Total 27	O 27	0
86	AF	10	Total 10	O 10	0
86	Wa	3	Total 3	O 3	0
86	Ta	7	Total 7	O 7	0
86	AZ	6	Total 6	O 6	0
86	BE	32	Total 32	O 32	0
86	Za	3	Total 3	O 3	0
86	AQ	4	Total 4	O 4	0
86	Oa	4	Total 4	O 4	0
86	Ua	33	Total 33	O 33	0
86	Ya	1	Total 1	O 1	0
86	AN	1	Total 1	O 1	0
86	BL	4	Total 4	O 4	0
86	Aa	9	Total 9	O 9	0
86	AY	74	Total 74	O 74	0
86	h1	1686	Total 1686	O 1686	0
86	B1	27	Total 27	O 27	0
86	W2	24	Total 24	O 24	0
86	Ba	3	Total 3	O 3	0
86	L3	1	Total 1	O 1	0

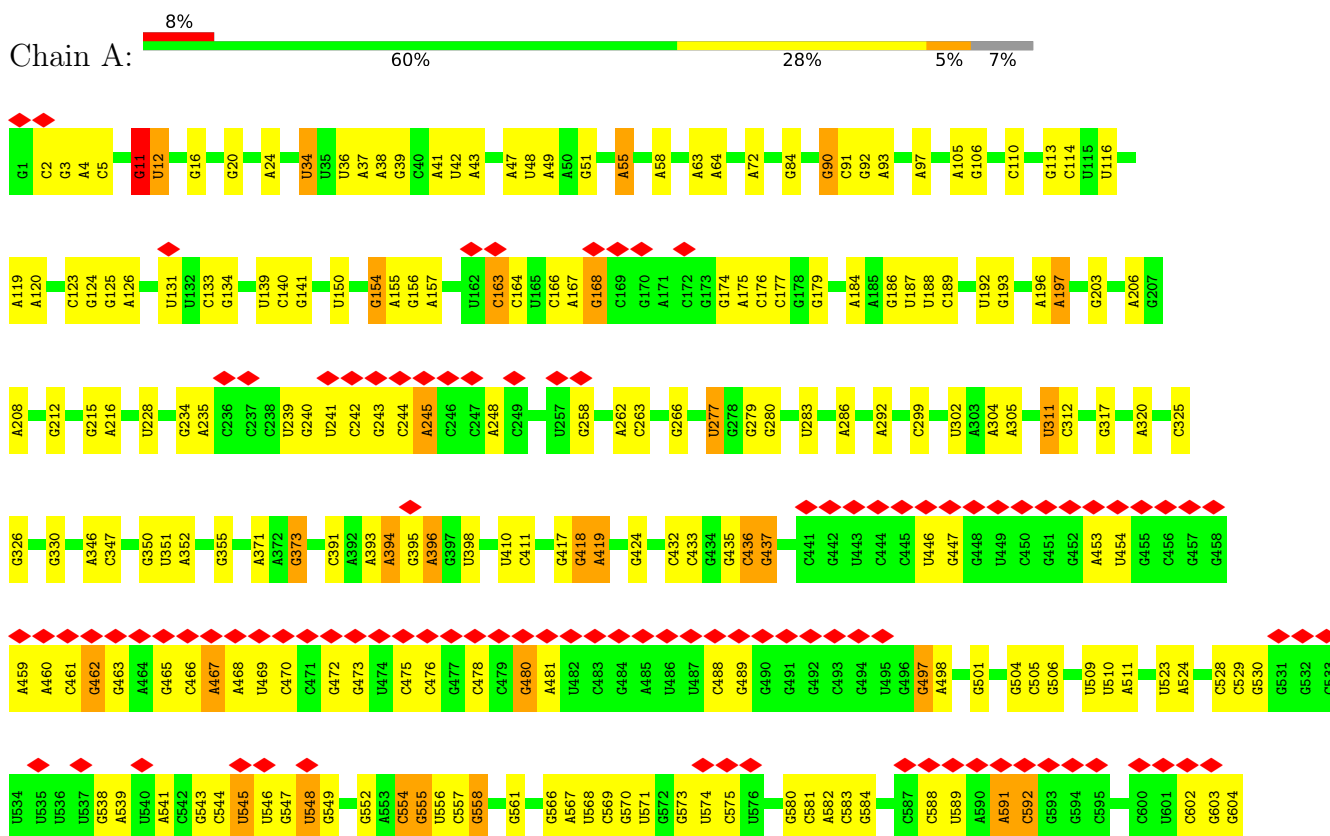
3 Residue-property plots

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

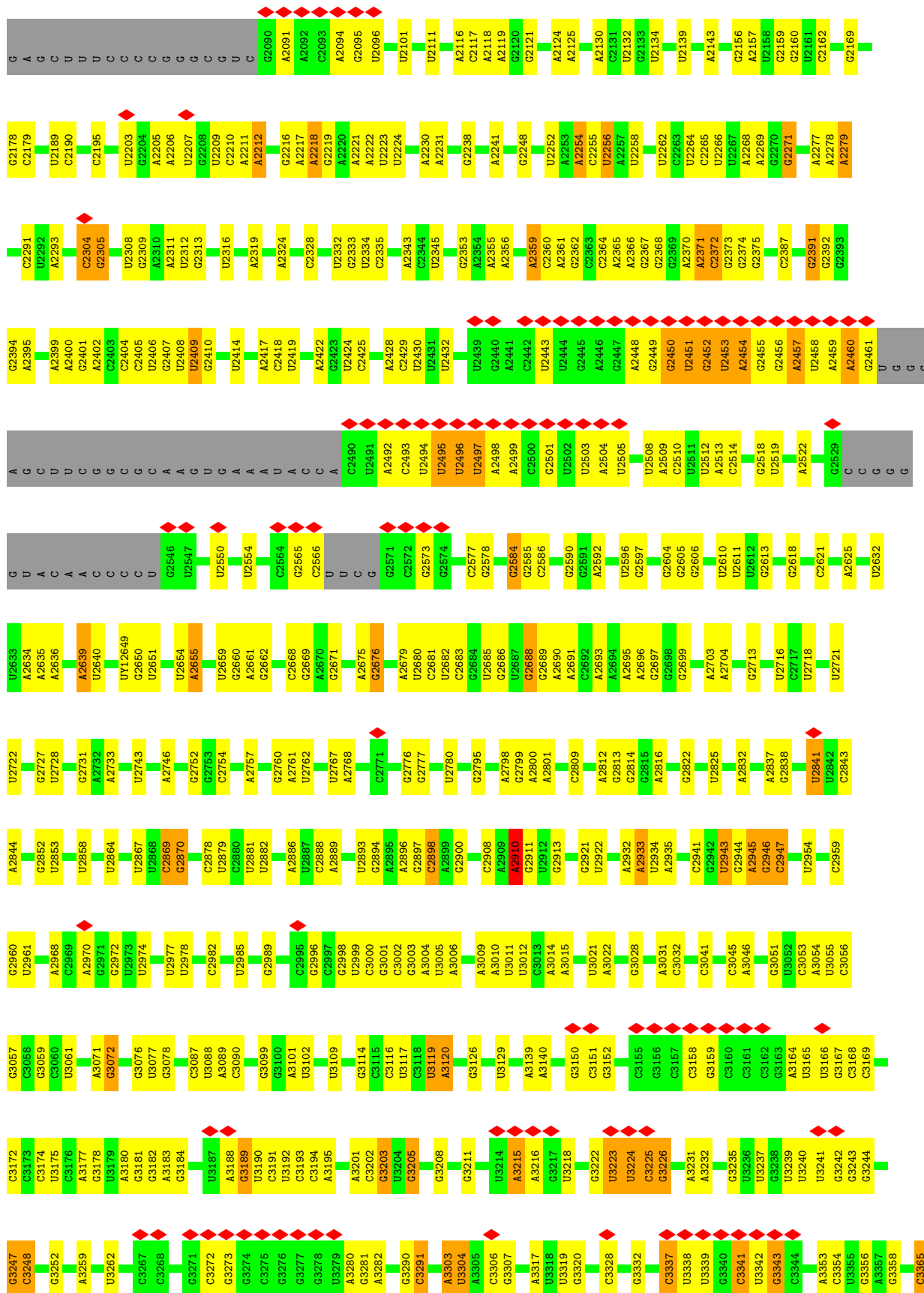
• Molecule 1: Ribosomal RNA 5.8S



• Molecule 2: Ribosomal RNA 25S

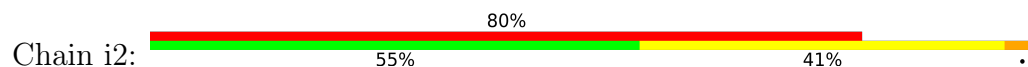




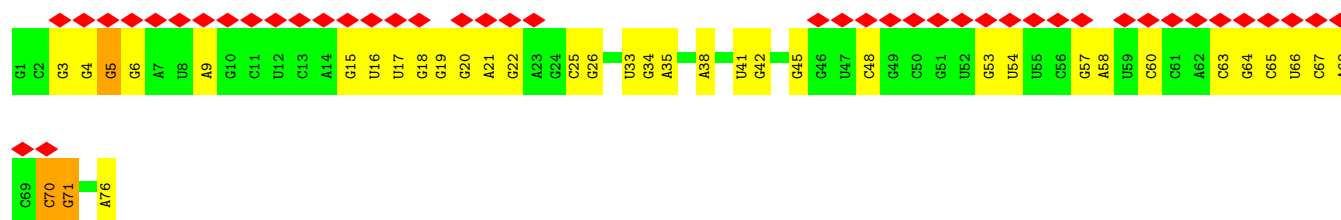




• Molecule 3: Transfer RNA Phe (GAA)



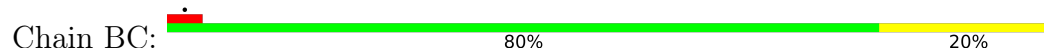
• Molecule 3: Transfer RNA Phe (GAA)



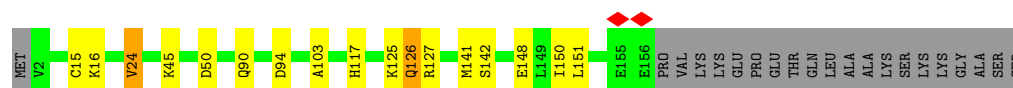
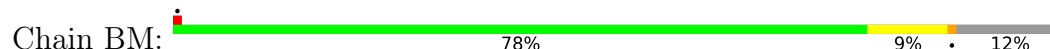
• Molecule 4: Ribosomal RNA 5S



• Molecule 5: Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v

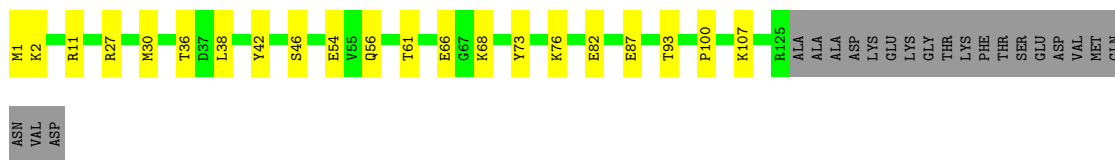


• Molecule 6: Large ribosomal subunit protein uL22z



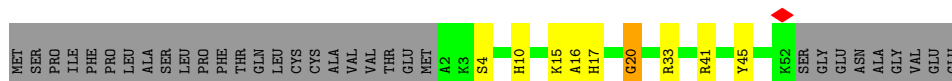
• Molecule 7: Large ribosomal subunit protein uL24z

Chain BO: 



- Molecule 8: 60S ribosomal protein L29

Chain AR: 



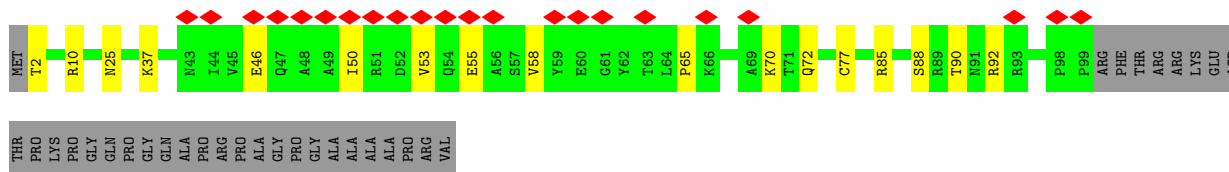
- Molecule 9: Large ribosomal subunit protein eL31y

Chain AU: 



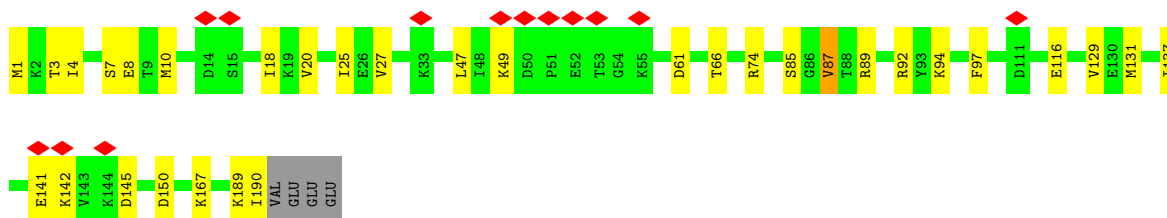
- Molecule 10: Small ribosomal subunit protein eS26y

Chain Ma: 



- Molecule 11: Large ribosomal subunit protein uL6z/uL6y

Chain Ia: 

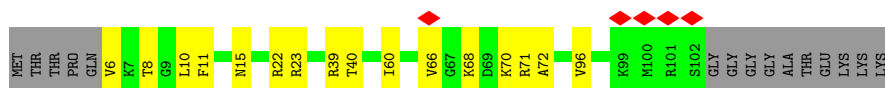
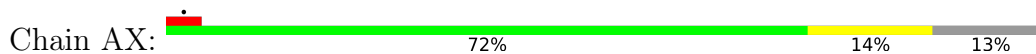


- Molecule 12: Small ribosomal subunit protein uS8z/uS8w

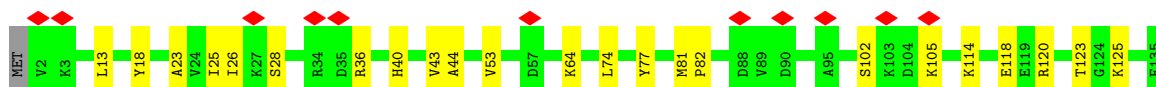
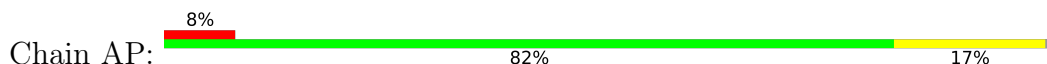
Chain AE: 



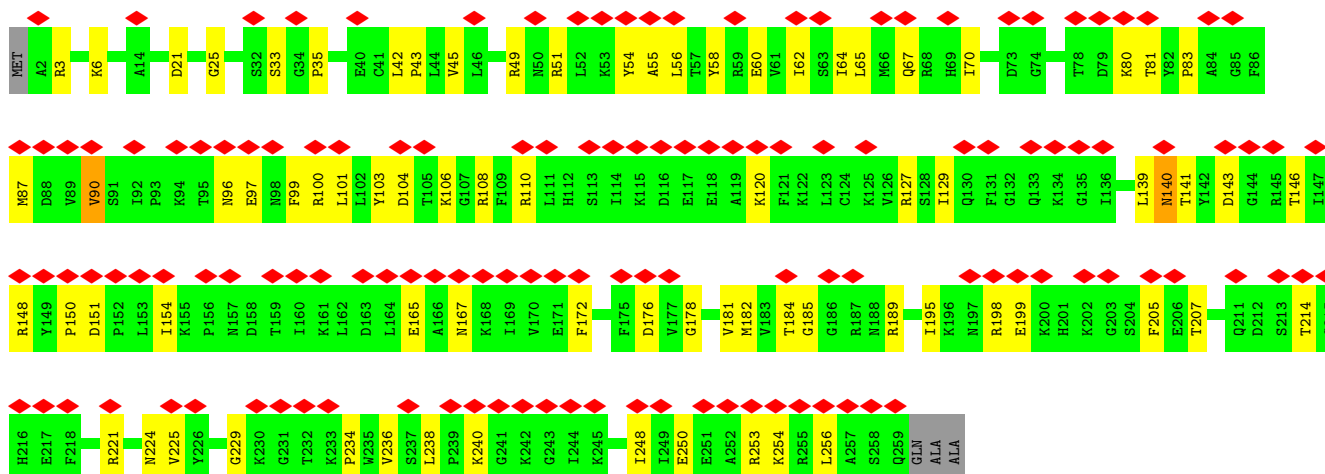
- Molecule 13: Large ribosomal subunit protein eL36y



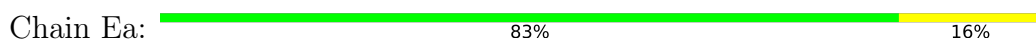
- Molecule 14: Large ribosomal subunit protein eL27x



- Molecule 15: Small ribosomal subunit protein eS4x



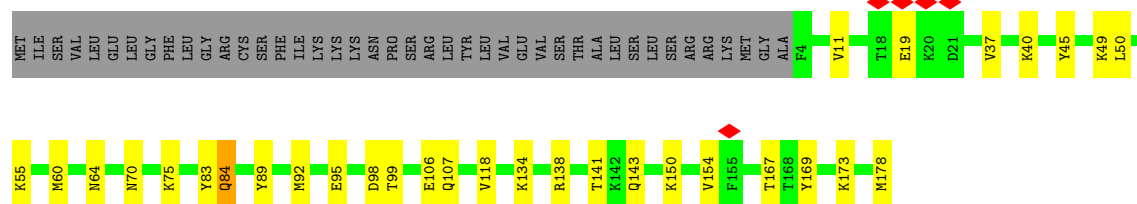
- Molecule 16: Large ribosomal subunit protein eL15z



- Molecule 17: Ribosomal protein L18ae/LX family protein

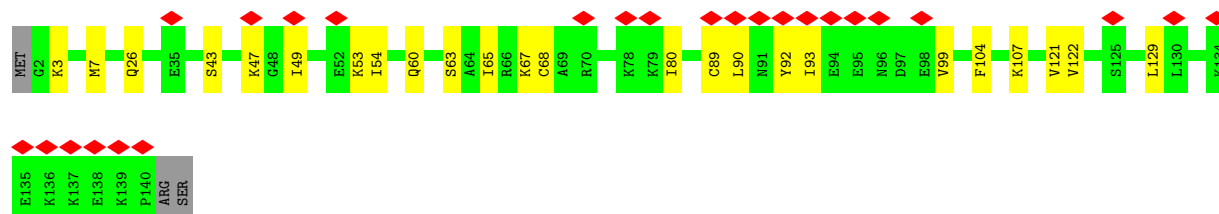


Chain AL: 



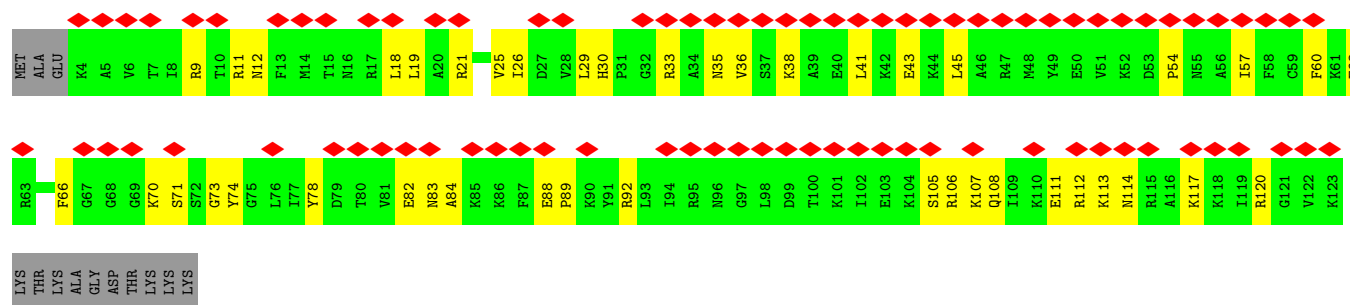
- Molecule 18: Small ribosomal subunit protein uS12y

Chain Va: 



- Molecule 19: Small ribosomal subunit protein eS24y

Chain Ka: 



- Molecule 20: Large ribosomal subunit protein eL33y

Chain AW: 



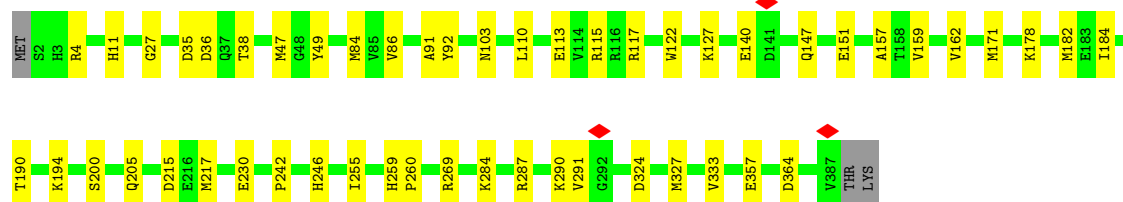
- Molecule 21: Large ribosomal subunit protein eL42z/eL42y

Chain BD: 



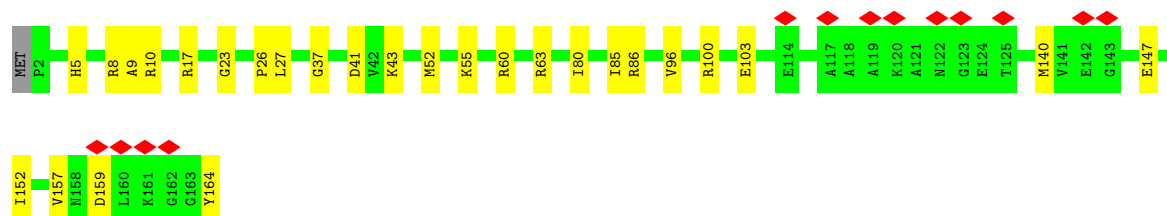
- Molecule 22: Large ribosomal subunit protein uL3z

Chain BS: 



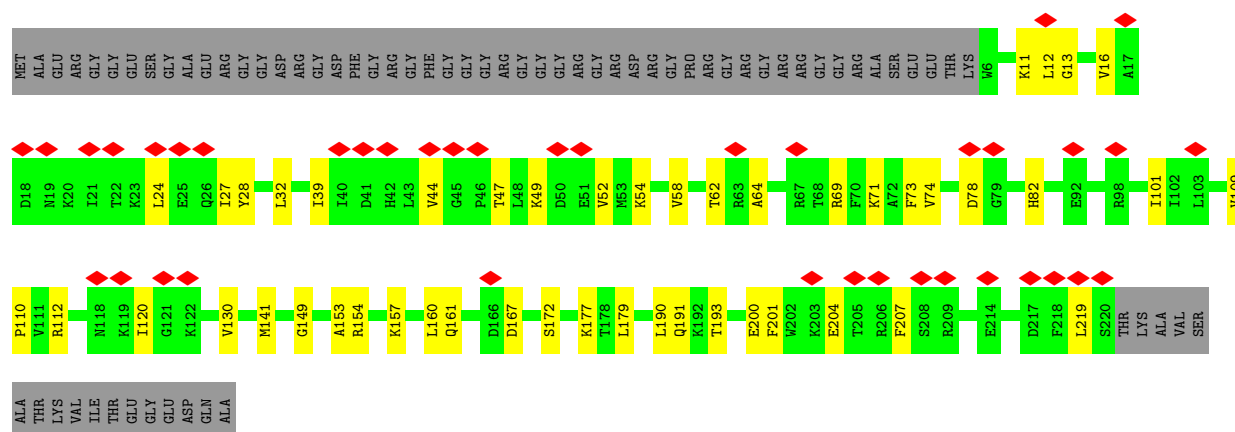
- Molecule 23: Large ribosomal subunit protein eL21z/eL21y

Chain AM: 



- Molecule 24: Small ribosomal subunit protein uS5y/uS5u/uS5v

Chain AC: 



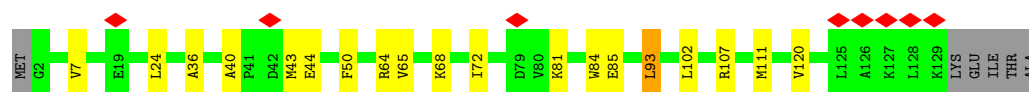
- Molecule 25: Large ribosomal subunit protein uL14x/uL14z/uL14y

Chain BI: 

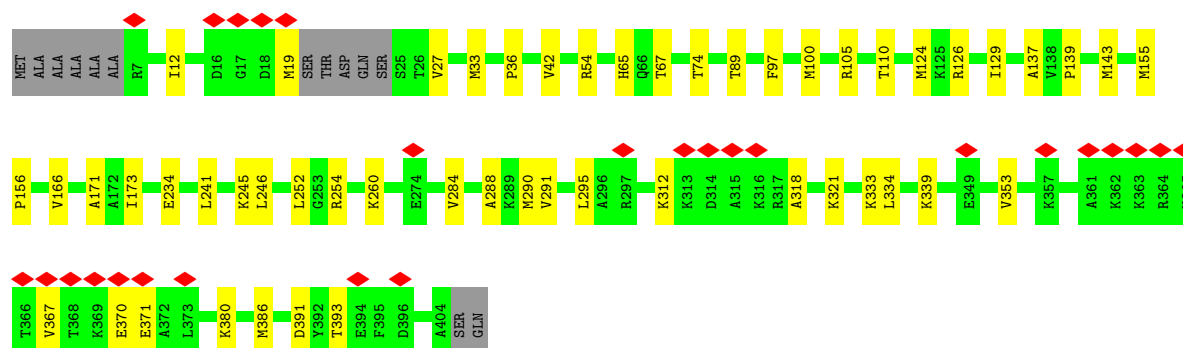
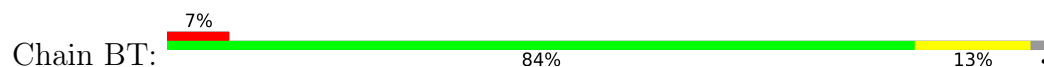


- Molecule 26: Large ribosomal subunit protein eL14y

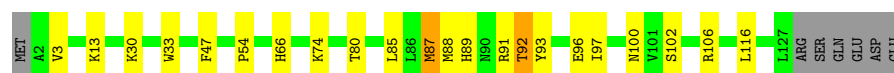
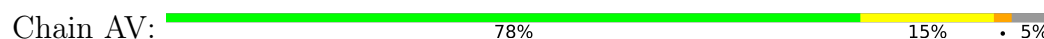
Chain AH: 



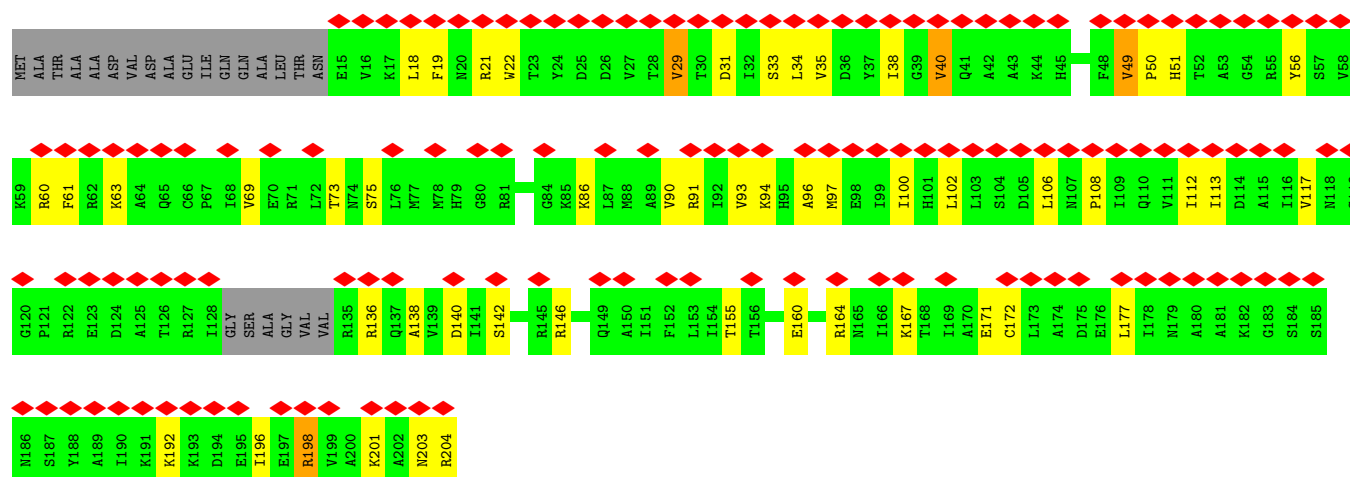
- Molecule 27: Large ribosomal subunit protein uL4z



- Molecule 28: Large ribosomal subunit protein eL32z



- Molecule 29: Small ribosomal subunit protein uS7y



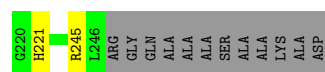
- Molecule 30: Large ribosomal subunit protein eL18x





- Molecule 31: Large ribosomal subunit protein uL2z

Chain BQ: 82% 12% 5%



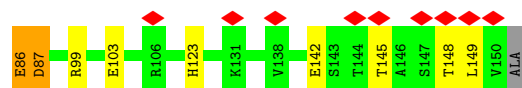
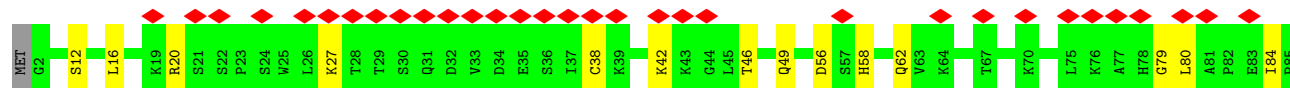
- Molecule 32: Large ribosomal subunit protein uL13y

Chain BH: 5% 88% 11%



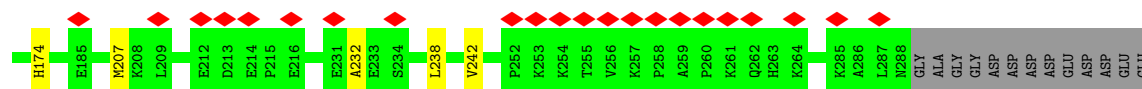
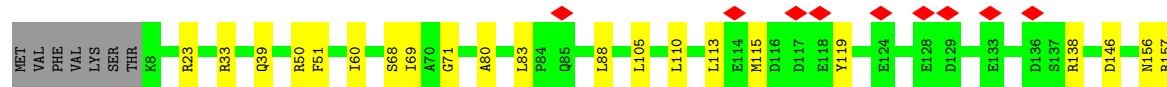
- Molecule 33: Small ribosomal subunit protein uS15y

Chain Da: 27% 83% 14% ..



- Molecule 34: Large ribosomal subunit protein uL18z

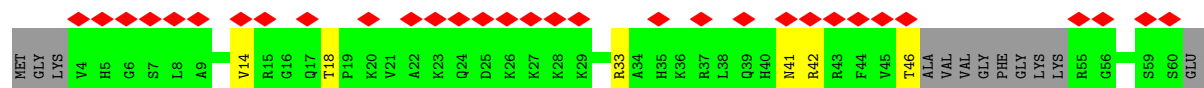
Chain BK: 10% 85% 9% 7%



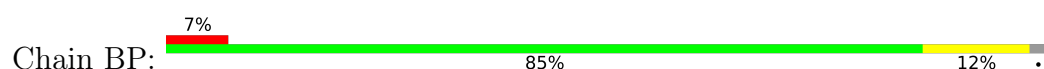
- Molecule 35: Large ribosomal subunit protein eL30y



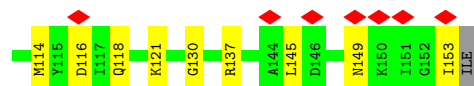
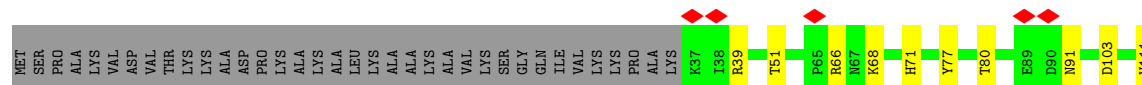
- Molecule 36: Small ribosomal subunit protein eS30z/eS30y/eS30x



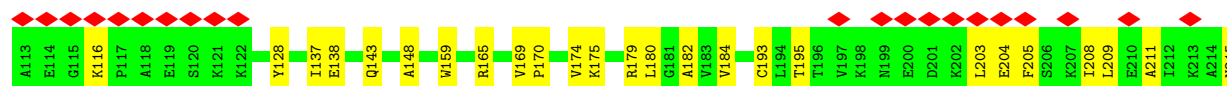
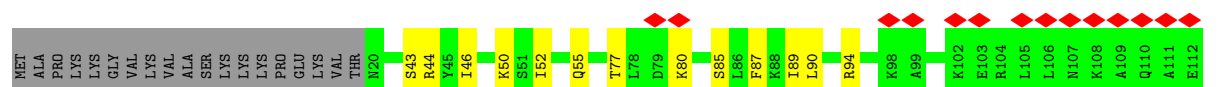
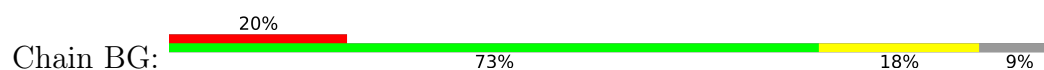
- Molecule 37: Large ribosomal subunit protein uL29x



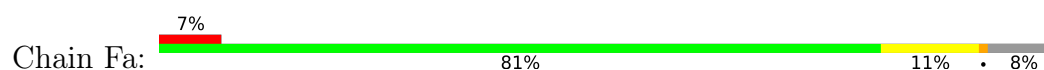
- Molecule 38: Large ribosomal subunit protein uL23y

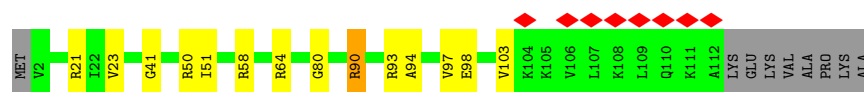


- Molecule 39: Large ribosomal subunit protein eL8y



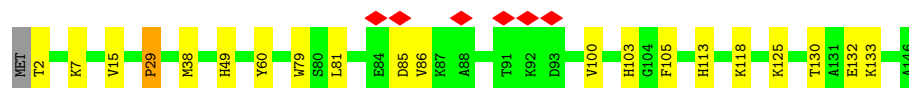
- Molecule 40: Large ribosomal subunit protein eL34z





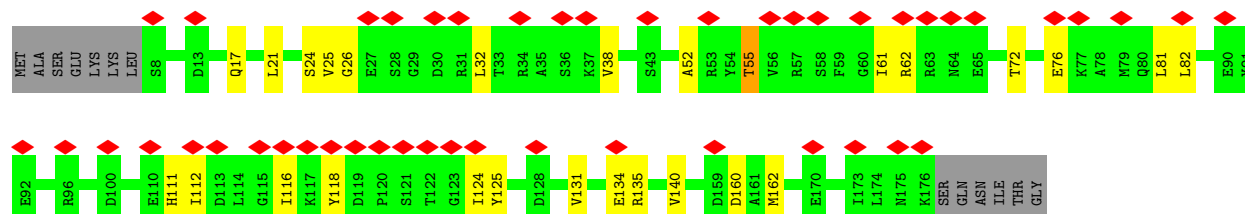
- Molecule 41: Large ribosomal subunit protein uL15x

Chain Ha: 86% 13% ..



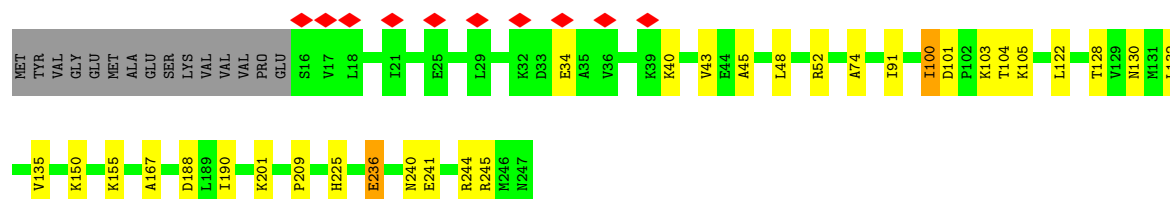
- Molecule 42: Large ribosomal subunit protein uL5z

Chain BU: 26% 78% 14% • 7%



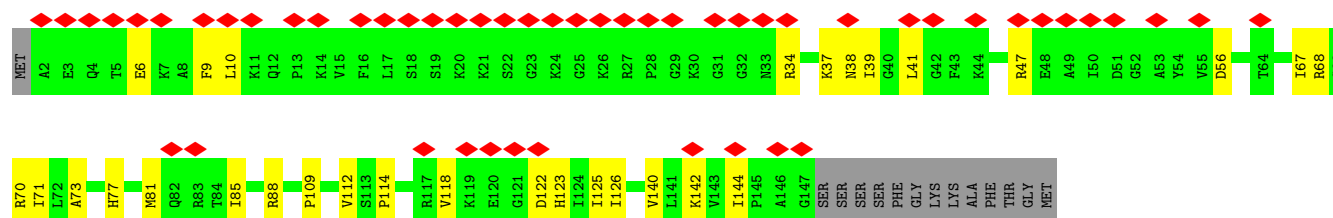
- Molecule 43: Ribosomal protein L30/L7 family protein

Chain BR: 81% 12% • 6%



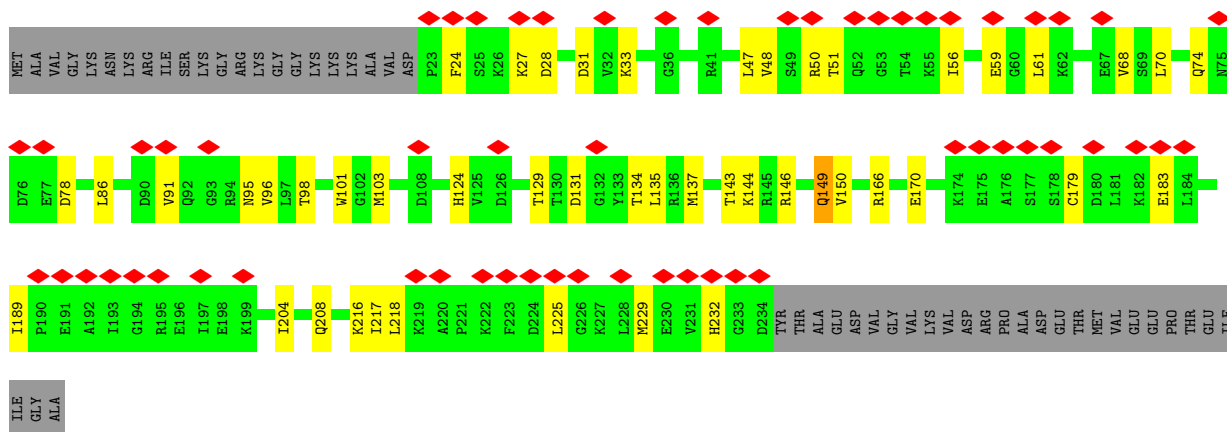
- Molecule 44: Small ribosomal subunit protein uS17z

Chain Xa: 32% 72% 19% 9%

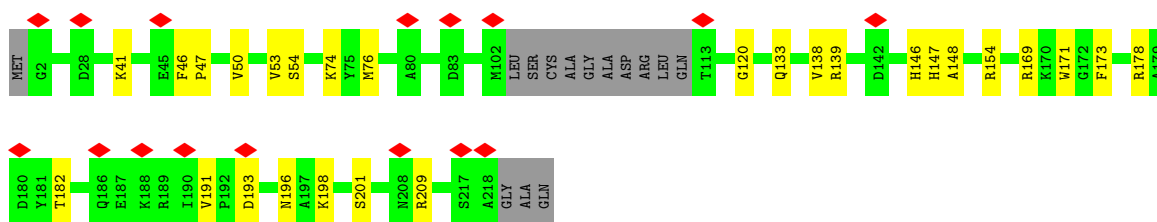
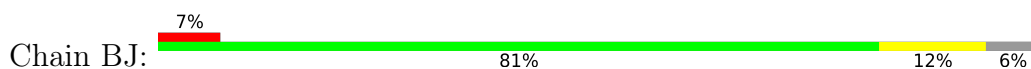


- Molecule 45: Small ribosomal subunit protein eS1y

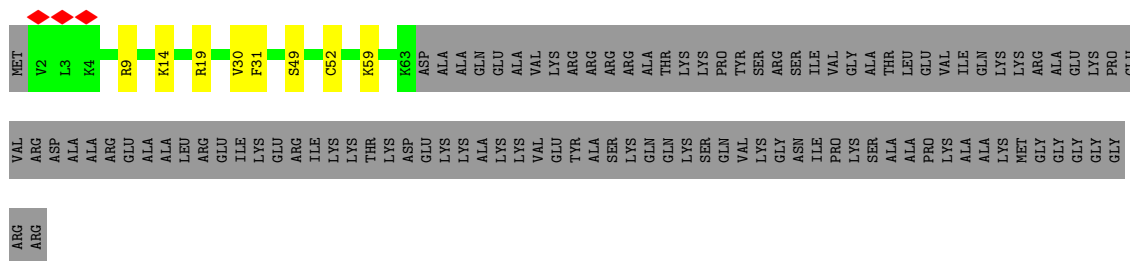
Chain BV: 22% 63% 18% 19%



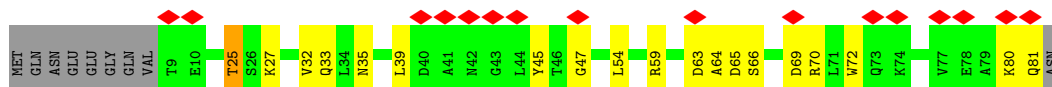
- Molecule 46: Large ribosomal subunit protein uL16y



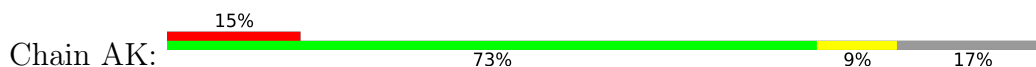
- Molecule 47: Large ribosomal subunit protein eL24z

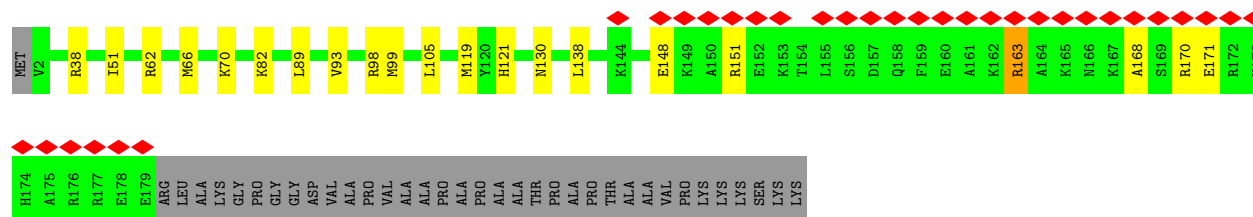


- Molecule 48: Small ribosomal subunit protein eS21y

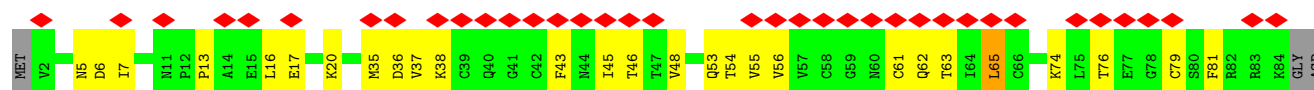
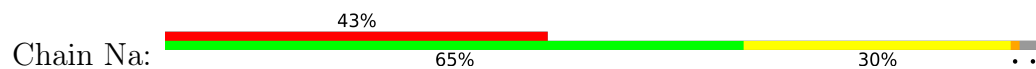


- Molecule 49: Large ribosomal subunit protein eL19x

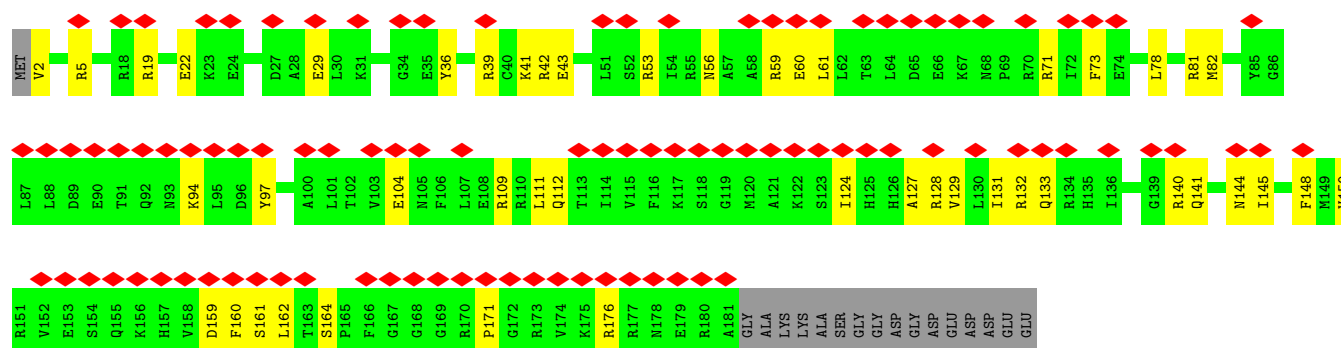




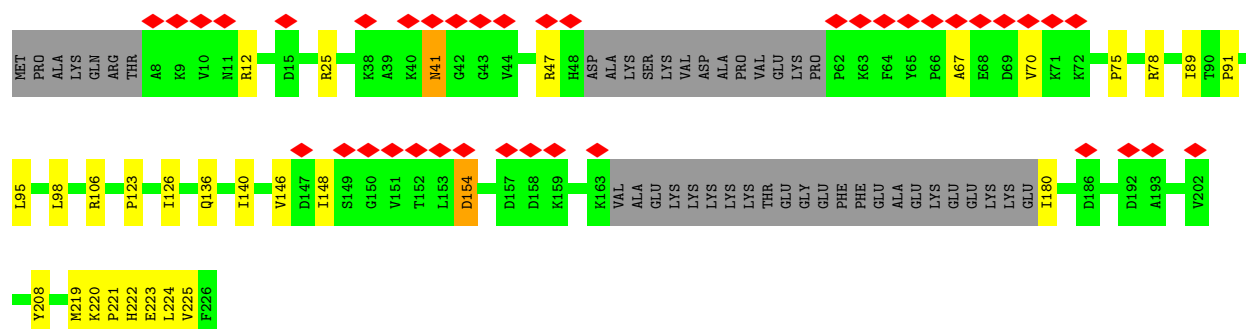
- Molecule 50: Small ribosomal subunit protein eS27y



- Molecule 51: Small ribosomal subunit protein uS4y



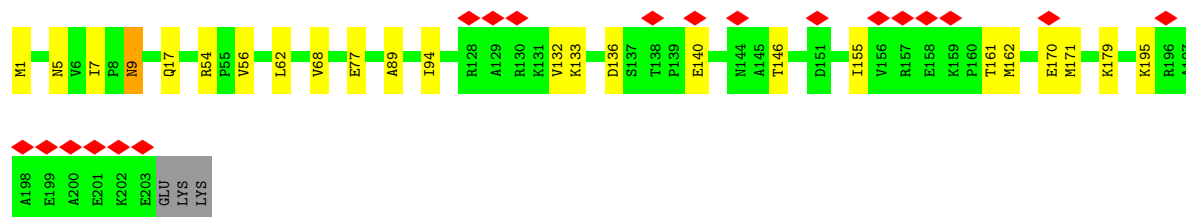
- Molecule 52: Large ribosomal subunit protein eL6y



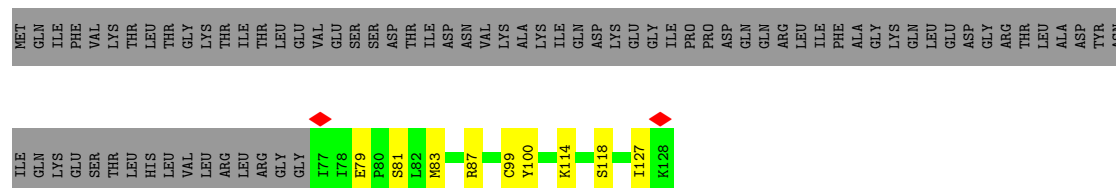
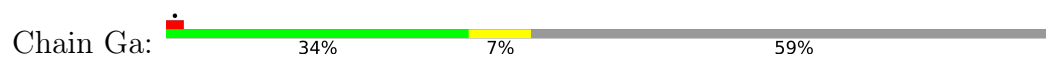
- Molecule 53: Small ribosomal subunit protein uS3z



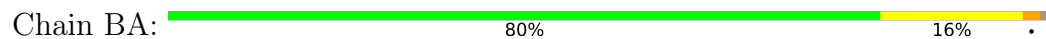
- Molecule 54: Large ribosomal subunit protein eL13z



- Molecule 55: Ubiquitin-ribosomal protein eL40z fusion protein.

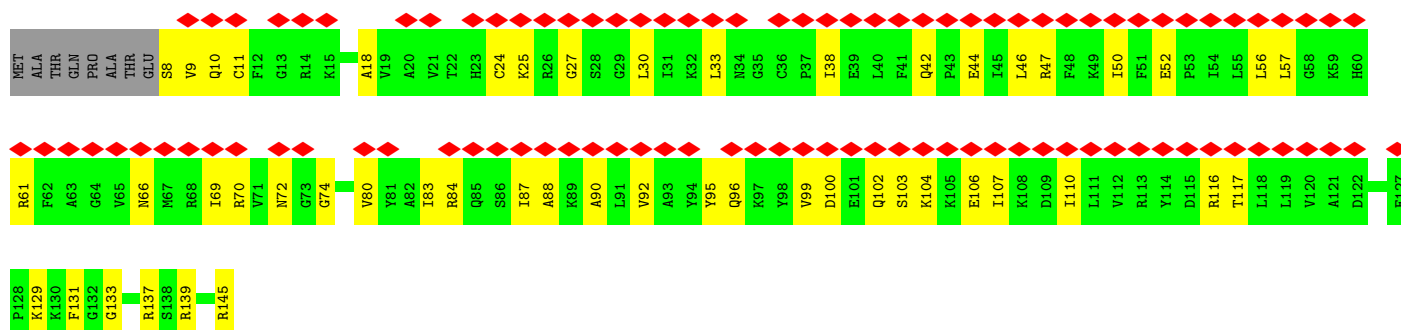


- Molecule 56: Large ribosomal subunit protein eL39z/eL39x

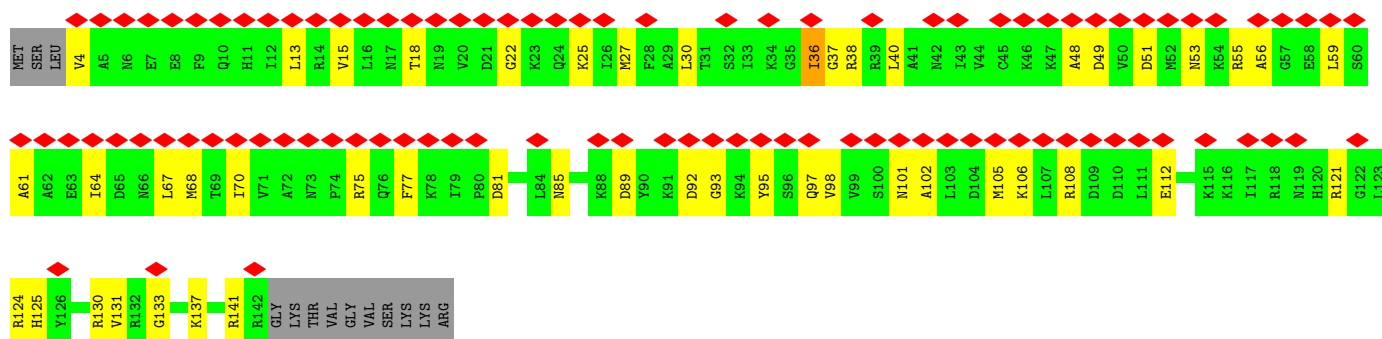


- Molecule 57: Small ribosomal subunit protein uS9z

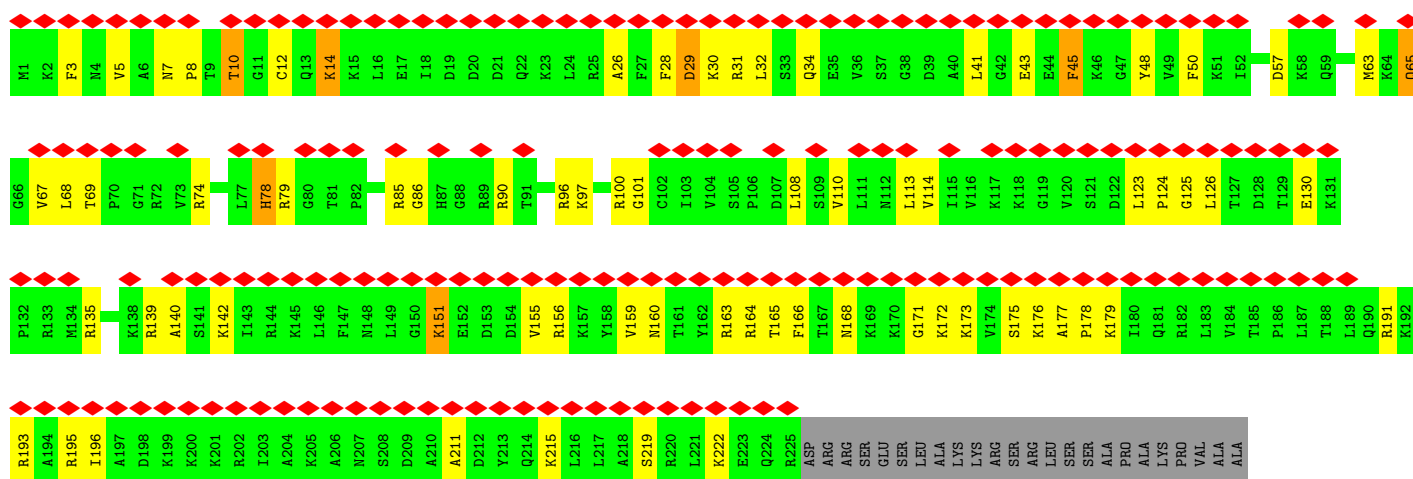
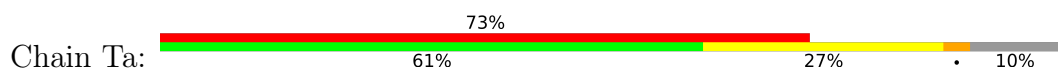




- Molecule 58: Small ribosomal subunit protein uS13z/uS13y/uS13x



- Molecule 59: Small ribosomal subunit protein eS6y



- Molecule 60: Large ribosomal subunit protein eL38z/eL38y

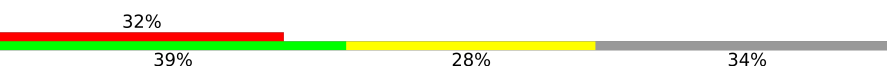


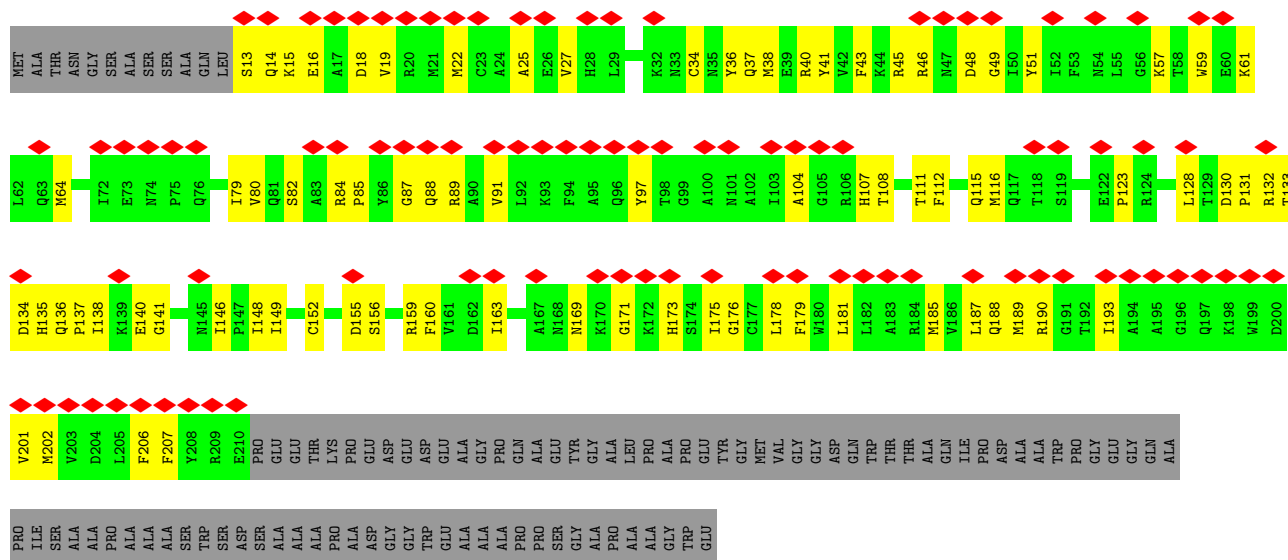
- Molecule 61: Large ribosomal subunit protein eL43y

Chain BE:  88% 10%



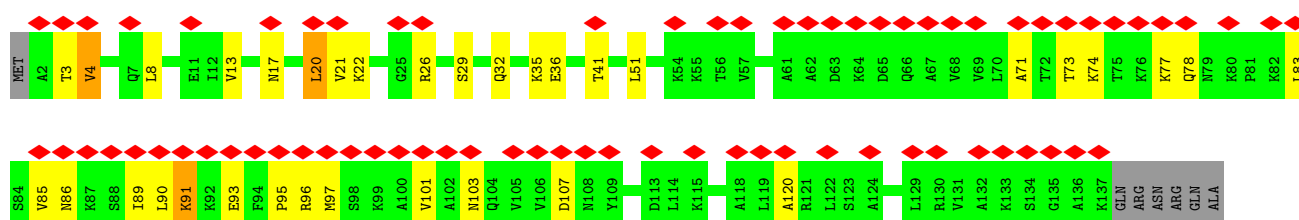
- Molecule 62: Small ribosomal subunit protein uS2z

Chain Za:  32% 39% 28% 34%



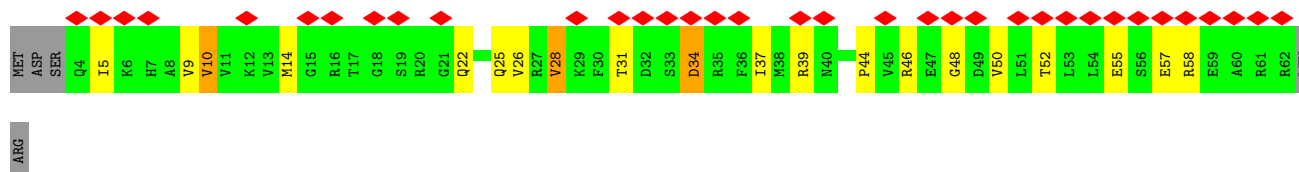
- Molecule 63: Large ribosomal subunit protein eL28z

Chain AQ:  51% 71% 22% 5%

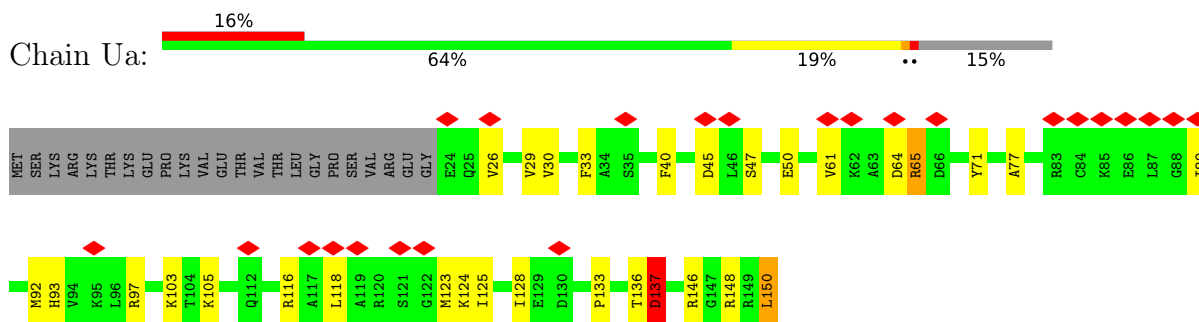


- Molecule 64: Small ribosomal subunit protein eS28x

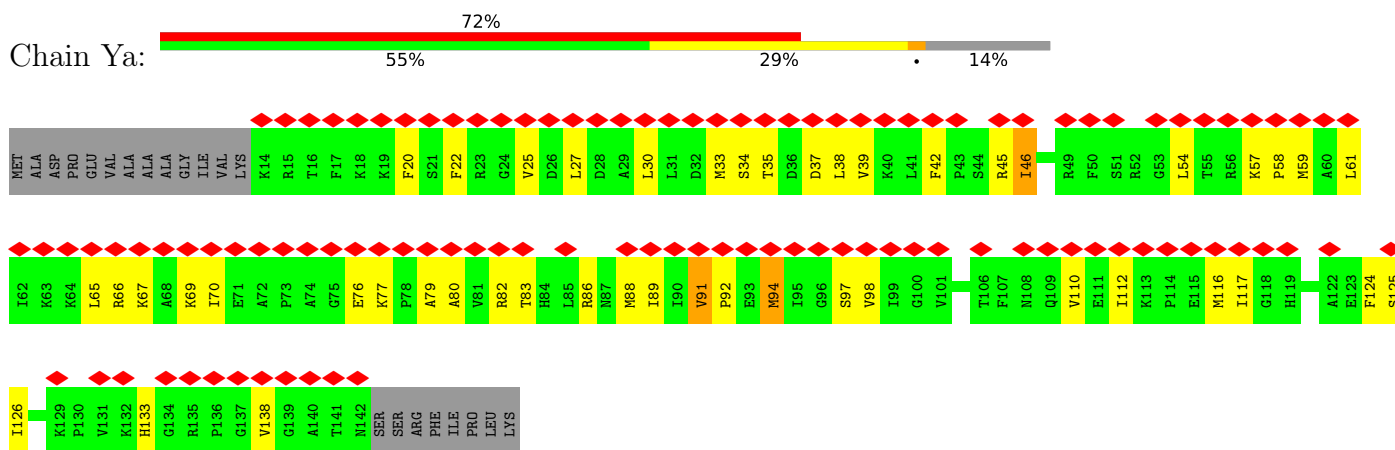
Chain Oa:  55% 61% 27% 5% 8%



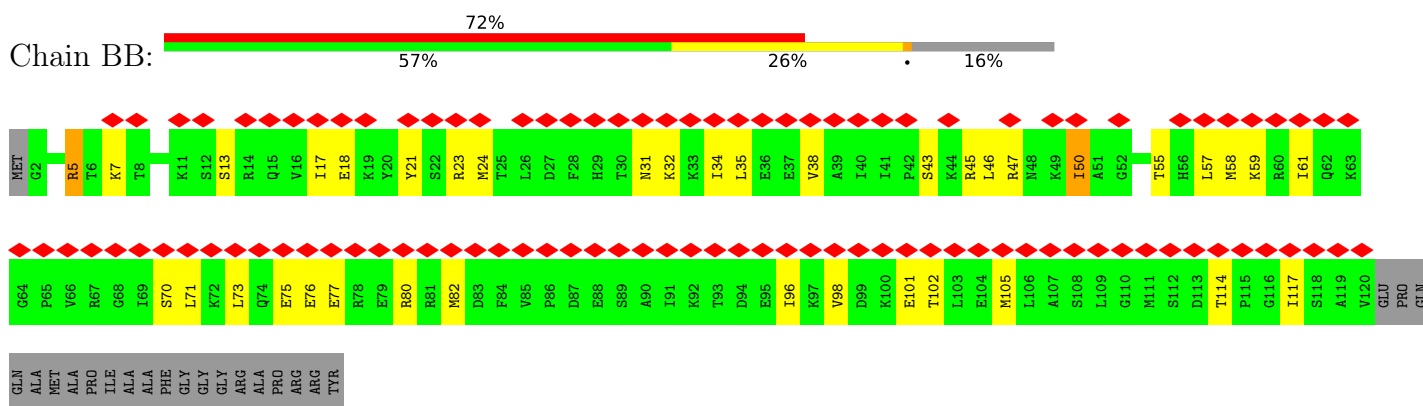
• Molecule 65: Small ribosomal subunit protein uS11y



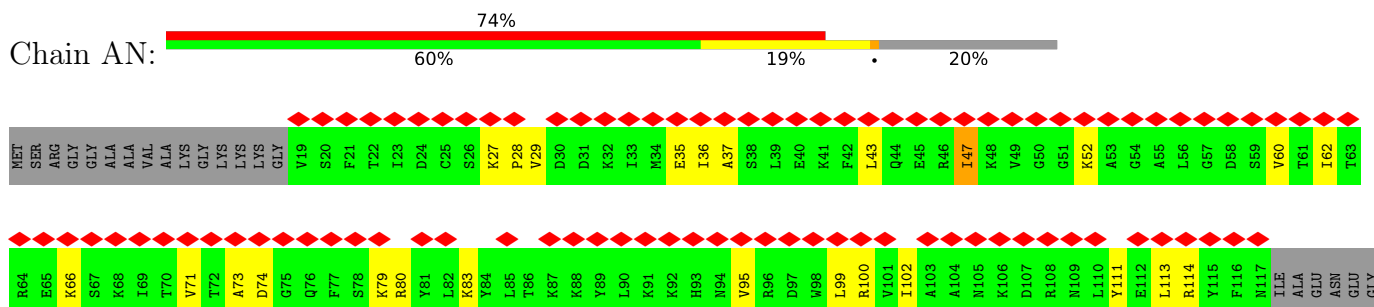
• Molecule 66: Small ribosomal subunit protein uS19y



• Molecule 67: Small ribosomal subunit protein eS17w

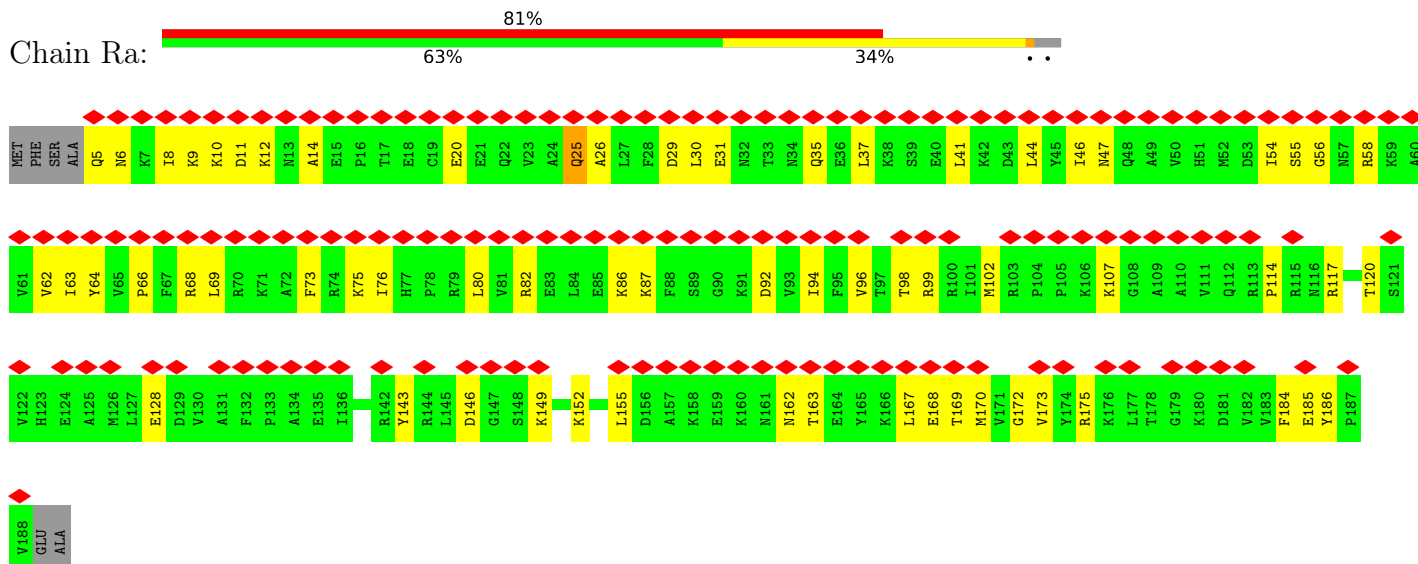


• Molecule 68: Large ribosomal subunit protein eL22z

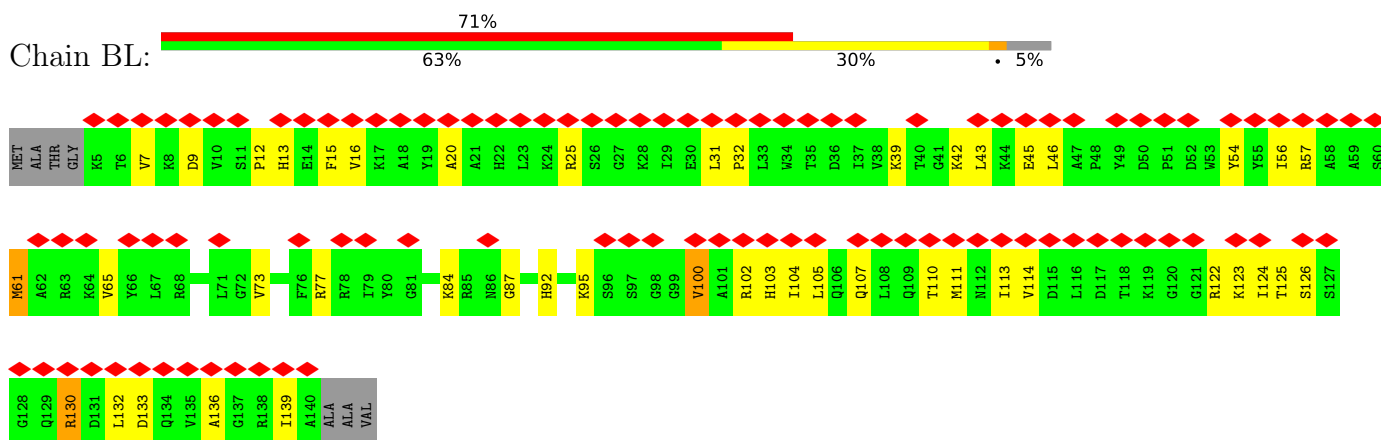


GLU
GLU
ASP

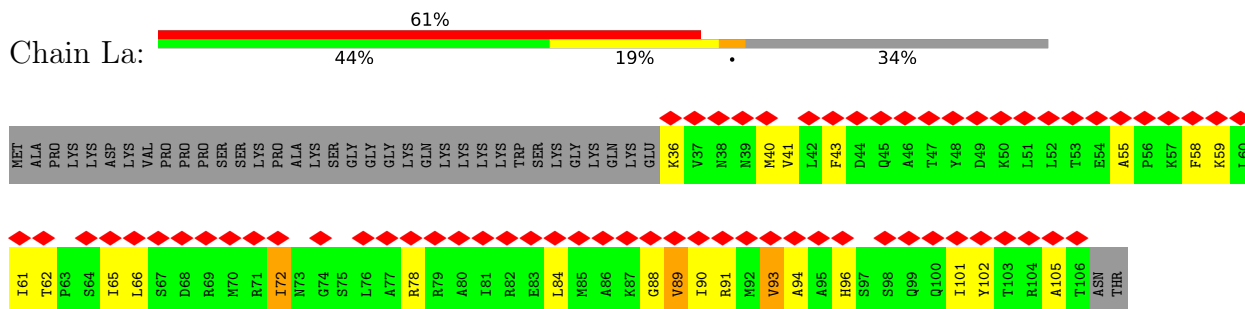
- Molecule 69: Small ribosomal subunit protein eS7x



- Molecule 70: Small ribosomal subunit protein eS19x

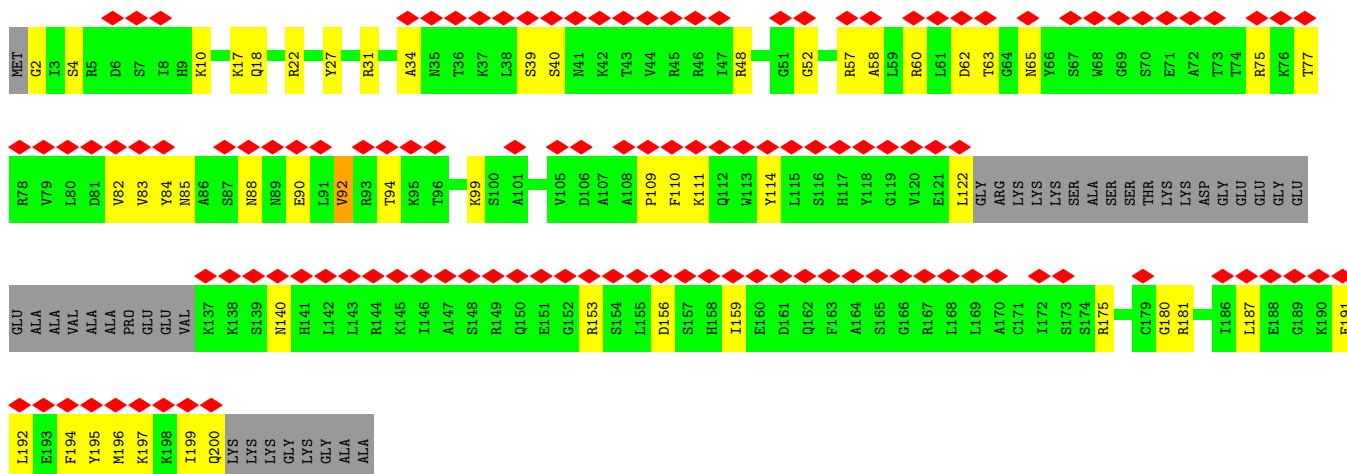


- Molecule 71: Small ribosomal subunit protein eS25w

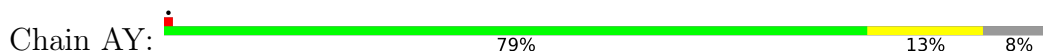


- Molecule 72: Small ribosomal subunit protein eS8z

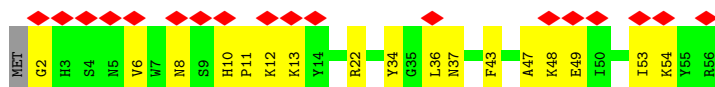




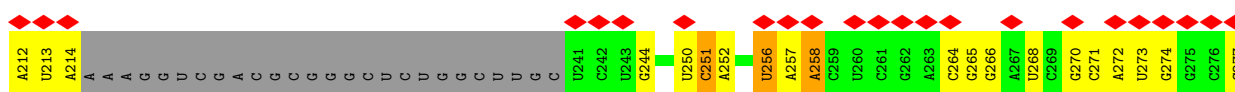
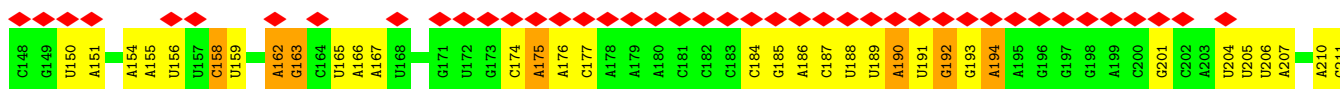
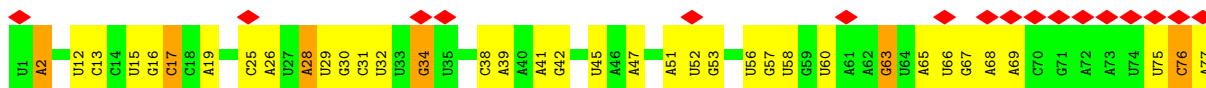
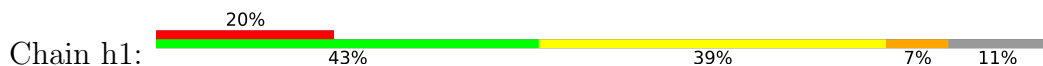
- Molecule 73: Large ribosomal subunit protein eL37z



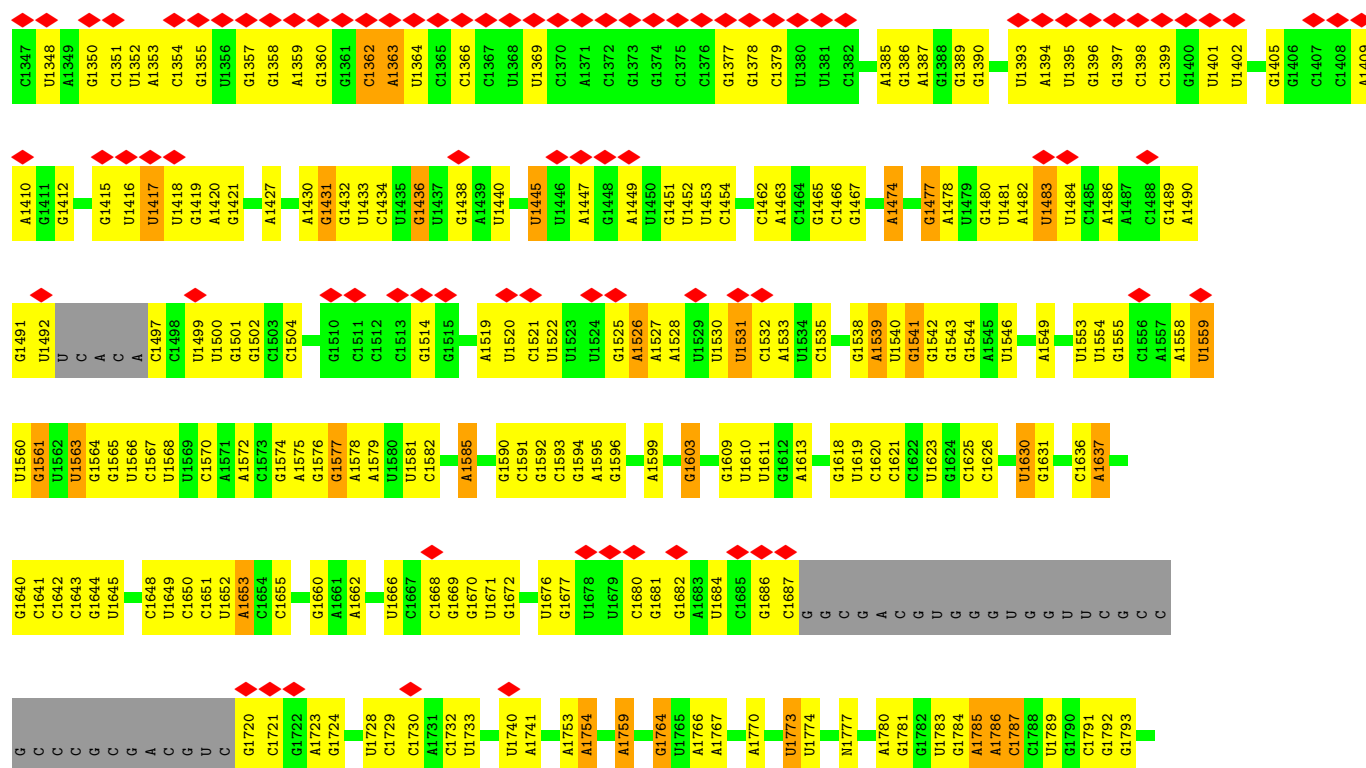
- Molecule 74: Small ribosomal subunit protein uS14z/uS14y/uS14x



- Molecule 75: Ribosomal RNA 18S



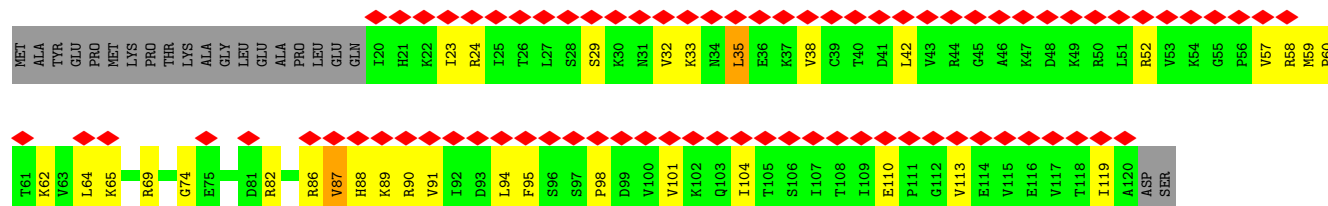




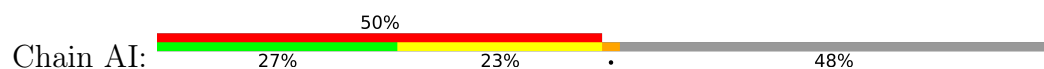
• Molecule 76: Messenger RNA (poly-U)

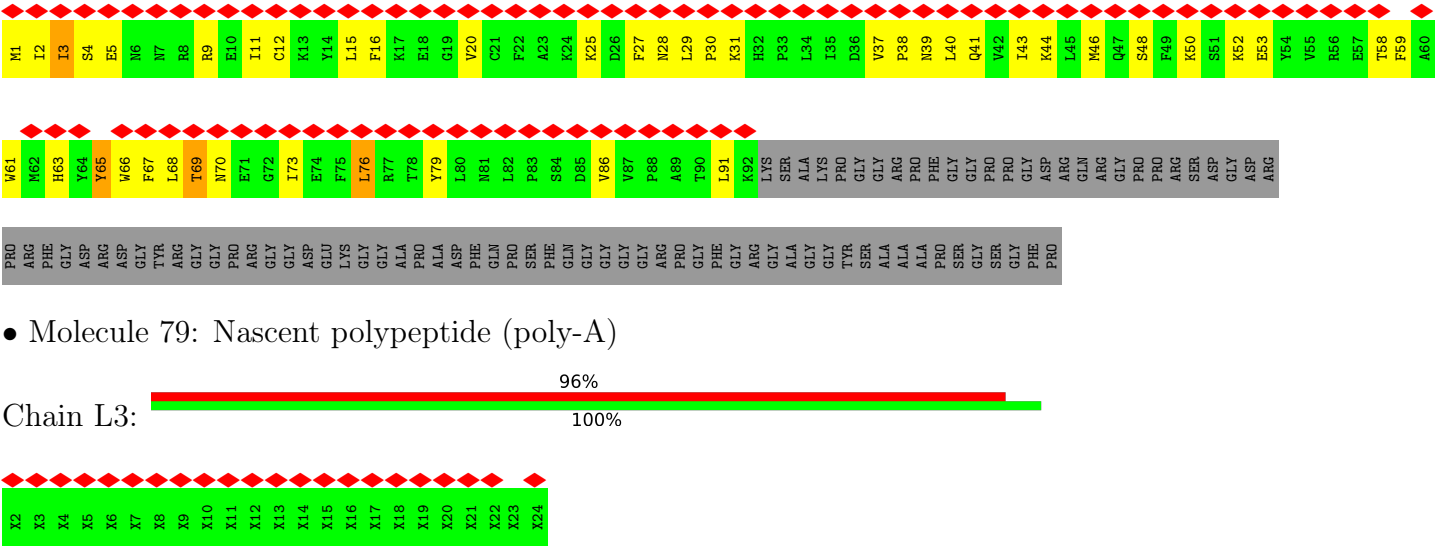


• Molecule 77: Small ribosomal subunit protein uS10y



• Molecule 78: Small ribosomal subunit protein eS10z





• Molecule 79: Nascent polypeptide (poly-A)

96%

Chain L3:

100%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58638	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 ($e^-/\text{\AA}^2$)	53.85	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.934	Depositor
Minimum map value	-0.382	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	500.094, 500.094, 500.094	wwPDB
Map dimensions	686, 686, 686	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.729, 0.729, 0.729	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, UY1, 6MZ, ZN, SPD, 5MC, MLY, 1MA, OMG, 4AC, 1MG, HIC, OMC, MG, G7M, MA6, K, C4J, TER, OMU, EPE, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	3	0.57	1/3713 (0.0%)	0.70	0/5784
2	A	0.58	9/72612 (0.0%)	0.71	4/113256 (0.0%)
3	W2	0.52	0/1822	0.63	0/2840
3	i2	0.52	0/1823	0.60	0/2840
4	C3	0.55	0/2834	0.67	0/4415
5	BC	0.51	0/238	0.69	0/302
6	BM	0.64	0/1269	0.75	0/1705
7	BO	0.56	0/1042	0.67	0/1390
8	AR	0.62	0/435	0.77	0/577
9	AU	0.57	0/900	0.69	0/1202
10	Ma	0.49	0/804	0.62	0/1081
11	Ia	0.49	0/1533	0.58	0/2050
12	AE	0.45	0/1051	0.59	0/1406
13	AX	0.54	0/793	0.73	0/1047
14	AP	0.53	0/1110	0.64	0/1477
15	Ja	0.43	0/2116	0.60	0/2841
16	Ea	0.66	0/1754	0.77	0/2349
17	AL	0.57	0/1523	0.67	0/2042
18	Va	0.49	0/1100	0.62	0/1465
19	Ka	0.43	0/1001	0.58	0/1329
20	AW	0.59	0/921	0.69	0/1234
21	BD	0.56	0/806	0.64	0/1065
22	BS	0.59	0/3165	0.68	0/4238
23	AM	0.57	0/1335	0.68	0/1789
24	AC	0.46	0/1709	0.61	0/2310
25	BI	0.61	0/1002	0.69	0/1347
26	AH	0.51	0/1054	0.60	0/1408
27	BT	0.59	0/3112	0.68	0/4187
28	AV	0.63	0/1045	0.73	0/1399
29	AD	0.43	0/1473	0.58	0/1985
30	AJ	0.62	0/1492	0.71	0/1995

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	BQ	0.65	0/1928	0.76	0/2594
32	BH	0.60	0/1664	0.68	0/2224
33	Da	0.48	0/1214	0.62	0/1630
34	BK	0.50	0/2321	0.60	0/3119
35	AT	0.54	0/731	0.60	0/982
36	Pa	0.48	0/394	0.68	0/519
37	BP	0.53	0/984	0.63	0/1306
38	BN	0.53	0/972	0.65	0/1309
39	BG	0.52	0/1908	0.66	1/2561 (0.0%)
40	Fa	0.62	0/909	0.79	1/1214 (0.1%)
41	Ha	0.67	0/1187	0.81	1/1584 (0.1%)
42	BU	0.45	0/1388	0.60	0/1858
43	BR	0.56	0/1931	0.69	1/2584 (0.0%)
44	Xa	0.47	0/1189	0.57	0/1590
45	BV	0.45	0/1746	0.57	0/2341
46	BJ	0.52	0/1691	0.59	0/2263
47	AO	0.52	0/541	0.68	0/718
48	BW	0.45	0/577	0.62	0/777
49	AK	0.56	0/1499	0.69	0/1975
50	Na	0.45	0/657	0.64	0/883
51	AB	0.42	0/1540	0.59	0/2061
52	BF	0.51	0/1521	0.61	0/2040
53	AA	0.44	0/1647	0.62	0/2212
54	AG	0.57	0/1680	0.70	0/2251
55	Ga	0.52	0/428	0.71	0/564
56	BA	0.61	0/456	0.71	0/603
57	AF	0.45	0/1133	0.60	0/1513
58	Wa	0.42	0/1152	0.61	0/1541
59	Ta	0.44	0/1819	0.65	0/2422
60	AZ	0.52	0/570	0.65	0/758
61	BE	0.57	0/711	0.74	0/942
62	Za	0.44	0/1609	0.58	0/2173
63	AQ	0.47	0/1070	0.62	0/1436
64	Oa	0.43	0/474	0.58	0/632
65	Ua	0.49	0/974	0.63	0/1305
66	Ya	0.45	0/1044	0.64	0/1398
67	BB	0.42	0/965	0.64	0/1287
68	AN	0.44	0/820	0.62	0/1097
69	Ra	0.43	0/1530	0.65	0/2052
70	BL	0.46	0/1086	0.59	0/1459
71	La	0.44	0/568	0.65	0/762
72	Aa	0.45	0/1517	0.59	0/2027
73	AY	0.69	0/717	0.87	0/951

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Ca	0.49	0/450	0.62	0/598
75	h1	0.53	4/36567 (0.0%)	0.62	0/56975
76	B1	0.58	0/263	0.68	0/404
77	Ba	0.45	0/809	0.61	0/1090
78	AI	0.41	0/801	0.62	0/1082
All	All	0.55	14/205939 (0.0%)	0.67	8/302021 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1
8	AR	0	1
16	Ea	0	1
19	Ka	0	1
22	BS	0	1
23	AM	0	1
25	BI	0	1
30	AJ	0	1
34	BK	0	1
39	BG	0	1
49	AK	0	2
53	AA	0	1
65	Ua	0	2
All	All	0	15

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2359	A2M	O3'-P	6.31	1.62	1.56
2	A	2279	A2M	O3'-P	5.93	1.62	1.56
2	A	2408	OMU	O3'-P	5.84	1.62	1.56
1	3	47	A2M	O3'-P	5.82	1.62	1.56
75	h1	794	A2M	O3'-P	5.37	1.61	1.56
2	A	1142	A2M	O3'-P	5.33	1.61	1.56
2	A	1066	OMU	O3'-P	5.33	1.61	1.56
75	h1	1754	A2M	O3'-P	5.23	1.61	1.56
75	h1	778	A2M	O3'-P	5.16	1.61	1.56
2	A	2124	A2M	O3'-P	5.10	1.61	1.56
2	A	2212	A2M	O3'-P	5.09	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	h1	799	A2M	O3'-P	5.09	1.61	1.56
2	A	885	A2M	O3'-P	5.06	1.61	1.56
2	A	48	OMU	O3'-P	5.05	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	Ha	29	PRO	CB-CA-C	6.43	117.28	111.87
40	Fa	58	ARG	NE-CZ-NH2	6.10	124.69	119.20
2	A	11	G	P-O5'-C5'	-5.97	111.94	120.90
2	A	676	OMU	OP1-P-O3'	5.50	117.30	105.20
43	BR	236	GLU	CB-CA-C	-5.42	110.31	116.54
2	A	2870	G	C4'-C3'-O3'	-5.41	104.88	113.00
2	A	826	A2M	OP1-P-O3'	5.21	116.66	105.20
39	BG	218	ASP	N-CA-C	-5.19	108.71	114.62

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	113	G	Sidechain
53	AA	42	THR	Peptide
30	AJ	180	ARG	Sidechain
49	AK	38	ARG	Sidechain
49	AK	62	ARG	Sidechain
23	AM	86	ARG	Sidechain
8	AR	20	GLY	Peptide
39	BG	44	ARG	Sidechain
25	BI	48	ARG	Sidechain
34	BK	23	ARG	Sidechain
22	BS	269	ARG	Sidechain
16	Ea	143	ARG	Sidechain
19	Ka	120	ARG	Sidechain
65	Ua	137	ASP	Peptide
65	Ua	148	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	3	3453	0	1754	38	0
2	A	67524	0	34113	660	0
3	W2	1629	0	823	21	0
3	i2	1630	0	822	24	0
4	C3	2536	0	1284	24	0
5	BC	237	0	289	4	0
6	BM	1246	0	1264	18	0
7	BO	1030	0	1110	10	0
8	AR	425	0	440	9	0
9	AU	888	0	933	8	0
10	Ma	789	0	810	10	0
11	Ia	1512	0	1598	21	0
12	AE	1033	0	1070	15	0
13	AX	786	0	888	11	0
14	AP	1092	0	1182	15	0
15	Ja	2074	0	2180	55	0
16	Ea	1713	0	1777	27	0
17	AL	1485	0	1547	27	0
18	Va	1082	0	1152	13	0
19	Ka	986	0	1053	35	0
20	AW	901	0	926	16	0
21	BD	792	0	843	9	0
22	BS	3111	0	3221	37	0
23	AM	1307	0	1359	18	0
24	AC	1672	0	1748	35	0
25	BI	986	0	1048	10	0
26	AH	1042	0	1119	16	0
27	BT	3056	0	3214	47	0
28	AV	1028	0	1105	21	0
29	AD	1454	0	1512	36	0
30	AJ	1468	0	1577	10	0
31	BQ	1881	0	1931	26	0
32	BH	1636	0	1752	18	0
33	Da	1190	0	1273	14	0
34	BK	2277	0	2311	19	0
35	AT	720	0	754	14	0
36	Pa	389	0	419	5	0
37	BP	975	0	1100	8	0
38	BN	955	0	1037	11	0
39	BG	1874	0	2015	30	0
40	Fa	896	0	975	10	0
41	Ha	1156	0	1207	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BU	1366	0	1407	15	0
43	BR	1898	0	2005	24	0
44	Xa	1163	0	1222	25	0
45	BV	1718	0	1774	30	0
46	BJ	1653	0	1707	22	0
47	AO	528	0	557	6	0
48	BW	568	0	566	14	0
49	AK	1480	0	1610	15	0
50	Na	647	0	663	19	0
51	AB	1514	0	1576	37	0
52	BF	1491	0	1596	19	0
53	AA	1625	0	1718	43	0
54	AG	1648	0	1755	18	0
55	Ga	433	0	475	4	0
56	BA	444	0	477	7	0
57	AF	1113	0	1169	38	0
58	Wa	1136	0	1177	42	0
59	Ta	1795	0	1920	62	0
60	AZ	562	0	606	15	0
61	BE	702	0	741	6	0
62	Za	1575	0	1578	55	0
63	AQ	1056	0	1128	27	0
64	Oa	471	0	497	12	0
65	Ua	962	0	994	28	0
66	Ya	1024	0	1090	31	0
67	BB	955	0	1012	34	0
68	AN	808	0	845	16	0
69	Ra	1506	0	1571	48	0
70	BL	1064	0	1097	35	0
71	La	562	0	599	20	0
72	Aa	1494	0	1538	36	0
73	AY	705	0	724	12	0
74	Ca	440	0	431	11	0
75	h1	34449	0	17391	602	0
76	B1	240	0	120	3	0
77	Ba	799	0	868	28	0
78	AI	779	0	790	35	0
79	L3	115	0	34	0	0
80	3	5	0	0	0	0
80	A	197	0	0	2	0
80	AC	1	0	0	0	0
80	AG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	AM	1	0	0	0	0
80	AY	2	0	0	0	0
80	BI	1	0	0	0	0
80	BM	1	0	0	0	0
80	BR	1	0	0	0	0
80	BS	4	0	0	0	0
80	BV	1	0	0	0	0
80	C3	4	0	0	0	0
80	Ja	1	0	0	0	0
80	Ta	1	0	0	0	0
80	h1	77	0	0	0	0
80	i2	1	0	0	0	0
81	3	4	0	0	0	0
81	A	125	0	0	0	0
81	AG	1	0	0	0	0
81	AJ	1	0	0	0	0
81	AR	1	0	0	0	0
81	AV	1	0	0	0	0
81	BD	1	0	0	0	0
81	BJ	1	0	0	0	0
81	BM	2	0	0	0	0
81	BQ	2	0	0	0	0
81	BS	2	0	0	0	0
81	C3	1	0	0	0	0
81	Ca	1	0	0	0	0
81	Ea	1	0	0	0	0
81	Fa	1	0	0	0	0
81	Ua	1	0	0	0	0
81	Va	2	0	0	0	0
81	Wa	1	0	0	0	0
81	h1	40	0	0	0	0
82	A	14	0	26	9	0
83	A	40	0	76	4	0
84	A	15	0	18	1	0
85	AY	1	0	0	0	0
85	BD	1	0	0	0	0
85	BE	1	0	0	0	0
85	Ca	1	0	0	0	0
85	Ga	1	0	0	0	0
85	Ma	1	0	0	0	0
86	3	328	0	0	12	0
86	A	7443	0	0	220	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	AA	2	0	0	0	0
86	AB	7	0	0	0	0
86	AC	21	0	0	4	0
86	AD	5	0	0	0	0
86	AE	15	0	0	1	0
86	AF	10	0	0	1	0
86	AG	87	0	0	4	0
86	AH	21	0	0	1	0
86	AJ	119	0	0	2	0
86	AK	47	0	0	3	0
86	AL	71	0	0	4	0
86	AM	86	0	0	7	0
86	AN	1	0	0	0	0
86	AO	23	0	0	2	0
86	AP	20	0	0	2	0
86	AQ	4	0	0	0	0
86	AR	43	0	0	2	0
86	AT	13	0	0	1	0
86	AU	27	0	0	0	0
86	AV	72	0	0	4	0
86	AW	65	0	0	7	0
86	AX	30	0	0	0	0
86	AY	74	0	0	4	0
86	AZ	6	0	0	0	0
86	Aa	9	0	0	1	0
86	B1	27	0	0	1	0
86	BA	27	0	0	4	0
86	BC	13	0	0	0	0
86	BD	74	0	0	4	0
86	BE	32	0	0	1	0
86	BF	18	0	0	1	0
86	BG	39	0	0	1	0
86	BH	84	0	0	5	0
86	BI	40	0	0	2	0
86	BJ	39	0	0	5	0
86	BK	69	0	0	5	0
86	BL	4	0	0	1	0
86	BM	74	0	0	7	0
86	BN	33	0	0	2	0
86	BO	34	0	0	0	0
86	BP	22	0	0	0	0
86	BQ	132	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	BR	79	0	0	5	0
86	BS	173	0	0	9	0
86	BT	146	0	0	9	0
86	BU	8	0	0	1	0
86	BV	16	0	0	0	0
86	BW	2	0	0	2	0
86	Ba	3	0	0	0	0
86	C3	180	0	0	12	0
86	Da	26	0	0	2	0
86	Ea	137	0	0	5	0
86	Fa	64	0	0	3	0
86	Ga	21	0	0	0	0
86	Ha	93	0	0	3	0
86	Ia	28	0	0	0	0
86	Ja	20	0	0	4	0
86	L3	1	0	0	0	0
86	Ma	32	0	0	0	0
86	Na	5	0	0	0	0
86	Oa	4	0	0	0	0
86	Pa	2	0	0	0	0
86	Ta	7	0	0	1	0
86	Ua	33	0	0	2	0
86	Va	33	0	0	2	0
86	W2	24	0	0	2	0
86	Wa	3	0	0	1	0
86	Xa	16	0	0	4	0
86	Ya	1	0	0	0	0
86	Za	3	0	0	0	0
86	h1	1686	0	0	117	0
86	i2	10	0	0	0	0
All	All	209233	0	145683	2661	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 8.

All (2661) 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)
2:A:277:PSU:OP2	82:A:3401:TER:N9	1.75	1.19
6:BM:141:MET:SD	86:BM:361:HOH:O	1.96	1.17
49:AK:121:HIS:ND1	86:AK:301:HOH:O	1.75	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:AY:76:THR:C	73:AY:77:CYS:N	2.04	1.15
3:W2:3:G:N7	86:W2:101:HOH:O	1.80	1.14
17:AL:60:MET:SD	86:AL:264:HOH:O	2.02	1.14
39:BG:232:MET:SD	86:BG:328:HOH:O	2.06	1.13
86:A:3889:HOH:O	27:BT:89:THR:CG2	2.00	1.08
2:A:1491:A:N7	86:A:3802:HOH:O	1.86	1.07
6:BM:24:VAL:HG12	86:BM:325:HOH:O	1.53	1.07
75:h1:58:U:O2	86:h1:2101:HOH:O	1.72	1.07
86:A:3889:HOH:O	27:BT:89:THR:HG22	1.53	1.07
19:Ka:84:ALA:O	19:Ka:88:GLU:HB2	1.52	1.06
2:A:554:C:O3'	86:A:3801:HOH:O	1.73	1.06
86:A:8756:HOH:O	38:BN:121:LYS:HD3	1.56	1.06
75:h1:1427:A:C8	86:h1:2339:HOH:O	2.10	1.03
75:h1:1206:C:OP2	86:h1:2102:HOH:O	1.78	1.02
86:A:3889:HOH:O	27:BT:89:THR:CB	2.08	0.98
4:C3:80:A:N7	86:C3:301:HOH:O	1.97	0.98
2:A:3071:A:N3	86:A:3806:HOH:O	1.96	0.98
75:h1:1563:PSU:O4	86:h1:2104:HOH:O	1.84	0.94
75:h1:274:G:H1	75:h1:285:U:H3	1.07	0.94
86:A:3889:HOH:O	27:BT:89:THR:HB	1.68	0.94
75:h1:584:U:O2'	86:h1:2103:HOH:O	1.79	0.93
2:A:3184:G:H1	2:A:3190:U:H3	1.15	0.92
49:AK:170:ARG:HH12	75:h1:817:A:H2'	1.32	0.92
2:A:710:G:N7	86:A:3815:HOH:O	2.03	0.91
27:BT:334:LEU:O	86:BT:501:HOH:O	1.88	0.91
75:h1:488:G:H1	75:h1:503:U:H3	1.19	0.90
22:BS:47:MET:HG3	22:BS:182:MET:HE2	1.51	0.90
2:A:1894:G:N7	86:A:3818:HOH:O	2.05	0.89
75:h1:1031:A:OP2	86:h1:2105:HOH:O	1.90	0.89
39:BG:170:PRO:HA	39:BG:217:ASN:HD21	1.37	0.89
44:Xa:70:ARG:NH1	75:h1:306:U:O2	2.07	0.87
19:Ka:114:ASN:HA	19:Ka:117:LYS:HD2	1.55	0.87
54:AG:62:LEU:HG	86:AG:454:HOH:O	1.75	0.86
75:h1:1348:U:OP1	77:Ba:24:ARG:NH2	2.09	0.86
15:Ja:181:VAL:HG11	15:Ja:225:VAL:HG13	1.58	0.86
2:A:1354:G:N7	86:A:3829:HOH:O	2.09	0.85
2:A:1808:A:N7	86:A:3827:HOH:O	2.09	0.85
2:A:1033:G:H22	2:A:1040:G:H1	1.22	0.85
6:BM:24:VAL:CG1	86:BM:325:HOH:O	2.11	0.85
22:BS:182:MET:SD	86:BS:642:HOH:O	2.35	0.84
22:BS:184:ILE:HB	86:BS:510:HOH:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3012:U:C6	86:A:5659:HOH:O	2.30	0.83
53:AA:42:THR:HG22	53:AA:43:PRO:HD2	1.61	0.83
70:BL:87:GLY:O	86:BL:201:HOH:O	1.96	0.83
75:h1:193:G:HO2'	75:h1:194:A:H8	1.26	0.83
2:A:424:G:H22	2:A:644:U:H3	1.25	0.83
2:A:1525:C:OP2	86:A:3804:HOH:O	1.94	0.83
8:AR:16:ALA:O	8:AR:20:GLY:HA2	1.78	0.83
75:h1:108:C:OP2	86:h1:2106:HOH:O	1.96	0.83
75:h1:1033:G:N7	86:h1:2126:HOH:O	2.10	0.82
2:A:3078:G:N7	86:A:3832:HOH:O	2.10	0.82
39:BG:77:THR:HG21	39:BG:175:LYS:HG3	1.60	0.82
59:Ta:156:ARG:HG2	75:h1:79:A:C8	2.15	0.82
2:A:3000:C:OP2	86:A:3808:HOH:O	1.97	0.82
70:BL:39:LYS:NZ	75:h1:1566:U:OP1	2.13	0.82
70:BL:102:ARG:HH12	75:h1:1504:C:H5	1.26	0.82
2:A:3223:U:H3	2:A:3240:U:H3	1.25	0.82
16:Ea:177:LYS:O	86:Ea:401:HOH:O	1.98	0.82
2:A:1507:A:N7	86:A:3842:HOH:O	2.13	0.81
58:Wa:40:LEU:HD22	58:Wa:97:GLN:HE21	1.46	0.81
2:A:3012:U:OP1	86:A:3807:HOH:O	1.96	0.81
49:AK:98:ARG:NH2	49:AK:130:ASN:OD1	2.13	0.81
16:Ea:50[B]:ARG:NH1	86:Ea:403:HOH:O	2.13	0.81
51:AB:5:ARG:HD2	75:h1:39:A:P	2.20	0.81
76:B1:24:U:H3	3:W2:34:G:H1	1.28	0.81
75:h1:390:OMG:OP1	86:h1:2107:HOH:O	1.97	0.81
2:A:2908:C:N3	86:A:3846:HOH:O	2.14	0.81
21:BD:67:LYS:NZ	86:BD:302:HOH:O	2.04	0.81
2:A:2697:G:N7	86:A:3843:HOH:O	2.14	0.80
2:A:1615:C:OP2	86:A:3809:HOH:O	1.97	0.80
75:h1:1590:G:H1	75:h1:1610:U:H3	1.26	0.80
2:A:847:G:O6	61:BE:4:ARG:NH2	2.13	0.80
2:A:49:A:H5''	86:A:4227:HOH:O	1.79	0.80
2:A:2514:C:OP2	86:A:3812:HOH:O	1.99	0.80
75:h1:1543:G:OP2	86:h1:2108:HOH:O	1.99	0.79
2:A:2211:A:P	86:A:3858:HOH:O	2.39	0.79
2:A:2970:A:H1'	3:i2:74:C:H5'	1.63	0.79
11:Ia:3:THR:HA	17:AL:143:GLN:HE22	1.48	0.79
75:h1:96:G:P	86:h1:2118:HOH:O	2.41	0.79
75:h1:607:A:OP2	86:h1:2110:HOH:O	2.00	0.79
75:h1:960:U:OP1	86:h1:2109:HOH:O	1.99	0.79
2:A:1210:A:N1	86:A:3855:HOH:O	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:736:G:N7	86:A:3854:HOH:O	2.15	0.79
43:BR:52:ARG:NH1	43:BR:188:ASP:OD2	2.16	0.78
75:h1:865:C:N3	86:h1:2143:HOH:O	2.16	0.78
2:A:1565:G:N7	86:A:3860:HOH:O	2.16	0.78
75:h1:809:A:OP1	86:h1:2111:HOH:O	2.02	0.78
70:BL:15:PHE:HZ	70:BL:132:LEU:HG	1.48	0.78
56:BA:51:PHE:O	86:BA:101:HOH:O	2.03	0.77
2:A:391:C:OP2	86:A:3813:HOH:O	2.00	0.77
4:C3:97:G:N7	86:C3:306:HOH:O	2.18	0.77
2:A:1013:A:O5'	86:A:3814:HOH:O	2.03	0.77
75:h1:19:A:N7	86:h1:2148:HOH:O	2.18	0.77
2:A:588:C:H2'	2:A:589:U:H2'	1.67	0.77
65:Ua:137:ASP:HA	86:Ua:327:HOH:O	1.85	0.77
20:AW:97:LYS:NZ	86:AW:202:HOH:O	2.19	0.76
27:BT:234:GLU:HG3	27:BT:254:ARG:HH22	1.50	0.76
75:h1:393:A:N3	86:h1:2145:HOH:O	2.17	0.76
75:h1:401:A:O2'	86:h1:2112:HOH:O	2.03	0.76
75:h1:869:G:H1	75:h1:961:U:H3	1.34	0.76
75:h1:1764:G:N7	86:h1:2144:HOH:O	2.17	0.76
78:AI:29:LEU:HD23	78:AI:39:ASN:HD22	1.50	0.76
2:A:3182:G:H1	2:A:3192:U:H3	1.34	0.76
14:AP:43:VAL:HB	86:AP:215:HOH:O	1.86	0.76
2:A:506:G:N7	86:A:3882:HOH:O	2.19	0.75
57:AF:145:ARG:NH2	3:W2:33:U:OP2	2.18	0.75
75:h1:979:A:N7	86:h1:2153:HOH:O	2.19	0.75
75:h1:407:C:O2	86:h1:2113:HOH:O	2.04	0.75
51:AB:29:GLU:HG3	51:AB:41:LYS:HE2	1.68	0.75
78:AI:12:CYS:HB3	78:AI:76:LEU:HD21	1.68	0.75
11:Ia:131:MET:HE3	11:Ia:137:ILE:HG21	1.69	0.75
75:h1:1753:A:N3	86:h1:2159:HOH:O	2.20	0.75
72:Aa:31:ARG:NH1	75:h1:334:U:OP1	2.19	0.75
2:A:844:A:N1	86:A:3879:HOH:O	2.19	0.74
2:A:1141:C:OP2	86:A:3816:HOH:O	2.04	0.74
18:Va:67:LYS:HB3	18:Va:90:LEU:HD22	1.68	0.74
66:Ya:46:ILE:HD12	66:Ya:89:ILE:HG21	1.70	0.74
2:A:352:A:N1	86:A:3889:HOH:O	2.20	0.74
2:A:1033:G:N2	2:A:1040:G:H1	1.85	0.74
2:A:1354:G:O6	86:A:3820:HOH:O	2.06	0.74
2:A:742:U:H3	2:A:747:G:H1	1.32	0.74
15:Ja:6:LYS:O	86:Ja:401:HOH:O	2.04	0.74
2:A:1880:G:N7	86:A:3897:HOH:O	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i2:20:G:C6	3:i2:59:U:O4	2.41	0.74
72:Aa:192:LEU:O	72:Aa:196:MET:HG3	1.88	0.74
75:h1:989:C:OP2	86:h1:2115:HOH:O	2.05	0.74
70:BL:133:ASP:OD2	75:h1:1359:A:O2'	2.04	0.74
75:h1:869:G:N3	86:h1:2167:HOH:O	2.21	0.74
23:AM:27:LEU:HB2	86:AM:375:HOH:O	1.86	0.74
64:Oa:39:ARG:NH2	64:Oa:55:GLU:O	2.21	0.74
2:A:1758:C:OP1	68:AN:100:ARG:NH2	2.21	0.73
2:A:2669:G:N7	86:A:3876:HOH:O	2.18	0.73
31:BQ:6:ARG:NH2	86:BQ:402:HOH:O	2.18	0.73
32:BH:90:ARG:HG3	32:BH:104:LEU:HD11	1.68	0.73
53:AA:37:VAL:HG23	53:AA:50:ILE:HG22	1.70	0.73
45:BV:48:VAL:HG21	45:BV:61:LEU:HG	1.69	0.73
75:h1:387:A:OP1	86:h1:2114:HOH:O	2.05	0.73
2:A:2699:G:O6	86:A:3817:HOH:O	2.05	0.73
8:AR:16:ALA:O	8:AR:20:GLY:CA	2.35	0.73
75:h1:381:U:OP2	86:h1:2117:HOH:O	2.06	0.73
75:h1:1296:G:N7	86:h1:2160:HOH:O	2.20	0.73
4:C3:113:G:O6	86:C3:302:HOH:O	2.07	0.73
75:h1:1648:C:O4'	86:h1:2116:HOH:O	2.06	0.73
75:h1:96:G:OP2	86:h1:2118:HOH:O	2.07	0.73
28:AV:13:LYS:O	86:AV:301:HOH:O	2.06	0.72
2:A:263:C:OP2	86:A:3821:HOH:O	2.06	0.72
2:A:609:A:N6	52:BF:25:ARG:O	2.23	0.72
4:C3:119:C:O3'	86:C3:303:HOH:O	2.07	0.72
2:A:778:A:N7	86:A:3903:HOH:O	2.22	0.72
86:A:7385:HOH:O	47:AO:52:CYS:SG	2.46	0.72
16:Ea:63:ARG:HD3	86:Ea:427:HOH:O	1.88	0.72
66:Ya:86:ARG:NH2	66:Ya:125:SER:O	2.22	0.72
75:h1:465:U:H2'	75:h1:466:A2M:H8	1.72	0.72
2:A:840:G:OP2	86:A:3819:HOH:O	2.06	0.72
15:Ja:108:ARG:NH2	75:h1:791:G:OP2	2.21	0.72
42:BU:55:THR:HG23	42:BU:62:ARG:HA	1.71	0.72
75:h1:945:A:N7	86:h1:2171:HOH:O	2.22	0.72
75:h1:385:G:O6	86:h1:2119:HOH:O	2.07	0.72
43:BR:45:ALA:HB2	86:BR:471:HOH:O	1.88	0.72
75:h1:1331:G:N7	86:h1:2172:HOH:O	2.22	0.72
44:Xa:142:LYS:HE2	44:Xa:144:ILE:HD11	1.71	0.71
15:Ja:151:ASP:HB3	15:Ja:154:ILE:HG12	1.72	0.71
71:La:91:ARG:HG2	71:La:105:ALA:HA	1.72	0.71
75:h1:274:G:N2	75:h1:285:U:O2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2407:OMG:OP2	86:A:3824:HOH:O	2.08	0.71
2:A:2921:OMG:N2	86:A:3921:HOH:O	2.23	0.71
34:BK:39:GLN:OE1	86:BK:401:HOH:O	2.08	0.71
2:A:110:C:OP2	86:A:3826:HOH:O	2.08	0.71
27:BT:370:GLU:OE2	27:BT:370:GLU:N	2.21	0.71
31:BQ:39:GLY:HA2	31:BQ:93:LYS:HD2	1.72	0.71
75:h1:113:A:N3	86:h1:2183:HOH:O	2.23	0.71
35:AT:32:SER:HB2	86:AT:203:HOH:O	1.90	0.71
2:A:3126:G:O6	86:A:3822:HOH:O	2.06	0.71
78:AI:46:MET:HA	78:AI:46:MET:HE3	1.71	0.71
22:BS:113:GLU:OE1	22:BS:113:GLU:N	2.23	0.71
59:Ta:168:ASN:HD21	59:Ta:172:LYS:HB3	1.54	0.71
1:3:70:G:N7	86:3:304:HOH:O	2.24	0.71
2:A:12:U:C6	86:A:7656:HOH:O	2.44	0.71
58:Wa:38:ARG:HG2	70:BL:46:LEU:HD21	1.72	0.71
75:h1:309:G:OP2	86:h1:2123:HOH:O	2.09	0.71
62:Za:38:MET:HE1	62:Za:152:CYS:HB2	1.71	0.70
75:h1:1655:C:OP1	86:h1:2121:HOH:O	2.09	0.70
2:A:3232:A:N7	86:A:3923:HOH:O	2.23	0.70
75:h1:112:U:O2	86:h1:2120:HOH:O	2.07	0.70
1:3:139:A:N7	86:3:305:HOH:O	2.24	0.70
31:BQ:36:GLU:OE2	86:BQ:401:HOH:O	2.09	0.70
31:BQ:137:ILE:HD11	31:BQ:149:LYS:HB2	1.73	0.70
2:A:1446:OMC:HM22	2:A:1447:U:H5'	1.73	0.70
2:A:2731:G:N7	86:A:3936:HOH:O	2.24	0.70
41:Ha:132:GLU:OE2	86:Ha:201:HOH:O	2.08	0.70
75:h1:1477:G:H2'	75:h1:1478:A:H8	1.56	0.70
78:AI:38:PRO:HB2	78:AI:41:GLN:HG3	1.72	0.70
2:A:34:PSU:OP2	86:A:3831:HOH:O	2.10	0.70
2:A:764:A:N7	86:A:3937:HOH:O	2.24	0.70
2:A:1021:G:N2	46:BJ:193:ASP:OD1	2.24	0.70
2:A:2762:U:OP1	86:A:3825:HOH:O	2.08	0.70
75:h1:129:U:OP2	75:h1:265:G:N2	2.22	0.70
2:A:1039:C:H2'	2:A:1040:G:C8	2.27	0.70
75:h1:1036:G:O2'	86:h1:2125:HOH:O	2.10	0.70
75:h1:1677:G:N7	86:h1:2192:HOH:O	2.25	0.70
16:Ea:30:TYR:OH	86:Ea:402:HOH:O	2.09	0.70
2:A:16:G:N7	86:A:3946:HOH:O	2.25	0.70
15:Ja:55:ALA:HB1	15:Ja:60:GLU:HB3	1.73	0.70
69:Ra:31:GLU:HB2	69:Ra:41:LEU:HD22	1.74	0.70
2:A:461:C:O2'	63:AQ:86:ASN:ND2	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:995:G:N7	86:A:3925:HOH:O	2.23	0.70
2:A:1035:G:N2	2:A:1038:A:OP2	2.24	0.70
15:Ja:129:ILE:HG22	75:h1:244:OMG:HM21	1.73	0.70
46:BJ:54:SER:O	86:BJ:401:HOH:O	2.10	0.70
75:h1:1774:U:OP2	86:h1:2122:HOH:O	2.09	0.70
2:A:1655:G:OP2	86:A:3828:HOH:O	2.09	0.70
4:C3:35:C:H1'	86:BK:457:HOH:O	1.90	0.70
22:BS:4:ARG:O	86:BS:501:HOH:O	2.10	0.70
1:3:161:A:H61	2:A:2:C:H42	1.39	0.69
2:A:1219:G:N7	86:A:3957:HOH:O	2.25	0.69
2:A:555:G:P	86:A:3801:HOH:O	2.46	0.69
2:A:3232:A:OP2	86:A:3833:HOH:O	2.10	0.69
13:AX:6:VAL:O	13:AX:15:ASN:ND2	2.25	0.69
75:h1:798:U:H2'	75:h1:799:A2M:H8	1.74	0.69
70:BL:15:PHE:CZ	70:BL:132:LEU:HG	2.26	0.69
59:Ta:10:THR:HG23	59:Ta:130:GLU:HA	1.75	0.69
75:h1:1295:G:N7	86:h1:2189:HOH:O	2.25	0.69
51:AB:81:ARG:NH2	75:h1:765:A:OP1	2.26	0.69
53:AA:9:ARG:NH1	75:h1:1491:G:OP1	2.26	0.69
65:Ua:26:VAL:HG12	65:Ua:89:ILE:HD13	1.73	0.69
75:h1:1477:G:H2'	75:h1:1478:A:C8	2.27	0.69
35:AT:19:LEU:HB3	35:AT:101:SER:HB2	1.74	0.69
4:C3:5:G:O6	86:C3:304:HOH:O	2.10	0.69
11:Ia:3:THR:HA	17:AL:143:GLN:NE2	2.08	0.69
2:A:1162:A:OP1	86:A:3834:HOH:O	2.11	0.68
2:A:2219:G:N1	86:A:3942:HOH:O	2.25	0.68
2:A:72:A:OP2	13:AX:22:ARG:NH2	2.25	0.68
1:3:150:G:N7	86:3:306:HOH:O	2.24	0.68
7:BO:1:MET:HE3	7:BO:2:LYS:H	1.59	0.68
69:Ra:167:LEU:HD23	69:Ra:170:MET:HE3	1.75	0.68
2:A:393:A:O2'	2:A:396:A:OP1	2.09	0.68
15:Ja:148:ARG:NH1	75:h1:126:U:H5'	2.08	0.68
44:Xa:41:LEU:HD13	44:Xa:71:ILE:HD11	1.74	0.68
75:h1:484:U:H2'	75:h1:485:A:H8	1.58	0.68
2:A:581:C:OP1	86:A:3836:HOH:O	2.11	0.68
2:A:3291:C:OP1	86:A:3835:HOH:O	2.11	0.68
29:AD:164:ARG:NH2	75:h1:1574:G:O2'	2.26	0.68
69:Ra:62:VAL:HG12	69:Ra:94:ILE:HB	1.73	0.68
72:Aa:99:LYS:HB3	75:h1:331:G:H5'	1.75	0.68
77:Ba:42:LEU:HD12	77:Ba:104:ILE:HG22	1.76	0.68
2:A:1152:A:OP1	86:A:3838:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1693:U:HO2'	2:A:1774:U:HO2'	1.38	0.67
51:AB:171:PRO:O	51:AB:176:ARG:NH1	2.27	0.67
2:A:701:A:N7	2:A:703:U:O2'	2.21	0.67
6:BM:24:VAL:CB	86:BM:325:HOH:O	2.38	0.67
24:AC:109:VAL:HG21	24:AC:191:GLN:HG3	1.75	0.67
2:A:197:A:OP2	86:A:3839:HOH:O	2.12	0.67
2:A:1192:C:O2'	86:A:3837:HOH:O	2.11	0.67
62:Za:79:ILE:HD13	62:Za:123:PRO:HB3	1.76	0.67
66:Ya:54:LEU:HB2	66:Ya:59:MET:HE1	1.75	0.67
2:A:548:U:N3	27:BT:367:VAL:O	2.27	0.67
2:A:1522:G:OP2	86:A:3840:HOH:O	2.12	0.67
2:A:1575:A:H2'	2:A:1576:A:O4'	1.94	0.67
45:BV:146:ARG:H	45:BV:149:GLN:HG3	1.59	0.67
53:AA:53:THR:HG23	53:AA:54:ARG:HG3	1.76	0.67
62:Za:112:PHE:HB2	62:Za:140:GLU:HG2	1.77	0.67
2:A:1493:A:H5''	86:A:5527:HOH:O	1.93	0.67
2:A:1572:C:H42	2:A:1576:A:H61	1.43	0.67
16:Ea:96:ARG:HH22	16:Ea:104:GLU:HG2	1.60	0.67
26:AH:107:ARG:NH2	52:BF:225:VAL:O	2.28	0.67
31:BQ:221:HIS:HB2	86:BQ:528:HOH:O	1.93	0.67
68:AN:28:PRO:HB3	68:AN:99:LEU:HD21	1.77	0.67
71:La:89:VAL:HG13	71:La:90:ILE:HG23	1.76	0.67
2:A:1526:A:OP2	86:A:3841:HOH:O	2.13	0.67
2:A:1656:A:N1	86:A:4001:HOH:O	2.28	0.67
75:h1:141:G:H2'	75:h1:142:G:C8	2.30	0.67
2:A:2356:A:N7	86:A:3982:HOH:O	2.27	0.67
2:A:2159:G:O6	86:A:3830:HOH:O	2.09	0.66
32:BH:127:ASP:OD2	86:BH:301:HOH:O	2.12	0.66
46:BJ:201:SER:O	46:BJ:209:ARG:NH2	2.28	0.66
2:A:330:G:N7	86:A:3988:HOH:O	2.28	0.66
2:A:1446:OMC:HM23	27:BT:100:MET:HG3	1.77	0.66
4:C3:85:G:N3	86:C3:310:HOH:O	2.27	0.66
7:BO:87:GLU:OE1	7:BO:93:THR:OG1	2.14	0.66
51:AB:127:ALA:O	51:AB:131:ILE:HG12	1.94	0.66
66:Ya:22:PHE:HB3	66:Ya:30:LEU:HD11	1.77	0.66
2:A:817:A:N7	86:A:4013:HOH:O	2.29	0.66
29:AD:60:ARG:NH1	75:h1:1618:G:OP1	2.29	0.66
53:AA:7:LYS:HA	53:AA:10:LYS:HE3	1.78	0.66
59:Ta:160:ASN:HA	59:Ta:163:ARG:HG3	1.78	0.66
67:BB:46:LEU:O	67:BB:50:ILE:HG22	1.94	0.66
2:A:12:U:C5	86:A:7656:HOH:O	2.49	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3183:A:H61	2:A:3191:C:H42	1.43	0.66
57:AF:46:LEU:HB3	57:AF:80:VAL:HG21	1.78	0.66
75:h1:1221:C:H2'	75:h1:1222:A:H8	1.60	0.66
75:h1:1436:G:OP1	86:h1:2131:HOH:O	2.14	0.66
2:A:713:A:N1	86:A:4012:HOH:O	2.29	0.66
68:AN:62:ILE:HG22	68:AN:71:VAL:HG22	1.77	0.66
75:h1:34:G:N2	86:h1:2173:HOH:O	2.22	0.66
34:BK:50:ARG:NH1	34:BK:146:ASP:OD2	2.29	0.66
57:AF:52:GLU:OE1	57:AF:84:ARG:NH1	2.28	0.66
72:Aa:10:LYS:O	72:Aa:18:GLN:NE2	2.27	0.66
75:h1:123:OMU:HM22	75:h1:124:G:H5'	1.77	0.66
75:h1:943:G:OP1	86:h1:2129:HOH:O	2.12	0.66
75:h1:1546:U:OP2	86:h1:2139:HOH:O	2.14	0.66
2:A:2841:U:OP1	2:A:2843:C:N4	2.27	0.65
49:AK:105:LEU:HD23	49:AK:138:LEU:HD23	1.77	0.65
49:AK:170:ARG:NH2	75:h1:819:G:N7	2.43	0.65
2:A:1492:G:O5'	86:A:3845:HOH:O	2.14	0.65
14:AP:28:SER:OG	14:AP:77:TYR:OH	2.13	0.65
59:Ta:57:ASP:OD2	59:Ta:100:ARG:NH1	2.29	0.65
69:Ra:64:TYR:HA	69:Ra:96:VAL:O	1.96	0.65
2:A:203:G:N7	86:A:4005:HOH:O	2.28	0.65
62:Za:82:SER:O	62:Za:88:GLN:NE2	2.29	0.65
75:h1:1084:G:HO2'	75:h1:1095:G:HO2'	1.44	0.65
27:BT:42:VAL:HG21	27:BT:252:LEU:HD21	1.78	0.65
75:h1:333:A:OP2	86:h1:2132:HOH:O	2.14	0.65
2:A:2451:U:N3	2:A:2453:U:OP1	2.30	0.65
2:A:2604:G:N7	86:A:4023:HOH:O	2.30	0.65
2:A:2760:G:OP1	86:A:3852:HOH:O	2.15	0.65
6:BM:50:ASP:OD2	86:BM:301:HOH:O	2.15	0.65
59:Ta:90:ARG:HD3	86:Ta:401:HOH:O	1.95	0.65
72:Aa:195:TYR:O	72:Aa:199:ILE:HG12	1.96	0.65
51:AB:56:ASN:O	51:AB:60:GLU:HG3	1.96	0.65
75:h1:879:G:N3	86:h1:2224:HOH:O	2.30	0.65
11:Ia:97:PHE:HB2	11:Ia:145:ASP:HB3	1.77	0.65
77:Ba:60:PRO:O	77:Ba:62:LYS:NZ	2.29	0.65
2:A:461:C:H2'	2:A:462:G:H8	1.61	0.65
2:A:2328:C:OP1	86:A:3851:HOH:O	2.15	0.65
62:Za:89:ARG:NH1	67:BB:82:MET:O	2.29	0.65
70:BL:77:ARG:HB3	70:BL:95:LYS:HG2	1.79	0.65
72:Aa:48:ARG:HE	72:Aa:52:GLY:HA2	1.61	0.65
75:h1:554:G:OP2	86:h1:2135:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:1623:U:O2	86:h1:2130:HOH:O	2.12	0.65
48:BW:63:ASP:OD1	62:Za:37:GLN:NE2	2.30	0.65
78:AI:3:ILE:HD13	78:AI:41:GLN:HB3	1.79	0.65
2:A:472:G:H2'	2:A:473:G:H8	1.61	0.65
39:BG:217:ASN:OD1	39:BG:217:ASN:N	2.30	0.65
75:h1:1567:C:OP1	86:h1:2133:HOH:O	2.14	0.65
2:A:1815:A:H1'	2:A:1818:G:H21	1.62	0.64
2:A:2238:G:N7	86:A:4003:HOH:O	2.28	0.64
6:BM:24:VAL:HB	86:BM:325:HOH:O	1.97	0.64
58:Wa:38:ARG:NH2	86:Wa:301:HOH:O	2.30	0.64
75:h1:564:G:N7	86:h1:2218:HOH:O	2.29	0.64
2:A:2387:C:OP2	86:A:3847:HOH:O	2.14	0.64
3:i2:67:C:H2'	3:i2:68:A:H8	1.62	0.64
3:i2:67:C:H2'	3:i2:68:A:C8	2.33	0.64
2:A:320:A:OP1	86:A:3844:HOH:O	2.14	0.64
2:A:3201:A:N7	86:A:4035:HOH:O	2.30	0.64
11:Ia:8:GLU:OE1	11:Ia:74:ARG:NH1	2.30	0.64
71:La:88:GLY:O	71:La:90:ILE:N	2.27	0.64
2:A:2503:U:H2'	2:A:2504:A:C8	2.33	0.64
19:Ka:54:PRO:HA	19:Ka:57:ILE:HD12	1.79	0.64
2:A:55:A:N7	86:A:4022:HOH:O	2.29	0.64
2:A:2422:A:OP1	86:A:3849:HOH:O	2.15	0.64
44:Xa:109:PRO:O	86:Xa:201:HOH:O	2.14	0.64
75:h1:1268:G:O2'	75:h1:1451:G:O2'	2.16	0.64
1:3:104:U:OP1	86:3:301:HOH:O	2.14	0.64
59:Ta:74:ARG:HG2	59:Ta:96:ARG:HG2	1.80	0.64
75:h1:474:U:O2'	75:h1:772:A:N3	2.31	0.64
75:h1:873:G:O2'	86:h1:2134:HOH:O	2.14	0.64
75:h1:941:A:N7	86:h1:2226:HOH:O	2.30	0.64
75:h1:1409:A:H2'	75:h1:1410:A:H8	1.62	0.64
2:A:580:G:O2'	27:BT:339:LYS:NZ	2.31	0.64
2:A:912:U:OP1	86:A:3853:HOH:O	2.15	0.64
2:A:923:A:OP2	86:A:3850:HOH:O	2.15	0.64
80:A:3600:MG:MG	86:A:4254:HOH:O	1.41	0.64
23:AM:37:GLY:HA2	23:AM:63:ARG:HD3	1.80	0.64
71:La:65:ILE:HD12	71:La:66:LEU:N	2.13	0.64
17:AL:11:VAL:HG13	17:AL:60:MET:HE1	1.80	0.64
71:La:93:VAL:HG23	71:La:101:ILE:HG13	1.78	0.64
75:h1:384:C:OP1	86:h1:2138:HOH:O	2.14	0.64
75:h1:749:A:H62	75:h1:806:G:H21	1.46	0.64
77:Ba:29:SER:HB2	77:Ba:113:VAL:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2293:A:O2'	86:A:3823:HOH:O	2.07	0.64
62:Za:43:PHE:CD2	67:BB:105:MET:HB3	2.33	0.64
69:Ra:99:ARG:HG3	75:h1:857:A:C6	2.33	0.64
2:A:3053:C:O4'	86:A:3856:HOH:O	2.15	0.63
7:BO:38:LEU:HD22	7:BO:42:TYR:HE2	1.63	0.63
75:h1:360:PSU:O2	86:h1:2127:HOH:O	2.11	0.63
75:h1:453:G:O2'	86:h1:2101:HOH:O	2.03	0.63
2:A:1605:A:N7	86:A:4038:HOH:O	2.30	0.63
69:Ra:9:LYS:O	69:Ra:47:ASN:ND2	2.30	0.63
2:A:1587:G:H2'	86:A:7647:HOH:O	1.98	0.63
44:Xa:68:ARG:NH1	75:h1:113:A:O2'	2.32	0.63
75:h1:1740:U:H2'	75:h1:1741:A:C8	2.33	0.63
86:A:7249:HOH:O	61:BE:17:ARG:HG2	1.98	0.63
2:A:661:A2M:OP2	2:A:2867:U:O2'	2.15	0.63
75:h1:1491:G:O2'	75:h1:1497:C:O2	2.16	0.63
2:A:611:C:O2'	52:BF:47:ARG:O	2.15	0.63
2:A:1233:A:OP2	2:A:1295:G:N2	2.31	0.63
31:BQ:102:LEU:HG	86:BQ:452:HOH:O	1.99	0.63
48:BW:72:TRP:CD1	62:Za:64:MET:HE2	2.34	0.63
75:h1:1260:C:H2'	75:h1:1261:OMU:H6	1.81	0.63
24:AC:11:LYS:HG3	24:AC:219:LEU:HD22	1.81	0.63
72:Aa:39:SER:HB3	72:Aa:60:ARG:HD3	1.81	0.63
75:h1:32:U:OP2	86:h1:2140:HOH:O	2.15	0.63
4:C3:95:C:OP2	86:C3:305:HOH:O	2.16	0.63
22:BS:200:SER:HA	86:BS:585:HOH:O	1.97	0.63
53:AA:45:ARG:HH21	53:AA:85:GLU:HG3	1.64	0.63
57:AF:57:LEU:HD11	57:AF:107:ILE:HG23	1.81	0.63
59:Ta:179:LYS:HG2	75:h1:79:A:H2	1.64	0.63
66:Ya:30:LEU:HA	66:Ya:33:MET:HG3	1.81	0.63
70:BL:100:VAL:O	70:BL:104:ILE:HG13	1.98	0.63
1:3:130:U:H6	1:3:134:G:H1	1.44	0.62
2:A:1039:C:H2'	2:A:1040:G:H8	1.62	0.62
59:Ta:123:LEU:HD12	59:Ta:124:PRO:HD2	1.81	0.62
75:h1:484:U:H2'	75:h1:485:A:C8	2.33	0.62
4:C3:22:A:H2'	4:C3:23:A:C8	2.35	0.62
50:Na:36:ASP:HB2	50:Na:45:ILE:HG12	1.80	0.62
75:h1:1804:G:N1	86:h1:2190:HOH:O	2.25	0.62
66:Ya:94:MET:HB3	66:Ya:112:ILE:HD12	1.81	0.62
75:h1:1172:A:H2'	75:h1:1173:G:C8	2.35	0.62
75:h1:1201:G:O6	86:h1:2124:HOH:O	2.09	0.62
57:AF:137:ARG:NH1	75:h1:1585:A:OP1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:BB:32:LYS:NZ	75:h1:1390:G:OP1	2.32	0.62
2:A:2169:G:N7	86:A:4050:HOH:O	2.31	0.62
69:Ra:175:ARG:NH1	69:Ra:175:ARG:O	2.32	0.62
2:A:1564:U:O2	39:BG:50:LYS:NZ	2.31	0.62
2:A:3014:A:H2'	2:A:3015:A:H8	1.64	0.62
8:AR:17:HIS:HA	8:AR:20:GLY:HA3	1.82	0.62
2:A:1204:G:H2'	2:A:1205:A:C8	2.35	0.61
33:Da:38:CYS:O	33:Da:42:LYS:HG3	2.00	0.61
48:BW:59:ARG:NH2	62:Za:160:PHE:O	2.33	0.61
75:h1:855:U:O4	75:h1:856:A:N6	2.33	0.61
57:AF:129:LYS:NZ	57:AF:133:GLY:O	2.31	0.61
78:AI:29:LEU:HD12	78:AI:30:PRO:HD2	1.82	0.61
2:A:3337:C:O2'	2:A:3339:U:OP2	2.18	0.61
23:AM:80:ILE:HD13	23:AM:85:ILE:HD12	1.81	0.61
75:h1:1352:U:H2'	75:h1:1353:A:C8	2.35	0.61
2:A:488:C:H2'	2:A:489:G:H8	1.66	0.61
67:BB:18:GLU:OE1	67:BB:70:SER:OG	2.19	0.61
2:A:1134:U:O2'	86:A:3859:HOH:O	2.16	0.61
2:A:3226:G:H1	2:A:3237:U:H3	1.49	0.61
23:AM:60:ARG:HD3	86:AM:307:HOH:O	2.01	0.61
59:Ta:166:PHE:HZ	59:Ta:176:LYS:HE3	1.65	0.61
65:Ua:146:ARG:HB2	65:Ua:150:LEU:HD12	1.82	0.61
2:A:1667:G:N7	86:A:4067:HOH:O	2.31	0.61
2:A:2900:G:O2'	2:A:3022:A:N1	2.31	0.61
2:A:3009:A:OP1	86:A:3861:HOH:O	2.16	0.61
75:h1:1352:U:H3	75:h1:1377:G:H1	1.48	0.61
4:C3:93:U:H2'	4:C3:94:C:C6	2.36	0.61
15:Ja:65:LEU:HD23	15:Ja:70:ILE:HD13	1.83	0.61
27:BT:139:PRO:O	27:BT:143:MET:HG3	2.00	0.61
56:BA:46:ARG:HD3	86:BA:127:HOH:O	2.00	0.61
66:Ya:59:MET:SD	66:Ya:59:MET:N	2.74	0.61
69:Ra:47:ASN:O	69:Ra:64:TYR:HB2	2.01	0.61
50:Na:56:VAL:HG13	50:Na:65:LEU:HB3	1.82	0.61
2:A:1707:C:O2	40:Fa:50:ARG:NH2	2.34	0.61
21:BD:55:LYS:NZ	86:BD:301:HOH:O	1.90	0.61
43:BR:91:ILE:HD13	43:BR:132:LEU:HD21	1.82	0.61
59:Ta:7:ASN:HB3	59:Ta:12:CYS:SG	2.41	0.61
65:Ua:33:PHE:HB3	65:Ua:40:PHE:HB2	1.82	0.61
84:A:3404:EPE:H21	16:Ea:65:ARG:HH22	1.66	0.60
18:Va:60:GLN:NE2	75:h1:1759:A:O4'	2.33	0.60
59:Ta:100:ARG:HB2	59:Ta:100:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:144:U:H2'	75:h1:145:A:H8	1.66	0.60
1:3:158:G:N7	86:3:313:HOH:O	2.32	0.60
27:BT:33:MET:HE3	27:BT:137:ALA:HB2	1.83	0.60
75:h1:1385:A:HO2'	75:h1:1386:G:H8	1.49	0.60
2:A:694:A:OP1	86:A:3857:HOH:O	2.16	0.60
2:A:2837:A:O2'	46:BJ:74:LYS:NZ	2.31	0.60
2:A:174:G:H2'	2:A:175:A:H8	1.66	0.60
2:A:3012:U:H3'	86:A:5659:HOH:O	2.02	0.60
69:Ra:82:ARG:NH2	69:Ra:162:ASN:OD1	2.34	0.60
2:A:1954:G:H2'	2:A:2091:A:H61	1.67	0.60
2:A:2304:C:O2'	2:A:2305:G:OP2	2.16	0.60
2:A:2621:C:N3	86:A:4059:HOH:O	2.31	0.60
2:A:2837:A:OP1	46:BJ:154:ARG:NH1	2.33	0.60
28:AV:87:MET:HG3	28:AV:116:LEU:HD22	1.83	0.60
65:Ua:137:ASP:OD2	75:h1:929:G:O3'	2.18	0.60
75:h1:1093:A:O4'	86:h1:2141:HOH:O	2.15	0.60
77:Ba:23:ILE:HG21	77:Ba:101:VAL:HG11	1.82	0.60
29:AD:192:LYS:O	29:AD:196:ILE:HG13	2.01	0.60
35:AT:16:ARG:HB3	35:AT:103:ILE:HG12	1.82	0.60
45:BV:129:THR:OG1	45:BV:131:ASP:OD1	2.19	0.60
55:Ga:99:CYS:HB2	55:Ga:114:LYS:HE3	1.82	0.60
80:A:3486:MG:MG	86:A:4015:HOH:O	1.44	0.60
15:Ja:3:ARG:HB3	75:h1:94:A:H1'	1.84	0.60
50:Na:35:MET:HG3	50:Na:48:VAL:HG23	1.82	0.60
51:AB:109:ARG:NH2	51:AB:150:VAL:O	2.33	0.60
77:Ba:52:ARG:HG3	77:Ba:95:PHE:HB2	1.82	0.60
2:A:472:G:O2'	63:AQ:103:ASN:OD1	2.20	0.60
2:A:876:G:N7	86:A:4053:HOH:O	2.31	0.60
2:A:1818:G:H2'	2:A:1819:C:C6	2.36	0.60
6:BM:127:ARG:HG3	6:BM:141:MET:HE1	1.84	0.60
29:AD:97:MET:HG3	29:AD:108:PRO:HB2	1.82	0.60
78:Al:11:ILE:HD11	78:Al:37:VAL:HG11	1.84	0.60
2:A:674:U:H2'	2:A:675:OMC:C6	2.37	0.60
2:A:1647:A:N1	86:A:4060:HOH:O	2.31	0.60
59:Ta:171:GLY:O	59:Ta:173:LYS:NZ	2.35	0.60
2:A:954:C:H2'	2:A:955:C:C6	2.37	0.59
18:Va:47:LYS:O	86:Va:301:HOH:O	2.17	0.59
23:AM:5:HIS:HD2	86:AM:380:HOH:O	1.83	0.59
72:Aa:181:ARG:NH1	75:h1:204:U:O2	2.34	0.59
1:3:120:G:N7	86:3:314:HOH:O	2.32	0.59
2:A:317:G:N7	86:A:4072:HOH:O	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:355:G:N7	86:A:4076:HOH:O	2.32	0.59
50:Na:46:THR:HG22	50:Na:48:VAL:HG13	1.83	0.59
65:Ua:89:ILE:HG22	65:Ua:123:MET:HE1	1.84	0.59
71:La:96:HIS:HE2	75:h1:1531:PSU:P	2.25	0.59
73:AY:76:THR:O	73:AY:77:CYS:HB2	2.02	0.59
75:h1:474:U:H2'	75:h1:475:A:C8	2.37	0.59
75:h1:886:G:H2'	75:h1:887:U:C6	2.37	0.59
75:h1:1221:C:OP1	78:AI:48:SER:OG	2.20	0.59
62:Za:131:PRO:HG2	62:Za:156:SER:HB2	1.84	0.59
2:A:506:G:O2'	52:BF:78:ARG:HD3	2.01	0.59
2:A:2125:A:N3	86:A:4057:HOH:O	2.31	0.59
75:h1:112:U:O2	86:h1:2137:HOH:O	2.14	0.59
2:A:3369:U:O2'	2:A:3371:G:N7	2.31	0.59
15:Ja:141:THR:OG1	15:Ja:143:ASP:OD1	2.12	0.59
58:Wa:133:GLY:HA3	75:h1:1561:G:H5''	1.83	0.59
72:Aa:65:ASN:ND2	75:h1:258:A:N3	2.51	0.59
75:h1:109:A:H2'	75:h1:110:G:C8	2.37	0.59
75:h1:342:U:H2'	75:h1:343:A:H8	1.67	0.59
75:h1:793:U:H2'	75:h1:794:A2M:H8	1.84	0.59
75:h1:872:A:H2'	75:h1:873:G:C8	2.38	0.59
75:h1:922:G:N7	86:h1:2240:HOH:O	2.32	0.59
2:A:1597:C:H2'	2:A:1598:C:C6	2.38	0.59
2:A:1814:G:H2'	2:A:1815:A:C8	2.37	0.59
17:AL:75:LYS:NZ	17:AL:99:THR:O	2.34	0.59
75:h1:96:G:HO2'	75:h1:462:A:HO2'	1.44	0.59
2:A:3061:U:OP2	86:A:3864:HOH:O	2.17	0.59
3:i2:58:A:O2'	3:i2:60:C:OP2	2.16	0.59
20:AW:14:VAL:HG23	20:AW:105:VAL:HB	1.83	0.59
20:AW:77:THR:HG22	20:AW:78:ARG:HG2	1.84	0.59
22:BS:117:ARG:HA	22:BS:178:LYS:HD2	1.84	0.59
29:AD:40:VAL:HG11	29:AD:113:ILE:HD11	1.85	0.59
48:BW:81:GLN:HE21	48:BW:81:GLN:H	1.51	0.59
58:Wa:51:ASP:OD1	58:Wa:53:ASN:N	2.35	0.59
59:Ta:32:LEU:HD12	59:Ta:63:MET:HG3	1.85	0.59
69:Ra:152:LYS:HD3	69:Ra:185:GLU:HG3	1.85	0.59
75:h1:76:C:O2'	75:h1:77:A:O4'	2.16	0.59
75:h1:327:G:H1'	86:h1:2723:HOH:O	2.01	0.59
29:AD:22:TRP:CD1	29:AD:97:MET:HE3	2.37	0.59
34:BK:119:TYR:OH	34:BK:138:ARG:O	2.19	0.59
37:BP:73:TYR:HB3	37:BP:79:LEU:HD22	1.85	0.59
2:A:2832:A:N7	86:A:4080:HOH:O	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ja:127:ARG:HB2	15:Ja:140:ASN:HB2	1.85	0.59
19:Ka:12:ASN:HB2	19:Ka:25:VAL:HG12	1.85	0.59
36:Pa:42:ARG:NH2	75:h1:591:C:OP1	2.35	0.59
45:BV:135:LEU:HD22	45:BV:217:ILE:HG12	1.83	0.59
75:h1:1409:A:H2'	75:h1:1410:A:C8	2.38	0.59
75:h1:1785:MA6:N7	86:h1:2234:HOH:O	2.31	0.59
19:Ka:106:ARG:NH2	75:h1:459:G:OP1	2.36	0.59
50:Na:35:MET:HE2	50:Na:81:PHE:CD2	2.37	0.59
63:AQ:97:MET:O	63:AQ:101:VAL:HG23	2.03	0.59
2:A:727:U:OP2	86:A:3862:HOH:O	2.16	0.58
2:A:2211:A:H2'	2:A:2212:A2M:C8	2.33	0.58
14:AP:123:THR:HG21	14:AP:125:LYS:HE2	1.85	0.58
22:BS:36:ASP:OD1	22:BS:38:THR:OG1	2.20	0.58
35:AT:30:TYR:OH	35:AT:58:GLU:OE1	2.16	0.58
42:BU:17:GLN:HB2	42:BU:134:GLU:HG3	1.84	0.58
59:Ta:139:ARG:HB3	59:Ta:142:LYS:HB2	1.85	0.58
66:Ya:80:ALA:HA	66:Ya:98:VAL:HG13	1.85	0.58
75:h1:212:A:H2'	75:h1:213:U:O4'	2.03	0.58
2:A:91:C:O2'	86:A:3805:HOH:O	1.95	0.58
32:BH:17:ARG:NH1	86:BH:304:HOH:O	2.36	0.58
44:Xa:77:HIS:HB2	44:Xa:88:ARG:HB2	1.85	0.58
66:Ya:67:LYS:O	66:Ya:70:ILE:HG13	2.03	0.58
75:h1:1042:G:H2'	75:h1:1043:G:C8	2.37	0.58
75:h1:1676:U:H2'	75:h1:1677:G:H8	1.68	0.58
57:AF:57:LEU:HG	57:AF:61:ARG:HD3	1.85	0.58
75:h1:1161:A:H2'	75:h1:1162:C:H6	1.67	0.58
77:Ba:57:VAL:HB	77:Ba:91:VAL:HG12	1.85	0.58
75:h1:515:U:H2'	75:h1:516:G:C8	2.39	0.58
2:A:2254:A2M:H4'	2:A:2255:C:H5''	1.86	0.58
43:BR:122:LEU:HD21	43:BR:128:THR:HB	1.84	0.58
51:AB:112:GLN:HE21	51:AB:124:ILE:HG13	1.69	0.58
59:Ta:191:ARG:O	59:Ta:195:ARG:HG2	2.03	0.58
60:AZ:9:LYS:H	60:AZ:9:LYS:HD3	1.68	0.58
75:h1:428:G:H1'	86:h1:2426:HOH:O	2.02	0.58
75:h1:1474:A:H2	75:h1:1477:G:N3	2.01	0.58
75:h1:1780:A:H2'	75:h1:1781:G:C8	2.39	0.58
35:AT:16:ARG:O	35:AT:20:VAL:HG23	2.02	0.58
38:BN:145:LEU:O	38:BN:149:ASN:ND2	2.36	0.58
53:AA:76:ARG:HD3	78:AI:63:HIS:CD2	2.39	0.58
58:Wa:36:ILE:HA	58:Wa:40:LEU:HD23	1.85	0.58
62:Za:84:ARG:NH2	62:Za:169:ASN:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:1297:A:N7	86:h1:2239:HOH:O	2.32	0.58
2:A:1043:U:H2'	2:A:1044:C:C6	2.39	0.58
2:A:2493:C:H2'	2:A:2494:U:C6	2.39	0.58
15:Ja:104:ASP:OD1	15:Ja:110:ARG:NE	2.37	0.58
41:Ha:113:HIS:N	86:Ha:204:HOH:O	2.36	0.58
64:Oa:22:GLN:OE1	64:Oa:22:GLN:N	2.32	0.58
75:h1:1357:G:H2'	75:h1:1358:G:H8	1.69	0.58
52:BF:67:ALA:HA	63:AQ:120:ALA:HB1	1.83	0.58
59:Ta:67:VAL:HG12	59:Ta:69:THR:HG22	1.86	0.58
67:BB:77:GLU:HA	67:BB:80:ARG:HD3	1.86	0.58
1:3:133:U:H2'	1:3:134:G:C8	2.39	0.58
34:BK:69:ILE:HB	86:BK:430:HOH:O	2.04	0.58
62:Za:149:ILE:HG12	62:Za:163:ILE:HD12	1.85	0.58
75:h1:593:A:H2'	75:h1:594:A:C8	2.38	0.58
2:A:1223:G:H4'	17:AL:92:MET:HG3	1.86	0.57
2:A:1576:A:H2'	2:A:1577:C:C6	2.39	0.57
2:A:1601:U:C6	86:A:6680:HOH:O	2.52	0.57
2:A:2733:A:OP1	86:A:3866:HOH:O	2.17	0.57
2:A:2852:G:N7	86:A:4096:HOH:O	2.32	0.57
43:BR:103:LYS:NZ	86:BR:403:HOH:O	2.37	0.57
50:Na:37:VAL:HG11	50:Na:65:LEU:HD11	1.86	0.57
53:AA:25:LEU:O	53:AA:29:LEU:HB2	2.05	0.57
69:Ra:168:GLU:H	69:Ra:168:GLU:CD	2.12	0.57
75:h1:29:U:H2'	75:h1:30:G:H8	1.69	0.57
2:A:1214:A:O3'	86:A:3863:HOH:O	2.17	0.57
4:C3:81:G:N7	86:C3:313:HOH:O	2.32	0.57
75:h1:30:G:N3	86:h1:2237:HOH:O	2.32	0.57
48:BW:66:SER:HB3	48:BW:70:ARG:HH12	1.69	0.57
2:A:1955:G:N2	2:A:2091:A:OP1	2.32	0.57
2:A:2205:A:H2'	2:A:2206:A:O4'	2.04	0.57
2:A:2291:OMC:O2	86:A:3848:HOH:O	2.15	0.57
2:A:3045:C:O2'	2:A:3046:A:H5'	2.04	0.57
16:Ea:64:VAL:HG21	16:Ea:106:ALA:HB2	1.87	0.57
26:AH:93:LEU:HB3	86:AH:206:HOH:O	2.04	0.57
69:Ra:94:ILE:HD13	69:Ra:173:VAL:HG11	1.86	0.57
75:h1:1593:C:H2'	75:h1:1594:G:H8	1.68	0.57
75:h1:1668:C:H2'	75:h1:1669:G:C8	2.40	0.57
29:AD:33:SER:HA	64:Oa:50:VAL:HB	1.86	0.57
48:BW:72:TRP:HD1	62:Za:64:MET:HE2	1.68	0.57
65:Ua:136:THR:C	65:Ua:137:ASP:OD1	2.48	0.57
2:A:3014:A:H2'	2:A:3015:A:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AL:169:TYR:OH	32:BH:31:GLU:HG3	2.04	0.57
69:Ra:99:ARG:HG3	75:h1:857:A:N6	2.20	0.57
75:h1:511:G:H2'	75:h1:512:G:C8	2.40	0.57
75:h1:1340:C:O2'	75:h1:1342:G:N7	2.37	0.57
75:h1:1526:A:H2'	75:h1:1527:A:C8	2.40	0.57
2:A:2212:A2M:H2	2:A:2428:A:O4'	2.04	0.57
2:A:2353:G:OP2	86:A:3867:HOH:O	2.17	0.57
2:A:2372:C:OP2	86:A:3868:HOH:O	2.17	0.57
2:A:2944:G:O2'	2:A:2947:OMC:OP2	2.22	0.57
34:BK:207:MET:HE2	34:BK:232:ALA:HB2	1.86	0.57
53:AA:132:LYS:HG3	53:AA:191:ASP:HA	1.85	0.57
75:h1:96:G:O2'	75:h1:462:A:O2'	2.17	0.57
3:W2:63:C:H2'	3:W2:64:G:H8	1.68	0.57
22:BS:35:ASP:OD2	22:BS:194:LYS:NZ	2.36	0.57
59:Ta:67:VAL:HB	59:Ta:101:GLY:HA2	1.86	0.57
2:A:2211:A:OP1	86:A:3858:HOH:O	2.16	0.57
64:Oa:9:VAL:HG22	64:Oa:50:VAL:HG22	1.86	0.57
75:h1:317:A:N1	75:h1:351:G:O2'	2.37	0.57
2:A:1865:G:OP2	86:A:3865:HOH:O	2.17	0.57
20:AW:50:LYS:O	86:AW:201:HOH:O	2.17	0.57
27:BT:290:MET:HE3	30:AJ:123:ASP:HB3	1.87	0.57
51:AB:42:ARG:NH2	75:h1:474:U:OP2	2.36	0.57
59:Ta:5:VAL:HG13	59:Ta:126:LEU:HD21	1.85	0.57
59:Ta:5:VAL:HG23	59:Ta:113:LEU:HB2	1.87	0.57
65:Ua:103:LYS:O	65:Ua:105:LYS:HE3	2.05	0.57
75:h1:1002:A:OP1	3:W2:38:A:O2'	2.21	0.57
75:h1:1230:G:N2	75:h1:1256:G:O2'	2.38	0.57
3:W2:63:C:H2'	3:W2:64:G:C8	2.40	0.57
2:A:1952:C:H2'	2:A:1953:U:C6	2.40	0.56
17:AL:40:LYS:HD3	17:AL:60:MET:HE2	1.87	0.56
20:AW:19:LEU:HD11	20:AW:36:GLN:HB2	1.87	0.56
2:A:244:C:H2'	2:A:245:A:C8	2.40	0.56
2:A:510:U:H2'	2:A:511:A:C8	2.41	0.56
3:i2:34:G:H1	76:B1:27:U:H3	1.52	0.56
51:AB:162:LEU:H	51:AB:162:LEU:HD12	1.70	0.56
53:AA:23:GLU:OE2	53:AA:27:ARG:NH2	2.38	0.56
64:Oa:28:VAL:HG23	64:Oa:37:ILE:HG22	1.86	0.56
3:W2:5:G:H22	3:W2:68:A:H2	1.52	0.56
2:A:472:G:H2'	2:A:473:G:C8	2.40	0.56
2:A:558:G:N7	86:A:4103:HOH:O	2.33	0.56
2:A:566:G:N7	86:A:4117:HOH:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2878:OMC:HM23	86:A:9544:HOH:O	2.05	0.56
15:Ja:35:PRO:HD2	15:Ja:83:PRO:HG2	1.85	0.56
18:Va:63:SER:OG	75:h1:567:C:O2	2.23	0.56
25:BI:32:THR:HG21	25:BI:105:ILE:HD12	1.86	0.56
27:BT:36:PRO:HB3	27:BT:288:ALA:HB2	1.87	0.56
43:BR:241:GLU:OE2	43:BR:245:ARG:NE	2.37	0.56
75:h1:1063:A:H3'	75:h1:1064:G:H8	1.70	0.56
2:A:465:G:N2	2:A:468:A:OP2	2.35	0.56
12:AE:113:HIS:NE2	12:AE:114:GLU:OE1	2.39	0.56
19:Ka:29:LEU:HD23	19:Ka:70:LYS:HG2	1.88	0.56
19:Ka:60:PHE:HE2	19:Ka:92:ARG:CZ	2.17	0.56
67:BB:13:SER:O	67:BB:17:ILE:HG22	2.06	0.56
75:h1:1059:U:H3'	75:h1:1060:U:C5'	2.35	0.56
77:Ba:82:ARG:HD2	77:Ba:82:ARG:H	1.68	0.56
2:A:2822:G:OP1	86:A:3870:HOH:O	2.18	0.56
44:Xa:34:ARG:N	44:Xa:34:ARG:HD3	2.21	0.56
58:Wa:15:VAL:HG13	58:Wa:68:MET:HE3	1.88	0.56
59:Ta:178:PRO:O	75:h1:79:A:O2'	2.19	0.56
69:Ra:30:LEU:HD12	69:Ra:37:LEU:HD12	1.86	0.56
69:Ra:35:GLN:OE1	69:Ra:35:GLN:N	2.39	0.56
75:h1:193:G:O2'	75:h1:194:A:H8	1.87	0.56
23:AM:157:VAL:HG21	46:BJ:169:ARG:HG3	1.86	0.56
75:h1:1128:G:N7	86:h1:2244:HOH:O	2.33	0.56
75:h1:1676:U:H2'	75:h1:1677:G:C8	2.41	0.56
20:AW:22:LYS:NZ	86:AW:206:HOH:O	2.38	0.56
33:Da:99:ARG:O	33:Da:103:GLU:HG2	2.06	0.56
2:A:11:G:H1'	86:A:4405:HOH:O	2.05	0.56
3:i2:69:C:H2'	3:i2:70:C:C6	2.40	0.56
9:AU:10:GLU:O	9:AU:81:ARG:NH1	2.34	0.56
25:BI:43:LYS:HE2	25:BI:62:MET:HE3	1.87	0.56
27:BT:321:LYS:NZ	86:BT:512:HOH:O	2.39	0.56
75:h1:1396:G:H2'	75:h1:1397:G:H8	1.70	0.56
2:A:488:C:H2'	2:A:489:G:C8	2.40	0.56
2:A:1952:C:H2'	2:A:1953:U:H6	1.71	0.56
2:A:2959:C:H2'	2:A:2960:G:C8	2.41	0.56
24:AC:191:GLN:HB3	86:AC:413:HOH:O	2.06	0.56
36:Pa:42:ARG:O	36:Pa:46:THR:OG1	2.23	0.56
78:AI:5:GLU:HB3	78:AI:9:ARG:HH21	1.71	0.56
15:Ja:49:ARG:NH2	75:h1:450:C:OP2	2.39	0.56
29:AD:34:LEU:O	29:AD:38:ILE:HG22	2.06	0.56
44:Xa:6:GLU:HG2	75:h1:329:U:O2'	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AF:27:GLY:HA3	57:AF:66:ASN:OD1	2.06	0.56
73:AY:65:ARG:HD3	86:AY:312:HOH:O	2.05	0.56
2:A:2268:A:H2'	2:A:2269:A:C8	2.40	0.55
65:Ua:45:ASP:OD2	65:Ua:47:SER:OG	2.24	0.55
74:Ca:22:ARG:NH2	74:Ca:36:LEU:O	2.33	0.55
3:W2:70:C:H2'	3:W2:71:G:C8	2.41	0.55
2:A:299:C:OP1	86:A:3872:HOH:O	2.18	0.55
45:BV:134:THR:HG22	45:BV:218:LEU:HD12	1.88	0.55
2:A:410:U:H2'	2:A:411:C:C6	2.41	0.55
2:A:890:C:OP1	86:A:3873:HOH:O	2.18	0.55
9:AU:45:GLU:HG3	9:AU:51:LYS:HA	1.89	0.55
17:AL:70:ASN:O	17:AL:75:LYS:NZ	2.38	0.55
27:BT:129:ILE:HD11	27:BT:246:LEU:HD12	1.87	0.55
44:XA:126:ILE:HG22	44:XA:140:VAL:HA	1.88	0.55
53:AA:56:GLN:NE2	53:AA:56:GLN:H	2.04	0.55
56:BA:44:TRP:CZ3	56:BA:45:ARG:HG3	2.42	0.55
75:h1:451:C:H2'	75:h1:452:U:C6	2.42	0.55
2:A:166:C:OP2	54:AG:133:LYS:NZ	2.40	0.55
31:BQ:103:PRO:HD3	86:BQ:519:HOH:O	2.05	0.55
46:BJ:133:GLN:N	86:BJ:401:HOH:O	2.30	0.55
57:AF:137:ARG:O	57:AF:139:ARG:NH1	2.40	0.55
69:Ra:76:ILE:HG12	69:Ra:80:LEU:HB2	1.87	0.55
73:AY:76:THR:O	73:AY:77:CYS:CB	2.55	0.55
2:A:1222:G:OP1	11:Ia:1:MET:N	2.32	0.55
2:A:3089:A:O4'	86:A:3871:HOH:O	2.18	0.55
63:AQ:83:LEU:HD12	63:AQ:83:LEU:O	2.07	0.55
64:Oa:34:ASP:OD1	64:Oa:34:ASP:N	2.32	0.55
75:h1:1171:G:OP1	86:h1:2149:HOH:O	2.18	0.55
2:A:1157:G:N7	86:A:4128:HOH:O	2.33	0.55
2:A:1704:G:O2'	2:A:1740:C:N4	2.40	0.55
2:A:2211:A:H2'	2:A:2212:A2M:H8	1.87	0.55
2:A:3011:U:H2'	2:A:3012:U:C6	2.41	0.55
22:BS:364:ASP:OD2	47:AO:19:ARG:NH2	2.35	0.55
29:AD:29:VAL:HG11	29:AD:35:VAL:HA	1.89	0.55
62:Za:18:ASP:O	62:Za:22:MET:HG3	2.07	0.55
2:A:591:A:H5''	2:A:592:C:OP1	2.07	0.55
10:Ma:37:LYS:HG2	10:Ma:72:GLN:HG2	1.88	0.55
28:AV:87:MET:SD	28:AV:88:MET:HE3	2.45	0.55
29:AD:61:PHE:CE2	64:Oa:46:ARG:HG3	2.41	0.55
43:BR:101:ASP:OD1	86:BR:402:HOH:O	2.18	0.55
66:Ya:54:LEU:HD12	66:Ya:58:PRO:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1032:G:H3'	2:A:1033:G:H8	1.72	0.55
2:A:1805:C:OP1	86:A:3874:HOH:O	2.18	0.55
3:i:20:G:O6	3:i:59:U:O4	2.24	0.55
6:BM:45:LYS:HB3	6:BM:45:LYS:NZ	2.21	0.55
15:Ja:185:GLY:HA2	15:Ja:189:ARG:HE	1.72	0.55
53:AA:115:VAL:HG21	53:AA:142:LEU:HD23	1.89	0.55
66:Ya:45:ARG:NH2	75:h1:1554:U:O4	2.38	0.55
1:3:115:G:C5	83:A:3402:SPD:H92	2.42	0.55
5:BC:14:LYS:HD2	86:h1:3756:HOH:O	2.06	0.55
6:BM:125:LYS:NZ	86:BM:306:HOH:O	2.34	0.55
18:Va:121:VAL:HG12	18:Va:129:LEU:HD11	1.88	0.55
75:h1:355:A:O2'	86:h1:2146:HOH:O	2.18	0.55
75:h1:1652:U:H2'	75:h1:1653:A:C8	2.42	0.55
2:A:583:C:H2'	2:A:584:G:H8	1.72	0.55
2:A:1676:A:H2	2:A:1692:G:H22	1.55	0.55
2:A:3119:U:H1'	2:A:3120:A:H5''	1.88	0.55
14:AP:53:VAL:HA	86:AP:203:HOH:O	2.07	0.55
15:Ja:108:ARG:NH1	75:h1:792:A:OP1	2.39	0.55
19:Ka:30:HIS:HE2	19:Ka:71:SER:HG	1.55	0.55
70:BL:7:VAL:HG21	70:BL:132:LEU:HD23	1.88	0.55
75:h1:999:A:H4'	86:h1:3454:HOH:O	2.07	0.55
24:AC:69:ARG:NH1	86:AC:402:HOH:O	2.39	0.54
31:BQ:105:ARG:NH1	31:BQ:144:ASP:OD1	2.40	0.54
68:AN:27:LYS:HE2	68:AN:114:ARG:HA	1.88	0.54
75:h1:129:U:H3'	75:h1:130:A:H5'	1.89	0.54
2:A:584:G:OP2	52:BF:12:ARG:NH2	2.40	0.54
2:A:2496:U:O2'	2:A:2497:U:OP1	2.24	0.54
83:A:3402:SPD:H52	86:A:8814:HOH:O	2.07	0.54
75:h1:99:U:OP2	86:h1:2147:HOH:O	2.18	0.54
2:A:1042:C:H2'	2:A:1043:U:C6	2.43	0.54
2:A:2271:G:O2'	2:A:2309:G:O6	2.22	0.54
2:A:2661:A:H2'	2:A:2662:G:C8	2.42	0.54
2:A:3303:A:O2'	2:A:3304:U:OP1	2.24	0.54
59:Ta:176:LYS:NZ	75:h1:69:A:N7	2.55	0.54
75:h1:1474:A:C8	75:h1:1542:G:H1'	2.42	0.54
75:h1:1577:G7M:H2'	75:h1:1578:A:C8	2.43	0.54
1:3:101:G:H5''	37:BP:66:LYS:HG3	1.88	0.54
15:Ja:64:ILE:HG12	19:Ka:19:LEU:HD21	1.90	0.54
42:BU:25:VAL:HG21	42:BU:32:LEU:HA	1.87	0.54
53:AA:65:ARG:O	53:AA:69:LEU:HG	2.07	0.54
58:Wa:85:ASN:N	58:Wa:97:GLN:OE1	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:BB:24:MET:HE3	67:BB:58:MET:HE3	1.90	0.54
71:La:40:MET:HE3	71:La:72:ILE:HD12	1.89	0.54
75:h1:51:A:OP2	75:h1:426:C:N4	2.35	0.54
2:A:1089:U:O2	34:BK:138:ARG:NH2	2.41	0.54
11:Ia:7:SER:OG	11:Ia:61:ASP:OD1	2.13	0.54
27:BT:12:ILE:HD13	27:BT:260:LYS:HD2	1.89	0.54
42:BU:112:ILE:HD12	42:BU:124:ILE:HD11	1.89	0.54
60:AZ:24:LYS:HG2	60:AZ:67:GLN:HB3	1.89	0.54
66:Ya:42:PHE:HB3	66:Ya:46:ILE:HG23	1.88	0.54
67:BB:24:MET:HB2	67:BB:58:MET:HE3	1.89	0.54
75:h1:15:U:H2'	75:h1:16:G:O4'	2.07	0.54
12:AE:4:ILE:HG23	75:h1:636:G:H5'	1.89	0.54
30:AJ:91:VAL:HG13	30:AJ:94:ILE:HD11	1.90	0.54
53:AA:105:LEU:HD12	53:AA:184:ILE:HD13	1.89	0.54
75:h1:824:C:H3'	75:h1:825:G:H21	1.71	0.54
75:h1:1417:U:O2'	75:h1:1419:G:OP2	2.17	0.54
2:A:2888:C:N4	2:A:2910:A2M:H2	2.23	0.54
38:BN:80:THR:HG23	38:BN:153:ILE:HG23	1.89	0.54
44:Xa:85:ILE:HD13	44:Xa:118:VAL:HG11	1.90	0.54
59:Ta:97:LYS:NZ	75:h1:158:C:O2'	2.41	0.54
60:AZ:11:PHE:CZ	60:AZ:34:PHE:HB3	2.43	0.54
75:h1:618:G:OP1	86:h1:2150:HOH:O	2.18	0.54
75:h1:939:G:N3	86:h1:2255:HOH:O	2.34	0.54
75:h1:1147:G:H2'	75:h1:1148:A:C8	2.43	0.54
2:A:2405:C:H2'	2:A:2406:U:C6	2.43	0.54
3:i2:69:C:H2'	3:i2:70:C:H6	1.73	0.54
51:AB:140:ARG:NH1	51:AB:141:GLN:HA	2.23	0.54
69:Ra:66:PRO:HG2	69:Ra:69:LEU:HB2	1.90	0.54
75:h1:139:U:H4'	75:h1:140:C:O5'	2.08	0.54
75:h1:1595:A:H2'	75:h1:1596:G:C8	2.43	0.54
2:A:3247:G:O2'	2:A:3248:C:OP1	2.23	0.54
2:A:3290:OMG:C4	86:A:4330:HOH:O	2.60	0.54
12:AE:28:ARG:NH2	75:h1:866:A:OP1	2.40	0.54
34:BK:110:LEU:HD22	34:BK:115:MET:HB2	1.89	0.54
78:AI:43:ILE:HG22	78:AI:44:LYS:HE3	1.88	0.54
2:A:1356:G:H5''	27:BT:312:LYS:HD2	1.90	0.54
86:A:4838:HOH:O	46:BJ:120:GLY:HA3	2.08	0.54
22:BS:11:HIS:O	86:BS:502:HOH:O	2.19	0.54
24:AC:120:ILE:HD12	24:AC:120:ILE:O	2.09	0.54
59:Ta:8:PRO:HD3	59:Ta:114:VAL:HG13	1.90	0.54
75:h1:390:OMG:HM22	75:h1:391:G:H5'	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:155:OMG:HM22	39:BG:52:ILE:HD11	1.90	0.53
2:A:304:A:H2'	2:A:305:A:C8	2.43	0.53
2:A:2119:A:N1	86:A:4114:HOH:O	2.33	0.53
33:Da:16:LEU:HG	33:Da:62:GLN:HE22	1.73	0.53
59:Ta:26:ALA:O	59:Ta:30:LYS:NZ	2.41	0.53
62:Za:85:PRO:HA	62:Za:88:GLN:OE1	2.08	0.53
2:A:1032:G:C6	2:A:1033:G:C6	2.96	0.53
86:A:4981:HOH:O	39:BG:232:MET:HE1	2.07	0.53
15:Ja:120:LYS:HG2	15:Ja:165:GLU:OE2	2.08	0.53
15:Ja:229:GLY:HA3	15:Ja:234:PRO:HA	1.90	0.53
47:AO:31:PHE:HA	86:AO:204:HOH:O	2.08	0.53
77:Ba:94:LEU:HD12	77:Ba:101:VAL:HG23	1.89	0.53
3:i:20:G:O6	3:i:59:U:C4	2.62	0.53
50:Na:48:VAL:HG11	50:Na:56:VAL:HG11	1.90	0.53
57:AF:10:GLN:OE1	57:AF:70:ARG:NH2	2.41	0.53
57:AF:18:ALA:HB2	57:AF:74:GLY:HA3	1.90	0.53
62:Za:45:ARG:HE	62:Za:49:GLY:HA2	1.73	0.53
75:h1:884:U:H3	75:h1:946:U:H3	1.56	0.53
2:A:2371:A:OP2	86:A:3877:HOH:O	2.18	0.53
7:BO:54:GLU:OE1	7:BO:68:LYS:HB2	2.09	0.53
14:AP:25:ILE:HA	14:AP:43:VAL:HG22	1.90	0.53
28:AV:88:MET:HG3	63:AQ:41:THR:HA	1.89	0.53
45:BV:47:LEU:O	65:Ua:50:GLU:HG3	2.08	0.53
63:AQ:20:LEU:HD12	63:AQ:22:LYS:HG3	1.89	0.53
74:Ca:11:PRO:HB3	74:Ca:13:LYS:NZ	2.24	0.53
75:h1:1161:A:H2'	75:h1:1162:C:C6	2.43	0.53
75:h1:1305:G:N2	86:h1:2142:HOH:O	2.16	0.53
1:3:151:C:H2'	1:3:152:C:C6	2.44	0.53
2:A:784:G:O2'	2:A:786:U:OP2	2.24	0.53
15:Ja:205:PHE:CD2	15:Ja:221:ARG:HD3	2.44	0.53
16:Ea:41:ARG:NH1	86:Ea:405:HOH:O	2.30	0.53
33:Da:123:HIS:HB3	86:Da:226:HOH:O	2.08	0.53
43:BR:104:THR:HG23	43:BR:135:VAL:HG12	1.90	0.53
46:BJ:193:ASP:OD2	46:BJ:198:LYS:HE3	2.08	0.53
51:AB:39:ARG:NH1	51:AB:43:GLU:OE2	2.41	0.53
67:BB:43:SER:OG	75:h1:1333:C:OP1	2.23	0.53
68:AN:43:LEU:O	68:AN:47:ILE:HG23	2.07	0.53
70:BL:123:LYS:NZ	70:BL:124:ILE:O	2.42	0.53
75:h1:128:G:OP1	75:h1:128:G:H2'	2.09	0.53
2:A:2972:G:O6	86:A:3880:HOH:O	2.19	0.53
2:A:3262:U:O2	20:AW:8:GLU:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3358:G:N7	86:A:4149:HOH:O	2.34	0.53
43:BR:241:GLU:OE1	86:BR:401:HOH:O	2.17	0.53
58:Wa:102:ALA:HA	58:Wa:105:MET:SD	2.49	0.53
75:h1:154:A:H2'	75:h1:155:A:O4'	2.08	0.53
86:A:6616:HOH:O	27:BT:74:THR:HG21	2.08	0.53
37:BP:89:ARG:O	37:BP:93:ARG:HG2	2.09	0.53
45:BV:86:LEU:HB3	45:BV:98:THR:HB	1.91	0.53
57:AF:33:LEU:HD23	57:AF:69:ILE:HB	1.91	0.53
65:Ua:137:ASP:OD1	65:Ua:137:ASP:N	2.41	0.53
67:BB:73:LEU:HD23	67:BB:73:LEU:H	1.73	0.53
75:h1:1360:G:OP2	75:h1:1363:A:N6	2.38	0.53
2:A:373:G:N7	86:A:4136:HOH:O	2.33	0.53
2:A:2219:G:N2	2:A:2222:A:OP2	2.28	0.53
2:A:2448:A:H2'	2:A:2449:G:O4'	2.08	0.53
69:Ra:75:LYS:HD2	69:Ra:75:LYS:C	2.33	0.53
75:h1:1395:U:H2'	75:h1:1396:G:H8	1.73	0.53
2:A:352:A:N1	27:BT:89:THR:HG22	2.24	0.53
2:A:1372:G:N7	86:A:4147:HOH:O	2.34	0.53
45:BV:28:ASP:OD1	45:BV:50:ARG:NH2	2.42	0.53
59:Ta:7:ASN:H	59:Ta:12:CYS:HB2	1.74	0.53
67:BB:76:GLU:HG3	67:BB:80:ARG:HD2	1.90	0.53
2:A:2837:A:H2'	2:A:2838:G:O4'	2.09	0.53
18:Va:53:LYS:NZ	18:Va:93:ILE:O	2.30	0.53
31:BQ:192:LYS:NZ	86:BQ:411:HOH:O	2.38	0.53
44:Xa:125:ILE:HB	44:Xa:142:LYS:HB3	1.91	0.53
60:AZ:9:LYS:O	60:AZ:13:LEU:HG	2.09	0.53
62:Za:87:GLY:O	62:Za:91:VAL:HG13	2.08	0.53
75:h1:1172:A:O2'	75:h1:1572:A:N3	2.36	0.53
75:h1:1396:G:H2'	75:h1:1397:G:C8	2.43	0.53
75:h1:1527:A:H2'	75:h1:1528:A:C8	2.44	0.53
1:3:118:G:OP1	2:A:1833:U:O2'	2.18	0.52
1:3:162:C:OP2	39:BG:80:LYS:NZ	2.43	0.52
2:A:242:C:H2'	2:A:243:G:H8	1.73	0.52
2:A:1210:A:C2	86:A:3855:HOH:O	2.60	0.52
13:AX:10:LEU:HD11	54:AG:179:LYS:HE3	1.91	0.52
20:AW:77:THR:HG21	86:AW:264:HOH:O	2.08	0.52
23:AM:9:ALA:O	23:AM:55:LYS:NZ	2.42	0.52
28:AV:97:ILE:HG21	28:AV:106:ARG:HG2	1.91	0.52
31:BQ:175:THR:OG1	86:BQ:403:HOH:O	2.18	0.52
49:AK:168:ALA:HA	49:AK:171:GLU:OE2	2.09	0.52
75:h1:1093:A:C1'	86:h1:2141:HOH:O	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ja:90:VAL:HG23	15:Ja:99:PHE:HB2	1.91	0.52
24:AC:27:ILE:HG23	24:AC:32:LEU:HB2	1.91	0.52
24:AC:62:THR:HG23	24:AC:64:ALA:H	1.75	0.52
29:AD:34:LEU:HD11	29:AD:146:ARG:HH21	1.74	0.52
42:BU:24:SER:N	86:BU:201:HOH:O	2.22	0.52
75:h1:1059:U:H3'	75:h1:1060:U:H5''	1.91	0.52
2:A:394:A:H4'	2:A:395:G:H3'	1.91	0.52
2:A:2503:U:H2'	2:A:2504:A:H8	1.75	0.52
18:Va:3:LYS:HB3	86:Va:317:HOH:O	2.09	0.52
24:AC:52:VAL:HG22	24:AC:74:VAL:HG22	1.90	0.52
39:BG:239:LYS:HG2	39:BG:243:LYS:NZ	2.24	0.52
59:Ta:196:ILE:HD11	75:h1:176:A:N9	2.25	0.52
62:Za:187:LEU:HD22	62:Za:190:ARG:HH12	1.74	0.52
75:h1:52:U:H2'	75:h1:53:G:C8	2.44	0.52
15:Ja:25:GLY:O	86:Ja:402:HOH:O	2.19	0.52
45:BV:61:LEU:HD22	45:BV:96:VAL:HG21	1.91	0.52
2:A:1371:C:H5''	27:BT:318:ALA:HB2	1.91	0.52
2:A:2405:C:H2'	2:A:2406:U:H6	1.73	0.52
44:Xa:38:ASN:N	86:Xa:202:HOH:O	2.43	0.52
51:AB:159:ASP:OD1	51:AB:160:PHE:N	2.43	0.52
2:A:2660:G:H2'	2:A:2661:A:C8	2.45	0.52
11:Ia:141:GLU:OE1	11:Ia:141:GLU:N	2.34	0.52
15:Ja:178:GLY:H	15:Ja:195:ILE:HG23	1.74	0.52
20:AW:78:ARG:NH2	86:AW:205:HOH:O	2.38	0.52
44:Xa:73:ALA:HB1	44:Xa:123:HIS:CE1	2.44	0.52
2:A:279:G:OP1	82:A:3401:TER:N1	2.40	0.52
2:A:668:A:H2'	2:A:669:A:C8	2.45	0.52
2:A:3241:U:H2'	2:A:3242:G:C8	2.45	0.52
19:Ka:108:GLN:OE1	19:Ka:112:ARG:NH2	2.43	0.52
74:Ca:43:PHE:O	74:Ca:47:ALA:HB2	2.09	0.52
75:h1:16:G:H2'	75:h1:17:C:C6	2.44	0.52
2:A:432:C:H2'	2:A:433:C:C6	2.45	0.52
2:A:469:U:H2'	2:A:470:C:C6	2.45	0.52
2:A:1576:A:H2'	2:A:1577:C:H6	1.74	0.52
2:A:2241:A:N7	31:BQ:245:ARG:HD2	2.24	0.52
2:A:2660:G:H2'	2:A:2661:A:H8	1.74	0.52
19:Ka:19:LEU:HD12	19:Ka:21:ARG:NH2	2.25	0.52
26:AH:64:ARG:HG2	26:AH:65:VAL:HG23	1.92	0.52
32:BH:68:ASN:HA	86:BH:319:HOH:O	2.09	0.52
32:BH:73:HIS:ND1	32:BH:73:HIS:O	2.42	0.52
39:BG:204:GLU:O	39:BG:208:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AA:32:ASP:C	53:AA:54:ARG:HD3	2.35	0.52
57:AF:103:SER:O	57:AF:107:ILE:HG12	2.10	0.52
58:Wa:102:ALA:O	58:Wa:106:LYS:HG2	2.10	0.52
74:Ca:34:TYR:OH	75:h1:1490:A:OP1	2.18	0.52
75:h1:124:G:N7	86:h1:2260:HOH:O	2.34	0.52
2:A:1056:A:H2'	2:A:1059:C:C5	2.45	0.52
11:Ia:129:VAL:HG22	11:Ia:167:LYS:HG3	1.91	0.52
16:Ea:167:GLU:HA	16:Ea:167:GLU:OE1	2.09	0.52
20:AW:15:ARG:NH1	20:AW:38:GLU:OE1	2.43	0.52
45:BV:179:CYS:HB3	45:BV:183:GLU:HB2	1.92	0.52
52:BF:136:GLN:HB3	86:BF:303:HOH:O	2.09	0.52
74:Ca:53:ILE:C	74:Ca:54:LYS:N	2.67	0.52
75:h1:342:U:H2'	75:h1:343:A:C8	2.44	0.52
75:h1:522:A:H2'	75:h1:523:A:C8	2.44	0.52
75:h1:821:U:H3	75:h1:854:G:H1	1.58	0.52
2:A:583:C:H2'	2:A:584:G:C8	2.45	0.52
2:A:1691:U:H2'	2:A:1692:G:C8	2.45	0.52
19:Ka:38:LYS:HA	19:Ka:41:LEU:HD12	1.92	0.52
27:BT:295:LEU:HD11	30:AJ:32:LEU:HB2	1.90	0.52
50:Na:74:LYS:HE2	50:Na:74:LYS:HA	1.92	0.52
75:h1:609:G:N2	75:h1:616:C:H5''	2.25	0.52
75:h1:1655:C:H5''	86:h1:2121:HOH:O	2.10	0.52
8:AR:4:SER:N	86:AR:201:HOH:O	2.36	0.51
18:Va:89:CYS:HA	18:Va:92:TYR:HD2	1.75	0.51
39:BG:165:ARG:HE	39:BG:220:TYR:HB3	1.75	0.51
59:Ta:165:THR:HG23	59:Ta:175:SER:HB2	1.92	0.51
72:Aa:90:GLU:O	72:Aa:94:THR:HG23	2.10	0.51
75:h1:1018:U:H2'	75:h1:1019:C:C6	2.46	0.51
75:h1:1630:PSU:H2'	75:h1:1631:G:C8	2.45	0.51
75:h1:1651:C:H2'	75:h1:1652:U:C6	2.45	0.51
2:A:1099:U:H2'	2:A:1100:C:C6	2.45	0.51
38:BN:39:ARG:HD3	39:BG:43:SER:HB3	1.93	0.51
2:A:277:PSU:P	82:A:3401:TER:H121	2.50	0.51
2:A:311:PSU:H2'	2:A:312:C:C6	2.45	0.51
2:A:2230:A:H2'	2:A:2231:A:C8	2.44	0.51
2:A:3002:C:H2'	2:A:3003:G:O4'	2.10	0.51
27:BT:241:LEU:HA	86:BT:507:HOH:O	2.09	0.51
29:AD:21:ARG:HB3	29:AD:22:TRP:CE2	2.44	0.51
67:BB:21:TYR:HD2	67:BB:73:LEU:HD11	1.76	0.51
75:h1:270:G:H2'	75:h1:271:C:C6	2.45	0.51
75:h1:1289:G:O6	86:h1:2154:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3242:G:H2'	2:A:3243:G:O4'	2.11	0.51
3:i:23:A:H2'	3:i:24:G:H8	1.75	0.51
42:BU:76:GLU:OE1	42:BU:76:GLU:HA	2.11	0.51
45:BV:91:VAL:HG22	45:BV:96:VAL:HG22	1.91	0.51
52:BF:123:PRO:HD2	52:BF:126:ILE:HD12	1.92	0.51
58:Wa:89:ASP:OD1	58:Wa:93:GLY:N	2.40	0.51
59:Ta:32:LEU:HD22	59:Ta:65:GLN:HE21	1.76	0.51
67:BB:17:ILE:HD11	67:BB:61:ILE:HD12	1.93	0.51
75:h1:12:U:H2'	75:h1:13:C:C6	2.45	0.51
75:h1:335:A:H2'	75:h1:336:G:C8	2.46	0.51
36:Pa:18:THR:HG21	75:h1:586:C:O2'	2.11	0.51
51:AB:111:LEU:HB2	51:AB:148:PHE:HB3	1.91	0.51
58:Wa:70:ILE:HG12	58:Wa:77:PHE:CD2	2.45	0.51
2:A:730:U:O4	41:Ha:133:LYS:HE3	2.10	0.51
2:A:2508:U:H2'	2:A:2509:A:H8	1.76	0.51
29:AD:204:ARG:NE	65:Ua:71:TYR:HB2	2.26	0.51
40:Fa:93:ARG:O	40:Fa:97:VAL:HG23	2.09	0.51
53:AA:106:ARG:HG2	53:AA:175:VAL:HG22	1.93	0.51
59:Ta:195:ARG:HH22	75:h1:268:U:H5	1.59	0.51
75:h1:452:U:H2'	75:h1:453:G:C8	2.45	0.51
2:A:1057:A:H5'	86:BJ:411:HOH:O	2.11	0.51
24:AC:54:LYS:HD2	24:AC:179:LEU:HD13	1.93	0.51
33:Da:142:GLU:N	33:Da:142:GLU:OE1	2.43	0.51
3:W2:67:C:H2'	3:W2:68:A:C8	2.45	0.51
2:A:2978:U:H3'	86:A:4435:HOH:O	2.10	0.51
15:Ja:248:ILE:HD11	51:AB:73:PHE:CE2	2.45	0.51
26:AH:81:LYS:O	26:AH:85:GLU:HG3	2.11	0.51
31:BQ:208:GLU:OE2	86:BQ:404:HOH:O	2.19	0.51
44:Xa:34:ARG:HD3	44:Xa:34:ARG:H	1.75	0.51
44:Xa:81:MET:HE2	86:h1:3381:HOH:O	2.09	0.51
53:AA:7:LYS:O	53:AA:10:LYS:HG2	2.10	0.51
53:AA:44:MET:O	53:AA:83:SER:OG	2.19	0.51
57:AF:145:ARG:NH1	3:W2:35:A:OP2	2.44	0.51
59:Ta:57:ASP:HA	59:Ta:108:LEU:HA	1.92	0.51
69:Ra:10:LYS:HE3	69:Ra:20:GLU:OE1	2.10	0.51
75:h1:188:U:O2	75:h1:192:G:O6	2.27	0.51
2:A:2881:U:H2'	2:A:2882:OMU:H6	1.93	0.51
3:i:70:C:H2'	3:i:71:G:H8	1.76	0.51
12:AE:23:ARG:NH1	50:Na:5:ASN:O	2.37	0.51
17:AL:167:THR:HB	86:AL:234:HOH:O	2.11	0.51
22:BS:217:MET:HE2	22:BS:284:LYS:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AC:74:VAL:HG11	24:AC:101:ILE:HG12	1.92	0.51
53:AA:17:PHE:HE2	53:AA:39:VAL:HG11	1.76	0.51
54:AG:9:ASN:ND2	86:AG:406:HOH:O	2.43	0.51
75:h1:437:C:H2'	75:h1:438:A2M:O4'	2.10	0.51
2:A:1213:A:H2'	2:A:1214:A:C8	2.46	0.51
2:A:2362:G:N7	86:A:4148:HOH:O	2.34	0.51
20:AW:41:ASN:ND2	86:AW:210:HOH:O	2.44	0.51
31:BQ:102:LEU:CD2	86:BQ:452:HOH:O	2.58	0.51
32:BH:126:PRO:HA	32:BH:129:LEU:HD12	1.93	0.51
34:BK:60:ILE:HB	34:BK:80:ALA:HB2	1.93	0.51
75:h1:79:A:H2'	75:h1:80:C:C6	2.46	0.51
2:A:2219:G:N3	86:A:4169:HOH:O	2.35	0.50
2:A:2432:U:OP1	86:A:3883:HOH:O	2.19	0.50
3:i2:5:G:H22	3:i2:68:A:H2	1.58	0.50
7:BO:56:GLN:HG3	7:BO:66:GLU:HG2	1.93	0.50
19:Ka:105:SER:HB3	19:Ka:108:GLN:HB3	1.92	0.50
27:BT:126:ARG:O	27:BT:129:ILE:HG22	2.10	0.50
54:AG:140:GLU:OE1	54:AG:140:GLU:HA	2.11	0.50
63:AQ:17:ASN:HB2	63:AQ:20:LEU:HD23	1.93	0.50
67:BB:61:ILE:HD13	67:BB:71:LEU:HD11	1.92	0.50
70:BL:105:LEU:HD22	70:BL:122:ARG:HG3	1.93	0.50
71:La:78:ARG:NH2	75:h1:1535:C:OP2	2.45	0.50
75:h1:175:A:H4'	75:h1:176:A:H5''	1.92	0.50
2:A:501:G:O2'	2:A:3259:A:N1	2.43	0.50
2:A:2404:C:H2'	2:A:2405:C:C6	2.46	0.50
2:A:2596:U:H2'	2:A:2597:G:C8	2.46	0.50
10:Ma:85:ARG:NH2	75:h1:1153:A:O3'	2.44	0.50
39:BG:203:LEU:HG	39:BG:204:GLU:OE2	2.11	0.50
1:3:81:A:H2'	1:3:82:G:C8	2.47	0.50
2:A:20:G:OP1	86:A:3881:HOH:O	2.19	0.50
2:A:642:A:H2'	2:A:643:U:C6	2.46	0.50
2:A:710:G:H5''	2:A:711:U:H5	1.77	0.50
2:A:1614:A:H3'	86:A:3809:HOH:O	2.11	0.50
2:A:1954:G:H2'	2:A:2091:A:N6	2.26	0.50
11:Ia:85:SER:HB3	11:Ia:189:LYS:HE2	1.92	0.50
53:AA:64:ARG:HD3	78:AI:91:LEU:HG	1.92	0.50
58:Wa:48:ALA:HB2	58:Wa:70:ILE:HD12	1.92	0.50
59:Ta:63:MET:HE1	59:Ta:108:LEU:HD11	1.93	0.50
59:Ta:68:LEU:H	59:Ta:68:LEU:HD12	1.77	0.50
67:BB:45:ARG:HH21	75:h1:1332:A:H5''	1.75	0.50
70:BL:130:ARG:HD2	75:h1:1360:G:OP1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Aa:84:TYR:HB2	72:Aa:199:ILE:HD11	1.94	0.50
75:h1:30:G:H2'	75:h1:31:C:C6	2.47	0.50
75:h1:65:A:H61	75:h1:84:G:H3'	1.76	0.50
77:Ba:62:LYS:HB2	77:Ba:87:VAL:HG12	1.92	0.50
2:A:729:A:OP1	41:Ha:130:THR:HB	2.10	0.50
2:A:1021:G:H22	2:A:1050:A:H2	1.59	0.50
2:A:1183:G:P	86:A:4240:HOH:O	2.69	0.50
13:AX:68:LYS:HB3	13:AX:71:ARG:HB2	1.93	0.50
19:Ka:33:ARG:HH12	19:Ka:36:VAL:HA	1.77	0.50
21:BD:92:GLU:OE1	21:BD:95:GLY:HA3	2.11	0.50
53:AA:166:GLU:HB3	53:AA:200:PRO:HB3	1.92	0.50
75:h1:609:G:H5'	75:h1:615:G:N2	2.26	0.50
75:h1:1610:U:C5'	86:h1:2307:HOH:O	2.59	0.50
2:A:2455:G:H1	2:A:2457:A:H3'	1.76	0.50
2:A:2590:G:N7	86:A:4157:HOH:O	2.34	0.50
2:A:3203:G:C8	26:AH:111:MET:HE3	2.46	0.50
86:A:6914:HOH:O	16:Ea:169:LYS:HD3	2.10	0.50
19:Ka:113:LYS:HG3	19:Ka:114:ASN:N	2.26	0.50
30:AJ:66:ARG:HD3	86:AJ:318:HOH:O	2.11	0.50
39:BG:85:SER:O	39:BG:89:ILE:HG13	2.12	0.50
51:AB:140:ARG:HH11	51:AB:141:GLN:HA	1.76	0.50
51:AB:145:ILE:CD1	75:h1:771:C:H1'	2.41	0.50
63:AQ:89:ILE:O	63:AQ:91:LYS:NZ	2.42	0.50
63:AQ:90:LEU:HB2	63:AQ:97:MET:HE2	1.93	0.50
67:BB:35:LEU:HD21	67:BB:50:ILE:HG23	1.93	0.50
75:h1:371:U:O2'	75:h1:372:A:OP1	2.26	0.50
75:h1:1071:G:N7	86:h1:2265:HOH:O	2.35	0.50
2:A:710:G:H5''	2:A:711:U:C5	2.46	0.50
2:A:2767:U:H2'	2:A:2768:A:H8	1.76	0.50
2:A:3174:C:N4	32:BH:172:LEU:HD13	2.27	0.50
10:Ma:58:VAL:HG13	65:Ua:124:LYS:HB3	1.94	0.50
16:Ea:101:VAL:O	16:Ea:104:GLU:HG3	2.12	0.50
28:AV:106:ARG:HD3	86:AV:322:HOH:O	2.11	0.50
33:Da:46:THR:HB	33:Da:86:GLU:CD	2.37	0.50
41:Ha:79:TRP:CZ2	41:Ha:118:LYS:HB3	2.46	0.50
59:Ta:139:ARG:HG2	59:Ta:140:ALA:H	1.77	0.50
75:h1:627:C:H2'	75:h1:628:U:C6	2.47	0.50
75:h1:826:A:H61	75:h1:849:U:H3	1.59	0.50
2:A:2757:A:N7	86:A:4181:HOH:O	2.35	0.50
24:AC:47:THR:HG22	24:AC:78:ASP:HB2	1.94	0.50
62:Za:169:ASN:C	62:Za:175:ILE:HD11	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:Ua:150:LEU:HD23	75:h1:1789:U:OP1	2.12	0.50
75:h1:428:G:C1'	86:h1:2426:HOH:O	2.56	0.50
75:h1:1145:U:H2'	75:h1:1146:U:C6	2.47	0.50
2:A:609:A:H4'	2:A:610:G:O5'	2.11	0.50
2:A:3059:G:O6	86:A:3886:HOH:O	2.20	0.50
16:Ea:103:GLU:OE2	16:Ea:118:SER:OG	2.29	0.50
32:BH:56:LYS:O	32:BH:60:MET:HG2	2.12	0.50
47:AO:9:ARG:NH1	47:AO:30:VAL:O	2.43	0.50
53:AA:105:LEU:O	53:AA:109:LEU:HG	2.12	0.50
70:BL:107:GLN:O	70:BL:110:THR:HG22	2.11	0.50
2:A:989:A:HO2'	2:A:991:G:H8	1.59	0.50
23:AM:100:ARG:HB3	23:AM:103:GLU:HG2	1.94	0.50
24:AC:141:MET:HE2	24:AC:160:LEU:HD11	1.94	0.50
29:AD:138:ALA:HB3	29:AD:204:ARG:HB3	1.93	0.50
50:Na:76:THR:OG1	50:Na:79:CYS:SG	2.70	0.50
57:AF:30:LEU:HD12	57:AF:66:ASN:ND2	2.27	0.50
75:h1:558:A:HO2'	75:h1:591:C:HO2'	1.58	0.50
1:3:116:U:H4'	86:3:450:HOH:O	2.12	0.49
2:A:63:A:H3'	86:A:8121:HOH:O	2.11	0.49
2:A:2094:A:H2'	2:A:2095:G:O4'	2.11	0.49
2:A:2680:U:H2'	2:A:2681:OMC:H6	1.76	0.49
26:AH:102:LEU:HD11	32:BH:204:ILE:HG21	1.93	0.49
35:AT:77:ASN:OD1	35:AT:77:ASN:N	2.45	0.49
57:AF:11:CYS:SG	57:AF:90:ALA:HA	2.52	0.49
58:Wa:81:ASP:HB3	58:Wa:95:TYR:CD2	2.47	0.49
62:Za:97:TYR:CE2	62:Za:201:VAL:HG11	2.47	0.49
70:BL:31:LEU:HD22	70:BL:31:LEU:H	1.77	0.49
19:Ka:113:LYS:O	19:Ka:117:LYS:HG3	2.12	0.49
42:BU:135:ARG:NH2	42:BU:160:ASP:OD2	2.45	0.49
75:h1:298:U:H2'	75:h1:299:U:C6	2.48	0.49
2:A:419:A:N1	2:A:2360:C:O2'	2.38	0.49
2:A:1458:A2M:HM'3	86:A:8467:HOH:O	2.11	0.49
19:Ka:62:PHE:CE1	19:Ka:73:GLY:HA3	2.47	0.49
44:Xa:9:PHE:CD2	72:Aa:191:GLU:HG3	2.46	0.49
46:BJ:139:ARG:NH1	86:BJ:402:HOH:O	2.29	0.49
65:Ua:137:ASP:OD1	75:h1:930:A:C8	2.65	0.49
68:AN:79:LYS:HG2	68:AN:111:TYR:CE2	2.47	0.49
69:Ra:62:VAL:HA	69:Ra:94:ILE:O	2.12	0.49
75:h1:1200:G:OP1	86:h1:2156:HOH:O	2.20	0.49
2:A:820:U:OP1	86:A:3869:HOH:O	2.18	0.49
2:A:909:G:H1'	2:A:1590:A:N6	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:979:U:OP2	86:A:3887:HOH:O	2.20	0.49
15:Ja:176:ASP:HA	15:Ja:198:ARG:HH22	1.77	0.49
29:AD:91:ARG:NH2	75:h1:1530:U:OP1	2.45	0.49
38:BN:130:GLY:HA2	86:BN:212:HOH:O	2.12	0.49
66:Ya:20:PHE:HD2	66:Ya:27:LEU:HG	1.78	0.49
75:h1:309:G:N7	86:h1:2268:HOH:O	2.35	0.49
2:A:2162:C:OP2	86:A:3878:HOH:O	2.18	0.49
2:A:2688:G:N3	2:A:2688:G:H2'	2.27	0.49
3:i2:20:G:H3'	3:i2:20:G:N3	2.28	0.49
22:BS:47:MET:HE2	22:BS:182:MET:HG2	1.94	0.49
59:Ta:156:ARG:HG2	75:h1:79:A:H8	1.66	0.49
72:Aa:140:ASN:HB2	75:h1:190:A:C2	2.48	0.49
75:h1:1176:PSU:H2'	75:h1:1177:G:C8	2.48	0.49
2:A:991:G:H1	2:A:1111:G:H2'	1.78	0.49
2:A:1616:C:H2'	2:A:1617:G:C8	2.47	0.49
2:A:3341:C:H4'	2:A:3342:U:H3'	1.93	0.49
4:C3:24:U:H2'	4:C3:25:G:O4'	2.13	0.49
16:Ea:6:TYR:OH	39:BG:138:GLU:OE2	2.22	0.49
23:AM:17:ARG:NH2	23:AM:23:GLY:O	2.45	0.49
49:AK:170:ARG:NH1	75:h1:817:A:N3	2.60	0.49
49:AK:170:ARG:NH1	75:h1:817:A:H2'	2.14	0.49
51:AB:19:ARG:HB2	51:AB:22:GLU:HG3	1.95	0.49
58:Wa:108:ARG:HH11	58:Wa:108:ARG:HG3	1.77	0.49
61:BE:71:MET:HE1	86:BE:221:HOH:O	2.11	0.49
62:Za:132:ARG:NH2	62:Za:155:ASP:O	2.45	0.49
66:Ya:116:MET:HB3	66:Ya:124:PHE:CZ	2.48	0.49
68:AN:35:GLU:HG3	68:AN:37:ALA:H	1.78	0.49
75:h1:890:U:H2'	75:h1:891:U:C6	2.48	0.49
75:h1:1028:A:OP1	75:h1:1793:G:O2'	2.26	0.49
75:h1:1594:G:H2'	75:h1:1595:A:H8	1.76	0.49
75:h1:1644:G:H2'	75:h1:1645:U:H6	1.78	0.49
2:A:1953:U:H2'	2:A:1954:G:H8	1.77	0.49
15:Ja:42:LEU:HD12	15:Ja:43:PRO:HD2	1.94	0.49
59:Ta:163:ARG:HG2	59:Ta:177:ALA:HB2	1.95	0.49
65:Ua:137:ASP:OD2	75:h1:929:G:C4'	2.60	0.49
75:h1:592:C:H2'	75:h1:593:A:H8	1.77	0.49
75:h1:1171:G:C2	75:h1:1172:A:C8	3.00	0.49
2:A:582:A:H2'	2:A:583:C:C6	2.48	0.49
2:A:733:G:O6	86:A:3875:HOH:O	2.18	0.49
2:A:3225:C:O2'	2:A:3226:G:OP1	2.27	0.49
12:AE:49:GLU:O	12:AE:64:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ja:21:ASP:HB2	75:h1:776:C:OP1	2.12	0.49
17:AL:19:GLU:OE1	17:AL:19:GLU:N	2.45	0.49
17:AL:95:GLU:HB3	17:AL:141:THR:HG21	1.94	0.49
20:AW:107:MET:HE3	52:BF:221:PRO:HB3	1.93	0.49
37:BP:36:VAL:HG21	38:BN:77:TYR:CD1	2.47	0.49
54:AG:170:GLU:HG2	54:AG:171:MET:N	2.28	0.49
74:Ca:2:GLY:O	74:Ca:6:VAL:HG13	2.12	0.49
75:h1:474:U:H2'	75:h1:475:A:H8	1.76	0.49
75:h1:1544:G:N2	75:h1:1570:C:H1'	2.28	0.49
2:A:544:C:C2'	2:A:545:U:H5'	2.43	0.49
2:A:985:U:H2'	2:A:986:C:O4'	2.13	0.49
2:A:1117:U:H2'	2:A:1118:C:C6	2.47	0.49
86:A:8756:HOH:O	38:BN:121:LYS:CD	2.35	0.49
11:Ia:150:ASP:HB3	11:Ia:190:ILE:HD11	1.94	0.49
13:AX:40:THR:HG23	16:Ea:5:LYS:HE2	1.95	0.49
15:Ja:54:TYR:OH	15:Ja:97:GLU:OE1	2.23	0.49
34:BK:83:LEU:HD13	34:BK:88:LEU:HD23	1.95	0.49
51:AB:78:LEU:O	51:AB:82:MET:HG2	2.13	0.49
66:Ya:25:VAL:HG12	66:Ya:30:LEU:HG	1.94	0.49
69:Ra:44:LEU:HD13	69:Ra:73:PHE:CZ	2.48	0.49
71:La:61:ILE:HB	71:La:102:TYR:HB2	1.94	0.49
1:3:56:A:H3'	86:3:440:HOH:O	2.12	0.49
2:A:991:G:N1	2:A:1111:G:H2'	2.28	0.49
24:AC:24:LEU:HD11	24:AC:44:VAL:HG21	1.94	0.49
27:BT:137:ALA:C	86:BT:537:HOH:O	2.56	0.49
51:AB:81:ARG:NH1	75:h1:766:G:OP2	2.46	0.49
58:Wa:124:ARG:NE	58:Wa:130:ARG:O	2.45	0.49
75:h1:94:A:H61	75:h1:398:G:H1'	1.78	0.49
75:h1:1648:C:H2'	75:h1:1649:U:C6	2.48	0.49
1:3:11:U:H2'	1:3:12:C:C6	2.47	0.48
2:A:2504:A:H2'	2:A:2505:U:C6	2.48	0.48
17:AL:84:GLN:HB2	17:AL:89:TYR:CE2	2.46	0.48
17:AL:154:VAL:HA	17:AL:178:MET:SD	2.53	0.48
22:BS:215:ASP:OD2	22:BS:357:GLU:HA	2.12	0.48
57:AF:96:GLN:HG3	57:AF:104:LYS:HG3	1.94	0.48
67:BB:71:LEU:O	67:BB:75:GLU:HG3	2.13	0.48
75:h1:1434:C:O2'	75:h1:1440:U:O4	2.31	0.48
75:h1:1785:MA6:H8	75:h1:1785:MA6:O5'	2.13	0.48
3:W2:67:C:H2'	3:W2:68:A:H8	1.77	0.48
2:A:174:G:C4	2:A:175:A:C8	3.02	0.48
2:A:1766:G:N2	2:A:1768:G:O2'	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2618:OMG:HM23	2:A:2618:OMG:H1'	1.61	0.48
16:Ea:119:TYR:OH	16:Ea:131:GLU:OE1	2.18	0.48
19:Ka:113:LYS:NZ	75:h1:57:G:O5'	2.45	0.48
29:AD:29:VAL:HG13	29:AD:35:VAL:HG22	1.95	0.48
29:AD:56:TYR:HB3	29:AD:63:LYS:HA	1.95	0.48
35:AT:98:PRO:HB3	35:AT:104:ILE:HD12	1.95	0.48
43:BR:240:ASN:O	43:BR:244:ARG:HG2	2.13	0.48
63:AQ:74:LYS:O	63:AQ:78:GLN:NE2	2.46	0.48
72:Aa:156:ASP:HB3	72:Aa:159:ILE:HG22	1.94	0.48
75:h1:321:U:H4'	75:h1:325:A:C8	2.48	0.48
2:A:988:G:H4'	2:A:989:A:C4	2.49	0.48
2:A:1423:G:N7	86:A:4194:HOH:O	2.35	0.48
86:A:7274:HOH:O	43:BR:201:LYS:HE3	2.13	0.48
6:BM:45:LYS:HB3	6:BM:45:LYS:HZ2	1.78	0.48
17:AL:98:ASP:OD2	17:AL:107:GLN:NE2	2.45	0.48
66:Ya:35:THR:O	66:Ya:39:VAL:HG13	2.13	0.48
67:BB:57:LEU:O	67:BB:61:ILE:HG13	2.14	0.48
75:h1:306:U:H2'	75:h1:307:C:C6	2.48	0.48
75:h1:940:A:H2'	75:h1:941:A:C8	2.47	0.48
2:A:1630:U:H2'	2:A:1631:G:C4	2.48	0.48
2:A:2417:A:H2'	2:A:2418:C:C6	2.47	0.48
32:BH:145:ARG:O	32:BH:149:GLU:HG2	2.13	0.48
66:Ya:91:VAL:HG13	66:Ya:92:PRO:HD2	1.94	0.48
75:h1:822:U:H2'	75:h1:823:U:C6	2.48	0.48
2:A:280:G:OP1	82:A:3401:TER:N1	2.42	0.48
2:A:459:A:H2'	2:A:460:A:C8	2.49	0.48
2:A:1787:C:OP1	86:A:3888:HOH:O	2.20	0.48
2:A:2116:A:OP1	86:A:3890:HOH:O	2.20	0.48
2:A:2156:G:N7	31:BQ:152:SER:OG	2.42	0.48
2:A:2361:A:N7	86:A:4192:HOH:O	2.35	0.48
2:A:3177:A:H2'	2:A:3178:G:C8	2.48	0.48
2:A:3317:A:H3'	86:A:4086:HOH:O	2.13	0.48
7:BO:54:GLU:HB2	7:BO:107:LYS:HB3	1.94	0.48
51:AB:5:ARG:HD2	75:h1:39:A:OP2	2.13	0.48
53:AA:5:ILE:HG23	53:AA:9:ARG:HB2	1.95	0.48
75:h1:875:C:H2'	75:h1:876:G:C8	2.48	0.48
75:h1:973:G:N7	86:h1:2262:HOH:O	2.35	0.48
2:A:1230:A:H4'	2:A:1232:G:H5''	1.96	0.48
53:AA:133:GLY:HA3	53:AA:156:TYR:O	2.13	0.48
59:Ta:41:LEU:HB3	59:Ta:45:PHE:CZ	2.49	0.48
69:Ra:10:LYS:HD3	69:Ra:14:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:BL:111:MET:HE3	70:BL:113:ILE:HG13	1.96	0.48
72:Aa:75:ARG:HB2	72:Aa:110:PHE:CE1	2.49	0.48
75:h1:117:U:H2'	75:h1:118:U:C6	2.48	0.48
2:A:1396:G:N7	86:A:4196:HOH:O	2.35	0.48
4:C3:12:U:OP2	4:C3:67:C:O2'	2.23	0.48
54:AG:56:VAL:HG22	54:AG:155:ILE:HG12	1.95	0.48
72:Aa:39:SER:OG	72:Aa:40:SER:N	2.45	0.48
75:h1:1452:U:H2'	75:h1:1453:U:H6	1.79	0.48
2:A:1897:A:O2'	2:A:3051:G:H4'	2.13	0.48
2:A:2610:U:H2'	2:A:2611:U:C6	2.49	0.48
2:A:2682:U:H2'	2:A:2683:C:C6	2.48	0.48
2:A:3158:C:H2'	2:A:3159:G:H8	1.78	0.48
19:Ka:88:GLU:OE2	19:Ka:92:ARG:HD2	2.14	0.48
20:AW:54:MET:HE2	20:AW:90:PHE:CZ	2.49	0.48
31:BQ:206:PRO:HG3	31:BQ:213:GLY:HA3	1.95	0.48
45:BV:204:ILE:O	75:h1:1065:G:O2'	2.32	0.48
57:AF:106:GLU:O	57:AF:110:ILE:HG12	2.14	0.48
63:AQ:3:THR:O	63:AQ:4:VAL:HB	2.12	0.48
67:BB:17:ILE:HG13	67:BB:58:MET:HE2	1.95	0.48
70:BL:125:THR:OG1	70:BL:126:SER:N	2.47	0.48
75:h1:448:A:N1	75:h1:463:G:O2'	2.43	0.48
75:h1:889:U:H2'	75:h1:890:U:C6	2.49	0.48
75:h1:1595:A:H2'	75:h1:1596:G:H8	1.79	0.48
2:A:795:A:H4'	2:A:796:G:H5'	1.94	0.48
2:A:1137:U:H2'	2:A:1138:A:O4'	2.13	0.48
2:A:2206:A:H2'	2:A:2207:U:C6	2.49	0.48
2:A:2362:G:H22	2:A:2394:G:H1'	1.79	0.48
2:A:2367:G:H2'	2:A:2368:G:C8	2.48	0.48
2:A:2888:C:H41	2:A:2910:A2M:H2	1.79	0.48
3:i2:70:C:H2'	3:i2:71:G:C8	2.48	0.48
11:Ia:92:ARG:HD3	11:Ia:94:LYS:NZ	2.29	0.48
67:BB:7:LYS:HG3	75:h1:1317:C:H5'	1.96	0.48
72:Aa:77:THR:HB	72:Aa:109:PRO:HG2	1.95	0.48
75:h1:336:G:H2'	75:h1:337:PSU:H6	1.79	0.48
75:h1:516:G:O2'	75:h1:517:A:H8	1.96	0.48
75:h1:1780:A:H2'	75:h1:1781:G:H8	1.76	0.48
75:h1:1791:C:H2'	75:h1:1792:G:C8	2.49	0.48
2:A:801:C:H2'	2:A:802:C:C6	2.49	0.48
3:i2:25:C:C2	3:i2:26:G:C8	3.01	0.48
15:Ja:80:LYS:HG2	15:Ja:81:THR:HG23	1.96	0.48
22:BS:86:VAL:HG13	22:BS:162:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:AV:30:LYS:CG	86:AV:365:HOH:O	2.62	0.48
28:AV:30:LYS:HG3	86:AV:365:HOH:O	2.14	0.48
29:AD:18:LEU:HD11	29:AD:50:PRO:HD3	1.96	0.48
44:XA:47:ARG:HH12	75:h1:847:G:C2'	2.26	0.48
49:AK:93:VAL:HG13	86:AK:303:HOH:O	2.14	0.48
49:AK:163:ARG:NH1	75:h1:817:A:O5'	2.47	0.48
60:AZ:14:THR:HA	60:AZ:17:ARG:HG3	1.96	0.48
65:UA:136:THR:O	75:h1:886:G:N2	2.35	0.48
67:BB:102:THR:HA	67:BB:105:MET:HG3	1.96	0.48
68:AN:29:VAL:HG21	68:AN:36:ILE:HD11	1.95	0.48
75:h1:1477:G:C2	75:h1:1478:A:C5	3.02	0.48
75:h1:1593:C:H2'	75:h1:1594:G:C8	2.49	0.48
75:h1:1720:G:H2'	75:h1:1721:C:C6	2.48	0.48
2:A:286:A:OP1	16:Ea:171:ASN:ND2	2.47	0.47
2:A:2216:G:H2'	2:A:2217:A:H8	1.78	0.47
2:A:2450:G:H5'	2:A:2452:G:OP2	2.13	0.47
2:A:2696:A:H2'	2:A:2697:G:C8	2.49	0.47
2:A:2894:G:O2'	55:Ga:100:TYR:O	2.31	0.47
29:AD:102:LEU:O	71:La:59:LYS:NZ	2.39	0.47
38:BN:66:ARG:NH1	86:BN:202:HOH:O	2.45	0.47
46:BJ:193:ASP:HB3	46:BJ:196:ASN:HB2	1.95	0.47
51:AB:129:VAL:HG13	51:AB:133:GLN:NE2	2.28	0.47
59:Ta:85:ARG:N	75:h1:159:U:OP1	2.47	0.47
75:h1:621:A2M:HM'3	75:h1:621:A2M:H1'	1.69	0.47
75:h1:940:A:N7	86:h1:2226:HOH:O	2.36	0.47
75:h1:1350:G:H2'	75:h1:1351:C:C6	2.49	0.47
75:h1:1354:C:H2'	75:h1:1355:G:H8	1.79	0.47
2:A:1629:U:O2'	2:A:1631:G:OP1	2.23	0.47
2:A:2117:C:H2'	2:A:2118:A:O4'	2.14	0.47
2:A:3101:A:H2'	2:A:3102:U:O4'	2.14	0.47
82:A:3401:TER:H112	86:A:6380:HOH:O	2.13	0.47
7:BO:30:MET:HB3	7:BO:100:PRO:HG2	1.95	0.47
15:Ja:64:ILE:CG1	19:Ka:19:LEU:HD21	2.43	0.47
27:BT:65:HIS:HA	27:BT:97:PHE:HE1	1.79	0.47
51:AB:78:LEU:HD12	51:AB:82:MET:HE3	1.96	0.47
51:AB:94:LYS:HD2	51:AB:97:TYR:HE2	1.79	0.47
53:AA:103:GLU:OE1	53:AA:173:ARG:NH1	2.47	0.47
57:AF:88:ALA:O	57:AF:92:VAL:HG22	2.14	0.47
59:Ta:196:ILE:HD11	75:h1:176:A:C4	2.49	0.47
62:Za:13:SER:O	62:Za:16:GLU:HG2	2.14	0.47
62:Za:25:ALA:HB3	62:Za:27:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ya:65:LEU:HD13	66:Ya:94:MET:HG2	1.95	0.47
75:h1:355:A:C2'	86:h1:2146:HOH:O	2.61	0.47
75:h1:389:A:O2'	86:h1:2162:HOH:O	2.20	0.47
75:h1:879:G:H1'	86:h1:2224:HOH:O	2.13	0.47
2:A:1510:U:O2'	2:A:1511:G:H5'	2.15	0.47
2:A:2841:U:O2	2:A:2841:U:H2'	2.14	0.47
2:A:3215:A:H2'	2:A:3216:A:O4'	2.14	0.47
3:i2:1:G:H2'	3:i2:2:C:H6	1.80	0.47
8:AR:33:ARG:HD3	86:AR:229:HOH:O	2.13	0.47
27:BT:245:LYS:HD3	86:BT:639:HOH:O	2.13	0.47
45:BV:124:HIS:HA	45:BV:137:MET:O	2.15	0.47
46:BJ:133:GLN:HA	86:BJ:431:HOH:O	2.13	0.47
58:Wa:75:ARG:O	58:Wa:75:ARG:HD3	2.14	0.47
62:Za:16:GLU:HA	62:Za:19:VAL:HG22	1.96	0.47
62:Za:41:TYR:OH	62:Za:61:LYS:NZ	2.43	0.47
69:Ra:114:PRO:HB2	69:Ra:117:ARG:HG2	1.96	0.47
75:h1:96:G:N7	86:h1:2266:HOH:O	2.35	0.47
75:h1:748:U:H2'	75:h1:749:A:H8	1.80	0.47
75:h1:1432:G:H2'	75:h1:1433:U:C6	2.49	0.47
2:A:2428:A:H2'	2:A:2429:C:C6	2.49	0.47
2:A:3193:C:OP2	2:A:3194:C:N4	2.42	0.47
82:A:3401:TER:H122	86:A:8158:HOH:O	2.14	0.47
16:Ea:135:VAL:HG21	16:Ea:151:ILE:HG21	1.97	0.47
20:AW:48:TRP:CD1	86:AW:237:HOH:O	2.68	0.47
21:BD:8:LYS:NZ	86:BD:306:HOH:O	2.46	0.47
24:AC:177:LYS:HD2	86:AC:407:HOH:O	2.14	0.47
26:AH:93:LEU:HD22	26:AH:93:LEU:H	1.79	0.47
69:Ra:8:ILE:HD13	69:Ra:46:ILE:HD11	1.96	0.47
72:Aa:62:ASP:OD1	72:Aa:63:THR:N	2.48	0.47
75:h1:1309:G:H2'	75:h1:1310:G:H8	1.78	0.47
75:h1:1335:U:O2'	77:Ba:86:ARG:NH2	2.44	0.47
77:Ba:24:ARG:HH11	77:Ba:24:ARG:HG2	1.79	0.47
77:Ba:98:PRO:O	77:Ba:101:VAL:HG12	2.13	0.47
2:A:569:C:O2'	2:A:570:G:H5'	2.15	0.47
2:A:1854:G:H1'	73:AY:9:GLY:HA3	1.95	0.47
2:A:3071:A:H2'	2:A:3072:G:O4'	2.14	0.47
19:Ka:89:PRO:HG2	19:Ka:92:ARG:HB2	1.96	0.47
41:Ha:100:VAL:HB	41:Ha:105:PHE:HB2	1.96	0.47
57:AF:131:PHE:HD2	77:Ba:82:ARG:HH21	1.63	0.47
62:Za:57:LYS:O	62:Za:61:LYS:HG2	2.15	0.47
72:Aa:58:ALA:HB2	72:Aa:180:GLY:HA2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:29:U:H2'	75:h1:30:G:C8	2.48	0.47
75:h1:1088:A:H2'	75:h1:1089:A:C8	2.50	0.47
75:h1:1261:OMU:HM22	75:h1:1262:A:H5'	1.95	0.47
75:h1:1345:A:H2'	75:h1:1346:A:C8	2.49	0.47
2:A:1953:U:H2'	2:A:1954:G:C8	2.49	0.47
83:A:3403:SPD:H72	86:A:7941:HOH:O	2.13	0.47
86:A:7274:HOH:O	43:BR:201:LYS:CE	2.63	0.47
29:AD:90:VAL:O	29:AD:93:VAL:HG12	2.14	0.47
68:AN:100:ARG:CZ	68:AN:102:ILE:HD11	2.45	0.47
75:h1:464:G:OP1	86:h1:2164:HOH:O	2.21	0.47
75:h1:482:A:H2'	75:h1:483:A:H8	1.79	0.47
75:h1:1248:U:C2	75:h1:1249:C:C5	3.03	0.47
75:h1:1452:U:H2'	75:h1:1453:U:C6	2.49	0.47
3:W2:18:G:O2'	3:W2:57:G:N2	2.41	0.47
77:Ba:29:SER:HB3	77:Ba:35:LEU:HB2	1.96	0.47
2:A:174:G:H2'	2:A:175:A:C8	2.48	0.47
2:A:728:G:H5''	86:A:5697:HOH:O	2.13	0.47
2:A:925:G:H5'	2:A:926:A:OP1	2.15	0.47
2:A:1079:U:H2'	2:A:1080:C:C6	2.50	0.47
2:A:1129:A:H2'	2:A:1130:U:H6	1.80	0.47
2:A:1696:A:H2'	2:A:1697:A:C8	2.49	0.47
2:A:1705:C:OP2	86:A:3884:HOH:O	2.20	0.47
2:A:1830:C:O2'	2:A:1831:G:H5'	2.14	0.47
2:A:2691:A:N7	86:A:4211:HOH:O	2.36	0.47
2:A:3239:U:H2'	2:A:3240:U:C6	2.50	0.47
10:Ma:70:LYS:NZ	75:h1:934:A:OP1	2.47	0.47
12:AE:14:MET:HG2	12:AE:25:VAL:HG11	1.96	0.47
12:AE:79:PHE:CD1	18:Va:7:MET:HE1	2.50	0.47
39:BG:143:GLN:HG3	39:BG:195:THR:O	2.15	0.47
45:BV:70:LEU:HD21	45:BV:189:ILE:HD13	1.96	0.47
48:BW:69:ASP:HA	62:Za:64:MET:HE1	1.96	0.47
51:AB:144:ASN:OD1	75:h1:770:U:N3	2.31	0.47
54:AG:54:ARG:NE	86:AG:403:HOH:O	2.33	0.47
57:AF:95:TYR:HA	57:AF:99:VAL:HB	1.96	0.47
57:AF:99:VAL:HG12	57:AF:100:ASP:N	2.29	0.47
59:Ta:179:LYS:HG2	75:h1:79:A:C2	2.46	0.47
60:AZ:8:ILE:HG12	60:AZ:45:LEU:HD21	1.96	0.47
60:AZ:55:LYS:O	60:AZ:59:SER:OG	2.28	0.47
62:Za:136:GLN:HB3	62:Za:137:PRO:HD3	1.97	0.47
75:h1:810:A:H2'	75:h1:811:C:H6	1.80	0.47
75:h1:1079:C:H2'	75:h1:1080:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:1221:C:H2'	75:h1:1222:A:C8	2.46	0.47
75:h1:1255:U:H2'	75:h1:1256:G:C8	2.48	0.47
75:h1:1358:G:H1	75:h1:1369:U:H3	1.62	0.47
75:h1:1386:G:OP1	77:Ba:88:HIS:CD2	2.68	0.47
75:h1:1566:U:H2'	75:h1:1567:C:C6	2.50	0.47
2:A:763:G:H2'	2:A:764:A:H8	1.79	0.47
2:A:787:C:H4'	30:AJ:186:LYS:HE2	1.97	0.47
2:A:826:A2M:H5''	86:A:9304:HOH:O	2.15	0.47
2:A:1385:G:H5'	63:AQ:26:ARG:HB3	1.95	0.47
2:A:2355:A:H2'	2:A:2356:A:C8	2.50	0.47
2:A:2767:U:H2'	2:A:2768:A:C8	2.50	0.47
15:Ja:250:GLU:O	15:Ja:254:LYS:HE2	2.14	0.47
31:BQ:108:PRO:HG3	61:BE:90:ILE:HD11	1.97	0.47
45:BV:216:LYS:NZ	75:h1:887:U:OP2	2.23	0.47
46:BJ:41:LYS:HD2	46:BJ:46:PHE:CZ	2.49	0.47
46:BJ:50:VAL:HG12	46:BJ:138:VAL:HB	1.97	0.47
51:AB:161:SER:HB3	51:AB:164:SER:HB2	1.97	0.47
52:BF:41:ASN:O	52:BF:41:ASN:ND2	2.48	0.47
53:AA:167:TYR:OH	53:AA:202:THR:O	2.22	0.47
71:La:36:LYS:HE2	75:h1:1538:G:H4'	1.95	0.47
75:h1:382:U:OP1	86:h1:2157:HOH:O	2.20	0.47
3:W2:25:C:C2	3:W2:26:G:C8	3.03	0.47
78:AI:25:LYS:HD3	78:AI:59:PHE:CZ	2.49	0.47
2:A:831:G:N7	86:A:4202:HOH:O	2.36	0.47
24:AC:13:GLY:HA2	24:AC:39:ILE:HD11	1.97	0.47
27:BT:54:ARG:NH2	86:BT:508:HOH:O	2.39	0.47
69:Ra:41:LEU:HG	69:Ra:44:LEU:HD11	1.95	0.47
70:BL:32:PRO:HG3	70:BL:103:HIS:NE2	2.30	0.47
75:h1:176:A:H2'	75:h1:177:C:O4'	2.15	0.47
75:h1:1385:A:O2'	75:h1:1386:G:H8	1.97	0.47
75:h1:1492:U:O3'	86:h1:2165:HOH:O	2.21	0.47
1:3:74:G:H5''	7:BO:27:ARG:CZ	2.45	0.47
2:A:168:G:C2	2:A:245:A:N1	2.84	0.47
11:Ia:20:VAL:HG22	11:Ia:25:ILE:HG13	1.97	0.47
39:BG:87:PHE:CE2	39:BG:179:ARG:HG2	2.50	0.47
62:Za:141:GLY:HA2	62:Za:146:ILE:HD12	1.96	0.47
75:h1:1270:OMU:H5''	75:h1:1270:OMU:H6	1.96	0.47
2:A:418:G:O6	32:BH:73:HIS:HE1	1.98	0.46
14:AP:40:HIS:HD2	14:AP:74:LEU:HD22	1.79	0.46
14:AP:81:MET:HE3	14:AP:82:PRO:HD2	1.96	0.46
29:AD:167:LYS:HE3	29:AD:172:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BA:43:HIS:CE1	56:BA:45:ARG:HB2	2.50	0.46
59:Ta:28:PHE:O	59:Ta:29:ASP:HB3	2.15	0.46
63:AQ:71:ALA:HA	63:AQ:86:ASN:O	2.15	0.46
70:BL:65:VAL:HG11	70:BL:114:VAL:HG22	1.95	0.46
78:AI:16:PHE:HE1	78:AI:86:VAL:HG12	1.79	0.46
2:A:192:U:H2'	2:A:193:G:O4'	2.15	0.46
2:A:239:U:H2'	2:A:240:G:H8	1.80	0.46
2:A:1630:U:O5'	86:A:3893:HOH:O	2.21	0.46
2:A:1697:A:OP1	40:Fa:21:ARG:NH2	2.48	0.46
15:Ja:240:LYS:HA	15:Ja:240:LYS:HD3	1.78	0.46
54:AG:5:ASN:HB2	86:AG:404:HOH:O	2.14	0.46
58:Wa:121:ARG:NH2	75:h1:1549:A:OP2	2.38	0.46
62:Za:91:VAL:HG12	62:Za:179:PHE:CZ	2.50	0.46
75:h1:52:U:H2'	75:h1:53:G:H8	1.80	0.46
75:h1:1196:C:H3'	86:h1:2462:HOH:O	2.15	0.46
2:A:371:A:N3	2:A:373:G:H5''	2.31	0.46
2:A:461:C:H2'	2:A:462:G:C8	2.48	0.46
2:A:528:C:C2	2:A:529:C:C5	3.04	0.46
2:A:905:A:H5'	31:BQ:183:GLY:HA2	1.96	0.46
2:A:1129:A:H2'	2:A:1130:U:C6	2.50	0.46
2:A:2565:G:H2'	2:A:2566:C:C6	2.50	0.46
4:C3:26:C:H2'	4:C3:27:A:O4'	2.15	0.46
15:Ja:146:THR:HG21	75:h1:124:G:H21	1.80	0.46
29:AD:75:SER:O	29:AD:155:THR:HG21	2.15	0.46
33:Da:56:ASP:OD2	50:Na:53:GLN:N	2.46	0.46
44:Xa:68:ARG:NE	86:Xa:203:HOH:O	2.47	0.46
52:BF:220:LYS:HB3	52:BF:222:HIS:CE1	2.51	0.46
59:Ta:3:PHE:HD2	59:Ta:113:LEU:HD21	1.80	0.46
62:Za:48:ASP:OD1	62:Za:49:GLY:N	2.48	0.46
69:Ra:102:MET:HG3	69:Ra:117:ARG:HB3	1.97	0.46
72:Aa:34:ALA:HB2	72:Aa:57:ARG:HG3	1.96	0.46
75:h1:29:U:O4	86:h1:2152:HOH:O	2.18	0.46
75:h1:810:A:H2'	75:h1:811:C:C6	2.50	0.46
75:h1:1108:G:O2'	75:h1:1109:G:H5'	2.15	0.46
75:h1:1579:A:H1'	86:h1:2308:HOH:O	2.14	0.46
75:h1:1680:C:H2'	75:h1:1681:G:O4'	2.16	0.46
75:h1:1728:U:H2'	75:h1:1729:C:C6	2.51	0.46
2:A:243:G:H2'	2:A:244:C:C6	2.50	0.46
2:A:944:U:OP1	86:A:3892:HOH:O	2.21	0.46
2:A:3005:U:H2'	2:A:3006:A:C8	2.50	0.46
2:A:3205:G:N3	2:A:3208:G:H2'	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:A:6804:HOH:O	32:BH:96:LYS:HE3	2.15	0.46
22:BS:230:GLU:OE2	86:BS:503:HOH:O	2.20	0.46
62:Za:34:CYS:HB2	62:Za:51:TYR:CD2	2.51	0.46
62:Za:36:TYR:CD1	75:h1:1041:G:H4'	2.50	0.46
78:AI:53:GLU:HG3	78:AI:53:GLU:O	2.15	0.46
2:A:1034:C:H2'	2:A:1035:G:C8	2.50	0.46
2:A:2212:A2M:HM'3	2:A:2212:A2M:H1'	1.73	0.46
2:A:2364:C:OP1	86:A:3895:HOH:O	2.21	0.46
2:A:2654:U:H4'	2:A:2655:A:O4'	2.14	0.46
2:A:2780:U:H4'	54:AG:195:LYS:HD2	1.97	0.46
17:AL:173:LYS:HE3	17:AL:173:LYS:HB2	1.66	0.46
24:AC:16:VAL:HG21	24:AC:39:ILE:HG23	1.96	0.46
29:AD:31:ASP:O	29:AD:35:VAL:HG23	2.15	0.46
33:Da:49:GLN:HG2	86:Da:224:HOH:O	2.14	0.46
49:AK:66:MET:HE3	49:AK:70:LYS:HD2	1.97	0.46
67:BB:35:LEU:HD23	67:BB:47:ARG:HG3	1.98	0.46
69:Ra:41:LEU:HD23	69:Ra:41:LEU:O	2.16	0.46
75:h1:87:A:H2'	75:h1:88:C:H6	1.80	0.46
75:h1:520:A:O2'	75:h1:521:C:H5''	2.16	0.46
75:h1:1121:U:H2'	75:h1:1122:C:C6	2.51	0.46
75:h1:1334:C:H2'	75:h1:1335:U:C6	2.50	0.46
75:h1:1344:U:H2'	75:h1:1345:A:C8	2.51	0.46
75:h1:1619:U:H2'	75:h1:1620:C:C6	2.51	0.46
1:3:151:C:H2'	1:3:152:C:H6	1.80	0.46
2:A:575:C:OP2	52:BF:75:PRO:HD3	2.15	0.46
17:AL:64:ASN:HB3	27:BT:386:MET:HE3	1.96	0.46
19:Ka:30:HIS:NE2	19:Ka:71:SER:OG	2.42	0.46
22:BS:110:LEU:O	22:BS:115:ARG:NH1	2.47	0.46
27:BT:12:ILE:HD13	27:BT:260:LYS:CD	2.46	0.46
28:AV:85:LEU:HD21	63:AQ:35:LYS:HG3	1.96	0.46
29:AD:51:HIS:HA	29:AD:86:LYS:HE2	1.97	0.46
58:Wa:81:ASP:HB3	58:Wa:95:TYR:HD2	1.79	0.46
75:h1:963:C:H2'	75:h1:964:A:O4'	2.16	0.46
75:h1:1686:G:H2'	75:h1:1687:C:C6	2.51	0.46
78:AI:1:MET:HE1	78:AI:41:GLN:HG2	1.97	0.46
2:A:1427:A:OP1	86:A:3894:HOH:O	2.21	0.46
2:A:1730:A:N6	61:BE:42:CYS:HA	2.30	0.46
16:Ea:20:ARG:HG2	16:Ea:20:ARG:HH11	1.81	0.46
50:Na:13:PRO:HB2	50:Na:16:LEU:HD13	1.97	0.46
60:AZ:12:LEU:HD13	60:AZ:16:ARG:NH2	2.31	0.46
75:h1:1072:C:H2'	75:h1:1073:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:1114:A:OP1	86:h1:2155:HOH:O	2.20	0.46
75:h1:1334:C:H2'	75:h1:1335:U:H6	1.81	0.46
75:h1:1466:C:H5''	86:h1:2510:HOH:O	2.15	0.46
75:h1:1787:C:OP1	86:h1:2166:HOH:O	2.21	0.46
2:A:466:C:O2'	2:A:467:A:O4'	2.34	0.46
2:A:858:C:H2'	2:A:859:U:C6	2.50	0.46
2:A:1675:G:H2'	2:A:1676:A:C8	2.50	0.46
2:A:3021:U:H2'	2:A:3022:A:H8	1.81	0.46
9:AU:15:GLU:HG3	9:AU:115:ILE:HD11	1.97	0.46
14:AP:114:LYS:O	14:AP:118:GLU:HG3	2.16	0.46
23:AM:140:MET:SD	43:BR:74:ALA:HB2	2.56	0.46
24:AC:27:ILE:HA	24:AC:32:LEU:HD12	1.96	0.46
26:AH:36:ALA:HB2	26:AH:50:PHE:CZ	2.51	0.46
29:AD:142:SER:OG	64:Oa:44:PRO:O	2.25	0.46
62:Za:202:MET:HA	62:Za:202:MET:HE2	1.97	0.46
65:Ua:77:ALA:HB1	65:Ua:118:LEU:HG	1.98	0.46
75:h1:1652:U:P	86:h1:2550:HOH:O	2.73	0.46
2:A:896:G:H2'	2:A:897:U:C6	2.51	0.46
2:A:1838:C:O2'	2:A:1844:A:N1	2.47	0.46
2:A:2639:A2M:HM'3	2:A:2639:A2M:H1'	1.71	0.46
2:A:2968:A:N7	31:BQ:215:ASN:ND2	2.63	0.46
2:A:3005:U:H2'	2:A:3006:A:H8	1.81	0.46
9:AU:88:ASP:OD1	9:AU:89:ALA:N	2.48	0.46
29:AD:19:PHE:CD2	29:AD:94:LYS:HG3	2.51	0.46
29:AD:204:ARG:HE	65:Ua:71:TYR:HB2	1.81	0.46
35:AT:101:SER:OG	35:AT:102:ASP:N	2.49	0.46
39:BG:250:GLU:OE2	45:BV:51:THR:OG1	2.30	0.46
86:Ha:264:HOH:O	54:AG:1:MET:HE3	2.15	0.46
63:AQ:95:PRO:HB2	63:AQ:96:ARG:HD2	1.97	0.46
2:A:4:A:H2'	2:A:5:C:O4'	2.16	0.46
2:A:1589:A:OP2	86:A:3896:HOH:O	2.21	0.46
4:C3:45:U:H2'	4:C3:46:C:C6	2.51	0.46
11:Ia:10:MET:HE2	11:Ia:10:MET:HB3	1.74	0.46
23:AM:52:MET:HE1	86:AM:327:HOH:O	2.16	0.46
35:AT:46:LEU:HD22	35:AT:71:HIS:HB3	1.97	0.46
43:BR:48:LEU:HD21	43:BR:52:ARG:HH21	1.81	0.46
45:BV:101:TRP:HA	45:BV:217:ILE:HD12	1.97	0.46
52:BF:98:LEU:HD11	52:BF:140:ILE:HG13	1.97	0.46
53:AA:7:LYS:HA	53:AA:10:LYS:HG2	1.98	0.46
58:Wa:40:LEU:HD22	58:Wa:97:GLN:NE2	2.24	0.46
59:Ta:14:LYS:HD3	59:Ta:125:GLY:HA3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Ta:45:PHE:HB2	59:Ta:48:TYR:HB2	1.98	0.46
72:Aa:181:ARG:HD3	86:Aa:303:HOH:O	2.16	0.46
73:AY:55:ARG:CB	86:AY:371:HOH:O	2.64	0.46
75:h1:38:OMC:HM23	75:h1:38:OMC:H1'	1.75	0.46
75:h1:884:U:H2'	75:h1:885:C:C6	2.51	0.46
75:h1:887:U:C2	75:h1:888:A:C8	3.04	0.46
75:h1:925:A:H2'	75:h1:926:G:C8	2.51	0.46
75:h1:1489:G:O6	75:h1:1525:G:N2	2.46	0.46
75:h1:1555:G:N1	75:h1:1558:A:OP2	2.49	0.46
2:A:610:G:H2'	2:A:611:C:C6	2.51	0.45
2:A:1338:C:H2'	2:A:1339:U:O4'	2.16	0.45
2:A:2095:G:H2'	2:A:2096:U:O4'	2.15	0.45
2:A:2695:A:H2'	2:A:2696:A:C8	2.51	0.45
2:A:3319:U:H2'	2:A:3320:G:O4'	2.16	0.45
86:A:8977:HOH:O	27:BT:67:THR:HG22	2.15	0.45
11:Ia:131:MET:HE3	11:Ia:137:ILE:CG2	2.41	0.45
15:Ja:42:LEU:HD21	15:Ja:51:ARG:HD2	1.98	0.45
29:AD:96:ALA:O	29:AD:100:ILE:HG13	2.16	0.45
54:AG:162:MET:HB2	54:AG:162:MET:HE3	1.74	0.45
66:Ya:34:SER:O	66:Ya:38:LEU:HG	2.16	0.45
75:h1:426:C:O2'	75:h1:428:G:OP1	2.19	0.45
75:h1:1385:A:H4'	77:Ba:58:ARG:HB3	1.96	0.45
77:Ba:58:ARG:HG3	77:Ba:90:ARG:CZ	2.46	0.45
2:A:754:C:H2'	2:A:755:C:C6	2.51	0.45
2:A:1169:A:O2'	2:A:1376:A2M:H5'	2.15	0.45
2:A:1712:U:H2'	2:A:1713:G:O4'	2.16	0.45
82:A:3401:TER:H71	86:A:5884:HOH:O	2.15	0.45
10:Ma:46:GLU:O	10:Ma:50:ILE:HG23	2.16	0.45
40:Fa:21:ARG:HD2	86:Fa:305:HOH:O	2.17	0.45
63:AQ:107:ASP:C	63:AQ:107:ASP:OD1	2.59	0.45
69:Ra:11:ASP:O	69:Ra:12:LYS:HG2	2.16	0.45
69:Ra:163:THR:HB	69:Ra:170:MET:HE1	1.98	0.45
2:A:880:U:P	86:A:4502:HOH:O	2.74	0.45
2:A:1004:G:N3	2:A:2636:A:H2'	2.32	0.45
4:C3:88:U:H2'	4:C3:89:G:O4'	2.15	0.45
29:AD:19:PHE:HE1	29:AD:49:VAL:HG12	1.81	0.45
35:AT:49:THR:HG23	35:AT:75:GLY:H	1.80	0.45
54:AG:89:ALA:HB1	54:AG:94:ILE:HB	1.99	0.45
58:Wa:125:HIS:CD2	58:Wa:131:VAL:HG11	2.51	0.45
59:Ta:211:ALA:O	59:Ta:215:LYS:HG3	2.17	0.45
62:Za:171:GLY:O	62:Za:175:ILE:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ya:33:MET:HE2	66:Ya:37:ASP:HB3	1.98	0.45
69:Ra:44:LEU:O	69:Ra:44:LEU:HD12	2.16	0.45
75:h1:332:G:H2'	75:h1:333:A:C8	2.51	0.45
75:h1:482:A:H2'	75:h1:483:A:C8	2.52	0.45
75:h1:788:C:H3'	75:h1:789:U:H5'	1.98	0.45
75:h1:821:U:H2'	75:h1:822:U:C6	2.52	0.45
75:h1:954:G:H2'	75:h1:955:G:C8	2.51	0.45
75:h1:1262:A:H2'	75:h1:1263:OMU:H6	1.98	0.45
75:h1:1481:U:C2	75:h1:1482:A:C8	3.05	0.45
2:A:51:G:H4'	2:A:821:G:H4'	1.99	0.45
2:A:2510:C:O2'	39:BG:232:MET:HE3	2.17	0.45
2:A:2659:U:H2'	2:A:2660:G:H8	1.82	0.45
2:A:2661:A:H2'	2:A:2662:G:H8	1.81	0.45
6:BM:15:CYS:SG	6:BM:151:LEU:HB2	2.56	0.45
15:Ja:58:TYR:O	15:Ja:62:ILE:HD13	2.16	0.45
19:Ka:66:PHE:O	51:AB:141:GLN:NE2	2.46	0.45
30:Aj:19:PRO:HG3	30:Aj:30:VAL:HG21	1.98	0.45
58:Wa:92:ASP:C	58:Wa:92:ASP:OD1	2.59	0.45
60:AZ:52:LYS:HA	60:AZ:55:LYS:HE3	1.97	0.45
70:BL:136:ALA:HA	70:BL:139:ILE:HG12	1.96	0.45
75:h1:534:U:H2'	75:h1:535:U:O4'	2.16	0.45
75:h1:1322:A:H4'	75:h1:1323:A:O5'	2.16	0.45
78:AI:39:ASN:O	78:AI:43:ILE:HD13	2.16	0.45
2:A:116:U:O2	2:A:119:A:H5''	2.17	0.45
2:A:242:C:H2'	2:A:243:G:C8	2.52	0.45
2:A:804:G:H2'	2:A:805:U:C6	2.51	0.45
2:A:1568:A:H5'	2:A:1569:G:OP2	2.16	0.45
15:Ja:167:ASN:ND2	75:h1:125:A:OP1	2.49	0.45
19:Ka:36:VAL:HG12	19:Ka:41:LEU:HG	1.98	0.45
22:BS:147:GLN:O	22:BS:151:GLU:HG2	2.17	0.45
40:Fa:64:ARG:NH1	86:Fa:303:HOH:O	2.28	0.45
43:BR:150:LYS:HG3	43:BR:190:ILE:HD13	1.98	0.45
63:AQ:93:GLU:O	63:AQ:97:MET:HG3	2.16	0.45
75:h1:413:C:H2'	75:h1:414:A:O4'	2.17	0.45
75:h1:1474:A:H2'	75:h1:1474:A:N3	2.31	0.45
3:W2:41:U:H2'	3:W2:42:G:H8	1.81	0.45
77:Ba:69:ARG:HH12	77:Ba:74:GLY:HA2	1.82	0.45
2:A:206:A:O2'	2:A:208:A:OP2	2.29	0.45
2:A:689:A:H4'	2:A:690:G:O5'	2.17	0.45
2:A:1032:G:H3'	2:A:1033:G:C8	2.50	0.45
2:A:3240:U:H2'	2:A:3241:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BQ:125:VAL:HG23	31:BQ:126:LEU:HG	1.98	0.45
37:BP:19:THR:O	37:BP:23:GLU:HG3	2.16	0.45
58:Wa:64:ILE:HA	58:Wa:67:LEU:HD12	1.98	0.45
72:Aa:111:LYS:HZ1	72:Aa:122:LEU:H	1.65	0.45
75:h1:1201:G:N2	86:h1:2461:HOH:O	2.50	0.45
75:h1:1649:U:H2'	75:h1:1650:C:C6	2.51	0.45
76:B1:21:U:OP2	86:B1:101:HOH:O	2.20	0.45
77:Ba:32:VAL:HG12	77:Ba:33:LYS:HE2	1.98	0.45
1:3:79:OMG:HM23	1:3:79:OMG:H1'	1.74	0.45
2:A:39:G:N7	83:A:3403:SPD:N10	2.64	0.45
2:A:466:C:O2'	2:A:467:A:O5'	2.34	0.45
12:AE:82:GLY:O	12:AE:86:ILE:HG13	2.17	0.45
22:BS:49:TYR:HB2	22:BS:171:MET:HE1	1.99	0.45
24:AC:112:ARG:H	24:AC:193:THR:HG21	1.82	0.45
49:AK:148:GLU:OE2	49:AK:151:ARG:NH2	2.36	0.45
59:Ta:163:ARG:NH2	59:Ta:175:SER:O	2.49	0.45
66:Ya:82:ARG:HB2	75:h1:1242:G:H5'	1.98	0.45
72:Aa:175:ARG:NH1	75:h1:334:U:O4	2.43	0.45
73:AY:55:ARG:HB3	86:AY:371:HOH:O	2.16	0.45
75:h1:206:U:H2'	75:h1:207:A:C8	2.51	0.45
75:h1:471:OMC:HM23	75:h1:471:OMC:H1'	1.76	0.45
75:h1:954:G:H2'	75:h1:955:G:H8	1.82	0.45
75:h1:1161:A:H3'	86:h1:2484:HOH:O	2.17	0.45
75:h1:1165:G:H2'	75:h1:1166:G:C8	2.51	0.45
2:A:945:A2M:HM'3	86:A:9342:HOH:O	2.17	0.45
2:A:1543:A:H2'	2:A:1544:A:C8	2.51	0.45
2:A:2221:A:H2'	2:A:2222:A:C8	2.52	0.45
2:A:2460:A:C6	2:A:2492:A:N6	2.85	0.45
86:A:4356:HOH:O	16:Ea:173:GLY:HA2	2.15	0.45
14:AP:13:LEU:HD12	14:AP:18:TYR:HB2	1.99	0.45
15:Ja:253:ARG:O	15:Ja:256:LEU:HG	2.16	0.45
52:BF:222:HIS:CD2	52:BF:223:GLU:HG2	2.52	0.45
58:Wa:4:VAL:O	71:La:43:PHE:HB2	2.17	0.45
70:BL:12:PRO:O	70:BL:16:VAL:HG23	2.16	0.45
75:h1:251:C:H2'	75:h1:252:A:H8	1.81	0.45
75:h1:488:G:N2	75:h1:503:U:O2	2.40	0.45
75:h1:1061:A:H2'	75:h1:1062:U:C6	2.52	0.45
75:h1:1398:C:H2'	75:h1:1399:C:H6	1.82	0.45
78:AI:69:THR:HG22	78:AI:70:ASN:H	1.81	0.45
2:A:419:A:C2	2:A:2361:A:H4'	2.52	0.45
2:A:1565:G:O2'	2:A:1582:A:N7	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2216:G:H2'	2:A:2217:A:C8	2.52	0.45
2:A:2814:OMG:H2'	2:A:2869:5MC:HM51	1.99	0.45
2:A:2945:A2M:HM'3	2:A:2945:A2M:H1'	1.74	0.45
10:Ma:65:PRO:HG2	65:Ua:128:ILE:O	2.17	0.45
24:AC:13:GLY:HA2	24:AC:39:ILE:CD1	2.47	0.45
27:BT:367:VAL:HG23	27:BT:371:GLU:HB2	1.98	0.45
29:AD:140:ASP:C	29:AD:140:ASP:OD1	2.60	0.45
36:Pa:41:ASN:O	36:Pa:46:THR:HG23	2.17	0.45
43:BR:209:PRO:HA	86:BR:422:HOH:O	2.17	0.45
49:AK:89:LEU:HB3	86:AK:338:HOH:O	2.17	0.45
51:AB:5:ARG:O	75:h1:39:A:H5''	2.17	0.45
57:AF:44:GLU:OE1	57:AF:47:ARG:NH2	2.49	0.45
57:AF:116:ARG:NH1	86:AF:201:HOH:O	2.33	0.45
59:Ta:43:GLU:OE2	59:Ta:45:PHE:HD1	1.99	0.45
67:BB:23:ARG:NH1	67:BB:23:ARG:HB3	2.31	0.45
69:Ra:26:ALA:HA	69:Ra:87:LYS:NZ	2.32	0.45
71:La:55:ALA:HA	71:La:58:PHE:CD2	2.52	0.45
75:h1:256:PSU:H2'	75:h1:257:A:H8	1.81	0.45
75:h1:1247:C:H2'	75:h1:1248:U:H6	1.82	0.45
75:h1:1649:U:H2'	75:h1:1650:C:H6	1.82	0.45
2:A:566:G:H2'	2:A:567:A:H8	1.82	0.45
11:Ia:142:LYS:HE2	11:Ia:142:LYS:HB2	1.66	0.45
15:Ja:45:VAL:HG23	15:Ja:80:LYS:O	2.16	0.45
15:Ja:172:PHE:C	15:Ja:172:PHE:CD1	2.94	0.45
19:Ka:9:ARG:N	19:Ka:9:ARG:HD2	2.32	0.45
29:AD:112:ILE:HG12	29:AD:177:LEU:HD13	1.99	0.45
39:BG:52:ILE:O	39:BG:55:GLN:HG2	2.17	0.45
45:BV:149:GLN:NE2	75:h1:1067:C:H5''	2.31	0.45
57:AF:102:GLN:O	57:AF:106:GLU:HG3	2.17	0.45
69:Ra:168:GLU:CD	69:Ra:168:GLU:N	2.74	0.45
75:h1:176:A:H8	75:h1:176:A:O5'	2.00	0.45
75:h1:1594:G:H2'	75:h1:1595:A:C8	2.51	0.45
2:A:139:U:H2'	2:A:140:C:C6	2.52	0.44
2:A:266:G:OP2	16:Ea:44:ARG:NH2	2.49	0.44
2:A:998:C:OP1	43:BR:130:ASN:ND2	2.45	0.44
4:C3:93:U:H2'	4:C3:94:C:H6	1.82	0.44
15:Ja:64:ILE:HG22	15:Ja:70:ILE:HD11	1.99	0.44
16:Ea:35:SER:HA	16:Ea:65:ARG:HG2	1.99	0.44
19:Ka:11:ARG:HB2	19:Ka:25:VAL:HG13	1.99	0.44
19:Ka:30:HIS:CE1	19:Ka:35:ASN:HA	2.52	0.44
24:AC:24:LEU:HD21	24:AC:44:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AC:149:GLY:O	24:AC:167:ASP:HA	2.17	0.44
31:BQ:36:GLU:OE1	31:BQ:163:ARG:NH1	2.50	0.44
34:BK:156:ASN:N	86:BK:405:HOH:O	2.51	0.44
37:BP:3:ARG:HE	37:BP:4:ILE:HG12	1.82	0.44
42:BU:82:LEU:HD13	42:BU:131:VAL:HG21	1.99	0.44
70:BL:73:VAL:O	70:BL:77:ARG:HG3	2.17	0.44
75:h1:187:C:H2'	75:h1:188:U:O4'	2.18	0.44
75:h1:412:A:H2'	75:h1:413:C:C6	2.52	0.44
75:h1:592:C:H2'	75:h1:593:A:C8	2.53	0.44
2:A:794:G:OP2	30:AJ:63:SER:OG	2.27	0.44
4:C3:7:G:OP1	34:BK:33:ARG:NH1	2.51	0.44
10:Ma:2:THR:N	75:h1:1143:A:OP1	2.50	0.44
22:BS:91:ALA:HB1	22:BS:157:ALA:HB2	1.99	0.44
29:AD:69:VAL:O	29:AD:73:THR:HG23	2.17	0.44
38:BN:68:LYS:HD3	38:BN:68:LYS:HA	1.78	0.44
39:BG:137:ILE:HG23	39:BG:169:VAL:HG21	1.99	0.44
58:Wa:4:VAL:HG22	71:La:43:PHE:HD2	1.80	0.44
67:BB:96:ILE:HD12	67:BB:117:ILE:HG12	1.98	0.44
72:Aa:109:PRO:C	72:Aa:111:LYS:H	2.24	0.44
75:h1:409:A:H2'	75:h1:410:C:C6	2.51	0.44
75:h1:432:G:H2'	75:h1:433:C:H6	1.81	0.44
75:h1:1544:G:OP2	86:h1:2108:HOH:O	2.20	0.44
2:A:2878:OMC:HM21	22:BS:242:PRO:HD3	2.00	0.44
2:A:3004:A:H2'	2:A:3005:U:O4'	2.17	0.44
35:AT:37:LEU:HD13	35:AT:62:TYR:HB3	1.99	0.44
50:Na:61:CYS:SG	50:Na:62:GLN:N	2.90	0.44
52:BF:89:ILE:HG23	52:BF:95:LEU:HD21	2.00	0.44
58:Wa:25:LYS:HE2	58:Wa:53:ASN:HA	2.00	0.44
62:Za:97:TYR:HE2	62:Za:201:VAL:HG11	1.82	0.44
62:Za:138:ILE:HD12	62:Za:148:ILE:HD12	2.00	0.44
70:BL:92:HIS:NE2	75:h1:1603:G:OP2	2.47	0.44
75:h1:907:A:H2'	75:h1:908:A:C8	2.52	0.44
75:h1:1351:C:H2'	75:h1:1352:U:O4'	2.17	0.44
75:h1:1559:U:O2'	75:h1:1560:U:H2'	2.18	0.44
78:AI:9:ARG:NH1	78:AI:79:TYR:OH	2.50	0.44
2:A:504:G:H2'	2:A:505:C:C6	2.53	0.44
2:A:1865:G:N1	2:A:1868:C:OP2	2.35	0.44
2:A:2217:A:H2'	2:A:2218:A2M:H8	1.98	0.44
2:A:2882:OMU:HM23	2:A:2882:OMU:H1'	1.76	0.44
2:A:3031:A:H2'	2:A:3032:C:H6	1.83	0.44
4:C3:39:C:O2	42:BU:72:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ja:184:THR:C	15:Ja:189:ARG:HG3	2.43	0.44
17:AL:150:LYS:HA	26:AH:7:VAL:O	2.18	0.44
22:BS:122:TRP:CE2	22:BS:127:LYS:HE3	2.52	0.44
28:AV:89:HIS:NE2	63:AQ:41:THR:O	2.49	0.44
62:Za:128:LEU:HD23	62:Za:148:ILE:HG23	2.00	0.44
62:Za:159:ARG:HG2	62:Za:160:PHE:CD2	2.53	0.44
66:Ya:83:THR:HA	75:h1:1242:G:H4'	1.98	0.44
72:Aa:2:GLY:N	75:h1:395:C:OP1	2.50	0.44
72:Aa:17:LYS:HD3	72:Aa:17:LYS:HA	1.78	0.44
75:h1:130:A:N6	75:h1:175:A:O2'	2.50	0.44
75:h1:1352:U:H2'	75:h1:1353:A:H8	1.81	0.44
75:h1:1501:G:H2'	75:h1:1502:G:H8	1.83	0.44
75:h1:1729:C:H2'	75:h1:1730:C:C6	2.52	0.44
1:3:87:C:H4'	1:3:89:G:N3	2.33	0.44
2:A:154:G:H1'	86:A:6225:HOH:O	2.17	0.44
2:A:1557:A:N6	86:A:3803:HOH:O	1.90	0.44
2:A:2365:A:H2'	2:A:2366:A:C8	2.52	0.44
17:AL:50:LEU:HD22	23:AM:152:ILE:HD11	1.97	0.44
34:BK:157:ARG:NE	86:BK:412:HOH:O	2.51	0.44
51:AB:132:ARG:NH1	51:AB:144:ASN:O	2.51	0.44
53:AA:28:GLU:OE2	78:AI:58:THR:OG1	2.29	0.44
53:AA:69:LEU:HD23	78:AI:67:PHE:HZ	1.82	0.44
60:AZ:55:LYS:O	60:AZ:58:GLN:HG2	2.17	0.44
66:Ya:61:LEU:HD23	66:Ya:88:MET:HG2	1.99	0.44
69:Ra:107:LYS:NZ	75:h1:747:U:OP2	2.50	0.44
75:h1:466:A2M:HM'3	75:h1:466:A2M:H1'	1.82	0.44
77:Ba:38:VAL:HG23	77:Ba:110:GLU:HG2	1.98	0.44
2:A:105:A:H2'	2:A:106:G:O4'	2.18	0.44
2:A:693:A:N6	2:A:709:C:H2'	2.32	0.44
2:A:866:G:OP1	86:A:3898:HOH:O	2.21	0.44
2:A:1752:G:C2	60:AZ:69:LEU:HD11	2.53	0.44
2:A:2210:C:H2'	86:A:6753:HOH:O	2.17	0.44
2:A:2279:A2M:H8	2:A:2279:A2M:H2'	1.62	0.44
24:AC:28:TYR:CZ	24:AC:110:PRO:HD3	2.53	0.44
39:BG:239:LYS:HG2	39:BG:243:LYS:HZ1	1.83	0.44
59:Ta:78:HIS:ND1	59:Ta:78:HIS:N	2.64	0.44
60:AZ:8:ILE:HG23	60:AZ:56:LEU:HD13	2.00	0.44
75:h1:87:A:H2'	75:h1:88:C:C6	2.53	0.44
75:h1:184:C:H2'	75:h1:185:G:O4'	2.17	0.44
75:h1:395:C:H2'	75:h1:396:C:C6	2.52	0.44
77:Ba:65:LYS:HE2	77:Ba:65:LYS:HB2	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:351:U:H2'	2:A:352:A:H8	1.83	0.44
2:A:858:C:H2'	2:A:859:U:H6	1.83	0.44
2:A:1112:A:H2'	2:A:1112:A:N3	2.33	0.44
2:A:2265:C:H2'	2:A:2266:U:C6	2.52	0.44
2:A:3164:A:H2'	2:A:3165:U:O4'	2.18	0.44
3:i2:1:G:H2'	3:i2:2:C:C6	2.53	0.44
6:BM:90:GLN:NE2	6:BM:94:ASP:OD1	2.48	0.44
13:AX:11:PHE:CD1	41:Ha:125:LYS:HD3	2.52	0.44
13:AX:60:ILE:HG23	13:AX:72:ALA:HB1	2.00	0.44
14:AP:23:ALA:HB1	14:AP:43:VAL:CG1	2.47	0.44
30:AJ:4:ASP:OD1	43:BR:105:LYS:HE2	2.18	0.44
33:Da:84:ILE:HD11	33:Da:149:LEU:HD21	1.99	0.44
48:BW:25:THR:HG22	48:BW:27:LYS:H	1.83	0.44
62:Za:176:GLY:HA2	62:Za:206:PHE:HB3	1.99	0.44
64:Oa:10:VAL:HG13	64:Oa:48:GLY:H	1.83	0.44
65:Ua:92:MET:HE3	65:Ua:92:MET:HB2	1.82	0.44
66:Ya:76:GLU:O	66:Ya:77:LYS:C	2.61	0.44
70:BL:54:TYR:CZ	70:BL:104:ILE:HG12	2.53	0.44
70:BL:114:VAL:HG13	70:BL:122:ARG:HB3	1.99	0.44
75:h1:438:A2M:H8	75:h1:438:A2M:O5'	2.17	0.44
75:h1:822:U:H2'	75:h1:823:U:H6	1.83	0.44
3:W2:3:G:C5	86:W2:101:HOH:O	2.48	0.44
78:AI:16:PHE:HB2	78:AI:76:LEU:CD1	2.47	0.44
2:A:794:G:H2'	2:A:794:G:N3	2.32	0.44
2:A:3272:C:H2'	2:A:3273:G:O4'	2.18	0.44
86:A:9431:HOH:O	49:AK:82:LYS:HE3	2.17	0.44
11:Ia:92:ARG:HD3	11:Ia:94:LYS:HZ2	1.81	0.44
22:BS:259:HIS:HA	22:BS:260:PRO:C	2.43	0.44
23:AM:43:LYS:NZ	86:AM:305:HOH:O	2.51	0.44
25:BI:86:LYS:NZ	86:BI:305:HOH:O	2.50	0.44
27:BT:391:ASP:OD2	27:BT:393:THR:OG1	2.23	0.44
44:Xa:9:PHE:HD1	72:Aa:194:PHE:HD2	1.66	0.44
63:AQ:17:ASN:HD21	63:AQ:51:LEU:HD11	1.83	0.44
63:AQ:71:ALA:HB1	63:AQ:85:VAL:HG13	2.00	0.44
69:Ra:54:ILE:HD13	69:Ra:169:THR:HG22	1.98	0.44
75:h1:384:C:P	86:h1:2138:HOH:O	2.76	0.44
75:h1:991:C:H2'	75:h1:992:G:O4'	2.18	0.44
78:AI:15:LEU:HG	78:AI:68:LEU:HD11	1.98	0.44
2:A:123:C:H2'	2:A:124:G:H8	1.83	0.44
2:A:480:G:H2'	2:A:481:A:O4'	2.18	0.44
2:A:990:C:C3'	2:A:991:G:H5''	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1129:A:N7	86:A:4235:HOH:O	2.36	0.44
2:A:1469:A:H5'	9:AU:55:VAL:O	2.18	0.44
2:A:2223:U:H2'	2:A:2224:U:C6	2.53	0.44
2:A:2335:OMC:HM23	2:A:2335:OMC:H1'	1.84	0.44
2:A:2682:U:H2'	2:A:2683:C:H6	1.82	0.44
2:A:3003:G:O2'	86:A:3899:HOH:O	2.21	0.44
2:A:3158:C:H2'	2:A:3159:G:C8	2.53	0.44
27:BT:321:LYS:HD2	43:BR:167:ALA:HB1	1.99	0.44
28:AV:92:THR:HG22	28:AV:93:TYR:CD2	2.53	0.44
32:BH:70:LYS:HD2	86:BH:309:HOH:O	2.18	0.44
42:BU:26:GLY:O	42:BU:61:ILE:HD11	2.18	0.44
51:AB:2:VAL:N	75:h1:463:G:OP1	2.51	0.44
53:AA:20:GLU:OE2	78:AI:61:TRP:CG	2.71	0.44
59:Ta:193:ARG:O	59:Ta:196:ILE:HG22	2.18	0.44
66:Ya:126:ILE:HD12	66:Ya:126:ILE:HA	1.79	0.44
69:Ra:170:MET:HA	69:Ra:173:VAL:HG22	2.00	0.44
70:BL:9:ASP:N	70:BL:9:ASP:OD1	2.51	0.44
71:La:62:THR:H	71:La:65:ILE:HG13	1.82	0.44
75:h1:1342:G:H22	75:h1:1387:A:H2	1.66	0.44
2:A:964:U:H2'	2:A:965:PSU:C6	2.52	0.43
2:A:2219:G:O6	13:AX:70:LYS:NZ	2.51	0.43
6:BM:117:HIS:NE2	6:BM:148:GLU:OE2	2.49	0.43
9:AU:70:GLY:N	9:AU:71:PRO:HD3	2.33	0.43
22:BS:190:THR:O	22:BS:194:LYS:HG3	2.17	0.43
24:AC:120:ILE:HD12	24:AC:120:ILE:C	2.42	0.43
50:Na:17:GLU:OE1	50:Na:20:LYS:HE2	2.18	0.43
59:Ta:79:ARG:NH2	59:Ta:86:GLY:O	2.50	0.43
59:Ta:135:ARG:NH2	75:h1:147:C:H1'	2.32	0.43
67:BB:96:ILE:HG22	67:BB:98:VAL:HG13	1.99	0.43
71:La:55:ALA:HA	71:La:58:PHE:CE2	2.52	0.43
75:h1:453:G:H2'	75:h1:455:C:O2	2.18	0.43
3:W2:67:C:C2	3:W2:68:A:C8	3.06	0.43
2:A:206:A:N6	27:BT:173:ILE:HD11	2.33	0.43
2:A:279:G:OP1	82:A:3401:TER:H32	2.18	0.43
2:A:2399:A:N3	86:A:4222:HOH:O	2.36	0.43
14:AP:120:ARG:HA	14:AP:120:ARG:HD3	1.83	0.43
25:BI:128:LEU:HD23	25:BI:128:LEU:HA	1.86	0.43
28:AV:66:HIS:CE1	63:AQ:29:SER:HB3	2.53	0.43
45:BV:33:LYS:HE2	45:BV:95:ASN:ND2	2.33	0.43
45:BV:150:VAL:HG23	75:h1:1068:U:H5''	2.00	0.43
50:Na:6:ASP:OD2	62:Za:40:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Ta:195:ARG:HG2	59:Ta:195:ARG:H	1.60	0.43
62:Za:173:HIS:ND1	62:Za:207:PHE:HE2	2.16	0.43
63:AQ:93:GLU:C	63:AQ:97:MET:HG3	2.43	0.43
75:h1:1018:U:H2'	75:h1:1019:C:H6	1.82	0.43
75:h1:1172:A:H2'	75:h1:1173:G:H8	1.80	0.43
75:h1:1302:PSU:N1	86:h1:2158:HOH:O	2.20	0.43
75:h1:1492:U:H1'	75:h1:1497:C:C4	2.53	0.43
2:A:240:G:H2'	2:A:241:U:C6	2.54	0.43
2:A:446:U:H2'	2:A:447:G:H8	1.84	0.43
2:A:1069:G:N7	86:A:4213:HOH:O	2.36	0.43
2:A:1166:G:H2'	2:A:1167:G:O4'	2.19	0.43
2:A:1373:A:H2'	2:A:1374:U:O4'	2.19	0.43
2:A:1594:G:H2'	2:A:1595:A:C8	2.53	0.43
2:A:2998:G:H2'	2:A:2999:U:C6	2.54	0.43
2:A:3139:A:N1	86:A:4228:HOH:O	2.36	0.43
2:A:3169:C:C2	20:AW:8:GLU:HG3	2.53	0.43
10:Ma:53:VAL:HA	65:Ua:125:ILE:HD11	1.99	0.43
17:AL:45:TYR:CZ	17:AL:49:LYS:HD2	2.54	0.43
28:AV:85:LEU:HD21	63:AQ:35:LYS:HA	2.00	0.43
44:Xa:10:LEU:H	44:Xa:10:LEU:HD12	1.82	0.43
48:BW:33:GLN:NE2	86:BW:101:HOH:O	2.51	0.43
50:Na:37:VAL:HG21	50:Na:65:LEU:HD11	2.00	0.43
57:AF:46:LEU:O	57:AF:50:ILE:HG22	2.18	0.43
58:Wa:108:ARG:O	58:Wa:112:GLU:HG3	2.18	0.43
75:h1:175:A:H5'	75:h1:177:C:OP2	2.18	0.43
75:h1:206:U:H2'	75:h1:207:A:H8	1.82	0.43
75:h1:210:A:H2'	75:h1:211:G:O4'	2.18	0.43
75:h1:302:A:H2'	75:h1:303:A:C8	2.53	0.43
75:h1:343:A:H2'	75:h1:344:C:C6	2.53	0.43
75:h1:1120:G:H2'	75:h1:1121:U:C6	2.54	0.43
75:h1:1653:A:N1	75:h1:1753:A:H2	2.16	0.43
2:A:639:C:H2'	2:A:640:C:C6	2.54	0.43
2:A:726:C:H2'	2:A:727:U:C6	2.54	0.43
2:A:957:C:OP1	86:A:3900:HOH:O	2.21	0.43
2:A:1675:G:H2'	2:A:1676:A:H8	1.83	0.43
2:A:2456:G:H21	2:A:2456:G:P	2.42	0.43
2:A:2518:G:H2'	2:A:2519:U:C6	2.54	0.43
2:A:2554:U:H5'	40:Fa:90:ARG:HH21	1.81	0.43
2:A:2881:U:H2'	2:A:2882:OMU:C6	2.49	0.43
2:A:2959:C:H2'	2:A:2960:G:H8	1.82	0.43
11:Ia:18:ILE:HG23	11:Ia:47:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BI:43:LYS:NZ	86:BI:307:HOH:O	2.51	0.43
86:AJ:416:HOH:O	41:Ha:38:MET:HG2	2.17	0.43
53:AA:48:ILE:HB	53:AA:86:LEU:HD12	1.99	0.43
60:AZ:40:ARG:HG2	60:AZ:41:TYR:CD2	2.53	0.43
69:Ra:55:SER:OG	69:Ra:56:GLY:N	2.51	0.43
75:h1:1259:U:H4'	78:AI:2:ILE:HG13	1.99	0.43
75:h1:1554:U:O2'	75:h1:1599:A:N3	2.32	0.43
2:A:643:U:H2'	2:A:644:U:C6	2.53	0.43
2:A:1359:A:H4'	2:A:1360:G:H5''	2.00	0.43
2:A:2455:G:N1	2:A:2457:A:H3'	2.33	0.43
2:A:3338:U:H3	2:A:3343:G:H21	1.65	0.43
24:AC:153:ALA:O	24:AC:157:LYS:HB2	2.18	0.43
40:Fa:41:GLY:HA2	86:Fa:331:HOH:O	2.17	0.43
53:AA:72:LEU:HD13	78:AI:65:TYR:CD2	2.53	0.43
57:AF:42:GLN:HG3	70:BL:13:HIS:HE1	1.83	0.43
58:Wa:137:LYS:O	58:Wa:141:ARG:NH1	2.51	0.43
66:Ya:112:ILE:HA	66:Ya:116:MET:HE2	1.99	0.43
67:BB:5:ARG:HG3	75:h1:1405:G:OP1	2.19	0.43
68:AN:60:VAL:HG22	68:AN:73:ALA:HB2	1.99	0.43
75:h1:397:U:H2'	75:h1:398:G:O4'	2.19	0.43
75:h1:1378:G:H2'	75:h1:1379:C:C6	2.53	0.43
2:A:1117:U:H2'	2:A:1118:C:H6	1.83	0.43
2:A:2943:PSU:H4'	86:BS:574:HOH:O	2.19	0.43
2:A:2960:G:H2'	2:A:2961:U:C6	2.54	0.43
3:i2:23:A:H2'	3:i2:24:G:C8	2.54	0.43
16:Ea:39:LEU:HD11	16:Ea:63:ARG:HB2	2.01	0.43
19:Ka:82:GLU:HG3	19:Ka:83:ASN:N	2.34	0.43
21:BD:37:ALA:O	21:BD:41:ARG:HG3	2.19	0.43
24:AC:190:LEU:O	24:AC:193:THR:HG22	2.19	0.43
27:BT:12:ILE:HD11	27:BT:260:LYS:HE3	2.00	0.43
38:BN:71:HIS:HD2	38:BN:114:MET:HE2	1.84	0.43
45:BV:78:ASP:OD1	45:BV:78:ASP:N	2.52	0.43
46:BJ:139:ARG:HB2	46:BJ:173:PHE:CE1	2.53	0.43
56:BA:6:SER:HB2	86:BA:106:HOH:O	2.19	0.43
59:Ta:173:LYS:HA	59:Ta:173:LYS:HD3	1.82	0.43
69:Ra:58:ARG:NH2	69:Ra:168:GLU:OE1	2.52	0.43
75:h1:28:A2M:HM'3	75:h1:28:A2M:H1'	1.72	0.43
75:h1:1641:OMC:H2'	75:h1:1642:C:O4'	2.19	0.43
78:AI:48:SER:O	78:AI:52:LYS:HG2	2.18	0.43
1:3:97:PSU:H2'	1:3:98:C:C6	2.53	0.43
2:A:437:G:O6	2:A:634:G:H1'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:710:G:N2	86:A:4064:HOH:O	2.31	0.43
2:A:2160:G:N7	86:A:4237:HOH:O	2.37	0.43
12:AE:42:GLN:NE2	12:AE:49:GLU:HA	2.33	0.43
13:AX:39:ARG:NH2	16:Ea:2:GLY:O	2.51	0.43
17:AL:154:VAL:HG12	17:AL:178:MET:HE1	2.00	0.43
24:AC:109:VAL:HG22	24:AC:110:PRO:HD2	1.99	0.43
29:AD:136:ARG:HB3	29:AD:203:ASN:OD1	2.19	0.43
41:Ha:49:HIS:CD2	54:AG:7:ILE:HD11	2.53	0.43
51:AB:78:LEU:CD1	51:AB:82:MET:HE3	2.48	0.43
59:Ta:168:ASN:ND2	59:Ta:172:LYS:HB3	2.29	0.43
62:Za:134:ASP:O	62:Za:138:ILE:HG12	2.18	0.43
62:Za:181:LEU:HG	62:Za:185:MET:HE3	2.00	0.43
72:Aa:62:ASP:OD1	72:Aa:63:THR:HG23	2.18	0.43
75:h1:77:A:O2'	75:h1:78:G:O4'	2.31	0.43
75:h1:257:A:H2'	75:h1:258:A:O4'	2.18	0.43
75:h1:469:G:N2	86:h1:2500:HOH:O	2.52	0.43
75:h1:1029:C:OP2	86:h1:2169:HOH:O	2.21	0.43
75:h1:1209:A:H5'	75:h1:1210:C:OP2	2.18	0.43
75:h1:1335:U:H2'	75:h1:1336:C:C6	2.54	0.43
78:AI:5:GLU:CB	78:AI:9:ARG:HH21	2.30	0.43
1:3:142:G:H5'	86:3:441:HOH:O	2.17	0.43
2:A:1335:G:H2'	2:A:1336:A:O4'	2.19	0.43
6:BM:126:GLN:HB2	6:BM:142:SER:OG	2.19	0.43
15:Ja:248:ILE:HD11	51:AB:73:PHE:CD2	2.54	0.43
27:BT:129:ILE:HD12	27:BT:129:ILE:HA	1.84	0.43
32:BH:67:MET:HE1	32:BH:73:HIS:CD2	2.53	0.43
50:Na:61:CYS:SG	50:Na:63:THR:OG1	2.77	0.43
58:Wa:30:LEU:HD11	58:Wa:67:LEU:HD13	1.99	0.43
64:Oa:57:GLU:O	65:Ua:116:ARG:NH2	2.52	0.43
70:BL:61:MET:O	70:BL:65:VAL:HG23	2.19	0.43
72:Aa:27:TYR:HB2	75:h1:335:A:N6	2.34	0.43
72:Aa:85:ASN:HB3	72:Aa:88:ASN:O	2.19	0.43
75:h1:526:U:H1'	75:h1:529:A:N7	2.34	0.43
75:h1:594:A:H2'	75:h1:595:U:O4'	2.19	0.43
75:h1:615:G:H4'	75:h1:616:C:OP1	2.18	0.43
75:h1:821:U:H2'	75:h1:822:U:H6	1.83	0.43
75:h1:1499:U:O2'	75:h1:1522:U:O2'	2.25	0.43
77:Ba:58:ARG:HG3	77:Ba:90:ARG:NE	2.33	0.43
2:A:1814:G:N7	14:AP:64:LYS:HE2	2.34	0.43
2:A:2659:U:H2'	2:A:2660:G:C8	2.53	0.43
19:Ka:26:ILE:HD11	19:Ka:45:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BS:291:VAL:HG23	22:BS:324:ASP:OD1	2.19	0.43
31:BQ:65:HIS:HB3	31:BQ:68:ARG:O	2.19	0.43
31:BQ:104:LEU:HD23	31:BQ:107:ILE:HD12	2.01	0.43
45:BV:146:ARG:N	45:BV:149:GLN:HG3	2.32	0.43
46:BJ:46:PHE:HB3	46:BJ:139:ARG:HG2	2.00	0.43
48:BW:35:ASN:OD1	48:BW:35:ASN:N	2.52	0.43
57:AF:9:VAL:HG23	57:AF:24:CYS:HB3	2.00	0.43
62:Za:45:ARG:NE	62:Za:49:GLY:HA2	2.34	0.43
69:Ra:5:GLN:N	69:Ra:5:GLN:CD	2.77	0.43
69:Ra:152:LYS:HE2	69:Ra:152:LYS:HB2	1.69	0.43
73:AY:71:PRO:HD2	86:AY:316:HOH:O	2.18	0.43
75:h1:416:OMC:HM23	75:h1:416:OMC:H1'	1.72	0.43
75:h1:1309:G:H2'	75:h1:1310:G:C8	2.53	0.43
75:h1:1431:OMG:HM23	75:h1:1431:OMG:H1'	1.64	0.43
1:3:35:G:O6	86:3:302:HOH:O	2.19	0.43
2:A:176:C:H2'	2:A:177:C:H6	1.84	0.43
2:A:186:G:N3	86:A:4199:HOH:O	2.35	0.43
2:A:833:C:O2'	2:A:1543:A:N3	2.52	0.43
2:A:1457:U:H2'	2:A:1458:A2M:H8	2.00	0.43
2:A:1636:C:OP1	14:AP:36:ARG:NH1	2.44	0.43
2:A:1833:U:H2'	2:A:1834:C:C6	2.54	0.43
2:A:3001:G:HO2'	22:BS:92:TYR:HH	1.66	0.43
2:A:3190:U:H2'	2:A:3191:C:C6	2.54	0.43
2:A:3224:U:H2'	2:A:3225:C:O4'	2.19	0.43
86:A:3909:HOH:O	43:BR:155:LYS:NZ	2.47	0.43
15:Ja:3:ARG:NH2	86:Ja:405:HOH:O	2.45	0.43
15:Ja:33:SER:OG	75:h1:299:U:O2	2.35	0.43
15:Ja:87:MET:SD	15:Ja:100:ARG:HD3	2.59	0.43
39:BG:94:ARG:NH2	39:BG:182:ALA:O	2.52	0.43
42:BU:118:TYR:O	58:Wa:101:ASN:HB3	2.19	0.43
53:AA:142:LEU:HD22	53:AA:150:MET:SD	2.59	0.43
62:Za:14:GLN:OE1	62:Za:14:GLN:N	2.51	0.43
66:Ya:45:ARG:NH1	75:h1:1553:U:O4	2.51	0.43
70:BL:57:ARG:NH1	75:h1:1482:A:OP1	2.49	0.43
71:La:94:ALA:HB3	71:La:101:ILE:HD11	2.01	0.43
75:h1:166:A:H2'	75:h1:167:A:C8	2.53	0.43
75:h1:450:C:H2'	75:h1:451:C:C6	2.53	0.43
75:h1:606:PSU:H2'	75:h1:607:A:O4'	2.18	0.43
75:h1:1445:OMU:HM23	75:h1:1445:OMU:H1'	1.65	0.43
75:h1:1581:U:H2'	75:h1:1582:C:C6	2.53	0.43
3:W2:58:A:H1'	3:W2:60:C:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:Ba:42:LEU:HD12	77:Ba:42:LEU:HA	1.81	0.43
2:A:243:G:C6	2:A:244:C:N4	2.87	0.42
2:A:277:PSU:OP1	82:A:3401:TER:H121	2.19	0.42
2:A:467:A:H2'	2:A:468:A:C8	2.54	0.42
2:A:567:A:H2'	2:A:568:U:C6	2.54	0.42
2:A:641:C:H2'	2:A:642:A:C8	2.54	0.42
2:A:754:C:H2'	2:A:755:C:H6	1.83	0.42
10:Ma:88:SER:O	10:Ma:92:ARG:HG3	2.19	0.42
19:Ka:21:ARG:HB3	19:Ka:78:TYR:CD1	2.54	0.42
25:BI:16:MET:HE1	25:BI:57:VAL:HB	2.01	0.42
27:BT:155:MET:HA	27:BT:156:PRO:C	2.44	0.42
35:AT:77:ASN:HB2	35:AT:89:ARG:HB3	2.01	0.42
50:Na:7:ILE:HG23	50:Na:13:PRO:HD3	2.01	0.42
70:BL:45:GLU:N	75:h1:1480:G:OP1	2.49	0.42
75:h1:1029:C:OP1	86:h1:2168:HOH:O	2.21	0.42
75:h1:1531:PSU:H2'	75:h1:1532:C:C6	2.54	0.42
1:3:63:A:OP2	86:3:303:HOH:O	2.21	0.42
2:A:1824:C:H2'	2:A:1825:A:C8	2.53	0.42
2:A:1835:G:OP1	56:BA:10:LYS:NZ	2.45	0.42
2:A:2812:A:H2'	2:A:2813:G:O4'	2.19	0.42
2:A:3374:G:N7	86:A:4252:HOH:O	2.37	0.42
12:AE:14:MET:HG3	12:AE:27:ILE:HD11	2.00	0.42
18:Va:107:LYS:HD2	75:h1:603:A:OP2	2.19	0.42
21:BD:24:LYS:NZ	21:BD:75:GLN:OE1	2.52	0.42
22:BS:333:VAL:N	86:BS:517:HOH:O	2.43	0.42
29:AD:192:LYS:HA	29:AD:192:LYS:HD3	1.81	0.42
32:BH:165:ARG:NH1	86:BH:306:HOH:O	2.39	0.42
38:BN:91:ASN:O	38:BN:137:ARG:HD2	2.19	0.42
53:AA:59:LEU:HA	53:AA:66:ILE:HG13	2.01	0.42
65:Ua:150:LEU:HB2	75:h1:1773:U:O2	2.19	0.42
66:Ya:66:ARG:O	66:Ya:70:ILE:HG23	2.19	0.42
75:h1:1248:U:H2'	75:h1:1249:C:H6	1.84	0.42
75:h1:1395:U:H2'	75:h1:1396:G:C8	2.52	0.42
75:h1:1671:U:H2'	75:h1:1672:G:O4'	2.18	0.42
75:h1:1723:A:H2'	75:h1:1724:G:O4'	2.19	0.42
2:A:239:U:H2'	2:A:240:G:C8	2.53	0.42
2:A:649:C:C2	2:A:650:C:C5	3.07	0.42
2:A:769:G:N2	2:A:779:G:O2'	2.40	0.42
2:A:1174:G:OP1	20:AW:89:LYS:NZ	2.52	0.42
2:A:1383:G:OP2	41:Ha:7:LYS:HE3	2.19	0.42
2:A:1953:U:C2	2:A:1954:G:C8	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BT:19:MET:SD	27:BT:19:MET:C	3.02	0.42
32:BH:118:ASP:OD1	32:BH:118:ASP:N	2.53	0.42
57:AF:83:ILE:O	57:AF:87:ILE:HG12	2.19	0.42
58:Wa:98:VAL:HG11	58:Wa:106:LYS:CG	2.49	0.42
67:BB:114:THR:HB	67:BB:117:ILE:HD12	2.02	0.42
75:h1:134:A:P	75:h1:134:A:H8	2.42	0.42
75:h1:1118:PSU:H2'	75:h1:1119:G:C8	2.54	0.42
75:h1:1535:C:H4'	75:h1:1541:G:O6	2.19	0.42
2:A:460:A:H2	2:A:473:G:H22	1.67	0.42
2:A:1010:G:N3	2:A:1013:A:N6	2.67	0.42
2:A:1507:A:H2'	2:A:1508:U:C6	2.54	0.42
2:A:2910:A2M:H8	2:A:2910:A2M:H2'	1.57	0.42
2:A:3053:C:O2	2:A:3055:U:H5'	2.19	0.42
12:AE:124:LYS:HE3	75:h1:808:PSU:O4	2.19	0.42
22:BS:140:GLU:OE1	22:BS:140:GLU:HA	2.19	0.42
27:BT:245:LYS:HE2	86:BT:639:HOH:O	2.19	0.42
44:Xa:56:ASP:OD2	44:Xa:114:PRO:HD3	2.19	0.42
45:BV:24:PHE:CD1	45:BV:27:LYS:HG3	2.54	0.42
57:AF:38:ILE:HD13	57:AF:50:ILE:HD11	2.02	0.42
57:AF:47:ARG:HA	57:AF:50:ILE:HG22	2.00	0.42
69:Ra:155:LEU:HB2	69:Ra:186:TYR:CE1	2.54	0.42
75:h1:579:G:H5''	86:h1:2422:HOH:O	2.19	0.42
75:h1:749:A:H62	75:h1:806:G:N2	2.16	0.42
75:h1:885:C:H2'	75:h1:886:G:H8	1.84	0.42
75:h1:1188:PSU:H2'	75:h1:1189:G:H8	1.85	0.42
75:h1:1453:U:H2'	75:h1:1454:C:H6	1.84	0.42
3:W2:65:C:C2	3:W2:66:U:C5	3.07	0.42
1:3:31:U:H2'	1:3:32:C:C6	2.55	0.42
1:3:148:C:OP1	16:Ea:62:TYR:OH	2.34	0.42
2:A:90:G:OP2	86:A:3901:HOH:O	2.22	0.42
2:A:1358:A:OP1	30:AJ:38:ARG:NH2	2.52	0.42
2:A:1678:G:OP2	68:AN:83:LYS:NZ	2.51	0.42
2:A:2374:G:H2'	2:A:2375:G:C8	2.55	0.42
2:A:2946:G:OP2	2:A:2946:G:H4'	2.19	0.42
17:AL:55:LYS:NZ	86:AL:215:HOH:O	2.52	0.42
18:Va:26:GLN:H	18:Va:26:GLN:HG2	1.63	0.42
23:AM:55:LYS:O	86:AM:301:HOH:O	2.21	0.42
33:Da:12:SER:HA	86:h1:2884:HOH:O	2.17	0.42
43:BR:40:LYS:O	43:BR:43:VAL:HG22	2.19	0.42
44:Xa:39:ILE:HG21	44:Xa:67:ILE:HD12	2.00	0.42
48:BW:80:LYS:O	48:BW:81:GLN:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:Wa:27:MET:HE1	58:Wa:38:ARG:HG3	2.00	0.42
58:Wa:61:ALA:HA	58:Wa:64:ILE:HD11	2.01	0.42
75:h1:256:PSU:H2'	75:h1:257:A:C8	2.54	0.42
75:h1:270:G:H2'	75:h1:271:C:H6	1.83	0.42
75:h1:568:C:H2'	75:h1:569:A:O4'	2.20	0.42
75:h1:819:G:C2	75:h1:820:A:C8	3.07	0.42
1:3:31:U:H2'	1:3:32:C:H6	1.83	0.42
2:A:125:G:H2'	2:A:126:A:C8	2.55	0.42
2:A:582:A:H2'	2:A:583:C:H6	1.83	0.42
2:A:667:C:H2'	2:A:668:A:C8	2.55	0.42
2:A:919:G:OP1	86:A:3904:HOH:O	2.22	0.42
2:A:2896:A:H2'	2:A:2898:C:H5''	2.02	0.42
5:BC:10:MET:HE3	5:BC:10:MET:O	2.19	0.42
9:AU:37:ILE:HD13	9:AU:63:ILE:HD13	2.01	0.42
12:AE:2:VAL:N	86:AE:202:HOH:O	2.52	0.42
15:Ja:35:PRO:HB3	75:h1:123:OMU:HM21	2.00	0.42
18:Va:54:ILE:CD1	18:Va:68:CYS:HB2	2.50	0.42
24:AC:200:GLU:HG3	24:AC:201:PHE:CD1	2.55	0.42
42:BU:21:LEU:HD11	42:BU:81:LEU:HD13	2.01	0.42
46:BJ:178:ARG:O	46:BJ:182:THR:HG23	2.19	0.42
51:AB:61:LEU:HD22	51:AB:71:ARG:HA	2.02	0.42
62:Za:84:ARG:HG2	62:Za:85:PRO:HD2	2.02	0.42
64:Oa:10:VAL:HA	64:Oa:28:VAL:HG12	2.01	0.42
65:Ua:97:ARG:HH21	65:Ua:133:PRO:HG3	1.85	0.42
67:BB:31:ASN:ND2	67:BB:55:THR:OG1	2.41	0.42
73:AY:25:ARG:HD2	73:AY:25:ARG:O	2.19	0.42
75:h1:41:A:H2'	75:h1:440:A:N7	2.34	0.42
75:h1:205:U:H2'	75:h1:206:U:C6	2.55	0.42
75:h1:361:G:OP2	75:h1:362:A:H5''	2.20	0.42
75:h1:856:A:C2	75:h1:858:U:H1'	2.55	0.42
75:h1:897:U:H2'	75:h1:898:C:C6	2.55	0.42
75:h1:1249:C:C2	75:h1:1250:U:C5	3.07	0.42
75:h1:1398:C:H2'	75:h1:1399:C:C6	2.54	0.42
1:3:108:A:N3	2:A:20:G:H1'	2.34	0.42
2:A:156:G:H2'	2:A:157:A:H8	1.84	0.42
2:A:1604:A:O2'	86:A:3810:HOH:O	1.97	0.42
2:A:1622:G:H2'	2:A:1623:U:C6	2.54	0.42
2:A:2970:A:N3	3:i2:74:C:H4'	2.35	0.42
4:C3:98:G:N7	86:C3:315:HOH:O	2.37	0.42
6:BM:127:ARG:HA	6:BM:141:MET:CE	2.49	0.42
11:Ia:4:ILE:H	17:AL:143:GLN:NE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AL:83:TYR:CD2	17:AL:118:VAL:HG21	2.55	0.42
22:BS:86:VAL:HG22	22:BS:162:VAL:HG11	2.02	0.42
24:AC:49:LYS:HB2	24:AC:49:LYS:HE2	1.82	0.42
24:AC:207:PHE:HD1	86:BW:101:HOH:O	2.02	0.42
27:BT:12:ILE:CD1	27:BT:260:LYS:HG3	2.49	0.42
34:BK:238:LEU:O	34:BK:242:VAL:HG23	2.20	0.42
46:BJ:46:PHE:CB	46:BJ:139:ARG:HG2	2.49	0.42
51:AB:56:ASN:OD1	51:AB:59:ARG:NH2	2.53	0.42
53:AA:29:LEU:HB3	53:AA:34:TYR:HB2	2.01	0.42
53:AA:45:ARG:HH11	53:AA:45:ARG:HG3	1.85	0.42
59:Ta:28:PHE:O	59:Ta:29:ASP:CB	2.67	0.42
63:AQ:13:VAL:HB	63:AQ:17:ASN:OD1	2.20	0.42
66:Ya:117:ILE:HD13	66:Ya:117:ILE:HA	1.90	0.42
69:Ra:54:ILE:HG23	69:Ra:172:GLY:HA3	2.02	0.42
75:h1:332:G:H2'	75:h1:333:A:H8	1.83	0.42
75:h1:597:OMG:HM23	75:h1:597:OMG:HI'	1.80	0.42
75:h1:823:U:H2'	75:h1:824:C:H6	1.85	0.42
75:h1:1184:A:H2'	75:h1:1185:A:C8	2.55	0.42
75:h1:1362:C:N4	75:h1:1366:C:N3	2.67	0.42
75:h1:1732:C:H2'	75:h1:1733:U:C6	2.55	0.42
2:A:801:C:H2'	2:A:802:C:H6	1.85	0.42
2:A:842:G:H2'	2:A:843:U:O4'	2.20	0.42
2:A:1183:G:H2'	2:A:1184:C:C6	2.55	0.42
13:AX:23:ARG:NH2	54:AG:77:GLU:OE1	2.52	0.42
69:Ra:146:ASP:OD1	69:Ra:146:ASP:N	2.51	0.42
72:Aa:85:ASN:HB2	72:Aa:92:VAL:HG23	2.02	0.42
75:h1:2:A:O4'	75:h1:372:A:C8	2.73	0.42
75:h1:823:U:H2'	75:h1:824:C:C6	2.54	0.42
75:h1:1420:A:H2'	75:h1:1421:G:O4'	2.20	0.42
75:h1:1564:G:C2	75:h1:1565:G:C8	3.07	0.42
2:A:990:C:H4'	2:A:991:G:OP2	2.18	0.42
2:A:1596:U:C2	2:A:1597:C:C5	3.08	0.42
2:A:2452:G:H2'	2:A:2455:G:O6	2.20	0.42
2:A:2676:G:N3	2:A:2676:G:H2'	2.35	0.42
2:A:3053:C:O2'	2:A:3055:U:OP2	2.36	0.42
3:i2:56:C:H2'	3:i2:57:G:O4'	2.20	0.42
4:C3:4:U:H2'	4:C3:5:G:C8	2.55	0.42
12:AE:104:LEU:HD23	12:AE:125:VAL:HA	2.01	0.42
15:Ja:97:GLU:HB3	15:Ja:99:PHE:CE2	2.55	0.42
15:Ja:103:TYR:HB2	15:Ja:182:MET:HE3	2.01	0.42
15:Ja:139:LEU:HB2	86:Ja:403:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BT:166:VAL:HG13	27:BT:171:ALA:HB3	2.02	0.42
28:AV:33:TRP:CZ2	28:AV:54:PRO:HD2	2.55	0.42
29:AD:198:ARG:HA	29:AD:201:LYS:HE3	2.01	0.42
35:AT:102:ASP:N	35:AT:102:ASP:OD1	2.52	0.42
45:BV:144:LYS:HG3	45:BV:208:GLN:HB3	2.01	0.42
46:BJ:47:PRO:HB3	46:BJ:171:TRP:CZ2	2.54	0.42
52:BF:154:ASP:OD1	52:BF:154:ASP:N	2.52	0.42
75:h1:396:C:H2'	75:h1:397:U:C6	2.55	0.42
75:h1:811:C:C2	75:h1:812:A:C8	3.07	0.42
75:h1:1482:A:C6	75:h1:1483:PSU:C2	3.08	0.42
75:h1:1539:A:C8	75:h1:1542:G:C6	3.08	0.42
75:h1:1567:C:H2'	75:h1:1568:U:O4'	2.20	0.42
2:A:2640:U:OP2	23:AM:10:ARG:NH2	2.52	0.42
2:A:2977[B]:U:O2'	2:A:2978:U:H5'	2.20	0.42
4:C3:27:A:H2'	4:C3:28:C:C6	2.55	0.42
19:Ka:18:LEU:O	19:Ka:19:LEU:HD23	2.19	0.42
24:AC:27:ILE:HD12	24:AC:27:ILE:H	1.85	0.42
24:AC:112:ARG:H	24:AC:193:THR:CG2	2.33	0.42
42:BU:111:HIS:ND1	42:BU:116:ILE:HG21	2.35	0.42
48:BW:45:TYR:CZ	48:BW:47:GLY:HA2	2.55	0.42
69:Ra:25:GLN:NE2	69:Ra:29:ASP:OD2	2.53	0.42
70:BL:43:LEU:HD23	70:BL:43:LEU:H	1.85	0.42
75:h1:31:C:O2'	75:h1:549:U:OP1	2.37	0.42
75:h1:794:A2M:H1'	75:h1:794:A2M:HM'3	1.58	0.42
75:h1:1147:G:N3	75:h1:1637:A:H2	2.17	0.42
75:h1:1273:U:O2'	75:h1:1276:A:OP2	2.26	0.42
75:h1:1651:C:H2'	75:h1:1652:U:H6	1.84	0.42
78:AI:27:PHE:HB3	78:AI:40:LEU:HD13	2.01	0.42
78:AI:50:LYS:HE2	78:AI:50:LYS:HB3	1.91	0.42
2:A:1033:G:C5	2:A:1034:C:C4	3.08	0.41
2:A:1759:G:P	68:AN:114:ARG:HH21	2.43	0.41
2:A:2407:OMG:HM21	2:A:2409:U:H5''	2.02	0.41
3:i2:29:A:H2'	3:i2:30:G:C8	2.55	0.41
6:BM:16:LYS:HG2	6:BM:150:ILE:HG12	2.01	0.41
16:Ea:99:ARG:HB3	16:Ea:167:GLU:HG2	2.01	0.41
16:Ea:114:ARG:NH1	16:Ea:151:ILE:O	2.54	0.41
31:BQ:144:ASP:OD1	31:BQ:160:SER:HB2	2.20	0.41
36:Pa:33:ARG:HD3	51:AB:128:ARG:HD3	2.01	0.41
39:BG:43:SER:HA	39:BG:46:ILE:HD12	2.02	0.41
42:BU:111:HIS:HB3	42:BU:125:TYR:O	2.19	0.41
52:BF:219:MET:HG2	52:BF:224:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Ta:164:ARG:NE	75:h1:66:U:O2	2.39	0.41
59:Ta:222:LYS:HD2	59:Ta:222:LYS:HA	1.86	0.41
67:BB:45:ARG:NH2	75:h1:1332:A:OP1	2.46	0.41
75:h1:251:C:H2'	75:h1:252:A:C8	2.54	0.41
75:h1:1272:OMG:H1'	75:h1:1272:OMG:HM23	1.74	0.41
75:h1:1359:A:H2'	75:h1:1360:G:H8	1.84	0.41
75:h1:1527:A:N3	75:h1:1591:C:O2'	2.44	0.41
75:h1:1610:U:H5''	86:h1:2307:HOH:O	2.20	0.41
2:A:212:G:H5''	7:BO:11:ARG:HG3	2.01	0.41
2:A:1800:A:H2'	2:A:1801:A:C8	2.55	0.41
2:A:1883:G:O6	86:A:3885:HOH:O	2.20	0.41
2:A:2695:A:N7	86:A:4260:HOH:O	2.37	0.41
2:A:2985:U:OP1	86:A:3905:HOH:O	2.22	0.41
2:A:3031:A:H2'	2:A:3032:C:C6	2.55	0.41
2:A:3189:G:H2'	2:A:3190:U:H6	1.85	0.41
22:BS:27:GLY:N	86:BS:508:HOH:O	2.39	0.41
23:AM:159:ASP:HB2	23:AM:164:TYR:HE2	1.83	0.41
26:AH:24:LEU:HD11	26:AH:84:TRP:CD1	2.55	0.41
35:AT:17:LEU:O	35:AT:21:MET:HG2	2.20	0.41
50:Na:38:LYS:HE2	50:Na:43:PHE:C	2.45	0.41
53:AA:56:GLN:CD	53:AA:56:GLN:N	2.78	0.41
56:BA:11:LYS:HG2	86:BA:126:HOH:O	2.19	0.41
57:AF:57:LEU:HD11	57:AF:107:ILE:HD12	2.02	0.41
57:AF:116:ARG:HA	57:AF:116:ARG:HD2	1.82	0.41
62:Za:188:GLN:HA	62:Za:193:ILE:HB	2.02	0.41
63:AQ:22:LYS:HG2	63:AQ:32:GLN:HG2	2.03	0.41
69:Ra:68:ARG:HG3	69:Ra:69:LEU:HD23	2.02	0.41
75:h1:295:U:H2'	75:h1:296:C:C6	2.54	0.41
2:A:1033:G:N2	2:A:1040:G:H22	2.18	0.41
2:A:2454:A:N3	2:A:2454:A:H2'	2.35	0.41
2:A:3174:C:H42	32:BH:172:LEU:HD13	1.84	0.41
15:Ja:106:LYS:NZ	75:h1:791:G:OP1	2.42	0.41
15:Ja:127:ARG:N	15:Ja:140:ASN:O	2.33	0.41
22:BS:84:MET:O	22:BS:205:GLN:HA	2.20	0.41
34:BK:110:LEU:HD23	34:BK:110:LEU:HA	1.90	0.41
45:BV:47:LEU:HD23	45:BV:47:LEU:C	2.45	0.41
75:h1:130:A:H8	75:h1:130:A:OP2	2.02	0.41
75:h1:162:A2M:O2'	75:h1:163:G:H5'	2.21	0.41
75:h1:387:A:O2'	86:h1:2170:HOH:O	2.21	0.41
75:h1:432:G:H2'	75:h1:433:C:C6	2.55	0.41
75:h1:962:U:H2'	75:h1:963:C:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:1216:OMC:HM23	75:h1:1216:OMC:H1'	1.62	0.41
75:h1:1500:U:C2	75:h1:1501:G:C8	3.08	0.41
77:Ba:59:MET:HG3	77:Ba:89:LYS:HG2	2.02	0.41
2:A:24:A:N3	2:A:325:C:O2'	2.48	0.41
2:A:764:A:OP1	86:A:3902:HOH:O	2.22	0.41
2:A:826:A2M:HM'3	2:A:929:A:C4	2.55	0.41
2:A:930:A:C6	73:AY:8:PHE:HE2	2.38	0.41
2:A:1548:U:H4'	86:A:4438:HOH:O	2.20	0.41
2:A:2685:U:H2'	2:A:2686:G:O4'	2.20	0.41
3:i2:16:U:H2'	3:i2:60:C:N3	2.36	0.41
18:Va:89:CYS:HA	18:Va:92:TYR:CD2	2.54	0.41
28:AV:116:LEU:HD23	28:AV:116:LEU:HA	1.91	0.41
31:BQ:135:ILE:HD12	31:BQ:149:LYS:HE3	2.02	0.41
44:Xa:38:ASN:OD1	44:Xa:38:ASN:C	2.63	0.41
45:BV:56:ILE:HB	45:BV:59:GLU:HG2	2.01	0.41
58:Wa:25:LYS:HA	58:Wa:55:ARG:HA	2.01	0.41
59:Ta:48:TYR:HB3	59:Ta:50:PHE:CE1	2.56	0.41
60:AZ:35:LYS:HA	60:AZ:43:TYR:O	2.20	0.41
74:Ca:48:LYS:HG3	74:Ca:49:GLU:N	2.35	0.41
75:h1:283:G:H2'	75:h1:284:C:C6	2.56	0.41
75:h1:422:A2M:HM'3	75:h1:422:A2M:H1'	1.67	0.41
75:h1:1143:A:H2'	75:h1:1144:A:C8	2.56	0.41
75:h1:1296:G:O6	86:h1:2161:HOH:O	2.20	0.41
75:h1:1412:G:N1	75:h1:1415:G:OP2	2.54	0.41
75:h1:1521:C:H2'	75:h1:1522:U:C6	2.56	0.41
75:h1:1539:A:N3	75:h1:1539:A:H2'	2.35	0.41
75:h1:1643:C:H2'	75:h1:1644:G:C8	2.55	0.41
75:h1:1670:G:H2'	75:h1:1671:U:C6	2.56	0.41
2:A:973:G:H5'	41:Ha:29:PRO:HB2	2.03	0.41
2:A:2345:OMU:H5	86:A:8715:HOH:O	2.20	0.41
2:A:2359:A2M:H2'	2:A:2360:C:C6	2.55	0.41
2:A:2424:U:H2'	2:A:2425:C:C6	2.55	0.41
2:A:3087:C:H2'	2:A:3088:U:O4'	2.21	0.41
2:A:3353:A:H2'	2:A:3354:C:C6	2.55	0.41
4:C3:4:U:H2'	4:C3:5:G:H8	1.84	0.41
86:C3:342:HOH:O	43:BR:225:HIS:HB2	2.19	0.41
6:BM:15:CYS:SG	6:BM:103:ALA:HB2	2.61	0.41
12:AE:56:HIS:CE1	33:Da:20:ARG:HD2	2.56	0.41
19:Ka:107:LYS:O	19:Ka:111:GLU:HG3	2.20	0.41
22:BS:92:TYR:HB2	22:BS:159:VAL:HB	2.02	0.41
33:Da:145:THR:HG22	33:Da:145:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BW:39:LEU:HD11	62:Za:189:MET:SD	2.61	0.41
53:AA:127:MET:HA	53:AA:127:MET:HE2	2.02	0.41
58:Wa:105:MET:HB2	58:Wa:106:LYS:NZ	2.35	0.41
62:Za:107:HIS:CE1	62:Za:111:THR:HB	2.55	0.41
71:La:61:ILE:HA	71:La:65:ILE:HD11	2.03	0.41
75:h1:412:A:H2'	75:h1:413:C:H6	1.86	0.41
75:h1:462:A:H3'	75:h1:463:G:H8	1.85	0.41
75:h1:754:G:H2'	75:h1:755:A:C8	2.55	0.41
75:h1:1218:A:C6	78:Al:40:LEU:HD22	2.56	0.41
1:3:84:A:H2'	1:3:85:U:H5'	2.02	0.41
2:A:556:U:H2'	2:A:557:C:C6	2.55	0.41
2:A:943:G:OP2	86:A:3906:HOH:O	2.22	0.41
2:A:1146:C:H5'	86:A:8852:HOH:O	2.19	0.41
4:C3:85:G:OP1	86:C3:308:HOH:O	2.21	0.41
12:AE:111:MET:HE2	12:AE:111:MET:HB3	1.97	0.41
14:AP:102:SER:OG	14:AP:105:LYS:HB2	2.20	0.41
15:Ja:199:GLU:HB2	15:Ja:207:THR:HG23	2.03	0.41
19:Ka:30:HIS:CD2	19:Ka:71:SER:HG	2.38	0.41
23:AM:8:ARG:CZ	86:AM:327:HOH:O	2.68	0.41
25:BI:30:ASP:OD1	25:BI:32:THR:HG22	2.20	0.41
26:AH:43:MET:HE3	26:AH:44:GLU:O	2.20	0.41
34:BK:88:LEU:HB2	34:BK:242:VAL:HG21	2.02	0.41
40:Fa:51:ILE:HG21	40:Fa:80:GLY:HA2	2.02	0.41
46:BJ:191:VAL:HG22	46:BJ:198:LYS:HB2	2.02	0.41
48:BW:54:LEU:HD13	48:BW:64:ALA:HB1	2.01	0.41
52:BF:91:PRO:HB3	52:BF:148:ILE:HD11	2.02	0.41
57:AF:52:GLU:O	57:AF:56:LEU:HG	2.21	0.41
62:Za:15:LYS:O	62:Za:19:VAL:HG13	2.20	0.41
69:Ra:170:MET:HB2	69:Ra:184:PHE:CE2	2.56	0.41
75:h1:410:C:H2'	75:h1:411:C:C6	2.56	0.41
75:h1:775:G:N2	75:h1:777:A:H1'	2.35	0.41
75:h1:820:A:H2'	75:h1:821:U:H6	1.86	0.41
75:h1:935:C:C4	75:h1:1078:C:H4'	2.56	0.41
2:A:92:G:H2'	2:A:93:A:C8	2.56	0.41
2:A:188:U:H2'	2:A:189:C:C6	2.56	0.41
2:A:436:C:O2'	2:A:437:G:H2'	2.21	0.41
2:A:1653:G:N7	86:A:4267:HOH:O	2.37	0.41
2:A:3365:C:H2'	2:A:3366:C:H6	1.86	0.41
24:AC:78:ASP:CG	24:AC:82:HIS:HB2	2.45	0.41
34:BK:68:SER:OG	34:BK:71:GLY:O	2.32	0.41
34:BK:113:LEU:HB2	34:BK:115:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BP:103:LYS:HE3	37:BP:107:GLU:HB3	2.03	0.41
47:AO:49:SER:N	86:AO:201:HOH:O	2.34	0.41
66:Ya:69:LYS:NZ	66:Ya:97:SER:OG	2.53	0.41
67:BB:31:ASN:HA	67:BB:34:ILE:HG22	2.03	0.41
67:BB:35:LEU:HA	67:BB:38:VAL:HG12	2.01	0.41
70:BL:42:LYS:HG2	75:h1:1565:G:H5'	2.01	0.41
72:Aa:114:TYR:HE2	72:Aa:153:ARG:HH21	1.68	0.41
75:h1:969:U:H2'	75:h1:970:C:O4'	2.21	0.41
75:h1:1483:PSU:O2'	75:h1:1484:U:H5'	2.21	0.41
78:AI:46:MET:HG3	78:AI:66:TRP:CD2	2.55	0.41
1:3:155:OMG:HM23	1:3:155:OMG:HI'	1.64	0.41
2:A:234:G:H2'	2:A:235:A:C8	2.56	0.41
2:A:469:U:H2'	2:A:470:C:H6	1.84	0.41
2:A:528:C:H5'	26:AH:68:LYS:HB2	2.03	0.41
2:A:780:A:H2'	2:A:781:A:O4'	2.21	0.41
2:A:977:G:O2'	8:AR:15:LYS:HE3	2.20	0.41
2:A:1534:G:H5'	2:A:1832:G:OP2	2.20	0.41
2:A:2721:U:H2'	2:A:2722:U:H6	1.86	0.41
2:A:2746:A:H5'	34:BK:174:HIS:HA	2.02	0.41
10:Ma:25:ASN:HB3	10:Ma:77:CYS:SG	2.61	0.41
15:Ja:127:ARG:HG3	15:Ja:141:THR:C	2.46	0.41
21:BD:68:ILE:HG12	86:BD:317:HOH:O	2.19	0.41
24:AC:161:GLN:HB3	86:AC:406:HOH:O	2.21	0.41
26:AH:24:LEU:HD11	26:AH:84:TRP:CG	2.55	0.41
31:BQ:211:HIS:CD2	31:BQ:219:ILE:HG23	2.56	0.41
33:Da:87:ASP:OD1	33:Da:87:ASP:N	2.52	0.41
39:BG:159:TRP:CD1	39:BG:159:TRP:H	2.36	0.41
41:Ha:81:LEU:HD22	41:Ha:103:HIS:CD2	2.56	0.41
44:Xa:47:ARG:HH12	75:h1:847:G:H2'	1.85	0.41
45:BV:131:ASP:OD1	45:BV:131:ASP:N	2.41	0.41
53:AA:205:PRO:HG2	75:h1:1332:A:C2	2.56	0.41
54:AG:9:ASN:HD22	54:AG:9:ASN:N	2.19	0.41
57:AF:100:ASP:OD1	57:AF:102:GLN:HB2	2.20	0.41
62:Za:46:ARG:HG2	67:BB:101:GLU:HG3	2.02	0.41
63:AQ:74:LYS:HB2	63:AQ:77:LYS:HB2	2.02	0.41
64:Oa:14:MET:HB2	64:Oa:25:GLN:HB3	2.02	0.41
68:AN:100:ARG:NH2	68:AN:102:ILE:HD11	2.36	0.41
70:BL:25:ARG:HB2	70:BL:25:ARG:HH11	1.86	0.41
75:h1:212:A:O5'	75:h1:212:A:H8	2.04	0.41
75:h1:1625:C:H2'	75:h1:1626:C:H6	1.86	0.41
3:W2:18:G:H4'	3:W2:60:C:C2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:163:C:H1'	2:A:164:C:H5	1.86	0.41
2:A:676:OMU:HM23	2:A:676:OMU:H1'	1.81	0.41
2:A:699:U:H2'	2:A:700:G:O4'	2.21	0.41
2:A:712:A:H3'	2:A:712:A:OP2	2.21	0.41
2:A:882:C:H5''	2:A:883:U:O5'	2.20	0.41
2:A:1223:G:H5'	17:AL:138:ARG:NH2	2.36	0.41
2:A:3169:C:H4'	86:A:5852:HOH:O	2.21	0.41
86:A:6128:HOH:O	54:AG:17:GLN:CD	2.64	0.41
3:i2:16:U:O2'	3:i2:19:G:OP2	2.38	0.41
86:C3:395:HOH:O	23:AM:26:PRO:HG3	2.21	0.41
9:AU:39:GLU:OE2	9:AU:42:LYS:NZ	2.53	0.41
15:Ja:181:VAL:HG11	15:Ja:225:VAL:CG1	2.41	0.41
19:Ka:60:PHE:HD1	19:Ka:74:TYR:HB3	1.85	0.41
22:BS:287:ARG:HB3	22:BS:327:MET:HB3	2.03	0.41
26:AH:68:LYS:HZ3	26:AH:72:ILE:HD11	1.86	0.41
28:AV:3:VAL:O	28:AV:91:ARG:NE	2.52	0.41
29:AD:34:LEU:HD12	29:AD:117:VAL:HG22	2.02	0.41
39:BG:116:LYS:H	39:BG:116:LYS:HD3	1.86	0.41
41:Ha:85:ASP:OD1	41:Ha:86:VAL:N	2.53	0.41
51:AB:53:ARG:NH2	75:h1:764:G:OP2	2.54	0.41
53:AA:56:GLN:H	53:AA:56:GLN:CD	2.28	0.41
54:AG:132:VAL:HG13	54:AG:136:ASP:HB2	2.03	0.41
58:Wa:15:VAL:O	58:Wa:18:THR:OG1	2.26	0.41
58:Wa:22:GLY:HA2	58:Wa:56:ALA:HB3	2.03	0.41
58:Wa:141:ARG:NH2	75:h1:1465:G:N7	2.61	0.41
60:AZ:61:PRO:HA	60:AZ:62:PRO:HD3	1.95	0.41
74:Ca:10:HIS:CE1	75:h1:1205:A:N3	2.89	0.41
75:h1:162:A2M:HM'3	75:h1:162:A2M:H1'	1.66	0.41
75:h1:754:G:H2'	75:h1:755:A:H8	1.86	0.41
75:h1:947:U:H2'	75:h1:948:PSU:C6	2.56	0.41
75:h1:987:G:H2'	75:h1:988:G:O4'	2.20	0.41
75:h1:1318:C:H2'	75:h1:1319:G:O4'	2.21	0.41
75:h1:1335:U:H2'	75:h1:1336:C:H6	1.86	0.41
75:h1:1640:G:H2'	75:h1:1641:OMC:O4'	2.21	0.41
75:h1:1754:A2M:H1'	75:h1:1754:A2M:HM'3	1.76	0.41
3:W2:9:A:H1'	3:W2:45:G:H2'	2.02	0.41
1:3:123:C:H2'	1:3:124:C:O4'	2.20	0.41
1:3:162:C:H2'	1:3:163:A:O4'	2.20	0.41
2:A:196:A:P	86:A:4248:HOH:O	2.79	0.41
2:A:475:C:H2'	2:A:476:C:C6	2.56	0.41
2:A:1678:G:O6	68:AN:80:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2343:A:H5'	2:A:3054:A:N6	2.36	0.41
2:A:2496:U:HO2'	2:A:2497:U:P	2.43	0.41
2:A:3009:A:N1	2:A:3041:C:O2'	2.47	0.41
17:AL:37:VAL:HG22	43:BR:236:GLU:HG3	2.03	0.41
22:BS:49:TYR:CD1	22:BS:171:MET:HE1	2.56	0.41
22:BS:103:ASN:N	22:BS:103:ASN:OD1	2.54	0.41
24:AC:154:ARG:HH11	24:AC:154:ARG:HG2	1.86	0.41
33:Da:79:GLY:O	33:Da:80:LEU:HD23	2.21	0.41
37:BP:80:PRO:O	37:BP:84:ARG:HG3	2.21	0.41
43:BR:100:ILE:HG22	43:BR:105:LYS:HB2	2.04	0.41
45:BV:166:ARG:O	45:BV:170:GLU:HG3	2.21	0.41
47:AO:14:LYS:HE2	47:AO:14:LYS:HB3	1.71	0.41
58:Wa:13:LEU:HG	58:Wa:15:VAL:HG23	2.02	0.41
59:Ta:195:ARG:NH2	75:h1:268:U:H5	2.19	0.41
61:BE:79:VAL:O	61:BE:83:ILE:HG12	2.21	0.41
65:Ua:64:ASP:OD1	65:Ua:64:ASP:N	2.53	0.41
68:AN:83:LYS:HB2	68:AN:111:TYR:CE2	2.56	0.41
70:BL:43:LEU:HA	70:BL:84:LYS:HG3	2.03	0.41
72:Aa:82:VAL:HG12	72:Aa:92:VAL:HG22	2.03	0.41
75:h1:60:U:N3	75:h1:63:G:OP1	2.45	0.41
75:h1:418:A:H3'	75:h1:419:A:H8	1.86	0.41
75:h1:466:A2M:C2	75:h1:467:G:C8	3.04	0.41
77:Ba:82:ARG:HD2	77:Ba:82:ARG:N	2.35	0.41
1:3:157:U:H2'	2:A:2584:G:N2	2.36	0.40
2:A:529:C:C2	2:A:530:G:C8	3.09	0.40
2:A:1057:A:N3	2:A:2632:U:O2'	2.53	0.40
2:A:1367:G:H2'	2:A:1368:C:C6	2.57	0.40
2:A:1581:A:N3	2:A:1581:A:H2'	2.36	0.40
2:A:1620:A:H2'	2:A:1621:C:O4'	2.21	0.40
2:A:2178:G:H2'	2:A:2179:C:C6	2.56	0.40
2:A:2577:C:H2'	2:A:2578:G:O4'	2.22	0.40
2:A:2634:A:H4'	2:A:2635:A:O5'	2.22	0.40
2:A:2668:C:H2'	2:A:2669:G:H8	1.86	0.40
2:A:2680:U:OP1	42:BU:52:ALA:HA	2.21	0.40
2:A:2721:U:H2'	2:A:2722:U:C6	2.56	0.40
5:BC:10:MET:HE1	5:BC:17:ARG:HH12	1.86	0.40
11:Ia:89:ARG:O	11:Ia:190:ILE:HB	2.21	0.40
13:AX:8:THR:HG23	13:AX:15:ASN:HB3	2.02	0.40
16:Ea:90:THR:O	21:BD:50:TYR:OH	2.34	0.40
27:BT:105:ARG:NH2	86:BT:520:HOH:O	2.48	0.40
27:BT:110:THR:HB	86:BT:557:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BG:211:ALA:O	39:BG:215:ASN:ND2	2.54	0.40
40:Fa:94:ALA:O	40:Fa:98:GLU:HG2	2.21	0.40
45:BV:229:MET:HE3	45:BV:232:HIS:O	2.21	0.40
58:Wa:37:GLY:H	75:h1:1568:U:H5''	1.86	0.40
58:Wa:55:ARG:HD2	71:La:41:VAL:HG11	2.02	0.40
58:Wa:55:ARG:O	58:Wa:59:LEU:HD23	2.21	0.40
59:Ta:151:LYS:HA	59:Ta:151:LYS:NZ	2.36	0.40
69:Ra:6:ASN:N	69:Ra:6:ASN:OD1	2.41	0.40
71:La:62:THR:H	71:La:65:ILE:CG1	2.34	0.40
72:Aa:187:LEU:HB3	72:Aa:192:LEU:HD12	2.02	0.40
75:h1:481:C:C2	75:h1:482:A:C8	3.10	0.40
75:h1:749:A:N6	75:h1:806:G:H21	2.14	0.40
75:h1:1177:G:C6	75:h1:1467:G:C6	3.09	0.40
75:h1:1219:G:N1	75:h1:1447:A:OP2	2.44	0.40
2:A:2889:A:O2'	2:A:2932:A:N3	2.46	0.40
2:A:3116:C:H2'	2:A:3117:U:O4'	2.20	0.40
6:BM:141:MET:HE2	6:BM:141:MET:HA	2.03	0.40
7:BO:73:TYR:CD1	7:BO:76:LYS:HG3	2.56	0.40
14:AP:26:ILE:HD11	14:AP:44:ALA:HB2	2.03	0.40
34:BK:51:PHE:CE1	34:BK:105:LEU:HD23	2.55	0.40
44:Xa:85:ILE:HG23	44:Xa:112:VAL:HG21	2.02	0.40
53:AA:69:LEU:HD23	78:AI:67:PHE:CZ	2.56	0.40
53:AA:195:THR:O	53:AA:201:LYS:HE2	2.21	0.40
55:Ga:83:MET:O	55:Ga:87:ARG:HD2	2.20	0.40
57:AF:8:SER:HB3	57:AF:25:LYS:NZ	2.36	0.40
57:AF:69:ILE:HG21	57:AF:83:ILE:HG12	2.02	0.40
62:Za:15:LYS:HG3	62:Za:59:TRP:CE3	2.56	0.40
65:Ua:65:ARG:HD3	86:Ua:324:HOH:O	2.20	0.40
67:BB:59:LYS:NZ	75:h1:1395:U:OP1	2.50	0.40
70:BL:20:ALA:CB	70:BL:56:ILE:HD13	2.51	0.40
72:Aa:22:ARG:NH1	86:h1:2114:HOH:O	2.54	0.40
74:Ca:22:ARG:HH12	74:Ca:37:ASN:HB2	1.85	0.40
75:h1:760:A:N6	86:h1:2498:HOH:O	2.54	0.40
75:h1:778:A2M:HM'3	75:h1:778:A2M:H1'	1.64	0.40
75:h1:1106:C:H2'	75:h1:1107:C:O4'	2.21	0.40
75:h1:1136:U:H2'	75:h1:1137:U:C6	2.56	0.40
75:h1:1191:C:H4'	75:h1:1192:C4J:O5'	2.22	0.40
75:h1:1385:A:O2'	75:h1:1386:G:H5''	2.22	0.40
75:h1:1385:A:H5'	77:Ba:60:PRO:HA	2.03	0.40
2:A:1003:G:O2'	2:A:1004:G:H5'	2.22	0.40
2:A:1341:U:H5''	86:A:5925:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1493:A:N7	86:A:4265:HOH:O	2.37	0.40
17:AL:134:LYS:HG3	86:AL:258:HOH:O	2.21	0.40
51:AB:36:TYR:OH	51:AB:104:GLU:HG2	2.21	0.40
68:AN:28:PRO:HG3	68:AN:113:LEU:HD23	2.02	0.40
69:Ra:169:THR:O	69:Ra:173:VAL:HG13	2.21	0.40
74:Ca:8:ASN:HB2	78:AI:28:ASN:HD22	1.86	0.40
75:h1:76:C:H2'	75:h1:77:A:C8	2.56	0.40
75:h1:1176:PSU:H2'	75:h1:1177:G:H8	1.86	0.40
75:h1:1320:U:H2'	75:h1:1321:U:O4'	2.21	0.40
78:AI:3:ILE:HD12	78:AI:4:SER:N	2.36	0.40
2:A:497:G:H2'	2:A:498:A:H8	1.87	0.40
2:A:873:G:N7	86:A:4250:HOH:O	2.37	0.40
2:A:985:U:OP2	30:AJ:50:LYS:NZ	2.51	0.40
2:A:1917:A:H5'	49:AK:82:LYS:O	2.21	0.40
2:A:2494:U:H2'	2:A:2495:U:C6	2.56	0.40
5:BC:10:MET:HE2	75:h1:1116:U:H4'	2.04	0.40
11:Ia:27:VAL:HG12	11:Ia:87:VAL:HG11	2.02	0.40
19:Ka:88:GLU:HA	19:Ka:88:GLU:OE1	2.21	0.40
22:BS:290:LYS:NZ	22:BS:324:ASP:OD2	2.55	0.40
25:BI:22:VAL:O	25:BI:23:ALA:HB3	2.20	0.40
26:AH:40:ALA:HB3	26:AH:43:MET:CG	2.51	0.40
26:AH:68:LYS:NZ	26:AH:72:ILE:HD11	2.37	0.40
27:BT:124:MET:HE2	27:BT:124:MET:HB3	1.95	0.40
27:BT:290:MET:HE2	27:BT:290:MET:HB3	1.96	0.40
28:AV:100:ASN:OD1	28:AV:100:ASN:N	2.52	0.40
31:BQ:3:ARG:NH2	86:BQ:416:HOH:O	2.43	0.40
39:BG:128:TYR:HB3	39:BG:184:VAL:HG11	2.03	0.40
39:BG:205:PHE:CE2	39:BG:209:LEU:HD11	2.57	0.40
40:Fa:98:GLU:OE2	40:Fa:98:GLU:HA	2.22	0.40
86:Xa:210:HOH:O	75:h1:338:G:H5''	2.20	0.40
45:BV:74:GLN:OE1	45:BV:189:ILE:HD12	2.21	0.40
46:BJ:146:HIS:CE1	46:BJ:147:HIS:CD2	3.10	0.40
53:AA:190:LEU:HD23	53:AA:190:LEU:H	1.85	0.40
59:Ta:31:ARG:H	59:Ta:34:GLN:HG3	1.85	0.40
59:Ta:155:VAL:O	59:Ta:159:VAL:HG23	2.22	0.40
62:Za:88:GLN:NE2	62:Za:104:ALA:O	2.34	0.40
65:Ua:29:VAL:HG22	65:Ua:93:HIS:HB2	2.04	0.40
73:AY:46:THR:CG2	73:AY:54:ILE:HG12	2.51	0.40
75:h1:1175:C:O2'	75:h1:1197:A:N6	2.54	0.40
3:W2:53:G:H2'	3:W2:54:U:C6	2.56	0.40
1:3:64:U:H4'	86:3:400:HOH:O	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:98:C:H3'	73:AY:72:ARG:HD3	2.03	0.40
2:A:36:U:H2'	2:A:37:A:O4'	2.22	0.40
2:A:954:C:H2'	2:A:955:C:H6	1.83	0.40
2:A:1398:U:H5''	28:AV:102:SER:HB3	2.03	0.40
2:A:1541:C:H2'	2:A:1542:U:C6	2.55	0.40
2:A:1659:U:H2'	2:A:1660:C:C6	2.56	0.40
2:A:2391:G:H4'	22:BS:255:ILE:HD13	2.04	0.40
2:A:2913:G:N3	2:A:2933:A2M:H2	2.37	0.40
8:AR:41:ARG:HG2	8:AR:45:TYR:CZ	2.56	0.40
15:Ja:55:ALA:HB2	15:Ja:64:ILE:HD12	2.04	0.40
24:AC:71:LYS:HD3	24:AC:73:PHE:CZ	2.56	0.40
25:BI:25:THR:HA	25:BI:37:LEU:O	2.22	0.40
25:BI:70:PRO:HG2	75:h1:1662:A:H5'	2.04	0.40
39:BG:148:ALA:HB2	39:BG:180:LEU:HD12	2.02	0.40
46:BJ:76:MET:SD	46:BJ:148:ALA:HA	2.61	0.40
52:BF:106:ARG:HD3	52:BF:208:TYR:CE2	2.57	0.40
55:Ga:79:GLU:OE1	55:Ga:81:SER:OG	2.31	0.40
57:AF:99:VAL:HG12	57:AF:100:ASP:H	1.86	0.40
62:Za:130:ASP:HB3	62:Za:133:THR:HG22	2.04	0.40
66:Ya:133:HIS:HB3	75:h1:1463:A:C8	2.56	0.40
69:Ra:143:TYR:CE2	69:Ra:149:LYS:HG2	2.56	0.40
72:Aa:197:LYS:HA	72:Aa:200:GLN:CD	2.46	0.40
74:Ca:34:TYR:CE2	77:Ba:64:LEU:HB3	2.57	0.40
75:h1:989:C:P	86:h1:2115:HOH:O	2.74	0.40
75:h1:1053:U:H2'	75:h1:1054:G:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BC	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	BM	153/176 (87%)	152 (99%)	1 (1%)	0	100	100
7	BO	123/146 (84%)	121 (98%)	2 (2%)	0	100	100
8	AR	49/83 (59%)	44 (90%)	5 (10%)	0	100	100
9	AU	107/119 (90%)	105 (98%)	2 (2%)	0	100	100
10	Ma	96/131 (73%)	95 (99%)	1 (1%)	0	100	100
11	Ia	188/194 (97%)	182 (97%)	6 (3%)	0	100	100
12	AE	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
13	AX	95/112 (85%)	93 (98%)	2 (2%)	0	100	100
14	AP	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
15	Ja	256/262 (98%)	246 (96%)	9 (4%)	1 (0%)	30	31
16	Ea	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
17	AL	173/217 (80%)	173 (100%)	0	0	100	100
18	Va	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
19	Ka	118/133 (89%)	113 (96%)	5 (4%)	0	100	100
20	AW	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
21	BD	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
22	BS	383/389 (98%)	378 (99%)	5 (1%)	0	100	100
23	AM	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
24	AC	213/284 (75%)	209 (98%)	4 (2%)	0	100	100
25	BI	129/140 (92%)	125 (97%)	4 (3%)	0	100	100
26	AH	126/134 (94%)	124 (98%)	2 (2%)	0	100	100
27	BT	389/406 (96%)	379 (97%)	10 (3%)	0	100	100
28	AV	124/133 (93%)	122 (98%)	2 (2%)	0	100	100
29	AD	180/207 (87%)	171 (95%)	9 (5%)	0	100	100
30	AJ	184/187 (98%)	178 (97%)	6 (3%)	0	100	100
31	BQ	244/258 (95%)	233 (96%)	11 (4%)	0	100	100
32	BH	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
33	Da	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
34	BK	279/301 (93%)	272 (98%)	7 (2%)	0	100	100
35	AT	92/112 (82%)	92 (100%)	0	0	100	100
36	Pa	45/62 (73%)	44 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BP	118/123 (96%)	115 (98%)	3 (2%)	0	100	100
38	BN	115/154 (75%)	112 (97%)	3 (3%)	0	100	100
39	BG	232/256 (91%)	225 (97%)	7 (3%)	0	100	100
40	Fa	109/120 (91%)	107 (98%)	2 (2%)	0	100	100
41	Ha	143/146 (98%)	137 (96%)	5 (4%)	1 (1%)	18	17
42	BU	167/182 (92%)	162 (97%)	5 (3%)	0	100	100
43	BR	230/247 (93%)	226 (98%)	4 (2%)	0	100	100
44	Xa	144/160 (90%)	137 (95%)	7 (5%)	0	100	100
45	BV	210/262 (80%)	210 (100%)	0	0	100	100
46	BJ	203/221 (92%)	199 (98%)	4 (2%)	0	100	100
47	AO	60/164 (37%)	58 (97%)	2 (3%)	0	100	100
48	BW	71/82 (87%)	68 (96%)	3 (4%)	0	100	100
49	AK	176/214 (82%)	175 (99%)	1 (1%)	0	100	100
50	Na	81/86 (94%)	70 (86%)	11 (14%)	0	100	100
51	AB	178/197 (90%)	169 (95%)	9 (5%)	0	100	100
52	BF	184/233 (79%)	178 (97%)	6 (3%)	0	100	100
53	AA	206/250 (82%)	197 (96%)	8 (4%)	1 (0%)	24	24
54	AG	201/206 (98%)	197 (98%)	4 (2%)	0	100	100
55	Ga	49/128 (38%)	49 (100%)	0	0	100	100
56	BA	48/51 (94%)	48 (100%)	0	0	100	100
57	AF	136/146 (93%)	128 (94%)	8 (6%)	0	100	100
58	Wa	137/152 (90%)	134 (98%)	3 (2%)	0	100	100
59	Ta	223/249 (90%)	206 (92%)	15 (7%)	2 (1%)	14	12
60	AZ	66/69 (96%)	63 (96%)	3 (4%)	0	100	100
61	BE	88/92 (96%)	83 (94%)	5 (6%)	0	100	100
62	Za	196/298 (66%)	187 (95%)	9 (5%)	0	100	100
63	AQ	134/143 (94%)	125 (93%)	7 (5%)	2 (2%)	8	4
64	Oa	57/64 (89%)	55 (96%)	2 (4%)	0	100	100
65	Ua	125/150 (83%)	119 (95%)	5 (4%)	1 (1%)	16	14
66	Ya	127/150 (85%)	115 (91%)	10 (8%)	2 (2%)	7	4
67	BB	117/141 (83%)	110 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	AN	97/124 (78%)	89 (92%)	7 (7%)	1 (1%)	12	10
69	Ra	182/190 (96%)	163 (90%)	19 (10%)	0	100	100
70	BL	134/143 (94%)	130 (97%)	4 (3%)	0	100	100
71	La	69/108 (64%)	67 (97%)	1 (1%)	1 (1%)	9	5
72	Aa	181/222 (82%)	171 (94%)	10 (6%)	0	100	100
73	AY	83/95 (87%)	80 (96%)	3 (4%)	0	100	100
74	Ca	51/56 (91%)	51 (100%)	0	0	100	100
77	Ba	99/122 (81%)	95 (96%)	4 (4%)	0	100	100
78	AI	90/177 (51%)	86 (96%)	4 (4%)	0	100	100
All	All	10399/11933 (87%)	10062 (97%)	325 (3%)	12 (0%)	49	56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
59	Ta	29	ASP
66	Ya	57	LYS
59	Ta	14	LYS
63	AQ	21	VAL
66	Ya	79	ALA
53	AA	5	ILE
65	Ua	137	ASP
71	La	89	VAL
68	AN	66	LYS
15	Ja	150	PRO
63	AQ	4	VAL
41	Ha	15	VAL

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	
5	BC	24/24 (100%)	22 (92%)	2 (8%)	10	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BM	131/148 (88%)	129 (98%)	2 (2%)	57	68
7	BO	116/133 (87%)	112 (97%)	4 (3%)	32	40
8	AR	44/71 (62%)	44 (100%)	0	100	100
9	AU	96/105 (91%)	95 (99%)	1 (1%)	68	77
10	Ma	87/110 (79%)	84 (97%)	3 (3%)	32	40
11	Ia	171/175 (98%)	167 (98%)	4 (2%)	44	55
12	AE	111/112 (99%)	109 (98%)	2 (2%)	51	63
13	AX	84/94 (89%)	82 (98%)	2 (2%)	43	54
14	AP	116/117 (99%)	116 (100%)	0	100	100
15	Ja	225/227 (99%)	215 (96%)	10 (4%)	25	29
16	Ea	180/180 (100%)	180 (100%)	0	100	100
17	AL	161/198 (81%)	159 (99%)	2 (1%)	63	74
18	Va	111/114 (97%)	104 (94%)	7 (6%)	16	16
19	Ka	104/114 (91%)	103 (99%)	1 (1%)	68	77
20	AW	97/98 (99%)	95 (98%)	2 (2%)	47	58
21	BD	87/93 (94%)	87 (100%)	0	100	100
22	BS	326/329 (99%)	326 (100%)	0	100	100
23	AM	137/138 (99%)	134 (98%)	3 (2%)	45	56
24	AC	183/225 (81%)	178 (97%)	5 (3%)	39	49
25	BI	104/110 (94%)	102 (98%)	2 (2%)	50	61
26	AH	112/117 (96%)	110 (98%)	2 (2%)	51	63
27	BT	323/331 (98%)	317 (98%)	6 (2%)	50	61
28	AV	114/121 (94%)	110 (96%)	4 (4%)	32	39
29	AD	156/171 (91%)	149 (96%)	7 (4%)	24	29
30	AJ	157/158 (99%)	155 (99%)	2 (1%)	61	72
31	BQ	192/197 (98%)	191 (100%)	1 (0%)	81	87
32	BH	176/177 (99%)	173 (98%)	3 (2%)	53	65
33	Da	132/133 (99%)	127 (96%)	5 (4%)	29	36
34	BK	238/254 (94%)	238 (100%)	0	100	100
35	AT	81/97 (84%)	81 (100%)	0	100	100
36	Pa	40/49 (82%)	39 (98%)	1 (2%)	42	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BP	108/110 (98%)	107 (99%)	1 (1%)	70	79
38	BN	108/136 (79%)	103 (95%)	5 (5%)	24	28
39	BG	200/219 (91%)	195 (98%)	5 (2%)	42	52
40	Fa	97/104 (93%)	94 (97%)	3 (3%)	35	44
41	Ha	120/121 (99%)	118 (98%)	2 (2%)	53	65
42	BU	147/158 (93%)	143 (97%)	4 (3%)	39	49
43	BR	199/212 (94%)	197 (99%)	2 (1%)	68	77
44	Xa	124/135 (92%)	122 (98%)	2 (2%)	55	66
45	BV	187/226 (83%)	181 (97%)	6 (3%)	34	43
46	BJ	170/179 (95%)	169 (99%)	1 (1%)	78	84
47	AO	58/137 (42%)	57 (98%)	1 (2%)	53	65
48	BW	60/68 (88%)	57 (95%)	3 (5%)	22	24
49	AK	158/181 (87%)	154 (98%)	4 (2%)	42	52
50	Na	76/78 (97%)	73 (96%)	3 (4%)	28	35
51	AB	161/172 (94%)	161 (100%)	0	100	100
52	BF	157/194 (81%)	152 (97%)	5 (3%)	34	43
53	AA	174/207 (84%)	163 (94%)	11 (6%)	16	16
54	AG	174/177 (98%)	170 (98%)	4 (2%)	44	55
55	Ga	47/114 (41%)	45 (96%)	2 (4%)	26	31
56	BA	47/48 (98%)	45 (96%)	2 (4%)	26	31
57	AF	117/123 (95%)	115 (98%)	2 (2%)	53	65
58	Wa	121/132 (92%)	119 (98%)	2 (2%)	53	65
59	Ta	193/213 (91%)	186 (96%)	7 (4%)	31	39
60	AZ	64/65 (98%)	60 (94%)	4 (6%)	16	16
61	BE	72/73 (99%)	70 (97%)	2 (3%)	38	48
62	Za	166/228 (73%)	160 (96%)	6 (4%)	31	39
63	AQ	116/122 (95%)	111 (96%)	5 (4%)	26	31
64	Oa	52/57 (91%)	44 (85%)	8 (15%)	2	1
65	Ua	100/121 (83%)	95 (95%)	5 (5%)	22	24
66	Ya	110/126 (87%)	105 (96%)	5 (4%)	24	29
67	BB	108/122 (88%)	106 (98%)	2 (2%)	50	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	AN	88/104 (85%)	84 (96%)	4 (4%)	24	29
69	Ra	165/169 (98%)	158 (96%)	7 (4%)	26	31
70	BL	110/113 (97%)	107 (97%)	3 (3%)	39	49
71	La	61/92 (66%)	58 (95%)	3 (5%)	22	24
72	Aa	158/183 (86%)	155 (98%)	3 (2%)	50	61
73	AY	73/78 (94%)	72 (99%)	1 (1%)	59	70
74	Ca	47/48 (98%)	46 (98%)	1 (2%)	47	58
77	Ba	93/110 (84%)	90 (97%)	3 (3%)	34	43
78	AI	87/139 (63%)	80 (92%)	7 (8%)	11	9
All	All	9089/10114 (90%)	8860 (98%)	229 (2%)	42	52

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	BC	16	LYS
5	BC	20	MET
6	BM	24	VAL
6	BM	126	GLN
7	BO	36	THR
7	BO	46	SER
7	BO	61	THR
7	BO	82	GLU
9	AU	90	LYS
10	Ma	10	ARG
10	Ma	55	GLU
10	Ma	90	THR
11	Ia	49	LYS
11	Ia	66	THR
11	Ia	87	VAL
11	Ia	116	GLU
12	AE	54	ASP
12	AE	65	LEU
13	AX	66	VAL
13	AX	96	VAL
15	Ja	56	LEU
15	Ja	67	GLN
15	Ja	90	VAL
15	Ja	96	ASN
15	Ja	101	LEU

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Mol	Chain	Res	Type
15	Ja	140	ASN
15	Ja	214	THR
15	Ja	224	ASN
15	Ja	236	VAL
15	Ja	238	LEU
17	AL	84	GLN
17	AL	106	GLU
18	Va	43	SER
18	Va	49	ILE
18	Va	65	ILE
18	Va	80	ILE
18	Va	99	VAL
18	Va	104	PHE
18	Va	122	VAL
19	Ka	43	GLU
20	AW	77	THR
20	AW	101	SER
23	AM	41	ASP
23	AM	96	VAL
23	AM	147	GLU
24	AC	12	LEU
24	AC	58	VAL
24	AC	130	VAL
24	AC	172	SER
24	AC	204	GLU
25	BI	71	ASP
25	BI	137	ASN
26	AH	93	LEU
26	AH	120	VAL
27	BT	27	VAL
27	BT	284	VAL
27	BT	291	VAL
27	BT	333	LYS
27	BT	353	VAL
27	BT	380	LYS
28	AV	80	THR
28	AV	87	MET
28	AV	92	THR
28	AV	96	GLU
29	AD	29	VAL
29	AD	40	VAL
29	AD	49	VAL

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Mol	Chain	Res	Type
29	AD	106	LEU
29	AD	160	GLU
29	AD	171	GLU
29	AD	198	ARG
30	AJ	57	VAL
30	AJ	72	THR
31	BQ	208	GLU
32	BH	174	GLU
32	BH	179	LEU
32	BH	203	SER
33	Da	27	LYS
33	Da	58	HIS
33	Da	86	GLU
33	Da	87	ASP
33	Da	148	THR
36	Pa	14	VAL
37	BP	67	SER
38	BN	51	THR
38	BN	103	ASP
38	BN	111	VAL
38	BN	116	ASP
38	BN	118	GLN
39	BG	90	LEU
39	BG	174	VAL
39	BG	193	CYS
39	BG	217	ASN
39	BG	246	VAL
40	Fa	23	VAL
40	Fa	90	ARG
40	Fa	103	VAL
41	Ha	2	THR
41	Ha	60	TYR
42	BU	38	VAL
42	BU	55	THR
42	BU	140	VAL
42	BU	162	MET
43	BR	34	GLU
43	BR	100	ILE
44	Xa	37	LYS
44	Xa	122	ASP
45	BV	31	ASP
45	BV	68	VAL

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Mol	Chain	Res	Type
45	BV	103	MET
45	BV	143	THR
45	BV	149	GLN
45	BV	225	LEU
46	BJ	53	VAL
47	AO	59	LYS
48	BW	25	THR
48	BW	32	VAL
48	BW	65	ASP
49	AK	51	ILE
49	AK	99	MET
49	AK	119	MET
49	AK	163	ARG
50	Na	54	THR
50	Na	55	VAL
50	Na	65	LEU
52	BF	41	ASN
52	BF	70	VAL
52	BF	146	VAL
52	BF	154	ASP
52	BF	180	ILE
53	AA	29	LEU
53	AA	61	GLU
53	AA	76	ARG
53	AA	79	PHE
53	AA	84	VAL
53	AA	105	LEU
53	AA	122	VAL
53	AA	137	ILE
53	AA	139	SER
53	AA	164	THR
53	AA	190	LEU
54	AG	9	ASN
54	AG	68	VAL
54	AG	146	THR
54	AG	161	THR
55	Ga	118	SER
55	Ga	127	ILE
56	BA	17	MET
56	BA	45	ARG
57	AF	72	ASN
57	AF	117	THR

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Mol	Chain	Res	Type
58	Wa	36	ILE
58	Wa	49	ASP
59	Ta	10	THR
59	Ta	45	PHE
59	Ta	65	GLN
59	Ta	78	HIS
59	Ta	110	VAL
59	Ta	151	LYS
59	Ta	219	SER
60	AZ	8	ILE
60	AZ	9	LYS
60	AZ	30	ASP
60	AZ	42	LEU
61	BE	52	VAL
61	BE	75	SER
62	Za	80	VAL
62	Za	108	THR
62	Za	115	GLN
62	Za	116	MET
62	Za	135	HIS
62	Za	178	LEU
63	AQ	8	LEU
63	AQ	20	LEU
63	AQ	36	GLU
63	AQ	73	THR
63	AQ	91	LYS
64	Oa	5	ILE
64	Oa	10	VAL
64	Oa	26	VAL
64	Oa	28	VAL
64	Oa	31	THR
64	Oa	34	ASP
64	Oa	52	THR
64	Oa	58	ARG
65	Ua	30	VAL
65	Ua	61	VAL
65	Ua	65	ARG
65	Ua	137	ASP
65	Ua	150	LEU
66	Ya	46	ILE
66	Ya	91	VAL
66	Ya	94	MET

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Mol	Chain	Res	Type
66	Ya	110	VAL
66	Ya	138	VAL
67	BB	5	ARG
67	BB	50	ILE
68	AN	47	ILE
68	AN	52	LYS
68	AN	74	ASP
68	AN	95	VAL
69	Ra	25	GLN
69	Ra	63	ILE
69	Ra	86	LYS
69	Ra	92	ASP
69	Ra	98	THR
69	Ra	120	THR
69	Ra	128	GLU
70	BL	61	MET
70	BL	100	VAL
70	BL	130	ARG
71	La	72	ILE
71	La	84	LEU
71	La	93	VAL
72	Aa	4	SER
72	Aa	83	VAL
72	Aa	92	VAL
73	AY	40	PRO
74	Ca	12	LYS
77	Ba	35	LEU
77	Ba	87	VAL
77	Ba	119	ILE
78	AI	3	ILE
78	AI	20	VAL
78	AI	31	LYS
78	AI	65	TYR
78	AI	69	THR
78	AI	73	ILE
78	AI	76	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
8	AR	6	ASN
12	AE	42	GLN

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Mol	Chain	Res	Type
13	AX	18	HIS
15	Ja	98	ASN
15	Ja	201	HIS
16	Ea	95	GLN
16	Ea	171	ASN
17	AL	143	GLN
20	AW	47	ASN
23	AM	158	ASN
24	AC	59	GLN
24	AC	66	GLN
24	AC	82	HIS
27	BT	43	ASN
27	BT	48	GLN
27	BT	94	GLN
27	BT	123	ASN
27	BT	151	ASN
28	AV	115	GLN
31	BQ	21	HIS
31	BQ	140	ASN
32	BH	18	HIS
33	Da	58	HIS
33	Da	62	GLN
33	Da	90	HIS
34	BK	251	ASN
35	AT	72	HIS
36	Pa	39	GLN
37	BP	65	GLN
38	BN	91	ASN
39	BG	185	HIS
40	Fa	56	HIS
41	Ha	103	HIS
42	BU	80	GLN
43	BR	98	ASN
43	BR	118	ASN
43	BR	164	GLN
45	BV	149	GLN
46	BJ	146	HIS
46	BJ	147	HIS
47	AO	13	GLN
47	AO	29	GLN
48	BW	61	GLN
49	AK	143	HIS

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Mol	Chain	Res	Type
51	AB	48	GLN
51	AB	178	ASN
52	BF	112	GLN
53	AA	101	GLN
54	AG	9	ASN
54	AG	58	HIS
54	AG	109	GLN
55	Ga	104	HIS
56	BA	19	GLN
57	AF	76	HIS
60	AZ	50	GLN
62	Za	117	GLN
62	Za	188	GLN
63	AQ	17	ASN
63	AQ	86	ASN
66	Ya	108	ASN
68	AN	93	HIS
68	AN	105	ASN
69	Ra	34	ASN
69	Ra	48	GLN
70	BL	103	HIS
72	Aa	104	GLN
74	Ca	3	HIS
77	Ba	78	ASN
78	AI	39	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	161/164 (98%)	25 (15%)	0
2	A	3142/3385 (92%)	411 (13%)	19 (0%)
3	W2	75/76 (98%)	14 (18%)	1 (1%)
3	i2	75/76 (98%)	13 (17%)	0
4	C3	118/121 (97%)	7 (5%)	0
75	h1	1604/1805 (88%)	254 (15%)	0
76	B1	11/12 (91%)	1 (9%)	0
All	All	5186/5639 (91%)	725 (13%)	20 (0%)

All (725) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	27	C
1	3	38	U
1	3	39	C
1	3	63	A
1	3	66	C
1	3	67	U
1	3	74	G
1	3	85	U
1	3	86	C
1	3	88	C
1	3	90	U
1	3	91	G
1	3	94	C
1	3	99	G
1	3	108	A
1	3	109	A
1	3	110	C
1	3	120	G
1	3	129	C
1	3	131	U
1	3	132	C
1	3	133	U
1	3	134	G
1	3	157	U
1	3	160	C
2	A	3	G
2	A	11	G
2	A	12	U
2	A	38	A
2	A	41	A
2	A	47	A
2	A	55	A
2	A	58	A
2	A	64	A
2	A	84	G
2	A	90	G
2	A	97	A
2	A	114	C
2	A	120	A
2	A	131	U
2	A	133	C
2	A	134	G
2	A	141	G

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Mol	Chain	Res	Type
2	A	154	G
2	A	155	A
2	A	163	C
2	A	167	A
2	A	168	G
2	A	179	G
2	A	184	A
2	A	187	U
2	A	197	A
2	A	215	G
2	A	216	A
2	A	245	A
2	A	248	A
2	A	258	G
2	A	262	A
2	A	283	U
2	A	292	A
2	A	302	U
2	A	326	G
2	A	346	A
2	A	347	C
2	A	350	G
2	A	373	G
2	A	394	A
2	A	396	A
2	A	398	U
2	A	417	G
2	A	418	G
2	A	419	A
2	A	435	G
2	A	436	C
2	A	437	G
2	A	453	A
2	A	454	U
2	A	462	G
2	A	463	G
2	A	467	A
2	A	478	C
2	A	480	G
2	A	497	G
2	A	523	U
2	A	524	A

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Mol	Chain	Res	Type
2	A	538	G
2	A	539	A
2	A	541	A
2	A	543	G
2	A	545	U
2	A	546	U
2	A	547	G
2	A	548	U
2	A	549	G
2	A	552	G
2	A	554	C
2	A	555	G
2	A	558	G
2	A	561	G
2	A	571	U
2	A	573	G
2	A	574	U
2	A	591	A
2	A	592	C
2	A	603	G
2	A	604	G
2	A	608	C
2	A	610	G
2	A	621	G
2	A	631	G
2	A	637	U
2	A	661	A2M
2	A	672	A
2	A	689	A
2	A	694	A
2	A	702	G
2	A	711	U
2	A	712	A
2	A	713	A
2	A	719	A
2	A	726	C
2	A	729	A
2	A	730	U
2	A	732	G
2	A	769	G
2	A	776	U
2	A	786	U

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Mol	Chain	Res	Type
2	A	789	A
2	A	790	G
2	A	793	U
2	A	794	G
2	A	817	A
2	A	824	G
2	A	826	A2M
2	A	839	G
2	A	858	C
2	A	866	G
2	A	870	C
2	A	878	G
2	A	883	U
2	A	888	U
2	A	905	A
2	A	916	G
2	A	917	OMG
2	A	923	A
2	A	925	G
2	A	926	A
2	A	930	A
2	A	932	C
2	A	934	A
2	A	946	G
2	A	953	C
2	A	968	C
2	A	969	PSU
2	A	983	G
2	A	986	C
2	A	989	A
2	A	990	C
2	A	991	G
2	A	992	C
2	A	993	G
2	A	995	G
2	A	1005	G
2	A	1012	C
2	A	1021	G
2	A	1024	G
2	A	1027	U
2	A	1036	C
2	A	1037	A

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Mol	Chain	Res	Type
2	A	1045	G
2	A	1046	A
2	A	1055	C
2	A	1057	A
2	A	1074	A
2	A	1075	C
2	A	1085	G
2	A	1091	U
2	A	1092	U
2	A	1104	C
2	A	1105	G
2	A	1106	G
2	A	1107	A
2	A	1112	A
2	A	1126	G
2	A	1140	G
2	A	1153	U
2	A	1162	A
2	A	1168	A
2	A	1183	G
2	A	1187	A
2	A	1189	C
2	A	1190	U
2	A	1191	G
2	A	1193	G
2	A	1203	A
2	A	1206	A
2	A	1210	A
2	A	1211	C
2	A	1212	A
2	A	1219	G
2	A	1295	G
2	A	1297	A
2	A	1317	G
2	A	1319	U
2	A	1326	U
2	A	1327	A
2	A	1341	U
2	A	1342	A
2	A	1358	A
2	A	1359	A
2	A	1360	G

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Mol	Chain	Res	Type
2	A	1361	A
2	A	1362	G
2	A	1363	C
2	A	1364	C
2	A	1408	A
2	A	1428	G
2	A	1443	G
2	A	1446	OMC
2	A	1455	A
2	A	1460	C
2	A	1490	A
2	A	1492	G
2	A	1493	A
2	A	1511	G
2	A	1534	G
2	A	1536	C
2	A	1545	G
2	A	1564	U
2	A	1569	G
2	A	1575	A
2	A	1576	A
2	A	1581	A
2	A	1588	A
2	A	1590	A
2	A	1594	G
2	A	1606	A
2	A	1621	C
2	A	1629	U
2	A	1645	G
2	A	1657	C
2	A	1676	A
2	A	1683	A
2	A	1688	U
2	A	1714	G
2	A	1725	G
2	A	1744	G
2	A	1751	A
2	A	1752	G
2	A	1759	G
2	A	1763	G
2	A	1764	U
2	A	1766	G

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Mol	Chain	Res	Type
2	A	1767	C
2	A	1768	G
2	A	1780	G
2	A	1799	A
2	A	1816	G
2	A	1817	U
2	A	1818	G
2	A	1821	G
2	A	1823	U
2	A	1844	A
2	A	1848	OMC
2	A	1849	A
2	A	1868	C
2	A	1880	G
2	A	1881	A
2	A	1882	U
2	A	1908	G
2	A	2101	U
2	A	2111	OMU
2	A	2121	G
2	A	2130	A
2	A	2139	U
2	A	2143	A
2	A	2157	A
2	A	2190	C
2	A	2203	U
2	A	2248	G
2	A	2256	PSU
2	A	2271	G
2	A	2277	A
2	A	2278	A
2	A	2305	G
2	A	2308	U
2	A	2311	A
2	A	2313	G
2	A	2332	U
2	A	2333	G
2	A	2334	U
2	A	2371	A
2	A	2372	C
2	A	2373	G
2	A	2391	G

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Mol	Chain	Res	Type
2	A	2392	G
2	A	2395	A
2	A	2400	A
2	A	2401	G
2	A	2402	A
2	A	2409	U
2	A	2410	G
2	A	2443	U
2	A	2450	G
2	A	2451	U
2	A	2452	G
2	A	2453	U
2	A	2454	A
2	A	2457	A
2	A	2458	U
2	A	2459	A
2	A	2460	A
2	A	2461	G
2	A	2495	U
2	A	2496	U
2	A	2497	U
2	A	2498	A
2	A	2499	A
2	A	2501	G
2	A	2512	U
2	A	2513	A
2	A	2522	A
2	A	2550	U
2	A	2573	G
2	A	2584	G
2	A	2586	C
2	A	2592	A
2	A	2605	G
2	A	2606	G
2	A	2613	G
2	A	2625	A
2	A	2651	U
2	A	2655	A
2	A	2671	G
2	A	2675	A
2	A	2676	G
2	A	2679	A

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Mol	Chain	Res	Type
2	A	2688	G
2	A	2689	G
2	A	2690	A
2	A	2693	A
2	A	2703	A
2	A	2704	A
2	A	2713	G
2	A	2718	U
2	A	2727	G
2	A	2728	U
2	A	2752	G
2	A	2754	C
2	A	2761	A
2	A	2776	G
2	A	2777	G
2	A	2795	G
2	A	2798	A
2	A	2799	G
2	A	2800	A
2	A	2801	A
2	A	2809	C
2	A	2816	A
2	A	2841	U
2	A	2844	A
2	A	2858	U
2	A	2870	G
2	A	2886	A
2	A	2897	G
2	A	2898	C
2	A	2910	A2M
2	A	2911	G
2	A	2934	U
2	A	2935	A
2	A	2941	C
2	A	2946	G
2	A	2982	C
2	A	2989	G
2	A	2996	G
2	A	3010	A
2	A	3028	G
2	A	3056	C
2	A	3057	G

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Mol	Chain	Res	Type
2	A	3072	G
2	A	3076	G
2	A	3077	U
2	A	3090	C
2	A	3099	G
2	A	3114	G
2	A	3120	A
2	A	3129	U
2	A	3140	A
2	A	3150	G
2	A	3151	C
2	A	3152	G
2	A	3166	U
2	A	3167	G
2	A	3168	C
2	A	3172	C
2	A	3175	U
2	A	3180	A
2	A	3181	G
2	A	3188	A
2	A	3189	G
2	A	3195	A
2	A	3202	C
2	A	3203	G
2	A	3205	G
2	A	3211	G
2	A	3215	A
2	A	3218	U
2	A	3222	G
2	A	3223	U
2	A	3224	U
2	A	3225	C
2	A	3226	G
2	A	3231	A
2	A	3235	G
2	A	3244	G
2	A	3248	C
2	A	3252	G
2	A	3280	A
2	A	3281	G
2	A	3282	A
2	A	3291	C

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Mol	Chain	Res	Type
2	A	3303	A
2	A	3304	U
2	A	3306	C
2	A	3307	G
2	A	3328	C
2	A	3332	G
2	A	3337	C
2	A	3341	C
2	A	3343	G
2	A	3356	G
2	A	3365	C
2	A	3369	U
2	A	3377	A
2	A	3379	G
2	A	3385	A
3	i2	5	G
3	i2	6	G
3	i2	9	A
3	i2	18	G
3	i2	20	G
3	i2	21	A
3	i2	22	G
3	i2	36	A
3	i2	47	U
3	i2	48	C
3	i2	73	A
3	i2	74	C
3	i2	76	A
4	C3	33	U
4	C3	38	U
4	C3	53	U
4	C3	64	G
4	C3	70	G
4	C3	110	G
4	C3	117	C
75	h1	2	A
75	h1	17	C
75	h1	25	C
75	h1	26	A
75	h1	34	G
75	h1	42	G
75	h1	45	U

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Mol	Chain	Res	Type
75	h1	47	A
75	h1	56	U
75	h1	63	G
75	h1	67	G
75	h1	68	A
75	h1	75	U
75	h1	76	C
75	h1	82	G
75	h1	84	G
75	h1	105	A
75	h1	115	A
75	h1	121	PSU
75	h1	124	G
75	h1	128	G
75	h1	129	U
75	h1	130	A
75	h1	132	C
75	h1	133	U
75	h1	135	C
75	h1	136	U
75	h1	138	C
75	h1	139	U
75	h1	140	C
75	h1	143	A
75	h1	150	U
75	h1	151	A
75	h1	156	U
75	h1	158	C
75	h1	163	G
75	h1	165	U
75	h1	174	C
75	h1	175	A
75	h1	186	A
75	h1	189	U
75	h1	190	A
75	h1	191	U
75	h1	192	G
75	h1	194	A
75	h1	201	G
75	h1	214	A
75	h1	250	U
75	h1	251	C

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Mol	Chain	Res	Type
75	h1	258	A
75	h1	264	C
75	h1	266	G
75	h1	272	A
75	h1	273	U
75	h1	277	C
75	h1	289	G
75	h1	301	A
75	h1	316	C
75	h1	318	A
75	h1	322	U
75	h1	324	G
75	h1	335	A
75	h1	339	G
75	h1	340	C
75	h1	361	G
75	h1	363	C
75	h1	368	A
75	h1	372	A
75	h1	391	G
75	h1	402	A
75	h1	403	A
75	h1	404	C
75	h1	413	C
75	h1	419	A
75	h1	424	G
75	h1	426	C
75	h1	427	A
75	h1	428	G
75	h1	436	G
75	h1	441	U
75	h1	446	C
75	h1	447	A
75	h1	460	G
75	h1	470	A
75	h1	479	A
75	h1	487	C
75	h1	488	G
75	h1	489	G
75	h1	503	U
75	h1	505	G
75	h1	509	U

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Mol	Chain	Res	Type
75	h1	512	G
75	h1	516	G
75	h1	517	A
75	h1	521	C
75	h1	536	A
75	h1	540	A
75	h1	542	G
75	h1	544	U
75	h1	545	C
75	h1	559	G
75	h1	567	C
75	h1	570	G
75	h1	580	OMU
75	h1	581	A
75	h1	583	PSU
75	h1	584	U
75	h1	596	A
75	h1	597	OMG
75	h1	608	A
75	h1	613	OMU
75	h1	621	A2M
75	h1	622	A
75	h1	625	A
75	h1	636	G
75	h1	641	U
75	h1	758	A
75	h1	759	A
75	h1	768	G
75	h1	769	C
75	h1	774	A
75	h1	778	A2M
75	h1	783	A
75	h1	784	C
75	h1	785	G
75	h1	788	C
75	h1	789	U
75	h1	792	A
75	h1	796	A
75	h1	815	A
75	h1	816	U
75	h1	817	A
75	h1	831	A

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Mol	Chain	Res	Type
75	h1	833	U
75	h1	856	A
75	h1	864	A
75	h1	877	G
75	h1	878	G
75	h1	887	U
75	h1	899	A
75	h1	934	A
75	h1	936	U
75	h1	952	A
75	h1	961	U
75	h1	967	A
75	h1	1005	U
75	h1	1006	A
75	h1	1027	A
75	h1	1029	C
75	h1	1033	G
75	h1	1040	A
75	h1	1054	G
75	h1	1060	U
75	h1	1061	A
75	h1	1063	A
75	h1	1077	A
75	h1	1082	A
75	h1	1084	G
75	h1	1088	A
75	h1	1093	A
75	h1	1098	U
75	h1	1139	A
75	h1	1147	G
75	h1	1151	G
75	h1	1156	G
75	h1	1159	C
75	h1	1166	G
75	h1	1168	G
75	h1	1184	A
75	h1	1186	U
75	h1	1192	C4J
75	h1	1193	C
75	h1	1195	A
75	h1	1197	A
75	h1	1200	G

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Mol	Chain	Res	Type
75	h1	1201	G
75	h1	1203	A
75	h1	1218	A
75	h1	1219	G
75	h1	1230	G
75	h1	1232	OMU
75	h1	1244	G
75	h1	1245	A
75	h1	1246	G
75	h1	1247	C
75	h1	1252	U
75	h1	1253	C
75	h1	1257	A
75	h1	1266	G
75	h1	1270	OMU
75	h1	1289	G
75	h1	1315	U
75	h1	1316	U
75	h1	1322	A
75	h1	1341	U
75	h1	1342	G
75	h1	1346	A
75	h1	1362	C
75	h1	1363	A
75	h1	1364	U
75	h1	1389	G
75	h1	1393	U
75	h1	1394	A
75	h1	1401	U
75	h1	1402	U
75	h1	1416	U
75	h1	1417	U
75	h1	1418	U
75	h1	1430	A
75	h1	1431	OMG
75	h1	1436	G
75	h1	1438	G
75	h1	1449	A
75	h1	1462	C
75	h1	1474	A
75	h1	1477	G
75	h1	1486	A

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Mol	Chain	Res	Type
75	h1	1514	G
75	h1	1519	A
75	h1	1526	A
75	h1	1533	A
75	h1	1539	A
75	h1	1540	U
75	h1	1541	G
75	h1	1559	U
75	h1	1561	G
75	h1	1576	G
75	h1	1585	A
75	h1	1592	G
75	h1	1603	G
75	h1	1609	G
75	h1	1613	A
75	h1	1621	C
75	h1	1636	C
75	h1	1637	A
75	h1	1653	A
75	h1	1660	G
75	h1	1666	U
75	h1	1682	G
75	h1	1684	U
75	h1	1759	A
75	h1	1764	G
75	h1	1766	A
75	h1	1770	A
75	h1	1773	U
75	h1	1784	G
75	h1	1786	MA6
75	h1	1787	C
75	h1	1796	G
75	h1	1797	G
75	h1	1798	A
75	h1	1799	U
75	h1	1800	C
75	h1	1803	U
76	B1	19	U
3	W2	4	G
3	W2	5	G
3	W2	6	G
3	W2	15	G

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Mol	Chain	Res	Type
3	W2	16	U
3	W2	17	U
3	W2	19	G
3	W2	20	G
3	W2	21	A
3	W2	22	G
3	W2	48	C
3	W2	70	C
3	W2	71	G
3	W2	76	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	547	G
2	A	554	C
2	A	591	A
2	A	602	C
2	A	609	A
2	A	882	C
2	A	917	OMG
2	A	925	G
2	A	990	C
2	A	1026	A
2	A	1848	OMC
2	A	2304	C
2	A	2370	A
2	A	2496	U
2	A	2585	G
2	A	3119	U
2	A	3225	C
2	A	3247	G
2	A	3303	A
3	W2	70	C

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

215 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
2	OMG	A	1853	2	23,26,27	0.50	0	33,38,41	0.46	0
2	OMG	A	2790	2	23,26,27	0.44	0	33,38,41	0.45	0
2	PSU	A	2974	2	18,21,22	1.03	2 (11%)	22,30,33	1.20	4 (18%)
75	OMU	h1	1381	80,75	19,22,23	0.70	0	26,31,34	0.64	0
75	PSU	h1	1000	75	18,21,22	0.85	1 (5%)	22,30,33	0.90	1 (4%)
75	UY1	h1	602	75	19,22,23	1.40	3 (15%)	22,31,34	0.92	1 (4%)
75	A2M	h1	466	75	22,25,26	0.75	0	31,36,39	2.31	9 (29%)
2	A2M	A	945	2	22,25,26	0.82	1 (4%)	31,36,39	2.04	11 (35%)
2	PSU	A	2943	81,80,2	18,21,22	0.87	1 (5%)	22,30,33	1.14	3 (13%)
2	OMC	A	1446	2	19,22,23	0.41	0	26,31,34	0.67	0
75	PSU	h1	948	75	18,21,22	0.92	2 (11%)	22,30,33	1.02	2 (9%)
22	HIC	BS	246	22	10,11,12	0.81	1 (10%)	8,14,16	0.79	0
2	A2M	A	2319	2	22,25,26	0.63	0	31,36,39	2.05	7 (22%)
2	OMU	A	2920	81,2	19,22,23	0.45	0	26,31,34	0.54	0
75	PSU	h1	360	75	18,21,22	0.80	1 (5%)	22,30,33	1.24	3 (13%)
2	OMG	A	2286	2	23,26,27	0.45	0	33,38,41	0.30	0
75	OMC	h1	38	75	19,22,23	0.36	0	26,31,34	0.34	0
2	A2M	A	2212	80,2	22,25,26	0.81	0	31,36,39	2.13	9 (29%)
2	OMC	A	1858	2	19,22,23	0.63	0	26,31,34	0.55	0
2	A2M	A	816	2	22,25,26	0.99	2 (9%)	31,36,39	2.48	9 (29%)
2	A2M	A	1376	80,2	22,25,26	0.80	1 (4%)	31,36,39	1.88	4 (12%)
2	OMG	A	2650	2	23,26,27	0.32	0	33,38,41	0.55	1 (3%)
75	PSU	h1	1215	75	18,21,22	0.84	1 (5%)	22,30,33	0.83	0
75	OMC	h1	1216	75	19,22,23	0.32	0	26,31,34	0.66	1 (3%)
75	PSU	h1	95	75	18,21,22	0.88	1 (5%)	22,30,33	0.83	0
2	OMC	A	2681	2	19,22,23	0.39	0	26,31,34	0.68	0
2	A2M	A	885	2	22,25,26	0.88	1 (4%)	31,36,39	1.96	8 (25%)
2	PSU	A	894	2	18,21,22	1.04	1 (5%)	22,30,33	1.04	1 (4%)
75	PSU	h1	1520	75	18,21,22	0.97	2 (11%)	22,30,33	0.95	1 (4%)
75	PSU	h1	256	75	18,21,22	0.90	1 (5%)	22,30,33	1.00	2 (9%)
2	PSU	A	828	2	18,21,22	0.82	1 (5%)	22,30,33	1.16	2 (9%)
75	A2M	h1	162	75	22,25,26	0.80	1 (4%)	31,36,39	2.26	10 (32%)
75	OMG	h1	1431	80,75	23,26,27	0.34	0	33,38,41	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A	1062	81,2	18,21,22	0.93	1 (5%)	22,30,33	1.00	1 (4%)
2	OMU	A	803	2	19,22,23	0.78	1 (5%)	26,31,34	0.85	0
75	PSU	h1	583	75	18,21,22	1.00	1 (5%)	22,30,33	0.87	0
75	OMU	h1	1270	80,75	19,22,23	0.63	0	26,31,34	0.76	1 (3%)
2	PSU	A	965	2	18,21,22	1.00	2 (11%)	22,30,33	1.00	1 (4%)
2	1MG	A	1646	2	22,26,27	1.20	3 (13%)	33,39,42	1.00	2 (6%)
75	4AC	h1	1281	75	21,24,25	1.44	2 (9%)	29,34,37	1.16	3 (10%)
2	PSU	A	975	81,2	18,21,22	1.00	2 (11%)	22,30,33	1.18	4 (18%)
2	OMU	A	676	2	19,22,23	0.60	0	26,31,34	0.91	0
75	OMU	h1	1263	75	19,22,23	0.96	2 (10%)	26,31,34	0.76	0
2	OMC	A	2363	2	19,22,23	0.45	0	26,31,34	0.54	0
75	C4J	h1	1192	75	24,29,30	1.23	3 (12%)	29,42,45	1.11	2 (6%)
2	OMC	A	1845	2	19,22,23	0.65	0	26,31,34	0.64	0
75	PSU	h1	1291	75	18,21,22	0.83	1 (5%)	22,30,33	1.07	3 (13%)
2	OMU	A	2716	2	19,22,23	0.70	0	26,31,34	0.79	1 (3%)
75	PSU	h1	1531	75	18,21,22	0.96	2 (11%)	22,30,33	1.00	2 (9%)
2	PSU	A	1015	81,2	18,21,22	0.77	1 (5%)	22,30,33	1.19	3 (13%)
75	PSU	h1	1208	75	18,21,22	0.89	1 (5%)	22,30,33	1.14	3 (13%)
2	PSU	A	2256	2	18,21,22	0.89	1 (5%)	22,30,33	0.86	1 (4%)
2	OMC	A	2878	2	19,22,23	0.60	0	26,31,34	0.45	0
2	OMG	A	814	2	23,26,27	0.52	0	33,38,41	0.50	0
2	OMC	A	2958	80,2	19,22,23	0.55	0	26,31,34	0.55	0
2	OMC	A	2335	2	19,22,23	0.41	0	26,31,34	0.53	0
2	OMU	A	48	2	19,22,23	0.66	0	26,31,34	0.72	0
75	A2M	h1	543	75	22,25,26	0.83	0	31,36,39	2.48	11 (35%)
2	PSU	A	1472	2	18,21,22	0.86	1 (5%)	22,30,33	0.97	1 (4%)
2	PSU	A	2853	2	18,21,22	0.84	1 (5%)	22,30,33	0.96	3 (13%)
2	5MC	A	2869	81,2	18,22,23	0.56	0	26,32,35	0.99	2 (7%)
75	OMU	h1	1261	75	19,22,23	0.94	2 (10%)	26,31,34	0.72	0
2	5MC	A	2276	80,2	18,22,23	0.50	0	26,32,35	0.57	0
75	PSU	h1	1783	75	18,21,22	1.08	2 (11%)	22,30,33	1.19	3 (13%)
2	OMG	A	2122	2	23,26,27	0.40	0	33,38,41	0.54	0
2	OMU	A	2419	2	19,22,23	0.84	1 (5%)	26,31,34	0.77	0
75	PSU	h1	1025	75	18,21,22	0.88	1 (5%)	22,30,33	1.29	5 (22%)
2	PSU	A	969	2	18,21,22	1.05	2 (11%)	22,30,33	1.21	3 (13%)
2	OMU	A	2111	2	19,22,23	0.55	0	26,31,34	0.58	0
2	OMC	A	2195	81,2	19,22,23	0.53	0	26,31,34	0.71	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	PSU	h1	121	75	18,21,22	0.79	1 (5%)	22,30,33	0.73	0
2	OMC	A	1517	80,2	19,22,23	0.53	0	26,31,34	0.60	0
2	OMG	A	2916	2	23,26,27	0.43	0	33,38,41	0.39	0
2	PSU	A	1480	2	18,21,22	0.85	1 (5%)	22,30,33	1.11	3 (13%)
2	PSU	A	2189	81,2	18,21,22	0.89	1 (5%)	22,30,33	1.20	2 (9%)
75	PSU	h1	1611	75	18,21,22	1.00	1 (5%)	22,30,33	1.13	3 (13%)
2	PSU	A	2316	80,2	18,21,22	0.89	1 (5%)	22,30,33	0.81	1 (4%)
75	A2M	h1	422	75	22,25,26	0.66	0	31,36,39	2.16	9 (29%)
75	A2M	h1	794	75	22,25,26	0.65	0	31,36,39	2.17	10 (32%)
75	PSU	h1	304	75	18,21,22	0.95	1 (5%)	22,30,33	1.01	2 (9%)
2	OMU	A	2734	80,2	19,22,23	0.64	0	26,31,34	0.79	0
75	PSU	h1	605	75	18,21,22	0.90	1 (5%)	22,30,33	1.22	3 (13%)
2	PSU	A	1681	2	18,21,22	0.99	2 (11%)	22,30,33	0.92	1 (4%)
2	PSU	A	1054	2	18,21,22	0.87	2 (11%)	22,30,33	0.92	1 (4%)
1	PSU	3	97	81,1	18,21,22	0.99	2 (11%)	22,30,33	1.04	3 (13%)
2	OMC	A	2291	2	19,22,23	0.50	0	26,31,34	0.51	0
2	OMG	A	1459	80,2	23,26,27	0.42	0	33,38,41	0.47	0
2	OMC	A	675	2	19,22,23	0.62	0	26,31,34	0.57	0
1	OMG	3	79	1	23,26,27	0.33	0	33,38,41	0.45	0
2	OMG	A	917	81,2	23,26,27	0.41	0	33,38,41	0.48	0
2	A2M	A	1458	80,2	22,25,26	0.88	1 (4%)	31,36,39	1.99	8 (25%)
2	A2M	A	2933	2	22,25,26	0.85	1 (4%)	31,36,39	1.91	6 (19%)
75	PSU	h1	1630	75	18,21,22	0.85	1 (5%)	22,30,33	1.08	3 (13%)
75	OMC	h1	416	75	19,22,23	0.32	0	26,31,34	0.55	0
2	PSU	A	2262	2	18,21,22	0.85	2 (11%)	22,30,33	1.08	2 (9%)
2	A2M	A	2279	2	22,25,26	0.84	0	31,36,39	2.27	12 (38%)
75	OMU	h1	580	75	19,22,23	0.63	0	26,31,34	0.63	0
2	PSU	A	311	81,2	18,21,22	1.00	2 (11%)	22,30,33	1.08	2 (9%)
2	PSU	A	2922	81,2	18,21,22	1.04	1 (5%)	22,30,33	1.07	2 (9%)
2	PSU	A	2264	2	18,21,22	0.94	1 (5%)	22,30,33	1.14	3 (13%)
2	PSU	A	42	81,2	18,21,22	0.86	1 (5%)	22,30,33	1.10	3 (13%)
2	PSU	A	1001	2	18,21,22	0.92	1 (5%)	22,30,33	1.22	3 (13%)
75	A2M	h1	1327	75	22,25,26	0.68	0	31,36,39	2.14	6 (19%)
75	PSU	h1	761	75	18,21,22	0.72	1 (5%)	22,30,33	0.88	1 (4%)
75	OMG	h1	1272	81,75	23,26,27	0.29	0	33,38,41	0.40	0
2	OMU	A	2345	2	19,22,23	0.74	0	26,31,34	0.89	0
2	PSU	A	34	2	18,21,22	1.20	2 (11%)	22,30,33	0.97	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	PSU	h1	606	75	18,21,22	1.08	2 (11%)	22,30,33	1.03	2 (9%)
75	PSU	h1	959	81,75	18,21,22	0.95	1 (5%)	22,30,33	1.00	1 (4%)
75	PSU	h1	762	75	18,21,22	0.82	1 (5%)	22,30,33	0.93	0
75	OMG	h1	390	81,75	23,26,27	0.32	0	33,38,41	0.41	0
75	MA6	h1	1786	75	23,26,27	0.51	0	34,38,41	2.00	5 (14%)
2	PSU	A	2252	2	18,21,22	0.84	1 (5%)	22,30,33	1.20	3 (13%)
2	PSU	A	1131	2	18,21,22	0.90	2 (11%)	22,30,33	1.00	1 (4%)
2	PSU	A	2132	81,2	18,21,22	1.03	2 (11%)	22,30,33	1.43	2 (9%)
2	A2M	A	2359	2	22,25,26	0.77	1 (4%)	31,36,39	1.96	8 (25%)
75	PSU	h1	604	75	18,21,22	0.79	1 (5%)	22,30,33	1.05	2 (9%)
2	PSU	A	2879	2	18,21,22	0.88	1 (5%)	22,30,33	1.06	1 (4%)
75	PSU	h1	1188	75	18,21,22	0.86	1 (5%)	22,30,33	1.15	3 (13%)
2	OMC	A	2835	2	19,22,23	0.51	0	26,31,34	0.60	0
75	6MZ	h1	1767	81,80,75	22,25,26	0.75	1 (4%)	30,36,39	0.85	2 (6%)
75	G7M	h1	1577	3,75	23,26,27	1.01	2 (8%)	35,39,42	1.19	4 (11%)
2	OMG	A	2393	80,2	23,26,27	0.56	0	33,38,41	0.57	0
2	A2M	A	2945	80,2	22,25,26	0.67	0	31,36,39	2.01	9 (29%)
75	OMU	h1	1232	75	19,22,23	0.91	1 (5%)	26,31,34	0.73	0
2	PSU	A	2134	2	18,21,22	0.95	1 (5%)	22,30,33	1.10	3 (13%)
2	PSU	A	2825	81,2	18,21,22	0.85	1 (5%)	22,30,33	1.10	1 (4%)
2	1MA	A	657	80,2	21,25,26	0.64	1 (4%)	31,37,40	0.82	0
2	OMG	A	2407	81,2	23,26,27	0.52	0	33,38,41	0.49	0
75	A2M	h1	438	75	22,25,26	0.75	0	31,36,39	2.15	9 (29%)
75	PSU	h1	1182	75	18,21,22	0.95	1 (5%)	22,30,33	1.00	2 (9%)
2	PSU	A	2414	80,2	18,21,22	0.98	2 (11%)	22,30,33	1.20	3 (13%)
2	OMG	A	2389	2	23,26,27	0.49	0	33,38,41	0.30	0
2	OMC	A	1478	2	19,22,23	0.44	0	26,31,34	0.56	0
75	PSU	h1	1563	75	18,21,22	0.95	1 (5%)	22,30,33	1.07	2 (9%)
75	PSU	h1	1118	75	18,21,22	0.92	1 (5%)	22,30,33	1.01	2 (9%)
2	PSU	A	3109	2	18,21,22	0.87	1 (5%)	22,30,33	1.08	3 (13%)
75	PSU	h1	337	81,75	18,21,22	0.85	1 (5%)	22,30,33	0.81	0
2	OMG	A	2618	2,3	23,26,27	0.47	0	33,38,41	0.41	0
2	A2M	A	2218	2	22,25,26	0.72	0	31,36,39	2.07	7 (22%)
1	A2M	3	47	1	22,25,26	0.72	0	31,36,39	2.14	10 (32%)
2	PSU	A	277	2	18,21,22	1.15	2 (11%)	22,30,33	1.02	1 (4%)
2	PSU	A	2312	81,2	18,21,22	0.93	2 (11%)	22,30,33	0.95	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	PSU	h1	468	75	18,21,22	0.85	1 (5%)	22,30,33	1.01	2 (9%)
75	PSU	h1	752	75	18,21,22	0.97	1 (5%)	22,30,33	1.02	2 (9%)
2	PSU	A	150	81,2	18,21,22	0.94	2 (11%)	22,30,33	0.82	1 (4%)
2	OMU	A	44	81,2	19,22,23	0.57	0	26,31,34	0.43	0
75	A2M	h1	28	75	22,25,26	0.66	0	31,36,39	2.15	9 (29%)
2	PSU	A	2893	2	18,21,22	1.02	2 (11%)	22,30,33	0.88	1 (4%)
2	PSU	A	2209	2	18,21,22	0.93	1 (5%)	22,30,33	1.12	3 (13%)
2	OMG	A	2792	2	23,26,27	0.47	0	33,38,41	0.38	0
75	PSU	h1	808	75	18,21,22	0.91	1 (5%)	22,30,33	0.99	2 (9%)
2	OMG	A	3290	80,2	23,26,27	0.35	0	33,38,41	0.59	0
2	PSU	A	228	2	18,21,22	0.89	1 (5%)	22,30,33	0.90	1 (4%)
75	A2M	h1	799	75	22,25,26	0.82	1 (4%)	31,36,39	2.22	9 (29%)
2	A2M	A	826	81,80,2	22,25,26	0.63	0	31,36,39	2.03	8 (25%)
2	PSU	A	901	81,2	18,21,22	1.04	2 (11%)	22,30,33	1.18	3 (13%)
75	OMU	h1	123	75	19,22,23	0.83	1 (5%)	26,31,34	0.75	0
2	A2M	A	2254	2	22,25,26	0.73	0	31,36,39	2.37	12 (38%)
2	OMC	A	1848	80,2	19,22,23	0.53	0	26,31,34	0.58	0
75	OMC	h1	1641	80,75	19,22,23	0.44	0	26,31,34	0.55	0
2	OMG	A	2921	2	23,26,27	0.28	0	33,38,41	0.33	0
2	PSU	A	1133	2	18,21,22	0.94	1 (5%)	22,30,33	0.95	1 (4%)
2	OMU	A	1066	2	19,22,23	0.62	0	26,31,34	0.84	0
75	A2M	h1	1575	75	22,25,26	0.74	0	31,36,39	2.47	13 (41%)
75	4AC	h1	1777	75	21,24,25	1.34	1 (4%)	29,34,37	1.30	5 (17%)
2	PSU	A	2258	2	18,21,22	0.94	1 (5%)	22,30,33	0.95	1 (4%)
2	A2M	A	2324	2	22,25,26	0.71	0	31,36,39	1.98	8 (25%)
75	A2M	h1	1754	75	22,25,26	0.58	0	31,36,39	2.11	9 (29%)
75	PSU	h1	308	80,75	18,21,22	1.00	2 (11%)	22,30,33	1.31	3 (13%)
75	MA6	h1	1785	75	23,26,27	0.48	0	34,38,41	1.92	5 (14%)
1	PSU	3	78	1	18,21,22	0.97	2 (11%)	22,30,33	0.95	1 (4%)
75	OMU	h1	613	75	19,22,23	0.65	0	26,31,34	0.69	0
75	PSU	h1	1104	75	18,21,22	0.82	1 (5%)	22,30,33	1.22	3 (13%)
75	OMG	h1	597	75	23,26,27	0.31	0	33,38,41	0.37	0
2	OMU	A	1890	2	19,22,23	0.65	0	26,31,34	0.79	0
2	A2M	A	2639	2	22,25,26	0.70	0	31,36,39	2.01	7 (22%)
2	A2M	A	2910	2	22,25,26	0.86	1 (4%)	31,36,39	2.13	10 (32%)
75	PSU	h1	1302	75	18,21,22	0.84	1 (5%)	22,30,33	0.95	1 (4%)
2	PSU	A	509	2	18,21,22	1.03	1 (5%)	22,30,33	1.09	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	PSU	h1	634	75	18,21,22	0.78	1 (5%)	22,30,33	1.13	2 (9%)
2	OMG	A	2814	2	23,26,27	0.42	0	33,38,41	0.39	0
75	OMC	h1	471	75	19,22,23	0.36	0	26,31,34	0.57	0
75	PSU	h1	1176	75	18,21,22	0.90	1 (5%)	22,30,33	1.07	3 (13%)
1	PSU	3	22	2,1	18,21,22	0.99	1 (5%)	22,30,33	0.94	1 (4%)
2	A2M	A	2124	2	22,25,26	0.67	0	31,36,39	1.92	9 (29%)
75	OMU	h1	1445	75	19,22,23	0.83	1 (5%)	26,31,34	0.67	0
2	A2M	A	661	2	22,25,26	0.86	1 (4%)	31,36,39	1.93	7 (22%)
2	PSU	A	2743	2	18,21,22	0.98	2 (11%)	22,30,33	1.04	3 (13%)
75	A2M	h1	621	80,75	22,25,26	0.83	1 (4%)	31,36,39	2.00	9 (29%)
75	A2M	h1	778	75	22,25,26	0.63	0	31,36,39	2.26	9 (29%)
75	PSU	h1	1483	75	18,21,22	0.94	1 (5%)	22,30,33	0.83	0
2	PSU	A	1132	2	18,21,22	0.80	1 (5%)	22,30,33	1.24	4 (18%)
55	MLY	Ga	113	55	9,10,11	0.43	0	6,11,13	0.44	0
2	PSU	A	2430	2	18,21,22	0.84	1 (5%)	22,30,33	1.15	3 (13%)
75	A2M	h1	975	75	22,25,26	0.71	1 (4%)	31,36,39	2.01	8 (25%)
2	PSU	A	685	2	18,21,22	1.00	2 (11%)	22,30,33	1.13	2 (9%)
75	PSU	h1	103	75	18,21,22	0.96	2 (11%)	22,30,33	0.87	0
2	OMG	A	2234	2	23,26,27	0.35	0	33,38,41	0.45	0
2	OMU	A	2408	81,2	19,22,23	0.76	0	26,31,34	0.88	0
2	OMU	A	2882	2	19,22,23	0.66	0	26,31,34	0.82	0
2	PSU	A	2954	2	18,21,22	0.87	1 (5%)	22,30,33	1.20	4 (18%)
75	OMG	h1	244	75	23,26,27	0.30	0	33,38,41	0.41	0
2	A2M	A	1142	2	22,25,26	0.77	1 (4%)	31,36,39	1.89	9 (29%)
2	OMC	A	2947	2	19,22,23	0.50	0	26,31,34	0.65	1 (3%)
1	OMG	3	155	2,1	23,26,27	0.36	0	33,38,41	0.34	0
2	OMU	A	3299	2	19,22,23	0.67	0	26,31,34	0.77	0
75	PSU	h1	415	75	18,21,22	0.88	1 (5%)	22,30,33	1.02	2 (9%)
2	UY1	A	2649	2	19,22,23	1.14	1 (5%)	22,31,34	0.92	1 (4%)
2	PSU	A	785	2	18,21,22	0.82	1 (5%)	22,30,33	0.82	0
75	PSU	h1	1306	75	18,21,22	0.90	1 (5%)	22,30,33	0.87	1 (4%)
2	OMU	A	144	81,2	19,22,23	0.38	0	26,31,34	0.68	0
75	PSU	h1	449	81,75	18,21,22	0.99	1 (5%)	22,30,33	1.05	2 (9%)
75	OMU	h1	1010	75	19,22,23	0.87	2 (10%)	26,31,34	0.75	0
2	PSU	A	2864	2	18,21,22	1.03	2 (11%)	22,30,33	0.88	1 (4%)

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
2	OMG	A	1853	2	-	0/9/27/28	0/3/3/3
2	OMG	A	2790	2	-	0/9/27/28	0/3/3/3
2	PSU	A	2974	2	-	0/7/25/26	0/2/2/2
75	OMU	h1	1381	80,75	-	1/9/27/28	0/2/2/2
75	PSU	h1	1000	75	-	0/7/25/26	0/2/2/2
75	UY1	h1	602	75	-	1/9/27/28	0/2/2/2
75	A2M	h1	466	75	-	2/9/27/28	0/3/3/3
2	A2M	A	945	2	-	0/9/27/28	0/3/3/3
2	PSU	A	2943	81,80,2	-	0/7/25/26	0/2/2/2
2	OMC	A	1446	2	-	2/9/27/28	0/2/2/2
75	PSU	h1	948	75	-	0/7/25/26	0/2/2/2
22	HIC	BS	246	22	-	0/5/6/8	0/1/1/1
2	A2M	A	2319	2	-	0/9/27/28	0/3/3/3
2	OMU	A	2920	81,2	-	0/9/27/28	0/2/2/2
75	PSU	h1	360	75	-	0/7/25/26	0/2/2/2
2	OMG	A	2286	2	-	0/9/27/28	0/3/3/3
75	OMC	h1	38	75	-	1/9/27/28	0/2/2/2
2	A2M	A	2212	80,2	-	1/9/27/28	0/3/3/3
2	OMC	A	1858	2	-	0/9/27/28	0/2/2/2
2	A2M	A	816	2	-	0/9/27/28	0/3/3/3
2	A2M	A	1376	80,2	-	1/9/27/28	0/3/3/3
2	OMG	A	2650	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	1215	75	-	0/7/25/26	0/2/2/2
75	OMC	h1	1216	75	-	1/9/27/28	0/2/2/2
75	PSU	h1	95	75	-	0/7/25/26	0/2/2/2
2	OMC	A	2681	2	-	0/9/27/28	0/2/2/2
2	A2M	A	885	2	-	0/9/27/28	0/3/3/3
2	PSU	A	894	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1520	75	-	1/7/25/26	0/2/2/2
75	PSU	h1	256	75	-	0/7/25/26	0/2/2/2
2	PSU	A	828	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	162	75	-	1/9/27/28	0/3/3/3
75	OMG	h1	1431	80,75	-	3/9/27/28	0/3/3/3
2	PSU	A	1062	81,2	-	1/7/25/26	0/2/2/2
2	OMU	A	803	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	583	75	-	3/7/25/26	0/2/2/2
75	OMU	h1	1270	80,75	-	2/9/27/28	0/2/2/2
2	PSU	A	965	2	-	0/7/25/26	0/2/2/2
2	1MG	A	1646	2	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	4AC	h1	1281	75	-	0/11/29/30	0/2/2/2
2	PSU	A	975	81,2	-	0/7/25/26	0/2/2/2
2	OMU	A	676	2	-	1/9/27/28	0/2/2/2
75	OMU	h1	1263	75	-	0/9/27/28	0/2/2/2
2	OMC	A	2363	2	-	0/9/27/28	0/2/2/2
75	C4J	h1	1192	75	-	4/16/34/35	0/2/2/2
2	OMC	A	1845	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	1291	75	-	0/7/25/26	0/2/2/2
2	OMU	A	2716	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	1531	75	-	0/7/25/26	0/2/2/2
2	PSU	A	1015	81,2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1208	75	-	1/7/25/26	0/2/2/2
2	PSU	A	2256	2	-	2/7/25/26	0/2/2/2
2	OMC	A	2878	2	-	0/9/27/28	0/2/2/2
2	OMG	A	814	2	-	0/9/27/28	0/3/3/3
2	OMC	A	2958	80,2	-	0/9/27/28	0/2/2/2
2	OMC	A	2335	2	-	0/9/27/28	0/2/2/2
2	OMU	A	48	2	-	0/9/27/28	0/2/2/2
75	A2M	h1	543	75	-	2/9/27/28	0/3/3/3
2	PSU	A	1472	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2853	2	-	0/7/25/26	0/2/2/2
2	5MC	A	2869	81,2	-	4/7/25/26	0/2/2/2
75	OMU	h1	1261	75	-	0/9/27/28	0/2/2/2
2	5MC	A	2276	80,2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1783	75	-	0/7/25/26	0/2/2/2
2	OMG	A	2122	2	-	0/9/27/28	0/3/3/3
2	OMU	A	2419	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	1025	75	-	0/7/25/26	0/2/2/2
2	PSU	A	969	2	-	3/7/25/26	0/2/2/2
2	OMU	A	2111	2	-	2/9/27/28	0/2/2/2
2	OMC	A	2195	81,2	-	4/9/27/28	0/2/2/2
75	PSU	h1	121	75	-	2/7/25/26	0/2/2/2
2	OMC	A	1517	80,2	-	0/9/27/28	0/2/2/2
2	OMG	A	2916	2	-	0/9/27/28	0/3/3/3
2	PSU	A	1480	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2189	81,2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1611	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2316	80,2	-	0/7/25/26	0/2/2/2
75	A2M	h1	422	75	-	3/9/27/28	0/3/3/3
75	A2M	h1	794	75	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	PSU	h1	304	75	-	0/7/25/26	0/2/2/2
2	OMU	A	2734	80,2	-	0/9/27/28	0/2/2/2
75	PSU	h1	605	75	-	0/7/25/26	0/2/2/2
2	PSU	A	1681	2	-	0/7/25/26	0/2/2/2
2	PSU	A	1054	2	-	0/7/25/26	0/2/2/2
1	PSU	3	97	81,1	-	0/7/25/26	0/2/2/2
2	OMC	A	2291	2	-	0/9/27/28	0/2/2/2
2	OMG	A	1459	80,2	-	0/9/27/28	0/3/3/3
2	OMC	A	675	2	-	0/9/27/28	0/2/2/2
1	OMG	3	79	1	-	1/9/27/28	0/3/3/3
2	OMG	A	917	81,2	-	0/9/27/28	0/3/3/3
2	A2M	A	1458	80,2	-	0/9/27/28	0/3/3/3
2	A2M	A	2933	2	-	1/9/27/28	0/3/3/3
75	PSU	h1	1630	75	-	0/7/25/26	0/2/2/2
75	OMC	h1	416	75	-	1/9/27/28	0/2/2/2
2	PSU	A	2262	2	-	0/7/25/26	0/2/2/2
2	A2M	A	2279	2	-	2/9/27/28	0/3/3/3
75	OMU	h1	580	75	-	4/9/27/28	0/2/2/2
2	PSU	A	311	81,2	-	0/7/25/26	0/2/2/2
2	PSU	A	2922	81,2	-	1/7/25/26	0/2/2/2
2	PSU	A	2264	2	-	0/7/25/26	0/2/2/2
2	PSU	A	42	81,2	-	0/7/25/26	0/2/2/2
2	PSU	A	1001	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	1327	75	-	0/9/27/28	0/3/3/3
75	PSU	h1	761	75	-	0/7/25/26	0/2/2/2
75	OMG	h1	1272	81,75	-	1/9/27/28	0/3/3/3
2	OMU	A	2345	2	-	0/9/27/28	0/2/2/2
2	PSU	A	34	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	606	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	959	81,75	-	0/7/25/26	0/2/2/2
75	PSU	h1	762	75	-	0/7/25/26	0/2/2/2
75	OMG	h1	390	81,75	-	1/9/27/28	0/3/3/3
75	MA6	h1	1786	75	-	1/11/29/30	0/3/3/3
2	PSU	A	2252	2	-	0/7/25/26	0/2/2/2
2	PSU	A	1131	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2132	81,2	-	0/7/25/26	0/2/2/2
2	A2M	A	2359	2	-	1/9/27/28	0/3/3/3
75	PSU	h1	604	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2879	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1188	75	-	1/7/25/26	0/2/2/2
2	OMC	A	2835	2	-	0/9/27/28	0/2/2/2
75	6MZ	h1	1767	81,80,75	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	G7M	h1	1577	3,75	-	0/7/25/26	0/3/3/3
2	OMG	A	2393	80,2	-	0/9/27/28	0/3/3/3
2	A2M	A	2945	80,2	-	1/9/27/28	0/3/3/3
75	OMU	h1	1232	75	-	2/9/27/28	0/2/2/2
2	PSU	A	2134	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2825	81,2	-	0/7/25/26	0/2/2/2
2	1MA	A	657	80,2	-	1/7/25/26	0/3/3/3
2	OMG	A	2407	81,2	-	0/9/27/28	0/3/3/3
75	A2M	h1	438	75	-	0/9/27/28	0/3/3/3
75	PSU	h1	1182	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2414	80,2	-	0/7/25/26	0/2/2/2
2	OMG	A	2389	2	-	0/9/27/28	0/3/3/3
2	OMC	A	1478	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	1563	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1118	75	-	0/7/25/26	0/2/2/2
2	PSU	A	3109	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	337	81,75	-	0/7/25/26	0/2/2/2
2	OMG	A	2618	2,3	-	3/9/27/28	0/3/3/3
2	A2M	A	2218	2	-	0/9/27/28	0/3/3/3
1	A2M	3	47	1	-	0/9/27/28	0/3/3/3
2	PSU	A	277	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2312	81,2	-	1/7/25/26	0/2/2/2
75	PSU	h1	468	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	752	75	-	0/7/25/26	0/2/2/2
2	PSU	A	150	81,2	-	0/7/25/26	0/2/2/2
2	OMU	A	44	81,2	-	0/9/27/28	0/2/2/2
75	A2M	h1	28	75	-	1/9/27/28	0/3/3/3
2	PSU	A	2893	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2209	2	-	0/7/25/26	0/2/2/2
2	OMG	A	2792	2	-	1/9/27/28	0/3/3/3
75	PSU	h1	808	75	-	0/7/25/26	0/2/2/2
2	OMG	A	3290	80,2	-	0/9/27/28	0/3/3/3
2	PSU	A	228	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	799	75	-	0/9/27/28	0/3/3/3
2	A2M	A	826	81,80,2	-	1/9/27/28	0/3/3/3
2	PSU	A	901	81,2	-	0/7/25/26	0/2/2/2
75	OMU	h1	123	75	-	3/9/27/28	0/2/2/2
2	A2M	A	2254	2	-	0/9/27/28	0/3/3/3
2	OMC	A	1848	80,2	-	1/9/27/28	0/2/2/2
75	OMC	h1	1641	80,75	-	1/9/27/28	0/2/2/2
2	OMG	A	2921	2	-	0/9/27/28	0/3/3/3
2	PSU	A	1133	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	A	1066	2	-	0/9/27/28	0/2/2/2
75	A2M	h1	1575	75	-	0/9/27/28	0/3/3/3
75	4AC	h1	1777	75	-	0/11/29/30	0/2/2/2
2	PSU	A	2258	2	-	0/7/25/26	0/2/2/2
2	A2M	A	2324	2	-	0/9/27/28	0/3/3/3
75	A2M	h1	1754	75	-	1/9/27/28	0/3/3/3
75	PSU	h1	308	80,75	-	0/7/25/26	0/2/2/2
75	MA6	h1	1785	75	-	0/11/29/30	0/3/3/3
1	PSU	3	78	1	-	0/7/25/26	0/2/2/2
75	OMU	h1	613	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	1104	75	-	0/7/25/26	0/2/2/2
75	OMG	h1	597	75	-	4/9/27/28	0/3/3/3
2	OMU	A	1890	2	-	0/9/27/28	0/2/2/2
2	A2M	A	2639	2	-	1/9/27/28	0/3/3/3
2	A2M	A	2910	2	-	4/9/27/28	0/3/3/3
75	PSU	h1	1302	75	-	0/7/25/26	0/2/2/2
2	PSU	A	509	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	634	75	-	0/7/25/26	0/2/2/2
2	OMG	A	2814	2	-	0/9/27/28	0/3/3/3
75	OMC	h1	471	75	-	1/9/27/28	0/2/2/2
75	PSU	h1	1176	75	-	0/7/25/26	0/2/2/2
1	PSU	3	22	2,1	-	0/7/25/26	0/2/2/2
2	A2M	A	2124	2	-	0/9/27/28	0/3/3/3
75	OMU	h1	1445	75	-	1/9/27/28	0/2/2/2
2	A2M	A	661	2	-	1/9/27/28	0/3/3/3
2	PSU	A	2743	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	621	80,75	-	4/9/27/28	0/3/3/3
75	A2M	h1	778	75	-	3/9/27/28	0/3/3/3
75	PSU	h1	1483	75	-	1/7/25/26	0/2/2/2
2	PSU	A	1132	2	-	0/7/25/26	0/2/2/2
55	MLY	Ga	113	55	-	1/8/9/11	-
2	PSU	A	2430	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	975	75	-	0/9/27/28	0/3/3/3
2	PSU	A	685	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	103	75	-	1/7/25/26	0/2/2/2
2	OMG	A	2234	2	-	0/9/27/28	0/3/3/3
2	OMU	A	2408	81,2	-	0/9/27/28	0/2/2/2
2	OMU	A	2882	2	-	1/9/27/28	0/2/2/2
2	PSU	A	2954	2	-	0/7/25/26	0/2/2/2
75	OMG	h1	244	75	-	0/9/27/28	0/3/3/3
2	A2M	A	1142	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	A	2947	2	-	0/9/27/28	0/2/2/2
1	OMG	3	155	2,1	-	1/9/27/28	0/3/3/3
2	OMU	A	3299	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	415	75	-	0/7/25/26	0/2/2/2
2	UY1	A	2649	2	-	0/9/27/28	0/2/2/2
2	PSU	A	785	2	-	3/7/25/26	0/2/2/2
75	PSU	h1	1306	75	-	1/7/25/26	0/2/2/2
2	OMU	A	144	81,2	-	1/9/27/28	0/2/2/2
75	PSU	h1	449	81,75	-	0/7/25/26	0/2/2/2
75	OMU	h1	1010	75	-	0/9/27/28	0/2/2/2
2	PSU	A	2864	2	-	0/7/25/26	0/2/2/2

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	h1	1281	4AC	C4-N4	4.82	1.46	1.39
75	h1	1777	4AC	C4-N4	4.79	1.46	1.39
75	h1	602	UY1	C6-C5	4.41	1.40	1.35
75	h1	1192	C4J	C6-C5	4.01	1.40	1.34
2	A	2649	UY1	C6-C5	4.00	1.40	1.35
75	h1	606	PSU	C6-C5	3.85	1.39	1.35
75	h1	1783	PSU	C6-C5	3.70	1.39	1.35
2	A	2922	PSU	C6-C5	3.53	1.39	1.35
75	h1	1611	PSU	C6-C5	3.52	1.39	1.35
75	h1	583	PSU	C6-C5	3.52	1.39	1.35
2	A	34	PSU	C6-C5	3.46	1.39	1.35
75	h1	1563	PSU	C6-C5	3.42	1.39	1.35
75	h1	449	PSU	C6-C5	3.36	1.39	1.35
75	h1	1531	PSU	C6-C5	3.35	1.39	1.35
75	h1	752	PSU	C6-C5	3.35	1.39	1.35
75	h1	1520	PSU	C6-C5	3.31	1.39	1.35
75	h1	304	PSU	C6-C5	3.29	1.39	1.35
2	A	2264	PSU	C6-C5	3.27	1.39	1.35
75	h1	1483	PSU	C6-C5	3.26	1.39	1.35
75	h1	959	PSU	C6-C5	3.24	1.39	1.35
2	A	969	PSU	C6-C5	3.23	1.39	1.35
75	h1	1182	PSU	C6-C5	3.20	1.39	1.35
75	h1	256	PSU	C6-C5	3.19	1.39	1.35
75	h1	1215	PSU	C6-C5	3.19	1.39	1.35
2	A	311	PSU	C6-C5	3.18	1.39	1.35
2	A	1001	PSU	C6-C5	3.15	1.39	1.35
75	h1	1025	PSU	C6-C5	3.14	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2258	PSU	C6-C5	3.13	1.39	1.35
75	h1	1176	PSU	C6-C5	3.12	1.39	1.35
75	h1	95	PSU	C6-C5	3.09	1.38	1.35
75	h1	308	PSU	C6-C5	3.09	1.38	1.35
2	A	1133	PSU	C6-C5	3.05	1.38	1.35
75	h1	415	PSU	C6-C5	3.05	1.38	1.35
75	h1	1188	PSU	C6-C5	3.04	1.38	1.35
1	3	78	PSU	C6-C5	3.03	1.38	1.35
75	h1	1208	PSU	C6-C5	3.00	1.38	1.35
2	A	277	PSU	C6-C5	2.97	1.38	1.35
2	A	2256	PSU	C6-C5	2.96	1.38	1.35
75	h1	605	PSU	C6-C5	2.94	1.38	1.35
75	h1	948	PSU	C6-C5	2.93	1.38	1.35
75	h1	1118	PSU	C6-C5	2.93	1.38	1.35
2	A	901	PSU	C4-C5	-2.93	1.35	1.44
75	h1	337	PSU	C6-C5	2.93	1.38	1.35
75	h1	808	PSU	C6-C5	2.90	1.38	1.35
75	h1	1306	PSU	C6-C5	2.90	1.38	1.35
75	h1	121	PSU	C6-C5	2.89	1.38	1.35
2	A	2954	PSU	C6-C5	2.89	1.38	1.35
75	h1	1630	PSU	C6-C5	2.87	1.38	1.35
2	A	1681	PSU	C6-C5	2.87	1.38	1.35
2	A	2209	PSU	C6-C5	2.85	1.38	1.35
2	A	2893	PSU	C6-C5	2.85	1.38	1.35
75	h1	468	PSU	C6-C5	2.83	1.38	1.35
75	h1	762	PSU	C6-C5	2.81	1.38	1.35
2	A	3109	PSU	C6-C5	2.80	1.38	1.35
75	h1	1291	PSU	C6-C5	2.80	1.38	1.35
2	A	277	PSU	C4-C5	-2.80	1.36	1.44
2	A	2252	PSU	C6-C5	2.80	1.38	1.35
2	A	228	PSU	C6-C5	2.80	1.38	1.35
2	A	2864	PSU	C6-C5	2.80	1.38	1.35
2	A	885	A2M	C3'-C2'	-2.79	1.46	1.52
2	A	1646	1MG	C2-N3	2.79	1.39	1.34
2	A	785	PSU	C6-C5	2.78	1.38	1.35
2	A	1458	A2M	C3'-C2'	-2.78	1.46	1.52
2	A	1646	1MG	C2-N2	2.78	1.39	1.34
2	A	2312	PSU	C6-C5	2.77	1.38	1.35
1	3	97	PSU	C6-C5	2.74	1.38	1.35
75	h1	1767	6MZ	C6-N6	2.74	1.37	1.34
75	h1	1000	PSU	C6-C5	2.73	1.38	1.35
2	A	685	PSU	C4-C5	-2.71	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1480	PSU	C6-C5	2.67	1.38	1.35
2	A	894	PSU	C6-C5	2.66	1.38	1.35
2	A	2974	PSU	C6-C5	2.66	1.38	1.35
2	A	1132	PSU	C6-C5	2.65	1.38	1.35
2	A	2825	PSU	C6-C5	2.65	1.38	1.35
75	h1	103	PSU	C6-C5	2.64	1.38	1.35
2	A	2316	PSU	C6-C5	2.64	1.38	1.35
75	h1	360	PSU	C6-C5	2.63	1.38	1.35
2	A	2743	PSU	C6-C5	2.62	1.38	1.35
2	A	1472	PSU	C6-C5	2.61	1.38	1.35
75	h1	1302	PSU	C6-C5	2.61	1.38	1.35
2	A	1062	PSU	C6-C5	2.60	1.38	1.35
2	A	150	PSU	C6-C5	2.60	1.38	1.35
2	A	509	PSU	C6-C5	2.59	1.38	1.35
2	A	2262	PSU	C6-C5	2.57	1.38	1.35
2	A	2414	PSU	C6-N1	-2.57	1.32	1.36
2	A	2743	PSU	C4-C5	-2.56	1.36	1.44
75	h1	602	UY1	C6-N1	2.56	1.40	1.36
2	A	2132	PSU	C4-C5	-2.55	1.36	1.44
75	h1	604	PSU	C6-C5	2.55	1.38	1.35
2	A	2933	A2M	C3'-C2'	-2.55	1.47	1.52
2	A	2853	PSU	C6-C5	2.53	1.38	1.35
2	A	1054	PSU	C6-C5	2.53	1.38	1.35
1	3	97	PSU	C4-C5	-2.52	1.37	1.44
2	A	816	A2M	C3'-C2'	-2.52	1.47	1.52
2	A	965	PSU	C4-C5	-2.50	1.37	1.44
2	A	965	PSU	C6-C5	2.47	1.38	1.35
2	A	1681	PSU	C4-C5	-2.46	1.37	1.44
2	A	42	PSU	C6-C5	2.46	1.38	1.35
2	A	34	PSU	C4-C5	-2.46	1.37	1.44
75	h1	634	PSU	C6-C5	2.45	1.38	1.35
75	h1	761	PSU	C6-C5	2.44	1.38	1.35
2	A	1131	PSU	C6-C5	2.43	1.38	1.35
2	A	2189	PSU	C6-C5	2.43	1.38	1.35
75	h1	602	UY1	O4-C4	2.40	1.28	1.23
75	h1	1577	G7M	C8-N7	2.40	1.37	1.33
75	h1	1232	OMU	C2-N3	2.39	1.42	1.38
1	3	22	PSU	C6-C5	2.39	1.38	1.35
2	A	685	PSU	C6-C5	2.38	1.38	1.35
75	h1	1104	PSU	C6-C5	2.37	1.38	1.35
75	h1	1263	OMU	C2-N3	2.36	1.42	1.38
75	h1	1192	C4J	C4-N3	2.36	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	969	PSU	C4-C5	-2.35	1.37	1.44
2	A	901	PSU	C6-C5	2.34	1.38	1.35
2	A	2430	PSU	C6-C5	2.34	1.38	1.35
75	h1	308	PSU	C4-C5	-2.34	1.37	1.44
75	h1	1261	OMU	C2-N3	2.34	1.42	1.38
2	A	2134	PSU	C6-C5	2.33	1.38	1.35
75	h1	103	PSU	C4-C5	-2.31	1.37	1.44
2	A	2359	A2M	C3'-C2'	-2.29	1.47	1.52
2	A	2943	PSU	C6-C5	2.27	1.38	1.35
2	A	2893	PSU	C4-C5	-2.26	1.37	1.44
2	A	828	PSU	C4-C5	-2.26	1.37	1.44
75	h1	162	A2M	C3'-C2'	-2.25	1.47	1.52
2	A	661	A2M	C8-N7	-2.25	1.27	1.31
2	A	150	PSU	C4-C5	-2.25	1.37	1.44
75	h1	1263	OMU	C2-N1	2.25	1.42	1.38
2	A	945	A2M	C3'-C2'	-2.22	1.48	1.52
75	h1	1445	OMU	C2-N1	2.22	1.42	1.38
2	A	1376	A2M	C3'-C2'	-2.21	1.48	1.52
75	h1	975	A2M	C3'-C2'	-2.21	1.48	1.52
75	h1	621	A2M	C3'-C2'	-2.20	1.48	1.52
75	h1	1281	4AC	C2-N3	2.19	1.40	1.36
2	A	2132	PSU	C6-C5	2.19	1.37	1.35
2	A	1646	1MG	C6-N1	2.19	1.45	1.40
2	A	975	PSU	C6-C5	2.19	1.37	1.35
22	BS	246	HIC	CD2-NE2	-2.17	1.33	1.36
75	h1	1261	OMU	C2-N1	2.17	1.41	1.38
2	A	1142	A2M	C3'-C2'	-2.17	1.48	1.52
2	A	2864	PSU	C4-C5	-2.16	1.38	1.44
75	h1	799	A2M	C3'-C2'	-2.16	1.48	1.52
2	A	2312	PSU	C4-C5	-2.16	1.38	1.44
1	3	78	PSU	C4-C5	-2.15	1.38	1.44
2	A	2879	PSU	C6-C5	2.15	1.37	1.35
75	h1	123	OMU	C2-N3	2.15	1.41	1.38
2	A	2910	A2M	C3'-C2'	-2.14	1.48	1.52
2	A	1015	PSU	C6-C5	2.14	1.37	1.35
75	h1	1010	OMU	C2-N3	2.14	1.41	1.38
75	h1	948	PSU	C4-C5	-2.13	1.38	1.44
2	A	2419	OMU	C2-N1	2.10	1.41	1.38
2	A	1054	PSU	C4-C5	-2.10	1.38	1.44
2	A	311	PSU	C4-C5	-2.10	1.38	1.44
75	h1	1010	OMU	C2-N1	2.09	1.41	1.38
2	A	1131	PSU	C4-C5	-2.08	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	975	PSU	C4-C5	-2.06	1.38	1.44
2	A	2974	PSU	C4-C5	-2.06	1.38	1.44
75	h1	1577	G7M	C6-N1	2.06	1.42	1.38
2	A	657	1MA	C5-C6	-2.04	1.38	1.43
75	h1	1520	PSU	C4-C5	-2.04	1.38	1.44
75	h1	1531	PSU	C4-C5	-2.03	1.38	1.44
2	A	816	A2M	C1'-N9	-2.03	1.40	1.46
2	A	803	OMU	C2-N3	2.02	1.41	1.38
75	h1	1783	PSU	C4-C5	-2.02	1.38	1.44
2	A	2262	PSU	C4-C5	-2.02	1.38	1.44
75	h1	606	PSU	C4-C5	-2.01	1.38	1.44
75	h1	1192	C4J	O4-C4	2.01	1.27	1.23
2	A	2414	PSU	C6-C5	2.01	1.37	1.35

All (524) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	1786	MA6	N1-C6-N6	-8.02	108.32	117.08
75	h1	1575	A2M	C1'-N9-C8	-7.68	109.79	127.14
75	h1	543	A2M	C1'-N9-C8	-7.67	109.81	127.14
2	A	816	A2M	C1'-N9-C8	-7.62	109.93	127.14
75	h1	1785	MA6	N1-C6-N6	-7.33	109.07	117.08
75	h1	466	A2M	C1'-N9-C8	-7.10	111.11	127.14
2	A	2254	A2M	C1'-N9-C8	-7.05	111.22	127.14
75	h1	438	A2M	C1'-N9-C8	-7.01	111.30	127.14
75	h1	778	A2M	C1'-N9-C8	-7.01	111.31	127.14
75	h1	1327	A2M	C1'-N9-C8	-6.87	111.62	127.14
2	A	2212	A2M	C1'-N9-C8	-6.81	111.76	127.14
75	h1	28	A2M	C1'-N9-C8	-6.81	111.76	127.14
75	h1	162	A2M	C1'-N9-C8	-6.76	111.87	127.14
2	A	2639	A2M	C1'-N9-C8	-6.63	112.17	127.14
75	h1	794	A2M	C1'-N9-C8	-6.62	112.19	127.14
2	A	885	A2M	C1'-N9-C8	-6.60	112.23	127.14
2	A	2359	A2M	C1'-N9-C8	-6.57	112.30	127.14
2	A	1376	A2M	C1'-N9-C8	-6.57	112.30	127.14
75	h1	799	A2M	C1'-N9-C8	-6.51	112.43	127.14
2	A	2218	A2M	C1'-N9-C8	-6.51	112.44	127.14
2	A	2910	A2M	C1'-N9-C8	-6.44	112.59	127.14
2	A	2319	A2M	C1'-N9-C8	-6.44	112.59	127.14
2	A	1458	A2M	C1'-N9-C8	-6.44	112.60	127.14
2	A	2279	A2M	C1'-N9-C8	-6.43	112.62	127.14
2	A	826	A2M	C1'-N9-C8	-6.36	112.77	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	1754	A2M	C1'-N9-C8	-6.34	112.82	127.14
2	A	661	A2M	C1'-N9-C8	-6.26	113.00	127.14
75	h1	422	A2M	C1'-N9-C8	-6.24	113.05	127.14
75	h1	975	A2M	C1'-N9-C8	-6.21	113.11	127.14
2	A	2324	A2M	C1'-N9-C8	-6.16	113.22	127.14
2	A	2933	A2M	C1'-N9-C8	-6.13	113.30	127.14
2	A	2945	A2M	C1'-N9-C8	-6.07	113.42	127.14
75	h1	621	A2M	C1'-N9-C8	-6.02	113.54	127.14
1	3	47	A2M	C1'-N9-C8	-5.98	113.64	127.14
75	h1	1575	A2M	C4-N9-C1'	5.95	140.77	126.59
2	A	945	A2M	C1'-N9-C8	-5.90	113.81	127.14
75	h1	1786	MA6	C5-C6-N6	5.87	135.52	125.30
2	A	816	A2M	C4-N9-C1'	5.77	140.33	126.59
2	A	2124	A2M	C1'-N9-C8	-5.66	114.36	127.14
2	A	1142	A2M	C1'-N9-C8	-5.63	114.43	127.14
75	h1	1785	MA6	C5-C6-N6	5.62	135.09	125.30
75	h1	543	A2M	C4-N9-C1'	5.54	139.79	126.59
2	A	2639	A2M	C4-N9-C1'	5.52	139.75	126.59
1	3	47	A2M	C2'-C1'-N9	-5.50	104.26	113.53
75	h1	778	A2M	C4-N9-C1'	5.46	139.60	126.59
2	A	2212	A2M	C4-N9-C1'	5.42	139.51	126.59
75	h1	466	A2M	C4-N9-C1'	5.39	139.44	126.59
2	A	2359	A2M	C4-N9-C1'	5.39	139.44	126.59
2	A	885	A2M	C4-N9-C1'	5.37	139.38	126.59
75	h1	1327	A2M	C4-N9-C1'	5.34	139.32	126.59
2	A	1376	A2M	C4-N9-C1'	5.31	139.25	126.59
75	h1	438	A2M	C4-N9-C1'	5.29	139.19	126.59
75	h1	28	A2M	C4-N9-C1'	5.28	139.17	126.59
2	A	2218	A2M	C4-N9-C1'	5.22	139.04	126.59
2	A	2254	A2M	C4-N9-C1'	5.22	139.03	126.59
75	h1	162	A2M	C4-N9-C1'	5.03	138.57	126.59
2	A	2319	A2M	C4-N9-C1'	5.02	138.55	126.59
75	h1	794	A2M	C4-N9-C1'	5.00	138.50	126.59
75	h1	1754	A2M	C4-N9-C1'	4.90	138.27	126.59
2	A	2945	A2M	C4-N9-C1'	4.84	138.12	126.59
2	A	2933	A2M	C4-N9-C1'	4.81	138.06	126.59
2	A	661	A2M	C4-N9-C1'	4.79	138.00	126.59
2	A	1458	A2M	C4-N9-C1'	4.77	137.95	126.59
75	h1	799	A2M	C4-N9-C1'	4.77	137.95	126.59
2	A	2910	A2M	C4-N9-C1'	4.74	137.89	126.59
2	A	2324	A2M	C4-N9-C1'	4.73	137.87	126.59
2	A	2279	A2M	O2'-C2'-C1'	4.71	118.26	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	422	A2M	C4-N9-C1'	4.70	137.79	126.59
75	h1	975	A2M	C4-N9-C1'	4.63	137.62	126.59
2	A	816	A2M	O4'-C1'-C2'	4.62	114.66	106.57
2	A	2279	A2M	C4-N9-C1'	4.53	137.38	126.59
75	h1	621	A2M	C4-N9-C1'	4.49	137.30	126.59
2	A	2124	A2M	C4-N9-C1'	4.37	136.99	126.59
1	3	47	A2M	C4-N9-C1'	4.35	136.96	126.59
2	A	826	A2M	C4-N9-C1'	4.29	136.81	126.59
2	A	1142	A2M	C4-N9-C1'	4.22	136.64	126.59
2	A	945	A2M	C4-N9-C1'	4.20	136.61	126.59
75	h1	799	A2M	C2'-C1'-N9	-4.11	106.61	113.53
2	A	826	A2M	C3'-C2'-C1'	-4.03	95.31	102.89
2	A	816	A2M	C4'-O4'-C1'	-3.91	100.84	109.47
75	h1	1785	MA6	C2-N1-C6	3.86	120.87	111.75
75	h1	1786	MA6	C2-N1-C6	3.86	120.86	111.75
75	h1	543	A2M	C4-N9-C8	3.85	109.90	105.73
75	h1	543	A2M	O4'-C1'-C2'	3.82	113.26	106.57
2	A	2945	A2M	O2'-C2'-C1'	3.81	116.51	109.08
2	A	2254	A2M	C4-N9-C8	3.71	109.75	105.73
75	h1	422	A2M	O2'-C2'-C1'	3.67	116.24	109.08
75	h1	1777	4AC	N4-C4-N3	3.67	120.01	113.85
2	A	2254	A2M	O2'-C2'-C1'	3.65	116.21	109.08
2	A	2132	PSU	C4-N3-C2	-3.65	121.08	126.34
2	A	2910	A2M	C4'-O4'-C1'	-3.62	101.49	109.47
2	A	2254	A2M	C2'-C1'-N9	-3.61	107.45	113.53
75	h1	543	A2M	N3-C4-N9	3.60	133.02	127.08
75	h1	1783	PSU	C6-C5-C4	3.55	120.68	118.20
2	A	945	A2M	C4'-O4'-C1'	-3.52	101.72	109.47
2	A	2279	A2M	C4-N9-C8	3.50	109.52	105.73
2	A	816	A2M	C4-N9-C8	3.49	109.51	105.73
75	h1	466	A2M	C2'-C1'-N9	-3.48	107.67	113.53
75	h1	438	A2M	C4-N9-C8	3.47	109.49	105.73
75	h1	1281	4AC	N4-C4-N3	3.45	119.65	113.85
75	h1	621	A2M	O2'-C2'-C1'	3.45	115.80	109.08
75	h1	778	A2M	O2'-C2'-C1'	3.44	115.79	109.08
2	A	1458	A2M	C4-N9-C8	3.44	109.45	105.73
75	h1	162	A2M	C4'-O4'-C1'	-3.42	101.92	109.47
75	h1	1575	A2M	C4-N9-C8	3.39	109.41	105.73
75	h1	162	A2M	C2'-C1'-N9	-3.39	107.83	113.53
2	A	2910	A2M	C4-N9-C8	3.38	109.39	105.73
2	A	2254	A2M	C4'-O4'-C1'	-3.37	102.03	109.47
75	h1	799	A2M	N3-C4-N9	3.37	132.63	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	799	A2M	C4-N9-C8	3.36	109.37	105.73
75	h1	162	A2M	N3-C4-N9	3.35	132.60	127.08
2	A	2189	PSU	C4-N3-C2	-3.34	121.53	126.34
2	A	2124	A2M	C2'-C1'-N9	-3.31	107.95	113.53
75	h1	794	A2M	C4-N9-C8	3.30	109.31	105.73
2	A	816	A2M	C5-C4-N9	-3.30	101.94	105.78
75	h1	162	A2M	C4-N9-C8	3.30	109.31	105.73
75	h1	466	A2M	O2'-C2'-C1'	3.30	115.52	109.08
75	h1	308	PSU	C6-C5-C4	3.29	120.50	118.20
75	h1	543	A2M	C5-C4-N9	-3.26	101.99	105.78
75	h1	1575	A2M	O3'-C3'-C2'	-3.25	101.92	111.17
75	h1	1208	PSU	C6-C5-C4	3.24	120.46	118.20
2	A	2279	A2M	C4'-O4'-C1'	-3.24	102.33	109.47
75	h1	1577	G7M	C2-N3-C4	3.23	118.06	112.30
2	A	2212	A2M	O2'-C2'-C1'	3.23	115.38	109.08
2	A	2319	A2M	N3-C4-N9	3.22	132.39	127.08
2	A	2945	A2M	C2'-C1'-N9	-3.22	108.11	113.53
2	A	816	A2M	N3-C4-N9	3.22	132.38	127.08
75	h1	975	A2M	C4-N9-C8	3.21	109.21	105.73
75	h1	466	A2M	N3-C4-N9	3.21	132.38	127.08
1	3	47	A2M	C4-N9-C8	3.20	109.19	105.73
75	h1	794	A2M	N3-C4-N9	3.19	132.34	127.08
75	h1	1192	C4J	C4-N3-C2	-3.19	121.43	125.46
2	A	826	A2M	O3'-C3'-C2'	-3.18	102.12	111.17
2	A	2319	A2M	C2'-C1'-N9	-3.18	108.18	113.53
75	h1	621	A2M	C4-N9-C8	3.17	109.16	105.73
75	h1	778	A2M	N3-C4-N9	3.16	132.30	127.08
2	A	1001	PSU	C6-C5-C4	3.16	120.41	118.20
75	h1	778	A2M	C2'-C1'-N9	-3.14	108.24	113.53
2	A	1646	1MG	C2-N3-C4	3.13	119.02	111.98
75	h1	422	A2M	C4-N9-C8	3.12	109.11	105.73
2	A	945	A2M	C4-N9-C8	3.11	109.10	105.73
75	h1	1575	A2M	C4'-O4'-C1'	-3.11	102.61	109.47
75	h1	778	A2M	C4-N9-C8	3.09	109.08	105.73
2	A	685	PSU	C4-N3-C2	-3.09	121.89	126.34
75	h1	605	PSU	C6-C5-C4	3.09	120.36	118.20
2	A	2910	A2M	O2'-C2'-C1'	3.08	115.10	109.08
75	h1	28	A2M	N3-C4-N9	3.08	132.16	127.08
2	A	828	PSU	C4-N3-C2	-3.08	121.91	126.34
75	h1	1327	A2M	N3-C4-N9	3.07	132.14	127.08
75	h1	466	A2M	C4-N9-C8	3.07	109.05	105.73
2	A	2324	A2M	N3-C4-N9	3.04	132.10	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2954	PSU	C6-C5-C4	3.04	120.32	118.20
75	h1	28	A2M	C4-N9-C8	3.02	109.01	105.73
75	h1	438	A2M	N3-C4-N9	3.02	132.06	127.08
2	A	2279	A2M	C3'-C2'-C1'	-3.02	97.22	102.89
75	h1	1754	A2M	N3-C4-N9	3.01	132.05	127.08
75	h1	1327	A2M	C4-N9-C8	3.01	108.99	105.73
2	A	661	A2M	C4-N9-C8	3.01	108.99	105.73
75	h1	422	A2M	N3-C4-N9	3.00	132.03	127.08
2	A	826	A2M	C4-N9-C8	3.00	108.98	105.73
75	h1	1104	PSU	C6-C5-C4	3.00	120.29	118.20
75	h1	799	A2M	C5-C4-N9	-2.98	102.31	105.78
2	A	1132	PSU	C4-N3-C2	-2.96	122.08	126.34
75	h1	799	A2M	C4'-O4'-C1'	-2.95	102.97	109.47
2	A	975	PSU	C4-N3-C2	-2.95	122.09	126.34
75	h1	1025	PSU	C4-N3-C2	-2.95	122.09	126.34
75	h1	1176	PSU	C6-C5-C4	2.94	120.25	118.20
75	h1	1327	A2M	C4'-O4'-C1'	-2.94	102.99	109.47
75	h1	1754	A2M	C2'-C1'-N9	-2.94	108.58	113.53
2	A	2922	PSU	C6-C5-C4	2.93	120.25	118.20
2	A	2218	A2M	N3-C4-N9	2.93	131.91	127.08
75	h1	1327	A2M	C5-C4-N9	-2.92	102.39	105.78
75	h1	1281	4AC	C6-C5-C4	2.91	120.52	116.96
2	A	2132	PSU	C5-C6-N1	-2.91	117.75	122.11
75	h1	543	A2M	C4'-O4'-C1'	-2.91	103.06	109.47
75	h1	1754	A2M	C4-N9-C8	2.90	108.87	105.73
75	h1	308	PSU	C4-N3-C2	-2.90	122.16	126.34
2	A	1458	A2M	C5-C4-N9	-2.89	102.42	105.78
2	A	2430	PSU	C4-N3-C2	-2.89	122.18	126.34
75	h1	1777	4AC	C5-C4-N3	-2.88	117.95	122.59
75	h1	360	PSU	C4-N3-C2	-2.88	122.19	126.34
2	A	945	A2M	C2'-C1'-N9	-2.87	108.69	113.53
75	h1	162	A2M	C5-C4-N9	-2.87	102.44	105.78
2	A	1142	A2M	C4-N9-C8	2.87	108.84	105.73
75	h1	1575	A2M	N3-C4-N9	2.87	131.81	127.08
2	A	2974	PSU	C4-N3-C2	-2.87	122.21	126.34
75	h1	422	A2M	C5-C4-N9	-2.86	102.45	105.78
75	h1	466	A2M	C4'-O4'-C1'	-2.86	103.15	109.47
2	A	2879	PSU	C4-N3-C2	-2.86	122.21	126.34
2	A	2319	A2M	C4-N9-C8	2.86	108.83	105.73
75	h1	422	A2M	C2'-C1'-N9	-2.86	108.72	113.53
75	h1	621	A2M	C4'-O4'-C1'	-2.85	103.18	109.47
75	h1	794	A2M	C5-C4-N9	-2.85	102.47	105.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	604	PSU	C6-C5-C4	2.85	120.19	118.20
75	h1	438	A2M	C5-C4-N9	-2.84	102.47	105.78
2	A	2825	PSU	C4-N3-C2	-2.82	122.28	126.34
75	h1	605	PSU	C4-N3-C2	-2.81	122.29	126.34
75	h1	1577	G7M	C1'-N9-C4	-2.80	118.18	126.50
75	h1	975	A2M	C4'-O4'-C1'	-2.80	103.30	109.47
75	h1	28	A2M	C5-C4-N9	-2.80	102.53	105.78
2	A	901	PSU	C4-N3-C2	-2.80	122.31	126.34
2	A	2414	PSU	C4-N3-C2	-2.79	122.31	126.34
2	A	661	A2M	C5-C4-N9	-2.79	102.53	105.78
75	h1	1754	A2M	C4'-O4'-C1'	-2.79	103.32	109.47
2	A	2359	A2M	N3-C4-N9	2.79	131.67	127.08
2	A	945	A2M	N3-C4-N9	2.78	131.67	127.08
75	h1	1754	A2M	O2'-C2'-C1'	2.78	114.50	109.08
75	h1	422	A2M	C4'-O4'-C1'	-2.78	103.34	109.47
75	h1	1575	A2M	O2'-C2'-C1'	2.78	114.49	109.08
75	h1	1767	6MZ	C1'-N9-C8	2.77	133.40	127.14
2	A	1458	A2M	C4'-O4'-C1'	-2.77	103.36	109.47
75	h1	466	A2M	C5-C4-N9	-2.77	102.56	105.78
2	A	2212	A2M	C4-N9-C8	2.77	108.73	105.73
2	A	2264	PSU	C6-C5-C4	2.76	120.13	118.20
2	A	2639	A2M	N3-C4-N9	2.76	131.64	127.08
75	h1	543	A2M	O2'-C2'-C1'	2.76	114.47	109.08
75	h1	360	PSU	C6-C5-C4	2.76	120.13	118.20
2	A	2218	A2M	C4'-O4'-C1'	-2.76	103.39	109.47
2	A	42	PSU	C4-N3-C2	-2.76	122.37	126.34
75	h1	975	A2M	N3-C4-N9	2.76	131.62	127.08
2	A	2324	A2M	C2'-C1'-N9	-2.75	108.90	113.53
2	A	2910	A2M	C2'-C1'-N9	-2.75	108.91	113.53
2	A	1015	PSU	C4-N3-C2	-2.75	122.38	126.34
75	h1	28	A2M	C2'-C1'-N9	-2.74	108.92	113.53
75	h1	778	A2M	C5-C4-N9	-2.74	102.60	105.78
2	A	2252	PSU	C6-C5-C4	2.74	120.11	118.20
75	h1	975	A2M	C5-C4-N9	-2.73	102.60	105.78
2	A	2945	A2M	N3-C4-N9	2.73	131.59	127.08
2	A	1142	A2M	N3-C4-N9	2.73	131.58	127.08
2	A	885	A2M	C2'-C1'-N9	-2.72	108.94	113.53
75	h1	975	A2M	C2'-C1'-N9	-2.72	108.95	113.53
75	h1	1777	4AC	C6-C5-C4	2.72	120.29	116.96
2	A	1015	PSU	C6-C5-C4	2.71	120.10	118.20
2	A	2324	A2M	C4-N9-C8	2.70	108.65	105.73
2	A	2933	A2M	C4-N9-C8	2.69	108.65	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	1520	PSU	C6-C5-C4	2.69	120.08	118.20
75	h1	634	PSU	C4-N3-C2	-2.69	122.47	126.34
2	A	2319	A2M	C5-C4-N9	-2.68	102.66	105.78
2	A	2124	A2M	C4-N9-C8	2.68	108.63	105.73
2	A	661	A2M	N3-C4-N9	2.68	131.50	127.08
2	A	2262	PSU	C4-N3-C2	-2.68	122.48	126.34
75	h1	1188	PSU	C4-N3-C2	-2.67	122.49	126.34
2	A	1142	A2M	C2'-C1'-N9	-2.66	109.05	113.53
2	A	2218	A2M	C5-C4-N9	-2.66	102.69	105.78
75	h1	1754	A2M	C5-C4-N9	-2.66	102.69	105.78
2	A	2209	PSU	C6-C5-C4	2.65	120.05	118.20
2	A	2252	PSU	C4-N3-C2	-2.65	122.52	126.34
75	h1	1575	A2M	C3'-C2'-C1'	-2.65	97.91	102.89
2	A	826	A2M	O4'-C1'-N9	-2.65	102.84	108.06
2	A	2252	PSU	C5-C6-N1	-2.64	118.14	122.11
2	A	2212	A2M	N3-C4-N9	2.64	131.44	127.08
2	A	1142	A2M	C4'-O4'-C1'	-2.63	103.67	109.47
2	A	2359	A2M	C2'-C1'-N9	-2.62	109.12	113.53
75	h1	959	PSU	C6-C5-C4	2.62	120.03	118.20
2	A	2279	A2M	C2'-C1'-N9	-2.62	109.12	113.53
2	A	2943	PSU	C5-C6-N1	-2.61	118.19	122.11
75	h1	1104	PSU	C5-C6-N1	-2.61	118.20	122.11
75	h1	1192	C4J	C3'-C2'-C1'	2.61	104.67	101.64
75	h1	794	A2M	C2'-C1'-N9	-2.61	109.14	113.53
1	3	47	A2M	N9-C8-N7	-2.61	110.35	113.91
1	3	97	PSU	C6-C5-C4	2.59	120.01	118.20
2	A	885	A2M	N3-C4-N9	2.59	131.35	127.08
75	h1	1575	A2M	O4'-C1'-N9	-2.59	102.96	108.06
2	A	945	A2M	O3'-C3'-C2'	-2.58	103.83	111.17
2	A	1480	PSU	C4-N3-C2	-2.58	122.62	126.34
75	h1	1104	PSU	C4-N3-C2	-2.57	122.63	126.34
75	h1	543	A2M	C2'-C1'-N9	-2.57	109.20	113.53
2	A	2218	A2M	C4-N9-C8	2.57	108.51	105.73
2	A	945	A2M	C5-C4-N9	-2.56	102.81	105.78
2	A	894	PSU	C4-N3-C2	-2.56	122.65	126.34
75	h1	1611	PSU	C4-N3-C2	-2.56	122.65	126.34
75	h1	308	PSU	C5-C6-N1	-2.56	118.27	122.11
75	h1	1575	A2M	C5-C4-N9	-2.55	102.82	105.78
2	A	2254	A2M	O3'-C3'-C2'	-2.55	103.92	111.17
1	3	47	A2M	N3-C4-N9	2.54	131.28	127.08
2	A	509	PSU	C4-N3-C2	-2.54	122.67	126.34
2	A	1001	PSU	C5-C6-N1	-2.54	118.30	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2743	PSU	C4-N3-C2	-2.54	122.68	126.34
75	h1	360	PSU	C5-C6-N1	-2.54	118.30	122.11
2	A	2279	A2M	N9-C8-N7	-2.54	110.44	113.91
75	h1	1291	PSU	C4-N3-C2	-2.54	122.68	126.34
2	A	2910	A2M	C3'-C2'-C1'	-2.53	98.12	102.89
2	A	277	PSU	C4-N3-C2	-2.53	122.70	126.34
2	A	969	PSU	C6-C5-C4	2.52	119.96	118.20
2	A	1376	A2M	N3-C4-N9	2.52	131.23	127.08
2	A	2254	A2M	C5-C4-N9	-2.52	102.86	105.78
2	A	2954	PSU	C4-N3-C2	-2.51	122.72	126.34
1	3	47	A2M	C4'-O4'-C1'	-2.51	103.94	109.47
2	A	945	A2M	O2'-C2'-C1'	2.51	113.97	109.08
1	3	22	PSU	C4-N3-C2	-2.51	122.73	126.34
75	h1	1281	4AC	C5-C4-N3	-2.50	118.58	122.59
75	h1	948	PSU	C6-C5-C4	2.50	119.94	118.20
2	A	2195	OMC	C3'-C2'-C1'	-2.50	98.20	102.89
75	h1	778	A2M	O4'-C1'-C2'	2.50	110.94	106.57
75	h1	415	PSU	C6-C5-C4	2.49	119.94	118.20
2	A	2189	PSU	C5-C6-N1	-2.49	118.37	122.11
75	h1	1575	A2M	N9-C8-N7	-2.49	110.51	113.91
2	A	1131	PSU	C4-N3-C2	-2.49	122.75	126.34
75	h1	1777	4AC	CM7-C7-N4	2.49	119.60	115.29
2	A	975	PSU	C6-C5-C4	2.49	119.94	118.20
2	A	1646	1MG	C5-C4-N3	-2.49	124.43	128.46
75	h1	1611	PSU	C6-C5-C4	2.49	119.94	118.20
2	A	945	A2M	O4'-C1'-C2'	2.48	110.92	106.57
2	A	2124	A2M	N3-C4-N9	2.48	131.18	127.08
2	A	965	PSU	C4-N3-C2	-2.48	122.76	126.34
75	h1	794	A2M	C4'-O4'-C1'	-2.48	104.00	109.47
75	h1	621	A2M	N9-C8-N7	-2.48	110.52	113.91
75	h1	1531	PSU	C6-C5-C4	2.48	119.93	118.20
75	h1	794	A2M	O2'-C2'-C1'	2.48	113.91	109.08
2	A	3109	PSU	C4-N3-C2	-2.47	122.77	126.34
75	h1	1188	PSU	C6-C5-C4	2.47	119.93	118.20
1	3	47	A2M	O2'-C2'-C1'	2.47	113.90	109.08
75	h1	438	A2M	N9-C8-N7	-2.46	110.54	113.91
2	A	2254	A2M	C3'-C2'-C1'	-2.46	98.27	102.89
2	A	1015	PSU	C5-C6-N1	-2.46	118.42	122.11
75	h1	28	A2M	C4'-O4'-C1'	-2.45	104.06	109.47
2	A	2134	PSU	C5-C6-N1	-2.45	118.43	122.11
2	A	969	PSU	C4-N3-C2	-2.44	122.82	126.34
2	A	885	A2M	C4-N9-C8	2.44	108.37	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2209	PSU	C5-C6-N1	-2.44	118.45	122.11
75	h1	1630	PSU	C6-C5-C4	2.43	119.90	118.20
2	A	311	PSU	C4-N3-C2	-2.43	122.83	126.34
2	A	1001	PSU	C4-N3-C2	-2.43	122.83	126.34
2	A	2324	A2M	C5-C4-N9	-2.43	102.95	105.78
75	h1	634	PSU	C6-C5-C4	2.43	119.90	118.20
75	h1	1118	PSU	C4-N3-C2	-2.43	122.84	126.34
2	A	2279	A2M	N3-C4-N9	2.43	131.09	127.08
75	h1	808	PSU	C4-N3-C2	-2.43	122.84	126.34
75	h1	28	A2M	O2'-C2'-C1'	2.42	113.80	109.08
75	h1	256	PSU	C6-C5-C4	2.42	119.89	118.20
75	h1	1182	PSU	C6-C5-C4	2.42	119.89	118.20
2	A	2943	PSU	C4-N3-C2	-2.41	122.87	126.34
2	A	311	PSU	C6-C5-C4	2.41	119.88	118.20
2	A	1376	A2M	C4-N9-C8	2.40	108.33	105.73
2	A	2954	PSU	C5-C6-N1	-2.40	118.51	122.11
75	h1	621	A2M	N3-C4-N9	2.39	131.03	127.08
2	A	2254	A2M	N9-C8-N7	-2.39	110.64	113.91
75	h1	1563	PSU	C6-C5-C4	2.39	119.87	118.20
2	A	1062	PSU	C4-N3-C2	-2.38	122.91	126.34
75	h1	605	PSU	C5-C6-N1	-2.38	118.54	122.11
2	A	228	PSU	C6-C5-C4	2.38	119.86	118.20
75	h1	1577	G7M	N9-C8-N7	-2.37	106.35	112.21
2	A	1132	PSU	C6-C5-C4	2.37	119.85	118.20
2	A	2974	PSU	C5-C6-N1	-2.36	118.56	122.11
75	h1	1630	PSU	C5-C6-N1	-2.36	118.57	122.11
2	A	2945	A2M	C4'-O4'-C1'	-2.36	104.27	109.47
75	h1	1302	PSU	C4-N3-C2	-2.36	122.94	126.34
2	A	2945	A2M	C4-N9-C8	2.36	108.28	105.73
2	A	2869	5MC	C5-C6-N1	-2.35	120.92	123.34
75	h1	1575	A2M	C2'-C3'-C4'	2.34	107.08	101.99
2	A	2124	A2M	O3'-C3'-C4'	2.34	117.81	111.05
75	h1	468	PSU	C6-C5-C4	2.34	119.83	118.20
2	A	1472	PSU	C4-N3-C2	-2.34	122.97	126.34
2	A	2264	PSU	C4-N3-C2	-2.34	122.97	126.34
75	h1	1630	PSU	C4-N3-C2	-2.33	122.98	126.34
2	A	1480	PSU	C6-C5-C4	2.33	119.83	118.20
2	A	2974	PSU	C6-C5-C4	2.33	119.83	118.20
2	A	2639	A2M	C2'-C1'-N9	-2.33	109.61	113.53
2	A	969	PSU	C3'-C2'-C1'	2.33	104.35	101.64
2	A	1458	A2M	N3-C4-N9	2.33	130.92	127.08
2	A	2316	PSU	C4-N3-C2	-2.33	122.99	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	1563	PSU	C4-N3-C2	-2.32	122.99	126.34
75	h1	1025	PSU	C5-C6-N1	-2.32	118.64	122.11
75	h1	304	PSU	C4-N3-C2	-2.32	123.00	126.34
2	A	2869	5MC	C1'-N1-C6	2.31	124.98	121.12
2	A	1132	PSU	C5-C6-N1	-2.31	118.64	122.11
75	h1	948	PSU	C4-N3-C2	-2.31	123.01	126.34
75	h1	449	PSU	C4-N3-C2	-2.31	123.01	126.34
75	h1	794	A2M	N9-C8-N7	-2.31	110.76	113.91
2	A	2134	PSU	C6-C5-C4	2.31	119.81	118.20
2	A	3109	PSU	C6-C5-C4	2.31	119.81	118.20
75	h1	1767	6MZ	C4-N9-C1'	-2.30	121.11	126.59
75	h1	543	A2M	N9-C8-N7	-2.30	110.77	113.91
2	A	2743	PSU	C6-C5-C4	2.30	119.81	118.20
2	A	34	PSU	C6-C5-C4	2.30	119.80	118.20
75	h1	752	PSU	C4-N3-C2	-2.29	123.03	126.34
2	A	1054	PSU	C4-N3-C2	-2.29	123.03	126.34
2	A	2864	PSU	C3'-C2'-C1'	2.29	104.30	101.64
2	A	2254	A2M	N3-C4-N9	2.29	130.86	127.08
75	h1	468	PSU	C4-N3-C2	-2.29	123.04	126.34
2	A	901	PSU	C6-C5-C4	2.28	119.80	118.20
75	h1	415	PSU	C4-N3-C2	-2.28	123.05	126.34
75	h1	1208	PSU	C4-N3-C2	-2.28	123.05	126.34
2	A	2639	A2M	O2'-C2'-C1'	2.28	113.53	109.08
1	3	97	PSU	C5-C6-N1	-2.27	118.70	122.11
2	A	816	A2M	C2'-C1'-N9	-2.27	109.70	113.53
2	A	826	A2M	O2'-C2'-C1'	2.27	113.51	109.08
2	A	885	A2M	C4'-O4'-C1'	-2.27	104.47	109.47
2	A	2124	A2M	C4'-O4'-C1'	-2.27	104.47	109.47
2	A	2124	A2M	C5-C4-N9	-2.27	103.15	105.78
75	h1	1306	PSU	C6-C5-C4	2.27	119.78	118.20
75	h1	752	PSU	C6-C5-C4	2.26	119.78	118.20
75	h1	1208	PSU	C5-C6-N1	-2.26	118.72	122.11
2	A	3109	PSU	C5-C6-N1	-2.26	118.72	122.11
2	A	2134	PSU	C4-N3-C2	-2.26	123.09	126.34
1	3	47	A2M	C5-N7-C8	2.25	106.71	103.51
2	A	2279	A2M	C5-C4-N9	-2.25	103.16	105.78
2	A	2430	PSU	C5-C6-N1	-2.25	118.73	122.11
2	A	1681	PSU	C6-C5-C4	2.25	119.77	118.20
75	h1	1785	MA6	C5-N7-C8	2.25	106.70	103.51
75	h1	162	A2M	O4'-C1'-C2'	2.25	110.51	106.57
2	A	2359	A2M	C4-N9-C8	2.24	108.16	105.73
1	3	47	A2M	C5-C4-N9	-2.24	103.18	105.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	1291	PSU	C6-C5-C4	2.24	119.76	118.20
75	h1	1575	A2M	C5-N7-C8	2.24	106.69	103.51
75	h1	1216	OMC	C1'-N1-C2	2.23	123.41	118.42
2	A	2359	A2M	C5-C4-N9	-2.23	103.19	105.78
2	A	2933	A2M	C4'-O4'-C1'	-2.23	104.55	109.47
75	h1	438	A2M	C5-N7-C8	2.23	106.68	103.51
75	h1	1786	MA6	C5-N7-C8	2.23	106.68	103.51
2	A	2910	A2M	C5-C4-N9	-2.23	103.19	105.78
2	A	1458	A2M	N9-C8-N7	-2.23	110.87	113.91
75	h1	1188	PSU	C5-C6-N1	-2.23	118.77	122.11
75	h1	1176	PSU	C5-C6-N1	-2.22	118.77	122.11
2	A	2853	PSU	C6-C5-C4	2.22	119.75	118.20
75	h1	1531	PSU	C4-N3-C2	-2.22	123.14	126.34
75	h1	1025	PSU	N1-C2-N3	2.22	117.65	115.13
75	h1	1182	PSU	C4-N3-C2	-2.21	123.15	126.34
2	A	2716	OMU	N3-C2-N1	2.21	117.82	114.89
2	A	2212	A2M	C4'-O4'-C1'	-2.21	104.60	109.47
2	A	2414	PSU	C6-C5-C4	2.20	119.74	118.20
75	h1	438	A2M	C2'-C1'-N9	-2.20	109.83	113.53
75	h1	1025	PSU	C3'-C2'-C1'	2.20	104.20	101.64
2	A	2933	A2M	O4'-C1'-N9	-2.20	103.73	108.06
75	h1	162	A2M	N9-C8-N7	-2.20	110.91	113.91
75	h1	1785	MA6	C4-C5-C6	2.20	118.34	115.88
75	h1	606	PSU	C4-N3-C2	-2.19	123.18	126.34
2	A	2743	PSU	C5-C6-N1	-2.19	118.82	122.11
2	A	975	PSU	C5-C6-N1	-2.19	118.83	122.11
75	h1	304	PSU	C6-C5-C4	2.19	119.73	118.20
2	A	1480	PSU	C5-C6-N1	-2.18	118.83	122.11
2	A	2947	OMC	C1'-N1-C2	2.18	123.29	118.42
2	A	661	A2M	C4'-O4'-C1'	-2.18	104.67	109.47
1	3	78	PSU	C6-C5-C4	2.18	119.72	118.20
2	A	1458	A2M	O4'-C1'-C2'	2.18	110.38	106.57
75	h1	1783	PSU	C4-N3-C2	-2.17	123.21	126.34
2	A	2893	PSU	C4-N3-C2	-2.17	123.21	126.34
2	A	2649	UY1	C4-N3-C2	-2.17	123.21	126.34
2	A	885	A2M	O4'-C1'-C2'	2.17	110.37	106.57
75	h1	761	PSU	C6-C5-C4	2.17	119.71	118.20
75	h1	621	A2M	C5-N7-C8	2.17	106.59	103.51
2	A	2639	A2M	C4-N9-C8	2.17	108.08	105.73
2	A	2650	OMG	C3'-C2'-C1'	-2.16	98.82	102.89
75	h1	422	A2M	N9-C8-N7	-2.16	110.96	113.91
2	A	661	A2M	C2'-C1'-N9	-2.16	109.89	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2933	A2M	N9-C8-N7	-2.15	110.97	113.91
75	h1	1118	PSU	C6-C5-C4	2.15	119.70	118.20
75	h1	256	PSU	C4-N3-C2	-2.15	123.25	126.34
2	A	885	A2M	C5-C4-N9	-2.14	103.29	105.78
2	A	1142	A2M	C5-C4-N9	-2.14	103.29	105.78
2	A	2209	PSU	C4-N3-C2	-2.14	123.25	126.34
2	A	2258	PSU	C4-N3-C2	-2.14	123.26	126.34
2	A	2212	A2M	O4'-C1'-C2'	2.14	110.32	106.57
2	A	2254	A2M	O4'-C1'-N9	-2.14	103.85	108.06
2	A	816	A2M	C3'-C2'-C1'	-2.14	98.87	102.89
75	h1	621	A2M	O4'-C1'-C2'	2.13	110.30	106.57
2	A	2414	PSU	O2-C2-N1	-2.13	120.45	122.79
2	A	2124	A2M	N9-C8-N7	-2.13	111.01	113.91
75	h1	604	PSU	C4-N3-C2	-2.12	123.28	126.34
2	A	2922	PSU	C5-C6-N1	-2.12	118.92	122.11
75	h1	778	A2M	O3'-C3'-C2'	-2.12	105.14	111.17
2	A	2212	A2M	C5-C4-N9	-2.12	103.32	105.78
75	h1	1025	PSU	C6-C5-C4	2.12	119.68	118.20
2	A	2910	A2M	O3'-C3'-C2'	-2.11	105.16	111.17
2	A	2256	PSU	C6-C5-C4	2.11	119.68	118.20
75	h1	466	A2M	O4'-C1'-C2'	2.11	110.26	106.57
2	A	1132	PSU	N1-C2-N3	2.11	117.52	115.13
75	h1	799	A2M	N9-C8-N7	-2.10	111.03	113.91
75	h1	1000	PSU	C4-N3-C2	-2.10	123.31	126.34
2	A	2910	A2M	N9-C8-N7	-2.10	111.04	113.91
2	A	2943	PSU	C6-C5-C4	2.10	119.67	118.20
75	h1	808	PSU	C6-C5-C4	2.10	119.67	118.20
2	A	2264	PSU	C5-C6-N1	-2.10	118.96	122.11
75	h1	1577	G7M	C5-C4-N3	-2.10	124.13	128.15
75	h1	1754	A2M	O3'-C3'-C4'	2.09	117.11	111.05
2	A	2853	PSU	C4-N3-C2	-2.09	123.32	126.34
2	A	1133	PSU	C4-N3-C2	-2.09	123.32	126.34
2	A	2218	A2M	C2'-C1'-N9	-2.09	110.01	113.53
75	h1	799	A2M	O4'-C1'-C2'	2.09	110.23	106.57
1	3	97	PSU	C4-N3-C2	-2.08	123.33	126.34
2	A	2312	PSU	C6-C5-C4	2.08	119.66	118.20
75	h1	606	PSU	C6-C5-C4	2.08	119.66	118.20
2	A	828	PSU	C6-C5-C4	2.08	119.65	118.20
75	h1	1783	PSU	C5-C6-N1	-2.08	118.99	122.11
2	A	1142	A2M	N9-C8-N7	-2.08	111.07	113.91
75	h1	449	PSU	C3'-C2'-C1'	2.07	104.05	101.64
75	h1	1270	OMU	C1'-N1-C2	2.07	121.33	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	438	A2M	O4'-C1'-C2'	2.07	110.20	106.57
75	h1	1291	PSU	C5-C6-N1	-2.07	119.00	122.11
2	A	2945	A2M	C5-C4-N9	-2.07	103.38	105.78
75	h1	1176	PSU	C4-N3-C2	-2.07	123.36	126.34
75	h1	794	A2M	O4'-C1'-C2'	2.07	110.19	106.57
75	h1	1611	PSU	C5-C6-N1	-2.07	119.01	122.11
2	A	2639	A2M	C5-N7-C8	2.06	106.44	103.51
75	h1	602	UY1	C4-N3-C2	-2.06	123.37	126.34
75	h1	543	A2M	C5-N7-C8	2.06	106.43	103.51
2	A	1142	A2M	O4'-C4'-C3'	-2.06	101.04	105.11
2	A	901	PSU	C2'-C3'-C4'	-2.06	98.64	102.64
2	A	2262	PSU	C5-C6-N1	-2.06	119.02	122.11
2	A	2324	A2M	O3'-C3'-C4'	2.05	116.99	111.05
75	h1	975	A2M	O4'-C1'-C2'	2.05	110.17	106.57
2	A	2945	A2M	O3'-C3'-C4'	2.05	116.97	111.05
2	A	2279	A2M	C5-N7-C8	2.05	106.42	103.51
2	A	2279	A2M	O3'-C3'-C4'	2.04	116.94	111.05
2	A	945	A2M	N9-C8-N7	-2.04	111.13	113.91
75	h1	1777	4AC	O7-C7-CM7	-2.03	118.29	122.06
2	A	826	A2M	C5-C4-N9	-2.03	103.42	105.78
2	A	2430	PSU	C6-C5-C4	2.03	119.61	118.20
2	A	42	PSU	C5-C6-N1	-2.02	119.08	122.11
2	A	2212	A2M	N9-C8-N7	-2.02	111.15	113.91
2	A	2319	A2M	O3'-C3'-C2'	-2.02	105.43	111.17
2	A	2324	A2M	C4'-O4'-C1'	-2.02	105.03	109.47
2	A	2974	PSU	C2'-C3'-C4'	-2.02	98.73	102.64
2	A	685	PSU	C5-C6-N1	-2.02	119.09	122.11
75	h1	1786	MA6	C4-C5-N7	-2.01	108.17	110.62
2	A	42	PSU	N1-C2-N3	2.01	117.41	115.13
2	A	975	PSU	N1-C2-N3	2.01	117.41	115.13
75	h1	28	A2M	N9-C8-N7	-2.01	111.16	113.91
2	A	2853	PSU	C5-C6-N1	-2.01	119.09	122.11
2	A	2359	A2M	O4'-C1'-C2'	2.01	110.09	106.57
2	A	2954	PSU	N1-C2-N3	2.01	117.40	115.13
2	A	2359	A2M	C4'-O4'-C1'	-2.00	105.05	109.47
2	A	150	PSU	C4-N3-C2	-2.00	123.45	126.34
75	h1	162	A2M	O2'-C2'-C1'	2.00	112.98	109.08

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	3	79	OMG	C1'-C2'-O2'-CM2
1	3	155	OMG	C1'-C2'-O2'-CM2
55	Ga	113	MLY	O-C-CA-CB
2	A	676	OMU	C1'-C2'-O2'-CM2
2	A	785	PSU	C2'-C1'-C5-C4
2	A	785	PSU	O4'-C1'-C5-C4
2	A	785	PSU	C2'-C1'-C5-C6
2	A	969	PSU	C2'-C1'-C5-C4
2	A	2111	OMU	C3'-C4'-C5'-O5'
2	A	2111	OMU	O4'-C4'-C5'-O5'
2	A	2195	OMC	C2'-C1'-N1-C6
2	A	2212	A2M	C1'-C2'-O2'-CM'
2	A	2256	PSU	C3'-C4'-C5'-O5'
2	A	2256	PSU	O4'-C4'-C5'-O5'
2	A	2279	A2M	O4'-C4'-C5'-O5'
2	A	2359	A2M	C1'-C2'-O2'-CM'
2	A	2618	OMG	C1'-C2'-O2'-CM2
2	A	2639	A2M	C1'-C2'-O2'-CM'
2	A	2882	OMU	C1'-C2'-O2'-CM2
2	A	2933	A2M	C1'-C2'-O2'-CM'
2	A	2945	A2M	C1'-C2'-O2'-CM'
75	h1	28	A2M	C1'-C2'-O2'-CM'
75	h1	38	OMC	C1'-C2'-O2'-CM2
75	h1	162	A2M	C1'-C2'-O2'-CM'
75	h1	416	OMC	C1'-C2'-O2'-CM2
75	h1	422	A2M	C1'-C2'-O2'-CM'
75	h1	466	A2M	C1'-C2'-O2'-CM'
75	h1	471	OMC	C1'-C2'-O2'-CM2
75	h1	580	OMU	O4'-C4'-C5'-O5'
75	h1	597	OMG	O4'-C4'-C5'-O5'
75	h1	597	OMG	C3'-C4'-C5'-O5'
75	h1	597	OMG	C1'-C2'-O2'-CM2
75	h1	621	A2M	C1'-C2'-O2'-CM'
75	h1	778	A2M	O4'-C4'-C5'-O5'
75	h1	778	A2M	C3'-C4'-C5'-O5'
75	h1	778	A2M	C1'-C2'-O2'-CM'
75	h1	794	A2M	C1'-C2'-O2'-CM'
75	h1	1216	OMC	C1'-C2'-O2'-CM2
75	h1	1232	OMU	C3'-C4'-C5'-O5'
75	h1	1232	OMU	O4'-C4'-C5'-O5'
75	h1	1272	OMG	C1'-C2'-O2'-CM2
75	h1	1381	OMU	C1'-C2'-O2'-CM2
75	h1	1431	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
75	h1	1445	OMU	C1'-C2'-O2'-CM2
75	h1	1754	A2M	C1'-C2'-O2'-CM'
75	h1	1767	6MZ	N1-C6-N6-C9
2	A	2195	OMC	C2'-C1'-N1-C2
75	h1	621	A2M	O4'-C4'-C5'-O5'
75	h1	621	A2M	C3'-C4'-C5'-O5'
75	h1	1192	C4J	C3'-C4'-C5'-O5'
75	h1	1192	C4J	O4'-C4'-C5'-O5'
75	h1	1192	C4J	C4'-C5'-O5'-P
2	A	2279	A2M	C3'-C4'-C5'-O5'
75	h1	123	OMU	C3'-C4'-C5'-O5'
75	h1	123	OMU	O4'-C4'-C5'-O5'
75	h1	422	A2M	O4'-C4'-C5'-O5'
75	h1	583	PSU	C3'-C4'-C5'-O5'
75	h1	583	PSU	O4'-C4'-C5'-O5'
75	h1	602	UY1	C1'-C2'-O2'-CM2
2	A	2910	A2M	O4'-C4'-C5'-O5'
2	A	2910	A2M	C3'-C4'-C5'-O5'
75	h1	543	A2M	C3'-C2'-O2'-CM'
2	A	2869	5MC	C2'-C1'-N1-C6
2	A	2922	PSU	C4'-C5'-O5'-P
75	h1	597	OMG	C4'-C5'-O5'-P
75	h1	1270	OMU	C4'-C5'-O5'-P
75	h1	422	A2M	C3'-C4'-C5'-O5'
2	A	2195	OMC	O4'-C1'-N1-C2
2	A	2312	PSU	C4'-C5'-O5'-P
75	h1	1431	OMG	C4'-C5'-O5'-P
2	A	1376	A2M	O4'-C4'-C5'-O5'
2	A	2195	OMC	O4'-C1'-N1-C6
2	A	2869	5MC	O4'-C1'-N1-C6
75	h1	1786	MA6	C4'-C5'-O5'-P
75	h1	1431	OMG	O4'-C4'-C5'-O5'
2	A	661	A2M	C4'-C5'-O5'-P
75	h1	1270	OMU	O4'-C4'-C5'-O5'
2	A	2618	OMG	C3'-C4'-C5'-O5'
75	h1	580	OMU	C3'-C4'-C5'-O5'
2	A	969	PSU	O4'-C1'-C5-C4
75	h1	1306	PSU	O4'-C1'-C5-C4
75	h1	1483	PSU	O4'-C1'-C5-C4
2	A	2792	OMG	C3'-C2'-O2'-CM2
2	A	2618	OMG	O4'-C4'-C5'-O5'
2	A	657	1MA	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
2	A	2869	5MC	O4'-C1'-N1-C2
75	h1	121	PSU	O4'-C4'-C5'-O5'
75	h1	1641	OMC	O4'-C4'-C5'-O5'
2	A	1062	PSU	O4'-C4'-C5'-O5'
75	h1	466	A2M	O4'-C4'-C5'-O5'
75	h1	1188	PSU	O4'-C4'-C5'-O5'
2	A	2910	A2M	C1'-C2'-O2'-CM'
75	h1	580	OMU	O4'-C1'-N1-C6
75	h1	390	OMG	C3'-C2'-O2'-CM2
2	A	1446	OMC	C2'-C1'-N1-C2
75	h1	123	OMU	C2'-C1'-N1-C2
2	A	1446	OMC	O4'-C4'-C5'-O5'
2	A	969	PSU	O4'-C1'-C5-C6
75	h1	583	PSU	O4'-C1'-C5-C6
75	h1	1192	C4J	C3-C31-C32-N33
75	h1	1208	PSU	O4'-C1'-C5-C6
75	h1	1520	PSU	O4'-C1'-C5-C6
2	A	2910	A2M	C4'-C5'-O5'-P
75	h1	543	A2M	O4'-C1'-N9-C8
2	A	826	A2M	O4'-C4'-C5'-O5'
75	h1	621	A2M	C2'-C1'-N9-C8
2	A	2869	5MC	C2'-C1'-N1-C2
2	A	1848	OMC	C3'-C2'-O2'-CM2
2	A	144	OMU	O4'-C4'-C5'-O5'
75	h1	103	PSU	O4'-C4'-C5'-O5'
75	h1	121	PSU	C3'-C4'-C5'-O5'
75	h1	580	OMU	C2'-C1'-N1-C6

There are no ring outliers.

81 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	h1	466	A2M	3	0
2	A	945	A2M	1	0
2	A	2943	PSU	1	0
2	A	1446	OMC	2	0
75	h1	948	PSU	1	0
75	h1	360	PSU	1	0
75	h1	38	OMC	1	0
2	A	2212	A2M	4	0
2	A	1376	A2M	1	0
75	h1	1216	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2681	OMC	1	0
75	h1	256	PSU	2	0
75	h1	162	A2M	2	0
75	h1	1431	OMG	1	0
75	h1	1270	OMU	1	0
2	A	965	PSU	1	0
2	A	676	OMU	1	0
75	h1	1263	OMU	1	0
75	h1	1192	C4J	1	0
75	h1	1531	PSU	2	0
2	A	2878	OMC	2	0
2	A	2335	OMC	1	0
2	A	2869	5MC	1	0
75	h1	1261	OMU	2	0
75	h1	422	A2M	1	0
75	h1	794	A2M	2	0
1	3	97	PSU	1	0
2	A	2291	OMC	1	0
2	A	675	OMC	1	0
1	3	79	OMG	1	0
2	A	1458	A2M	2	0
2	A	2933	A2M	1	0
75	h1	1630	PSU	1	0
75	h1	416	OMC	1	0
2	A	2279	A2M	1	0
2	A	311	PSU	1	0
75	h1	1272	OMG	1	0
2	A	2345	OMU	1	0
2	A	34	PSU	1	0
75	h1	606	PSU	1	0
75	h1	390	OMG	2	0
2	A	2359	A2M	1	0
75	h1	1188	PSU	1	0
75	h1	1577	G7M	1	0
2	A	2945	A2M	1	0
2	A	2407	OMG	2	0
75	h1	438	A2M	2	0
75	h1	1563	PSU	1	0
75	h1	1118	PSU	1	0
75	h1	337	PSU	1	0
2	A	2618	OMG	1	0
2	A	2218	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	277	PSU	3	0
75	h1	28	A2M	1	0
75	h1	808	PSU	1	0
2	A	3290	OMG	1	0
75	h1	799	A2M	1	0
2	A	826	A2M	2	0
75	h1	123	OMU	2	0
2	A	2254	A2M	1	0
75	h1	1641	OMC	2	0
2	A	2921	OMG	1	0
75	h1	1754	A2M	1	0
75	h1	1785	MA6	2	0
75	h1	597	OMG	1	0
2	A	2639	A2M	1	0
2	A	2910	A2M	3	0
75	h1	1302	PSU	1	0
2	A	2814	OMG	1	0
75	h1	471	OMC	1	0
75	h1	1176	PSU	2	0
75	h1	1445	OMU	1	0
2	A	661	A2M	1	0
75	h1	621	A2M	1	0
75	h1	778	A2M	1	0
75	h1	1483	PSU	2	0
2	A	2882	OMU	3	0
75	h1	244	OMG	1	0
2	A	2947	OMC	1	0
1	3	155	OMG	2	0
2	A	785	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 500 ligands modelled in this entry, 494 are monoatomic - leaving 6 for Mogul analysis.

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
82	TER	A	3401	-	13,13,13	0.34	0	12,12,12	0.63	0
83	SPD	A	3403	-	9,9,9	0.21	0	8,8,8	0.43	0
83	SPD	A	3402	-	9,9,9	0.19	0	8,8,8	0.16	0
84	EPE	A	3404	-	15,15,15	0.67	1 (6%)	18,20,20	0.75	0
83	SPD	A	3406	-	9,9,9	0.14	0	8,8,8	0.17	0
83	SPD	A	3405	-	9,9,9	0.18	0	8,8,8	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	TER	A	3401	-	-	6/11/11/11	-
83	SPD	A	3403	-	-	2/7/7/7	-
83	SPD	A	3402	-	-	2/7/7/7	-
84	EPE	A	3404	-	-	6/9/19/19	0/1/1/1
83	SPD	A	3406	-	-	3/7/7/7	-
83	SPD	A	3405	-	-	1/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	A	3404	EPE	O3S-S	2.41	1.56	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	A	3404	EPE	C8-C7-N4-C3
84	A	3404	EPE	S-C10-C9-N1
84	A	3404	EPE	C9-C10-S-O1S
82	A	3401	TER	C6-C7-C8-N9
83	A	3403	SPD	N6-C7-C8-C9
83	A	3402	SPD	C8-C7-N6-C5

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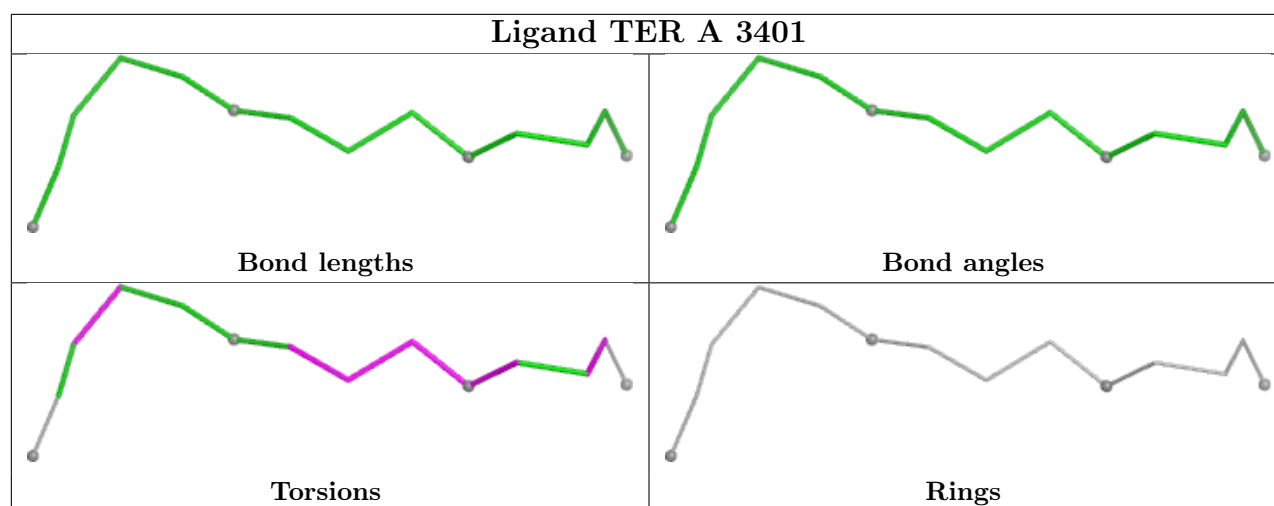
Mol	Chain	Res	Type	Atoms
83	A	3406	SPD	C3-C4-C5-N6
82	A	3401	TER	N5-C6-C7-C8
84	A	3404	EPE	N4-C7-C8-O8
82	A	3401	TER	C10-C11-C12-C13
84	A	3404	EPE	C9-C10-S-O3S
82	A	3401	TER	C3-C4-N5-C6
82	A	3401	TER	C7-C6-N5-C4
83	A	3406	SPD	C8-C7-N6-C5
82	A	3401	TER	N1-C2-C3-C4
83	A	3403	SPD	C7-C8-C9-N10
83	A	3406	SPD	C2-C3-C4-C5
84	A	3404	EPE	C9-C10-S-O2S
83	A	3405	SPD	C2-C3-C4-C5
83	A	3402	SPD	N1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	A	3401	TER	9	0
83	A	3403	SPD	2	0
83	A	3402	SPD	2	0
84	A	3404	EPE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
74	Ca	1
73	AY	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ca	53:ILE	C	54:LYS	N	2.67
1	AY	76:THR	C	77:CYS	N	2.04

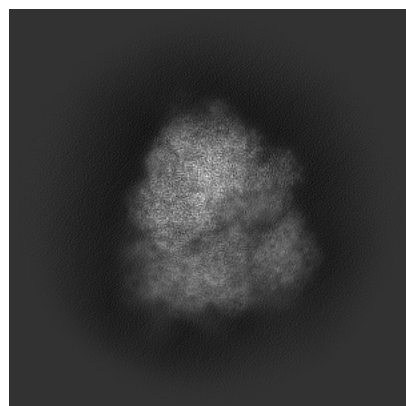
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52299. These allow visual inspection of the internal detail of the map and identification of artifacts.

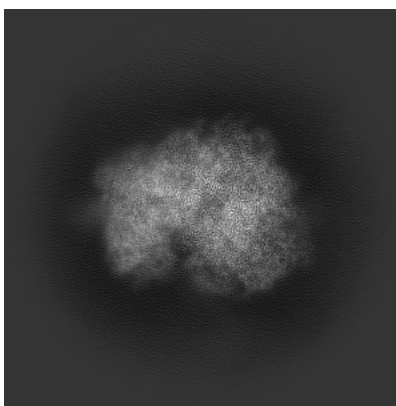
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

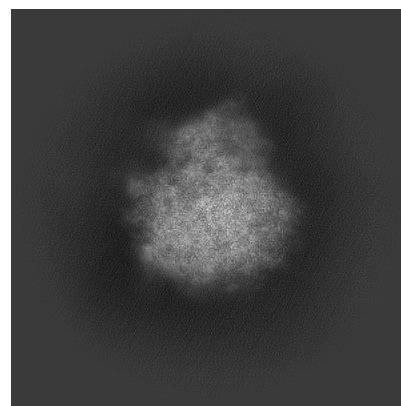
6.1.1 Primary map



X

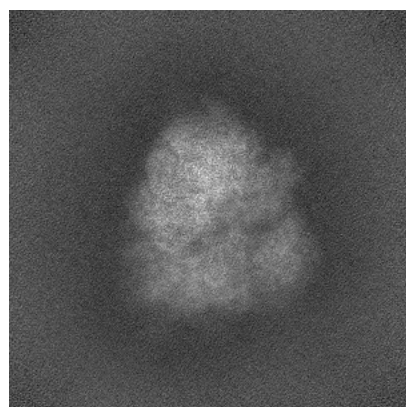


Y

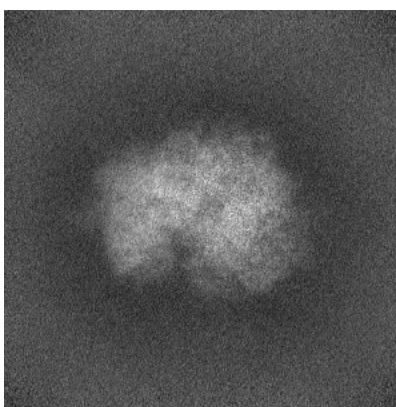


Z

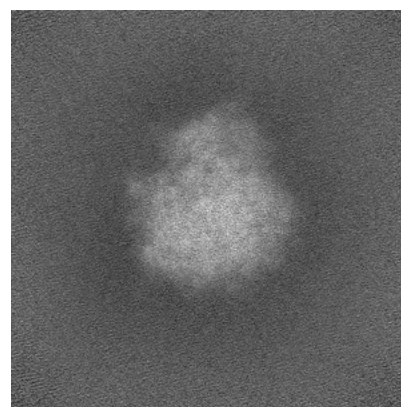
6.1.2 Raw map



X



Y

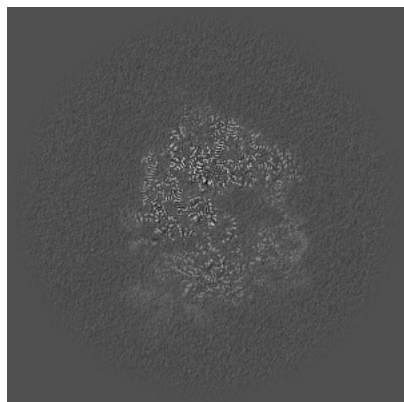


Z

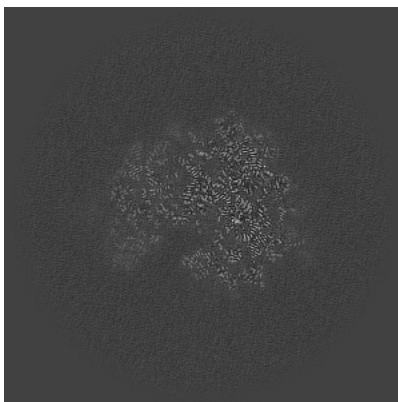
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

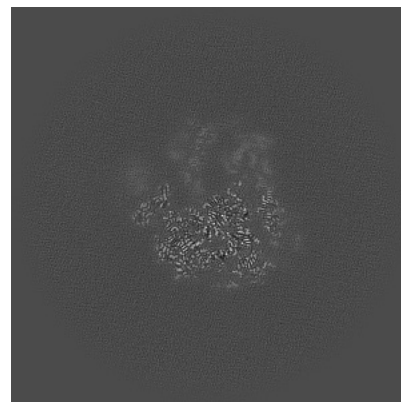
6.2.1 Primary map



X Index: 343

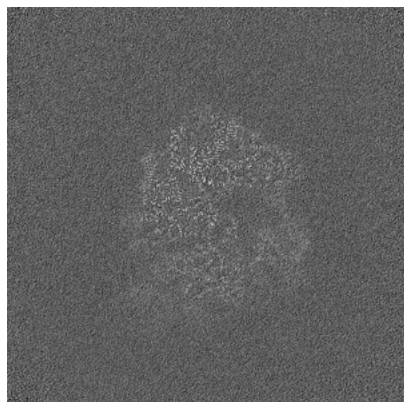


Y Index: 343

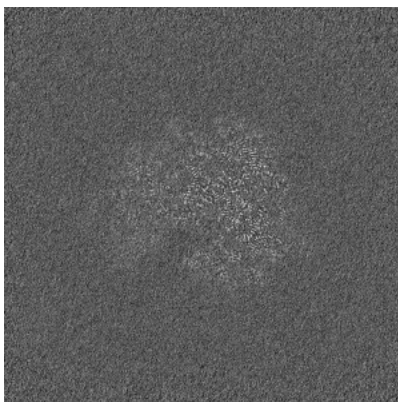


Z Index: 343

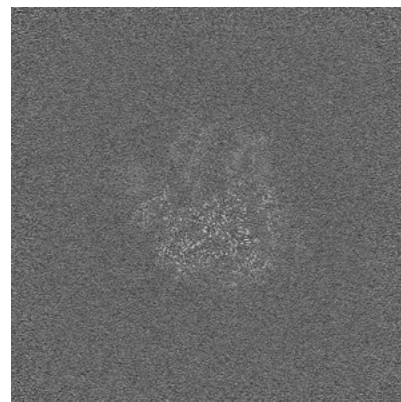
6.2.2 Raw map



X Index: 343



Y Index: 343

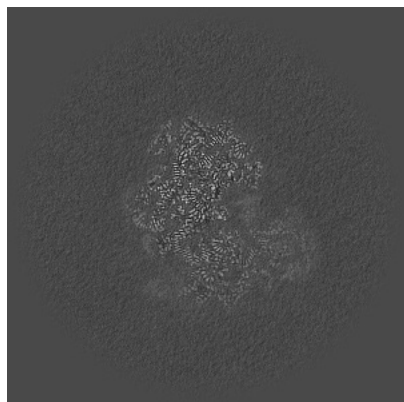


Z Index: 343

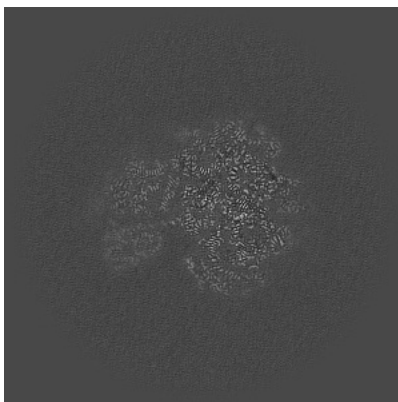
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

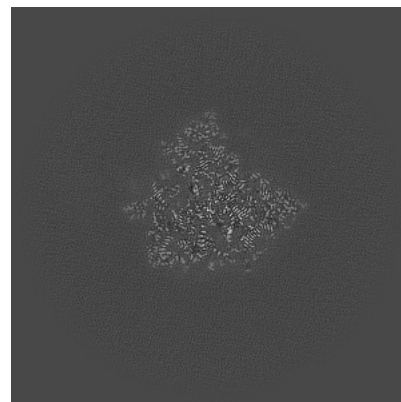
6.3.1 Primary map



X Index: 371

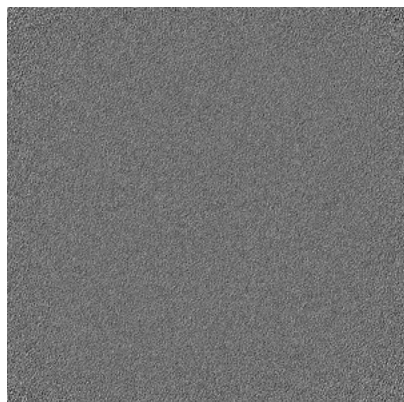


Y Index: 331

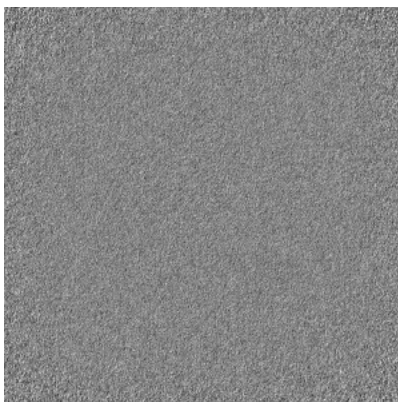


Z Index: 393

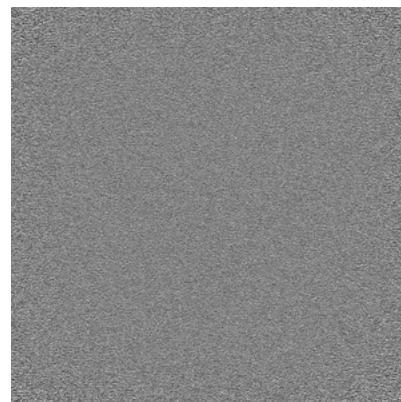
6.3.2 Raw map



X Index: 0



Y Index: 0

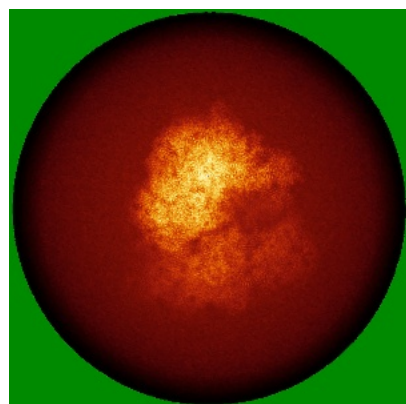


Z Index: 0

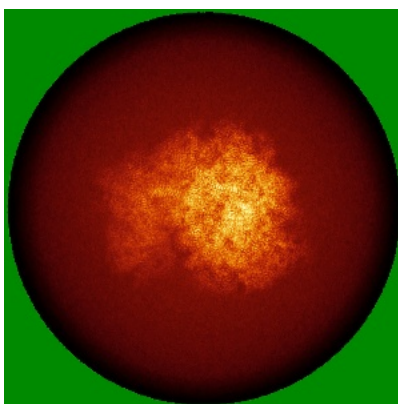
The images above show the largest variance slices of the map in three orthogonal directions.

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

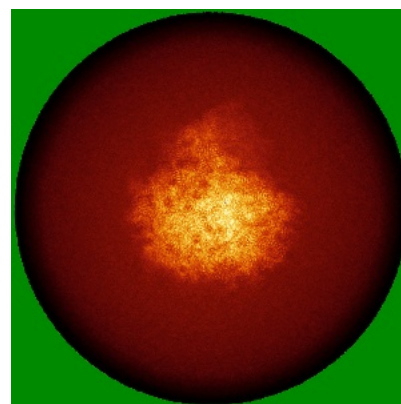
6.4.1 Primary map



X

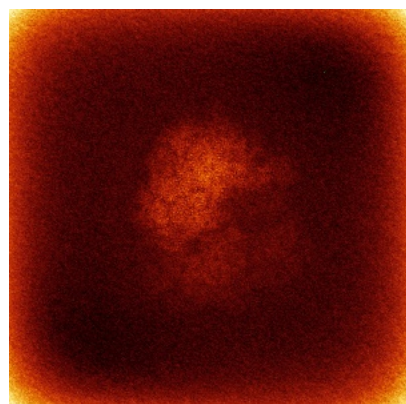


Y

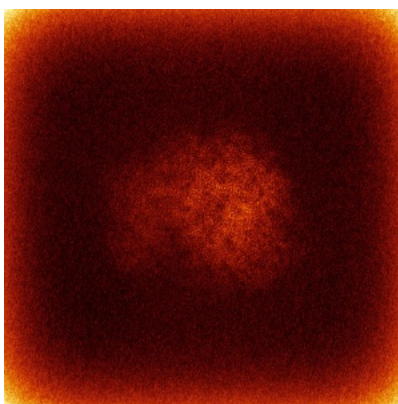


Z

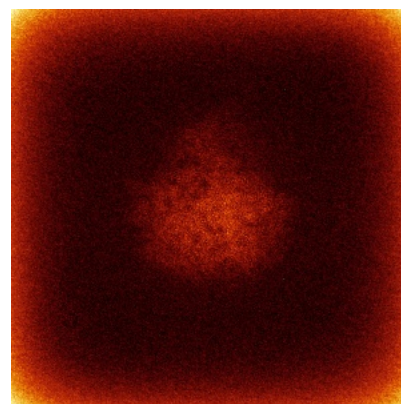
6.4.2 Raw map



X



Y

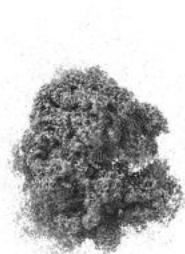


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



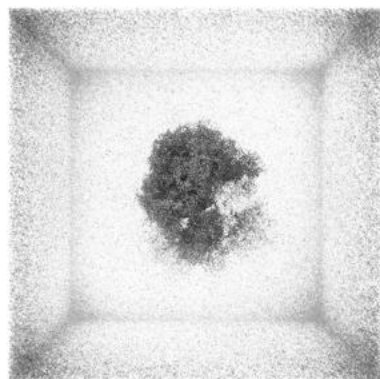
Y



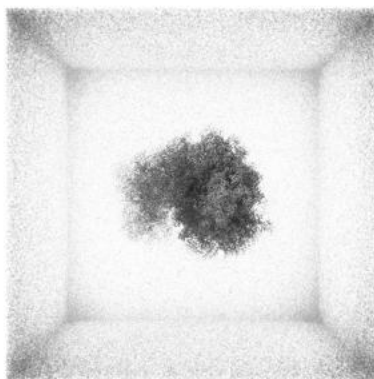
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

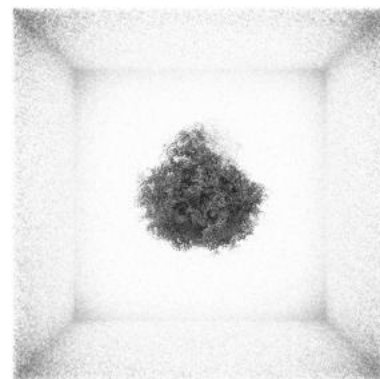
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

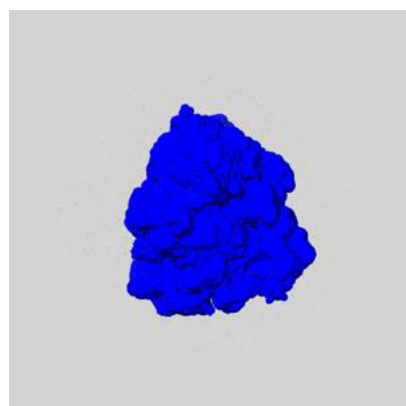
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

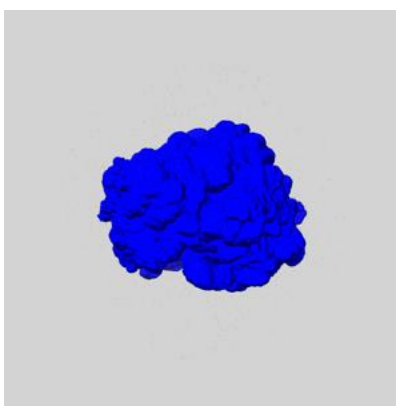
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

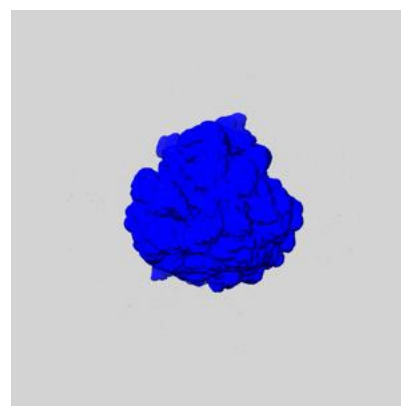
6.6.1 emd_52299_msk_1.map [i](#)



X



Y

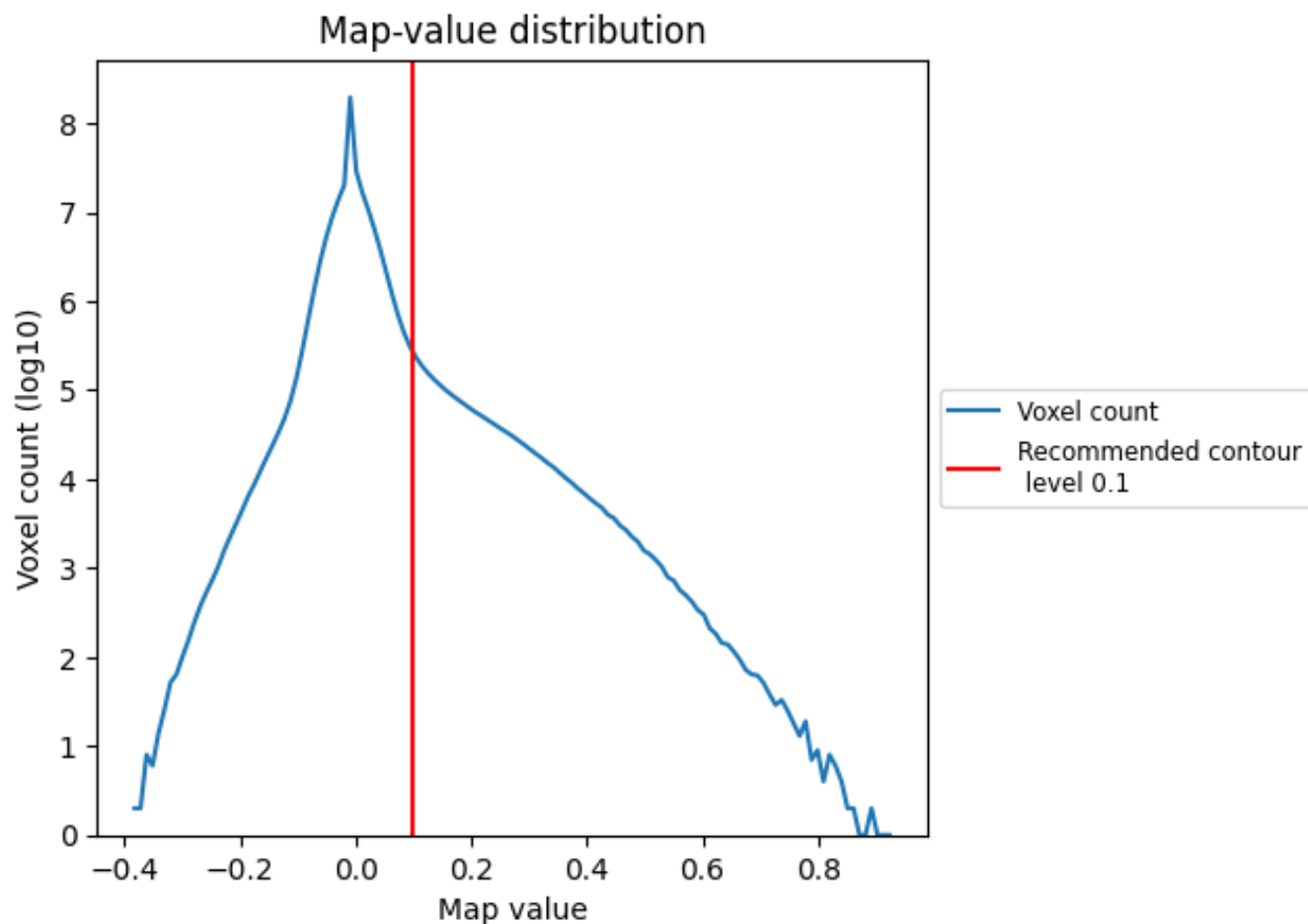


Z

7 Map analysis [i](#)

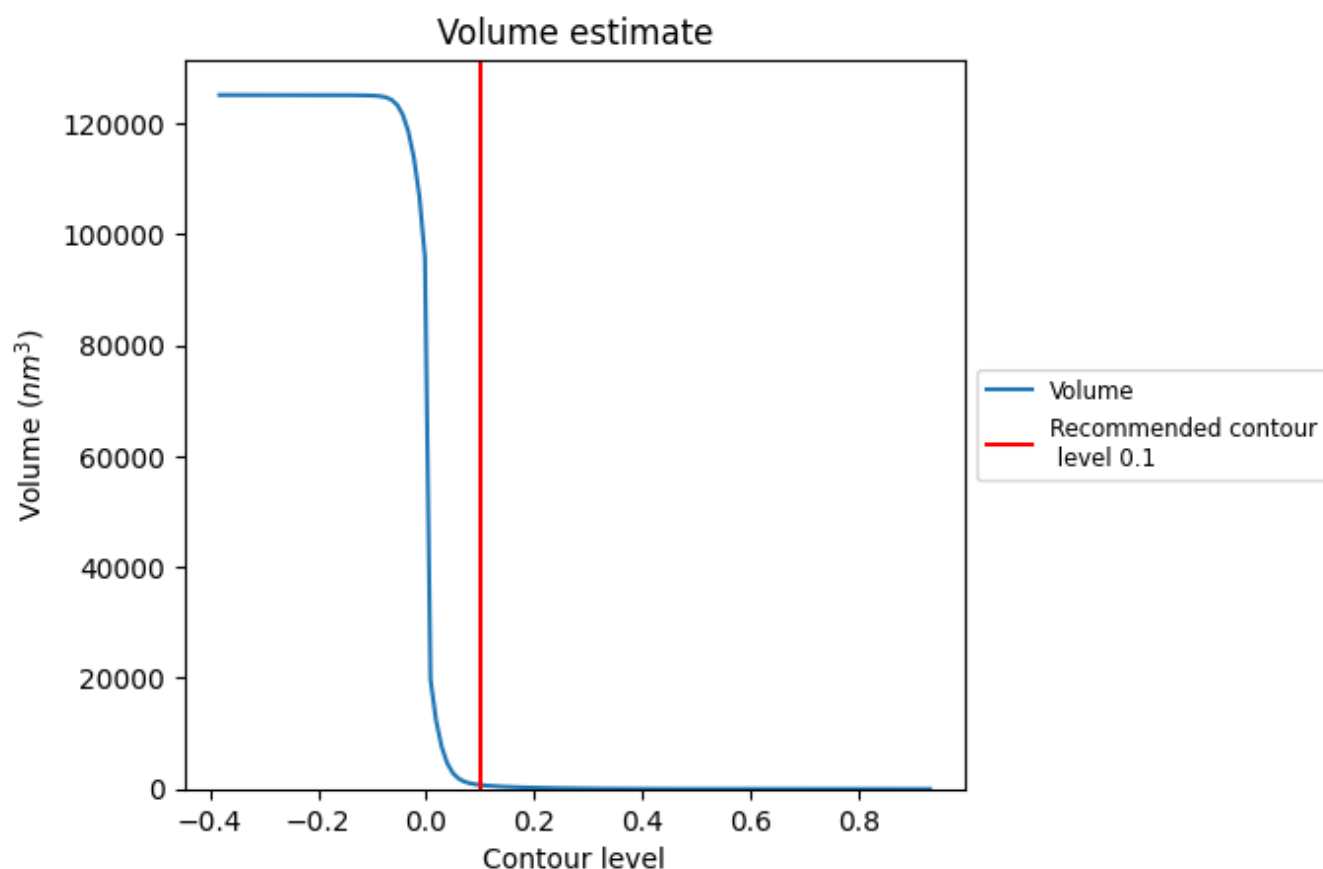
This section contains the results of statistical analysis of the map.

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.

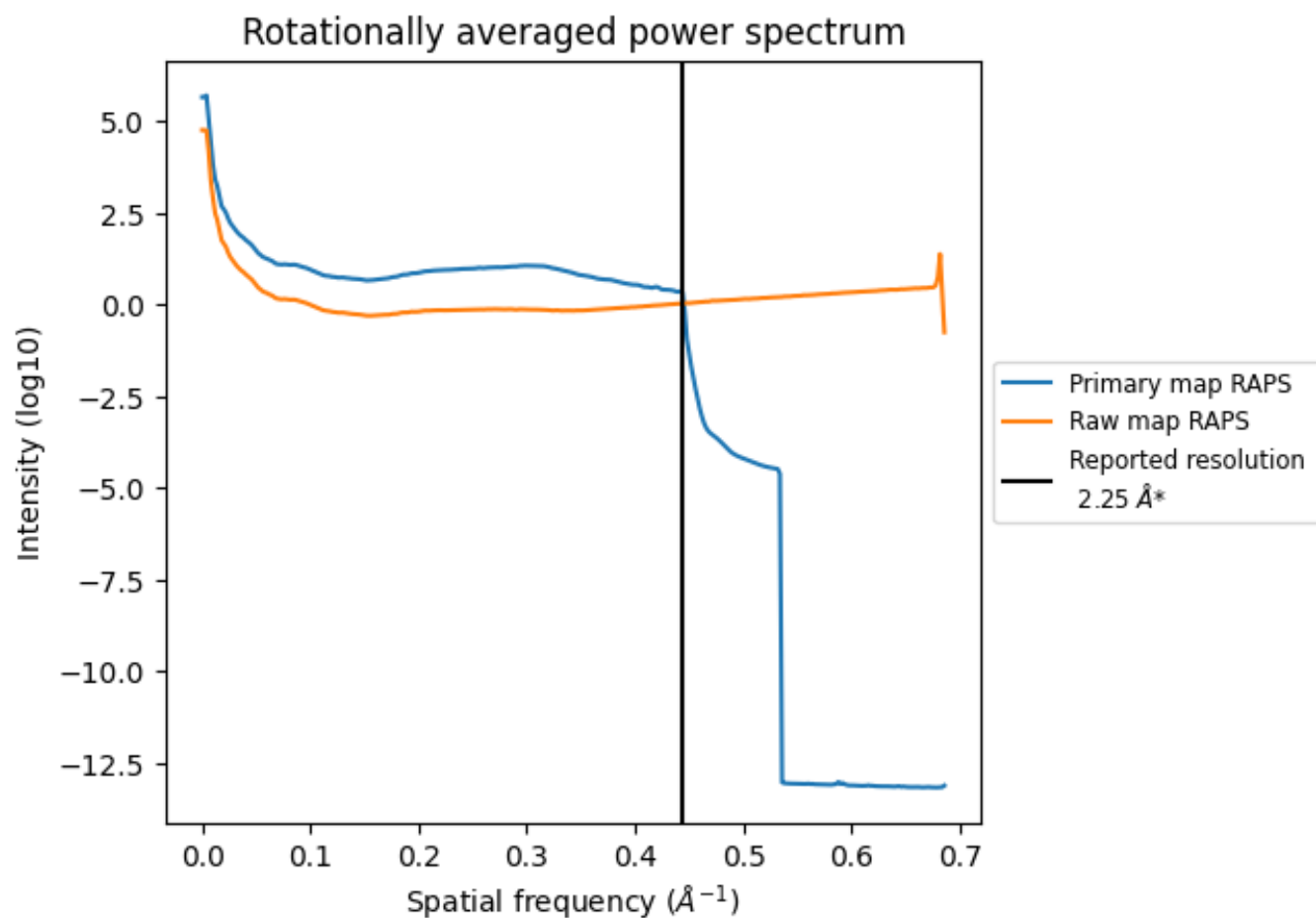
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 726 nm^3 ; this corresponds to an approximate mass of 656 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 ⓘ

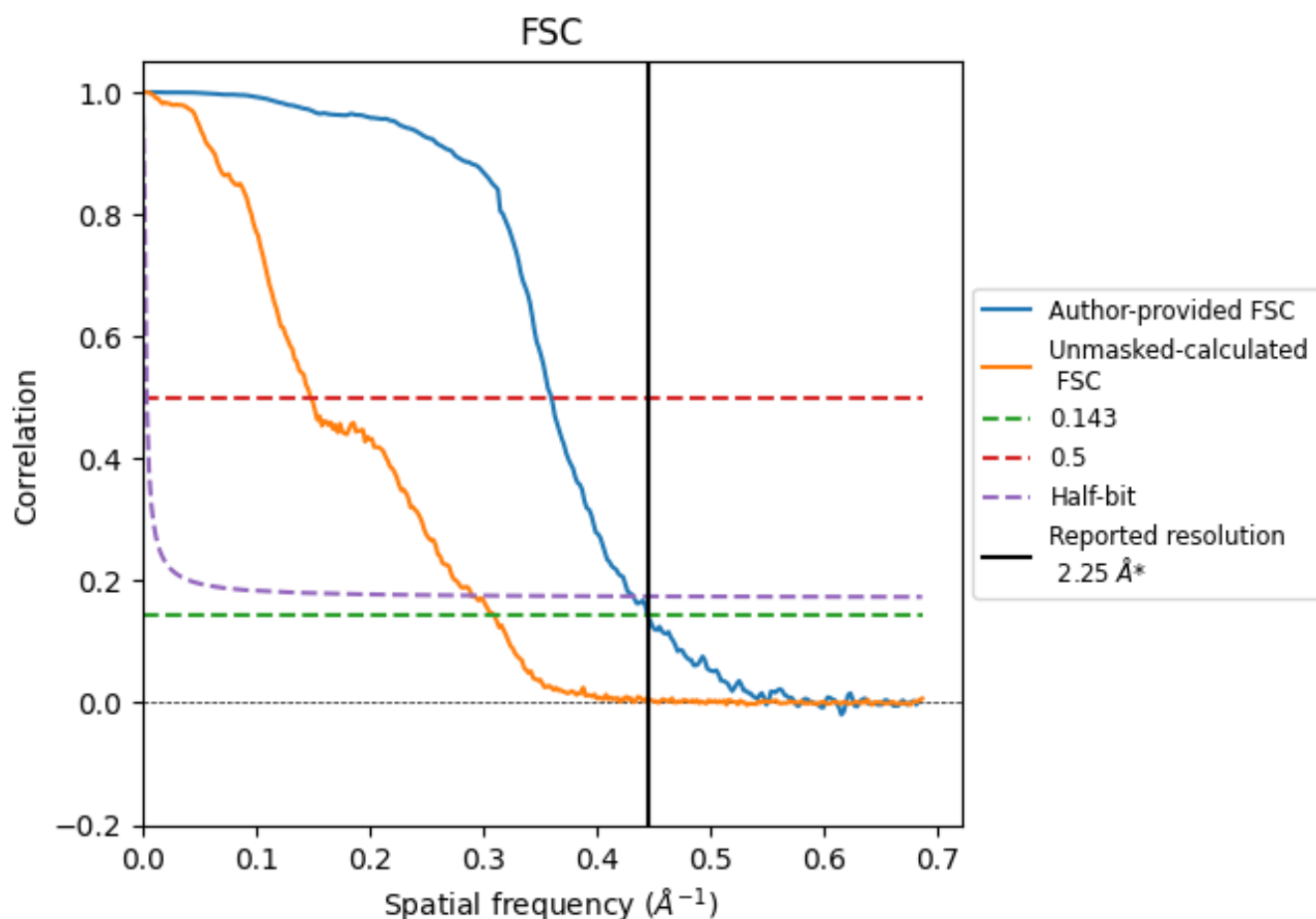


*Reported resolution corresponds to spatial frequency of 0.444 Å⁻¹

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 0.444 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

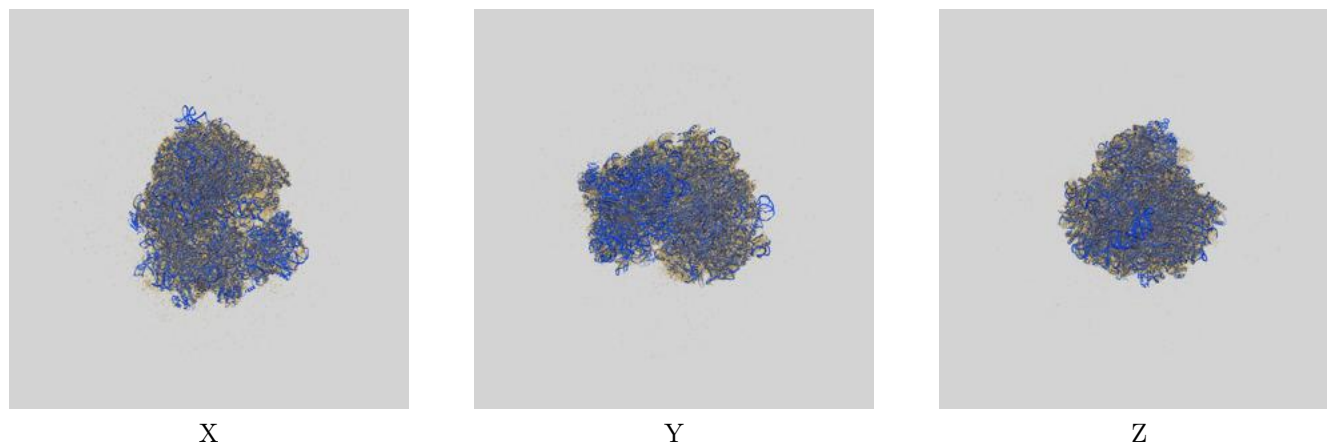
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.25	2.78	2.32
Unmasked-calculated*	3.23	6.76	3.45

*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 3.23 differs from the reported value 2.25 by more than 10 %

9 Map-model fit [i](#)

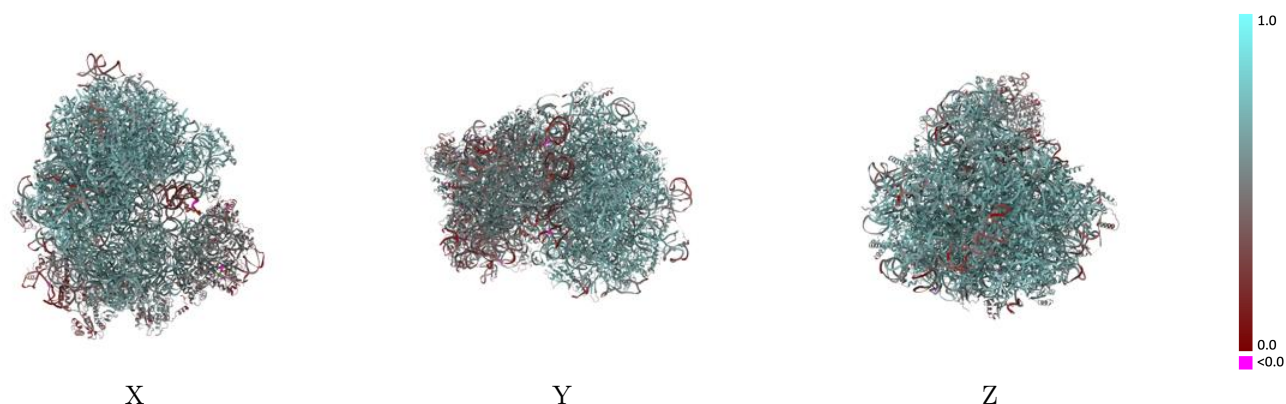
This section contains information regarding the fit between EMDB map EMD-52299 and PDB model 9HMW. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)



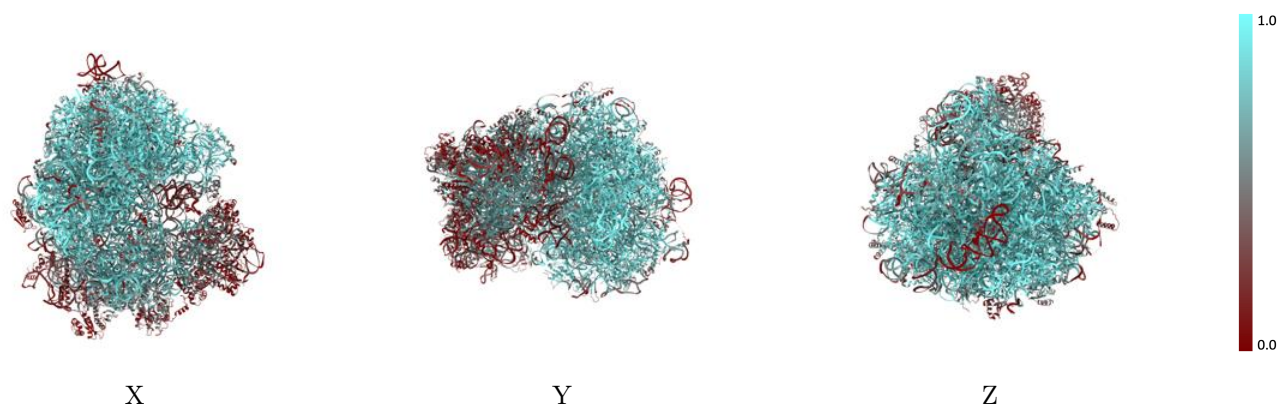
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



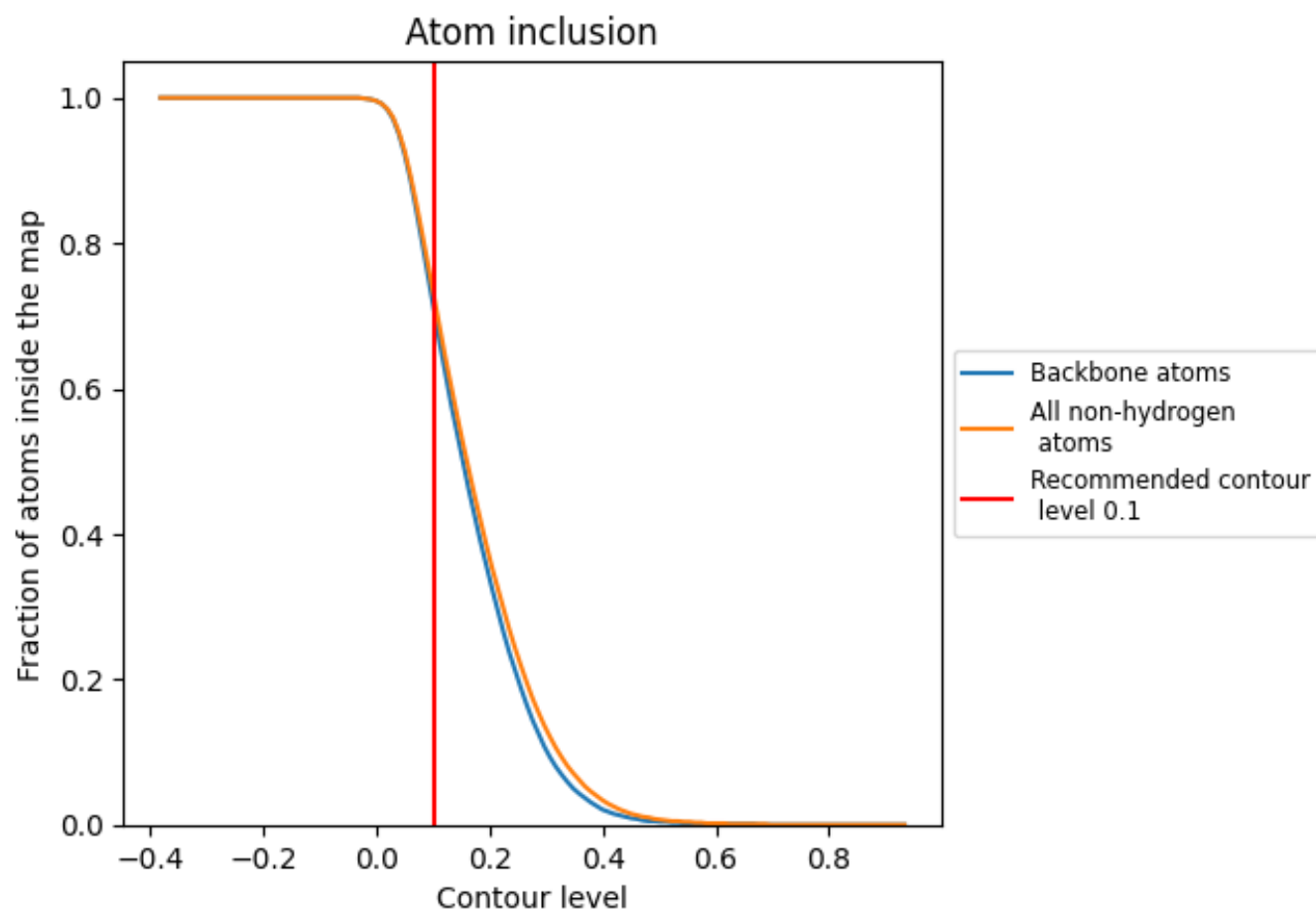
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7320	 0.5990
3	 0.8700	 0.6350
A	 0.8770	 0.6440
AA	 0.2440	 0.4470
AB	 0.4070	 0.5060
AC	 0.6470	 0.6080
AD	 0.2810	 0.4730
AE	 0.7680	 0.6420
AF	 0.2780	 0.4310
AG	 0.8380	 0.6640
AH	 0.8040	 0.6400
AI	 0.1110	 0.3630
AJ	 0.9490	 0.7010
AK	 0.7590	 0.6130
AL	 0.9080	 0.6860
AM	 0.8430	 0.6670
AN	 0.0930	 0.4190
AO	 0.8810	 0.6840
AP	 0.7830	 0.6350
AQ	 0.3940	 0.5840
AR	 0.8980	 0.6860
AT	 0.8140	 0.6510
AU	 0.7810	 0.6330
AV	 0.9310	 0.6970
AW	 0.9390	 0.7050
AX	 0.8070	 0.6430
AY	 0.9540	 0.7070
AZ	 0.5950	 0.5930
Aa	 0.3320	 0.4730
B1	 0.7250	 0.5550
BA	 0.9500	 0.6950
BB	 0.1350	 0.3620
BC	 0.7940	 0.6470
BD	 0.9150	 0.6960
BE	 0.8990	 0.6920



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Chain	Atom inclusion	Q-score
BF	 0.6850	 0.6100
BG	 0.6880	 0.6000
BH	 0.8770	 0.6860
BI	 0.8900	 0.6910
BJ	 0.7840	 0.6390
BK	 0.7610	 0.6270
BL	 0.2670	 0.4760
BM	 0.9110	 0.6910
BN	 0.7750	 0.6470
BO	 0.8890	 0.6790
BP	 0.7760	 0.6430
BQ	 0.9610	 0.7100
BR	 0.8560	 0.6760
BS	 0.9130	 0.6960
BT	 0.8490	 0.6730
BU	 0.5940	 0.5800
BV	 0.5710	 0.5720
BW	 0.5420	 0.5730
Ba	 0.2110	 0.3950
C3	 0.9460	 0.6620
Ca	 0.4650	 0.5340
Da	 0.5940	 0.5720
Ea	 0.9780	 0.7160
Fa	 0.8770	 0.6730
Ga	 0.8610	 0.6630
Ha	 0.9210	 0.6920
Ia	 0.7820	 0.6430
Ja	 0.4040	 0.5090
Ka	 0.2890	 0.4530
L3	 0.0430	 0.1450
La	 0.1260	 0.3920
Ma	 0.6640	 0.6190
Na	 0.4620	 0.5190
Oa	 0.3330	 0.4850
Pa	 0.3320	 0.5120
Ra	 0.1820	 0.3820
Ta	 0.2170	 0.4000
Ua	 0.6260	 0.5910
Va	 0.6410	 0.6170
W2	 0.4340	 0.4060
Wa	 0.2930	 0.4690
Xa	 0.5520	 0.5490

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Chain	Atom inclusion	Q-score
Ya	 0.1990	 0.4120
Za	 0.4340	 0.5170
h1	 0.6570	 0.5390
i2	 0.2820	 0.3710