



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 06:35 PM JST

PDB ID : 8JDL / pdb_00008jdl
EMDB ID : EMD-36180
Title : Structure of the Human cytoplasmic Ribosome with human tRNA
Tyr(GalQ34) and mRNA(UAU) (non-rotated state)
Authors : Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.
Deposited on : 2023-05-14
Resolution : 2.42 Å(reported)
Based on initial model : 6Y0G

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:

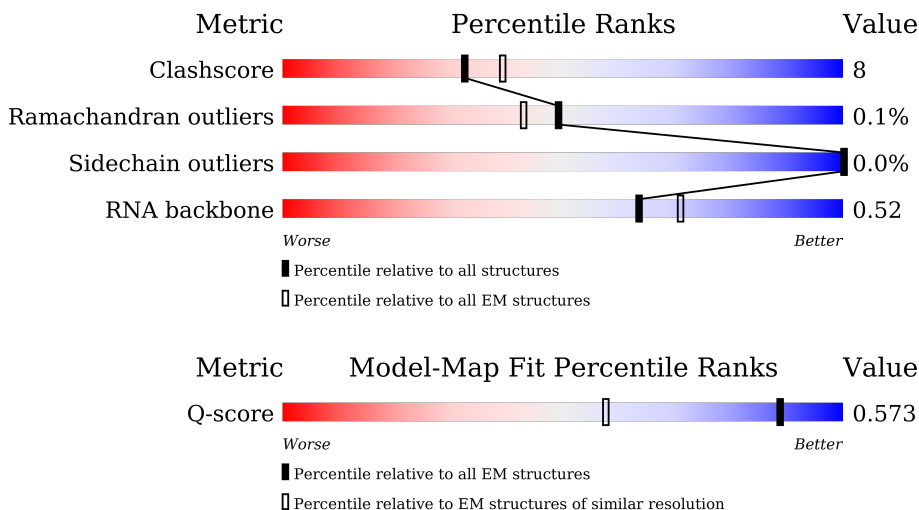
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

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

The reported resolution of this entry is 2.42 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.















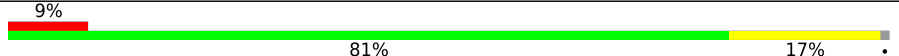
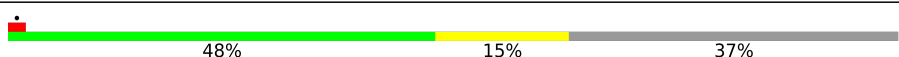
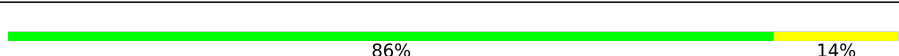

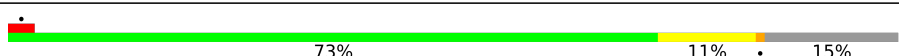
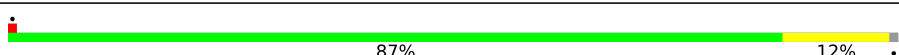
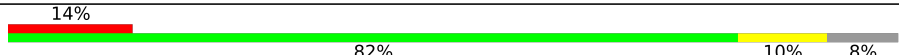
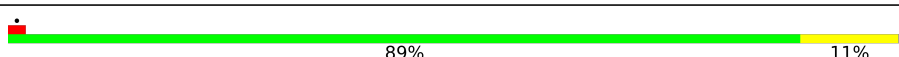
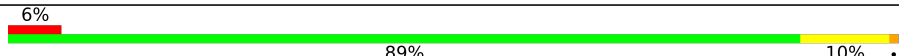



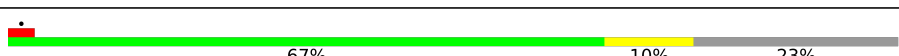
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5729 (1.92 - 2.92)

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	A	14	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>36%</p> </div> <div style="text-align: center;"> <p>43%</p> </div> <div style="text-align: center;"> <p>36%</p> </div> <div style="text-align: center;"> <p>21%</p> </div> </div>
2	B	76	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>74%</p> </div> <div style="text-align: center;"> <p>42%</p> </div> <div style="text-align: center;"> <p>38%</p> </div> <div style="text-align: center;"> <p>16%</p> </div> <div style="text-align: center;"> <p>.</p> </div> </div>
3	D	5070	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>8%</p> </div> <div style="text-align: center;"> <p>43%</p> </div> <div style="text-align: center;"> <p>21%</p> </div> <div style="text-align: center;"> <p>5%</p> </div> <div style="text-align: center;"> <p>31%</p> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	120	
5	F	156	
6	G	257	
7	H	403	
8	I	427	
9	J	297	
10	K	288	
11	L	248	
12	M	266	
13	N	192	
14	O	214	
15	P	178	
16	Q	211	
17	R	215	
18	S	204	
19	T	203	
20	U	184	
21	V	188	
22	W	196	
23	X	176	
24	Y	160	
25	Z	128	
26	a	140	
27	b	157	
28	c	156	

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Mol	Chain	Length	Quality of chain
29	d	145	6% 77% 16% 8%
30	e	136	77% 22%
31	f	148	80% 19%
32	g	159	15% 55% 9% 35%
33	h	115	70% 15% 16%
34	i	125	8% 77% 9% 14%
35	j	135	87% 7% 5%
36	k	110	85% 15%
37	l	117	9% 83% 13%
38	m	123	86% 12%
39	n	105	10% 87% 10%
40	o	97	76% 10% 11%
41	p	70	20% 86% 13%
42	q	51	75% 24%
43	r	128	34% 6% 59%
44	s	25	100%
45	t	106	12% 82% 17%
46	u	92	5% 91% 8%
47	v	137	76% 15% 9%
48	w	1869	20% 37% 38% 12% 13%
49	x	295	28% 58% 14% 27%
50	y	264	24% 62% 18% 20%
51	z	293	13% 57% 15% 28%
52	0	243	63% 57% 30% 13%
53	1	263	67% 62% 37%

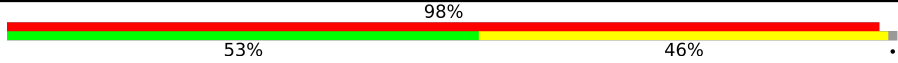
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Mol	Chain	Length	Quality of chain
54	2	204	53% 67% 25% 8%
55	3	249	79% 58% 37% 5%
56	4	194	74% 63% 33%
57	5	208	32% 72% 27%
58	6	194	71% 44% 49% 6%
59	7	165	58% 35% 23% 42%
60	8	158	15% 78% 12% 10%
61	9	151	22% 79% 20%
62	AA	151	15% 64% 25% 11%
63	AB	145	87% 68% 25% 8%
64	AC	146	65% 65% 32%
65	AD	135	71% 70% 26%
66	AE	152	72% 65% 30% 5%
67	AF	145	71% 74% 25%
68	AG	119	66% 47% 39% 14%
69	AH	83	40% 81% 19%
70	AI	130	7% 78% 22%
71	AJ	143	17% 79% 20%
72	AK	133	86% 45% 47% 8%
73	AL	125	62% 51% 18% 31%
74	AM	115	16% 71% 15% 14%
75	AN	84	52% 73% 26%
76	AO	69	52% 75% 13% 12%
77	AP	56	27% 43% 38% 20%
78	AQ	59	86% 68% 29%

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Mol	Chain	Length	Quality of chain
79	AR	317	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment on the left labeled '53%', a yellow segment in the middle labeled '46%', and a small grey segment on the right. Above the bar, the text '98%' is centered, indicating the total quality percentage.</p>

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 207902 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 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	11	226	102	31	82	11	0	0

- Molecule 2 is a RNA chain called tRNA (Tyr).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	76	1647	746	288	538	75	0	0

- Molecule 3 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	D	3512	75336	33585	13757	24482	3512	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	E	120	2558	1141	456	842	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	F	156	3315	1481	585	1094	155	0	0

- Molecule 6 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	247	1891	1185	388	312	6	0	0

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	398	3211	2045	604	548	14	0	0

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	363	2884	1815	577	478	14	0	0

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	293	2379	1506	434	425	14	0	0

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	217	1751	1128	332	287	4	0	0

- Molecule 11 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	225	1870	1202	358	301	9	0	0

- Molecule 12 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	227	1832	1168	352	308	4	0	0

- Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	190	1518	956	284	272	6	0	0

- Molecule 14 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	206	1660	1053	319	275	13	0	0

- Molecule 15 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	170	1362	861	254	241	6	0	0

- Molecule 16 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	208	1682	1052	348	278	4	0	0

- Molecule 17 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	136	1120	719	215	179	7	0	0

- Molecule 18 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	203	1701	1072	359	266	4	0	0

- Molecule 19 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	200	1641	1058	320	258	5	0	0

- Molecule 20 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	U	157	1273	797	246	221	9	0	0

- Molecule 21 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 22 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 23 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 24 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 25 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	101	Total	C	N	O	S	0	0
			821	526	143	150	2		

- Molecule 26 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 27 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 28 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	120	981	628	185	167	1	0	0

- Molecule 29 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	134	1115	700	226	186	3	0	0

- Molecule 30 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	135	1107	714	208	182	3	0	0

- Molecule 31 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	147	1162	736	237	186	3	0	0

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	104	832	515	182	132	3	0	0

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	97	755	479	133	137	6	0	0

- Molecule 34 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	107	888	560	171	155	2	0	0

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	128	1053	667	216	165	5	0	0

- Molecule 36 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	109	876	555	174	144	3	0	0

- Molecule 37 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	112	888	555	183	144	6	0	0

- Molecule 38 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	m	121	1010	638	204	167	1	0	0

- Molecule 39 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	102	832	521	177	129	5	0	0

- Molecule 40 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	86	705	434	155	111	5	0	0

- Molecule 41 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	69	569	366	103	99	1	0	0

- Molecule 42 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 43 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 44 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 45 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 46 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 47 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 48 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	1634	Total	C	N	O	P	0	0
			34933	15622	6267	11411	1633		

- Molecule 49 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	215	Total	C	N	O	S	0	0
			1695	1077	297	313	8		

- Molecule 50 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	212	Total	C	N	O	S	0	0
			1725	1096	308	307	14		

- Molecule 51 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	212	Total	C	N	O	S	0	0
			1633	1059	279	285	10		

- Molecule 52 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	212	Total	C	N	O	S	0	0
			1646	1050	299	290	7		

- Molecule 53 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	262	Total	C	N	O	S	0	0
			2070	1321	383	358	8		

- Molecule 54 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	187	Total	C	N	O	S	0	0
			1464	916	276	265	7		

- Molecule 55 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	237	Total	C	N	O	S	0	0
			1917	1197	384	329	7		

- Molecule 56 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	187	Total	C	N	O	S	0	0
			1510	963	278	268	1		

- Molecule 57 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	206	Total	C	N	O	S	0	0
			1674	1049	329	291	5		

- Molecule 58 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	6	182	Total	C	N	O	S	0	0
			1506	959	300	245	2		

- Molecule 59 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	7	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 60 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	8	142	Total	C	N	O	S	0	0
			1150	732	215	197	6		

- Molecule 61 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	9	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 62 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AA	134	Total	C	N	O	S	0	0
			1002	612	197	187	6		

- Molecule 63 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	AB	134	1103	703	208	185	7	0	0

- Molecule 64 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	AC	142	1128	717	213	195	3	0	0

- Molecule 65 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	AD	131	1057	665	197	191	4	0	0

- Molecule 66 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	AE	144	1169	731	236	201	1	0	0

- Molecule 67 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	AF	143	1111	696	213	198	4	0	0

- Molecule 68 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	AG	102	799	501	153	141	4	0	0

- Molecule 69 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	AH	83	636	393	117	121	5	0	0

- Molecule 70 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	AI	129	1034	659	193	176	6	0	0

- Molecule 71 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	AJ	141	1098	693	219	183	3	0	0

- Molecule 72 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	AK	123	1002	634	196	167	5	0	0

- Molecule 73 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	AL	86	680	436	127	116	1	0	0

- Molecule 74 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	AM	99	792	492	165	130	5	0	0

- Molecule 75 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	AN	83	643	402	119	115	7	0	0

- Molecule 76 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	AO	61	479	292	95	90	2	0	0

- Molecule 77 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AP	45	Total	C	N	O	S	0	0
			370	228	77	60	5		

- Molecule 78 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AQ	57	Total	C	N	O	S	0	0
			452	279	99	73	1		

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AR	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

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

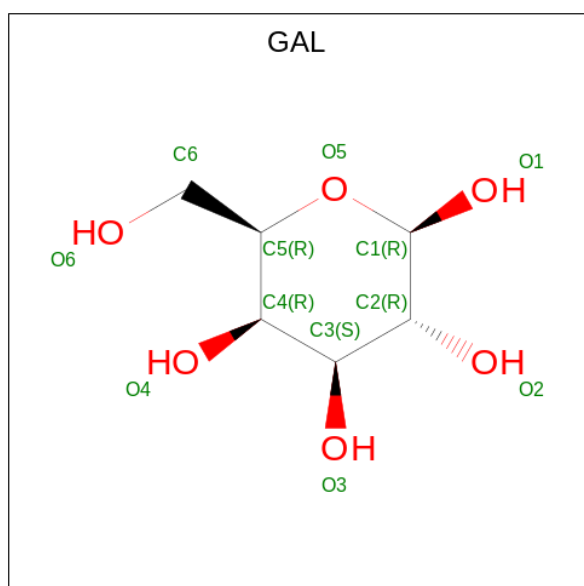
Mol	Chain	Residues	Atoms		AltConf
80	A	1	Total	Mg	0
			1	1	
80	D	401	Total	Mg	0
			401	401	
80	E	10	Total	Mg	0
			10	10	
80	F	5	Total	Mg	0
			5	5	
80	G	2	Total	Mg	0
			2	2	
80	H	1	Total	Mg	0
			1	1	
80	I	1	Total	Mg	0
			1	1	
80	N	1	Total	Mg	0
			1	1	
80	O	1	Total	Mg	0
			1	1	
80	S	1	Total	Mg	0
			1	1	
80	U	2	Total	Mg	0
			2	2	
80	V	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
80	X	1	Total 1	Mg 1	0
80	a	1	Total 1	Mg 1	0
80	g	1	Total 1	Mg 1	0
80	j	1	Total 1	Mg 1	0
80	k	1	Total 1	Mg 1	0
80	l	1	Total 1	Mg 1	0
80	w	100	Total 100	Mg 100	0
80	8	1	Total 1	Mg 1	0
80	AA	1	Total 1	Mg 1	0
80	AF	1	Total 1	Mg 1	0
80	AJ	1	Total 1	Mg 1	0
80	AM	1	Total 1	Mg 1	0

- Molecule 81 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
81	B	1	Total	C	O	0
			11	6	5	

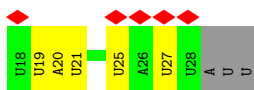
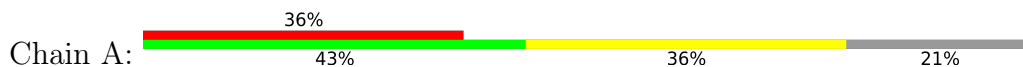
- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	o	1	Total	Zn	0
			1	1	
82	r	1	Total	Zn	0
			1	1	
82	t	1	Total	Zn	0
			1	1	
82	u	1	Total	Zn	0
			1	1	
82	AM	1	Total	Zn	0
			1	1	
82	AP	1	Total	Zn	0
			1	1	

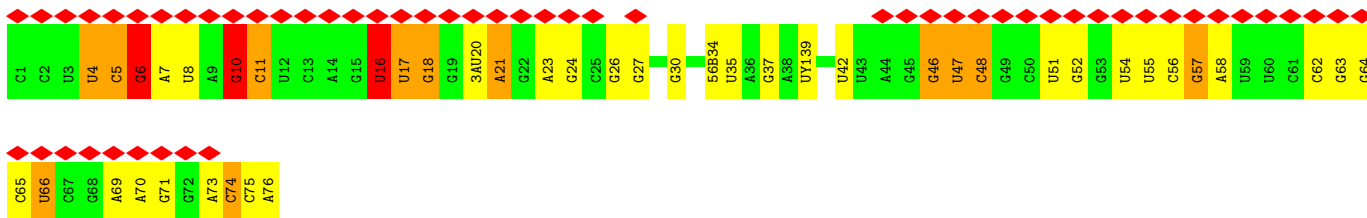
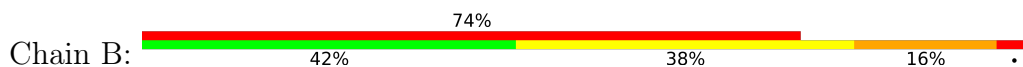
3 Residue-property plots [i](#)

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

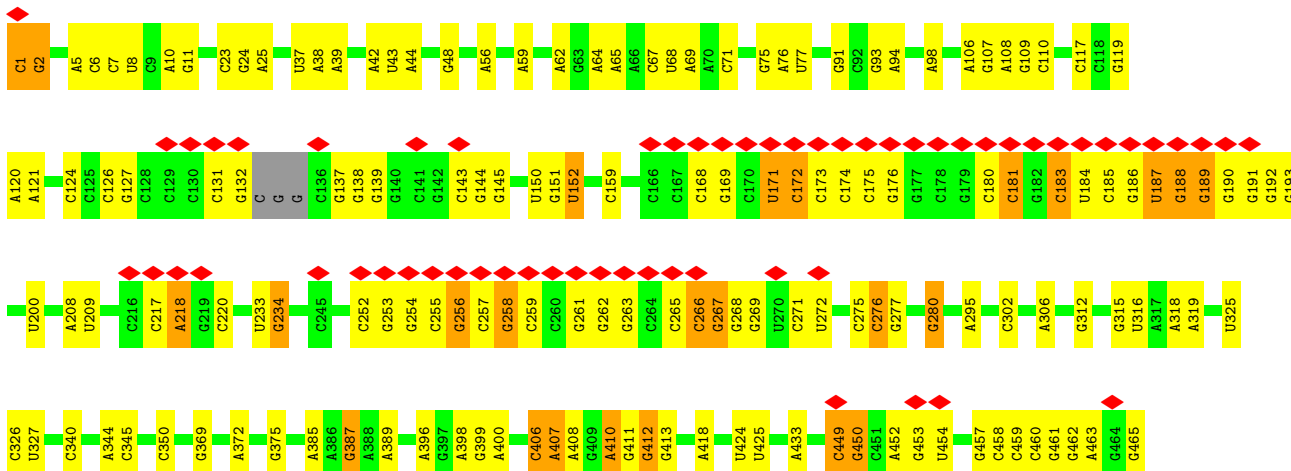
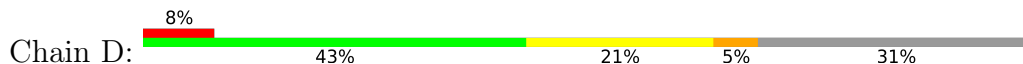
- Molecule 1: mRNA

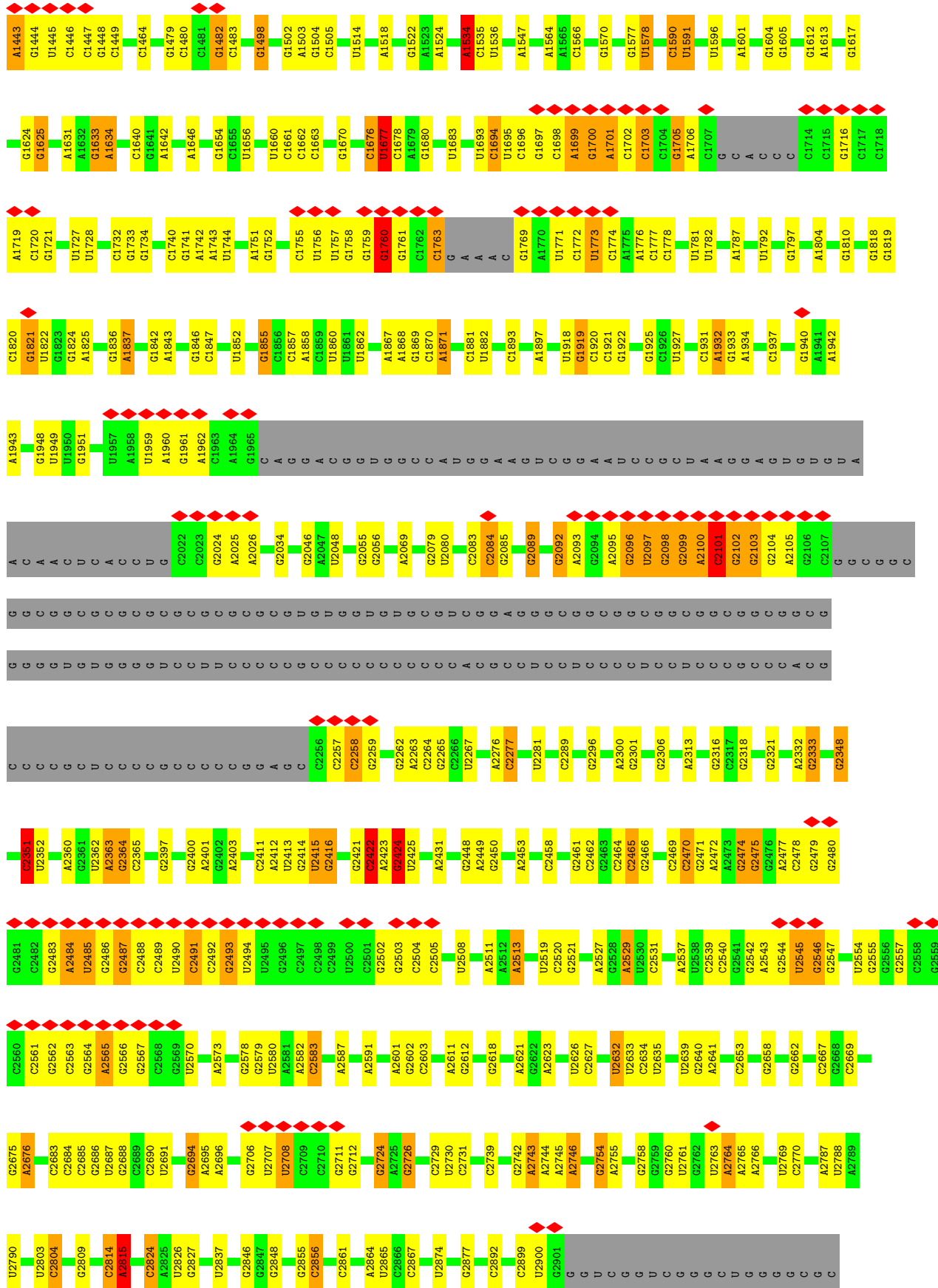


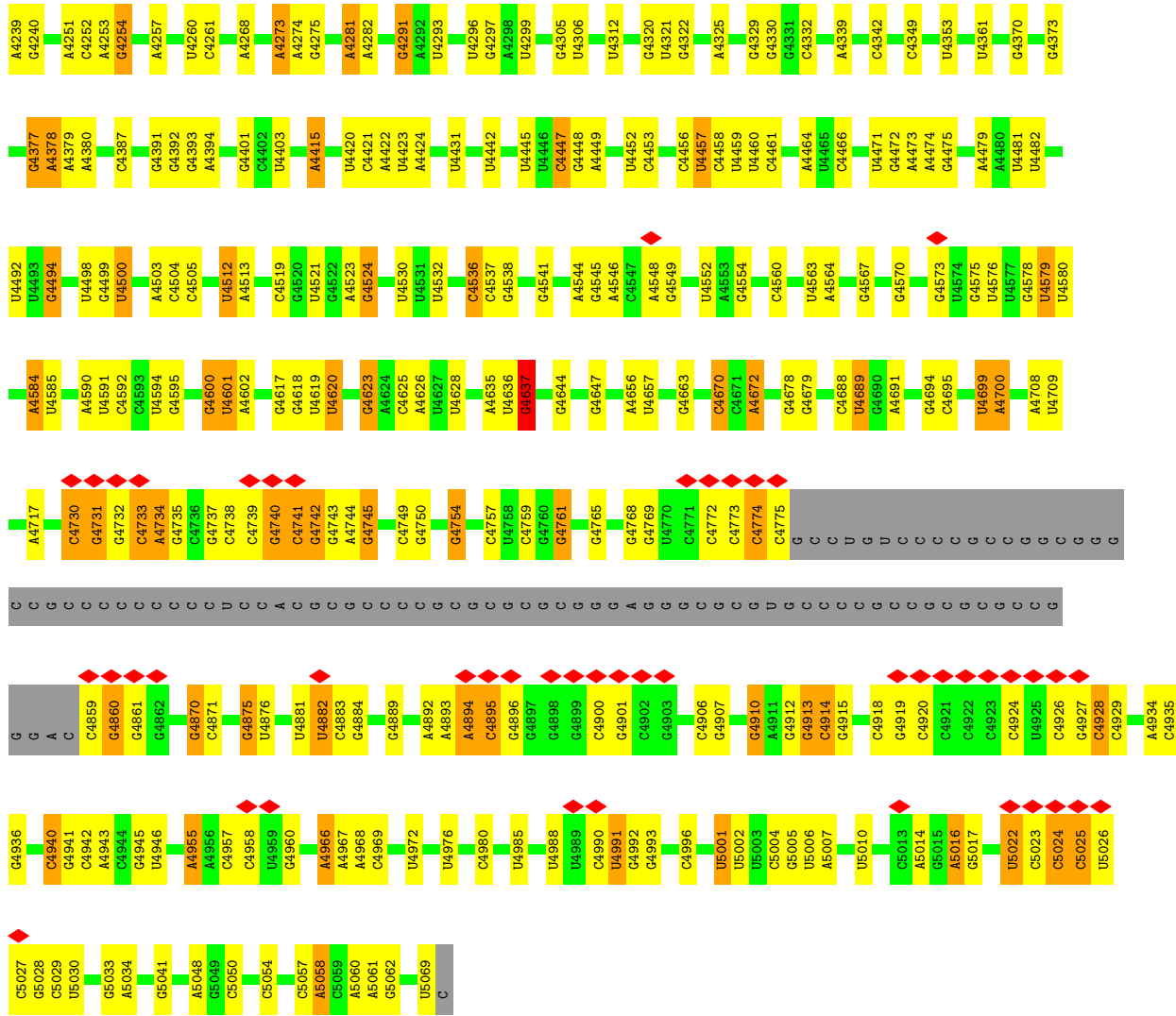
- Molecule 2: tRNA (Tyr)



- Molecule 3: 28S ribosomal RNA



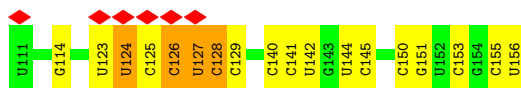
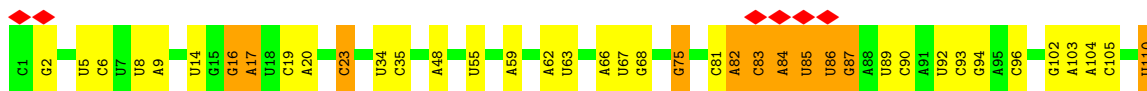


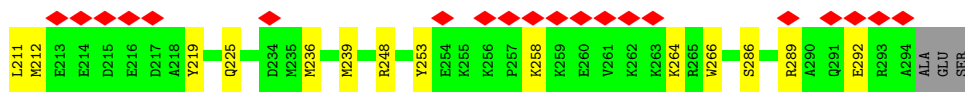


• Molecule 4: 5S ribosomal RNA

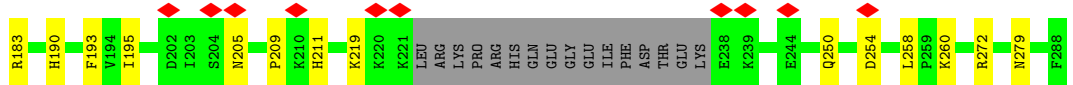
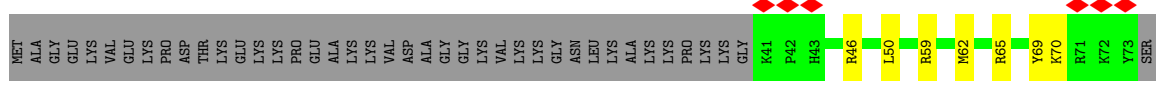


• Molecule 5: 5.8S ribosomal RNA

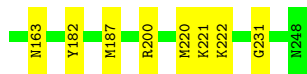
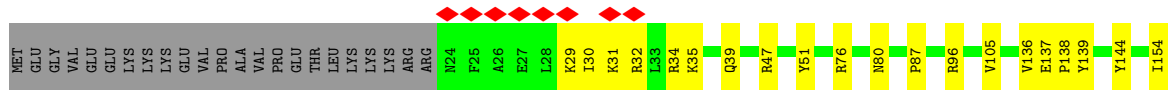
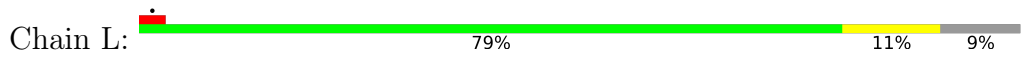




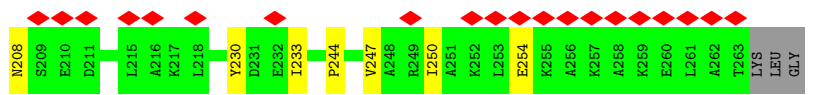
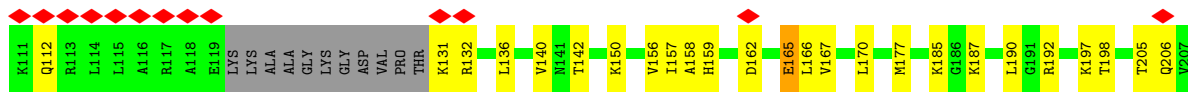
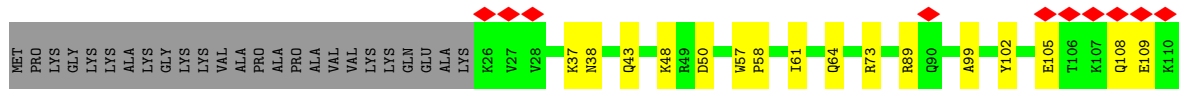
• Molecule 10: 60S ribosomal protein L6



• Molecule 11: 60S ribosomal protein L7

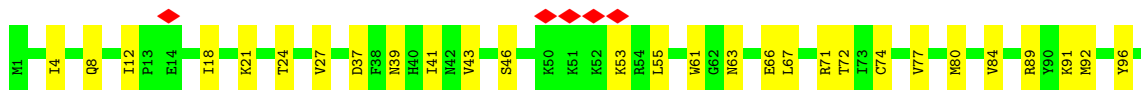


• Molecule 12: 60S ribosomal protein L7a

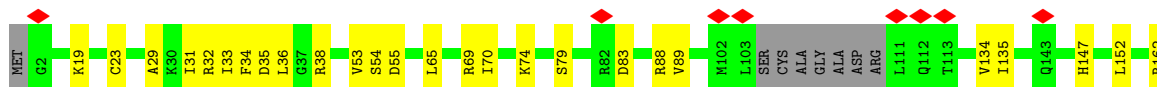
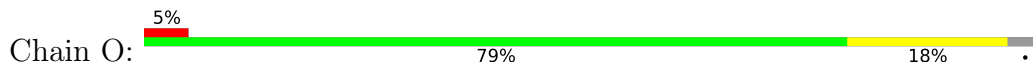


• Molecule 13: 60S ribosomal protein L9

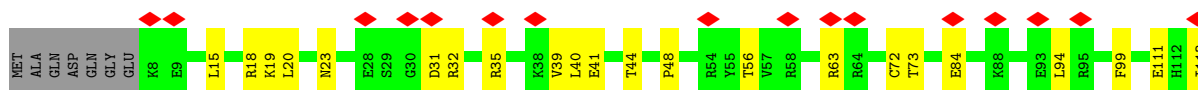




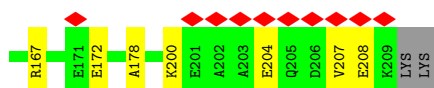
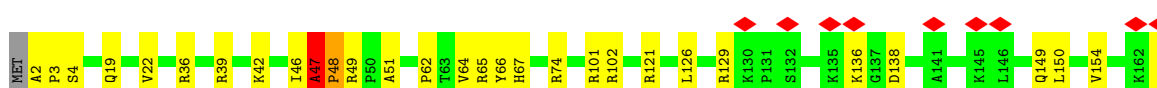
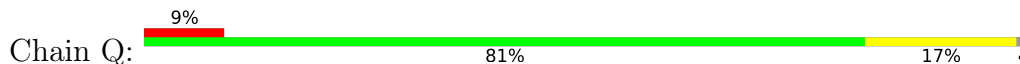
• Molecule 14: 60S ribosomal protein L10-like



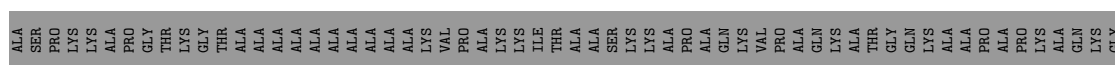
• Molecule 15: 60S ribosomal protein L11



• Molecule 16: 60S ribosomal protein L13

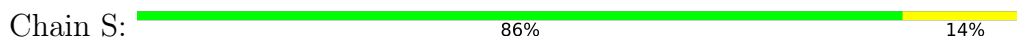


• Molecule 17: 60S ribosomal protein L14

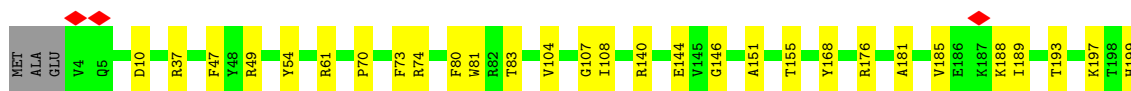
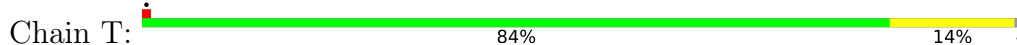


GLN
LYS
ALA
PRO
GLN
LYS
ALA
PRO
ALA
PRO
LYS
ALA
SER
GLY
LYS
LYS
ALA

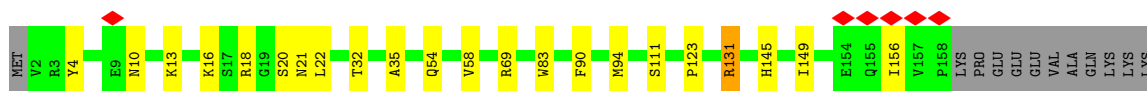
• Molecule 18: 60S ribosomal protein L15



• Molecule 19: 60S ribosomal protein L13a

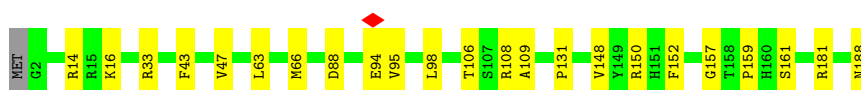


• Molecule 20: 60S ribosomal protein L17

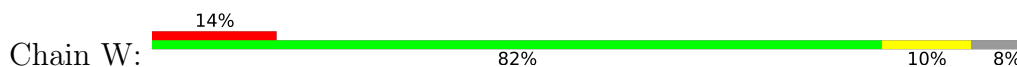


I1E
SER
GLN
LYS
LEU
LYS
GLN
LEU
MET
ALA
ARG
GLU

• Molecule 21: 60S ribosomal protein L18



• Molecule 22: 60S ribosomal protein L19



K180
K181
GLU
GLU
ILE
LYS
THR
LEU
SER
LYS
GLU
GLU
THR
LYS
LYS

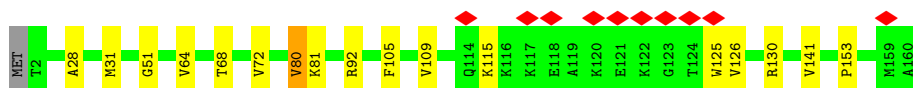
• Molecule 23: 60S ribosomal protein L18a

Chain X: 89% 11%



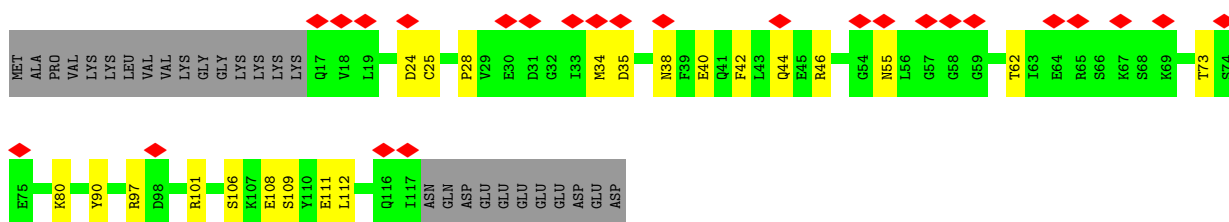
• Molecule 24: 60S ribosomal protein L21

Chain Y: 6% 89% 10%



• Molecule 25: 60S ribosomal protein L22

Chain Z: 20% 62% 17% 21%



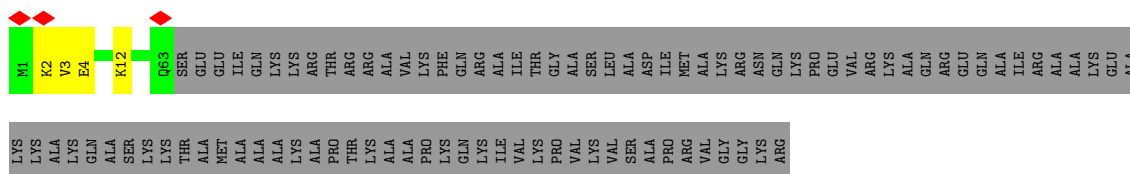
• Molecule 26: 60S ribosomal protein L23

Chain a: 81% 12% 6%



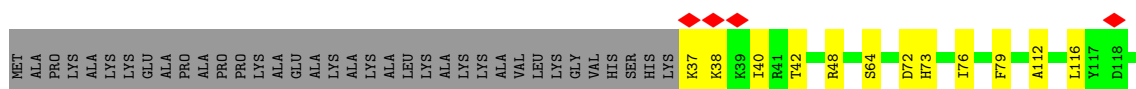
• Molecule 27: 60S ribosomal protein L24

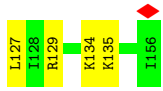
Chain b: 38% 60%



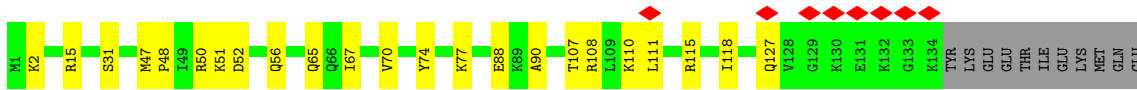
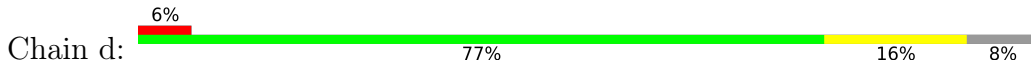
• Molecule 28: 60S ribosomal protein L23a

Chain c: 67% 10% 23%

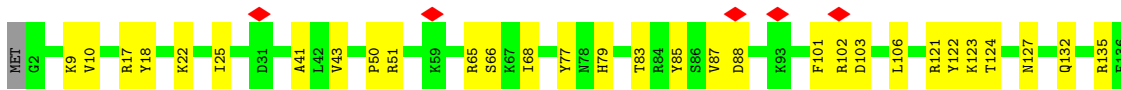
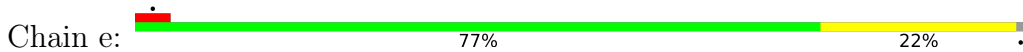




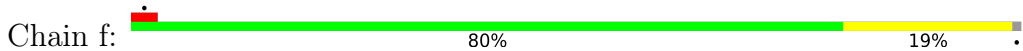
• Molecule 29: 60S ribosomal protein L26



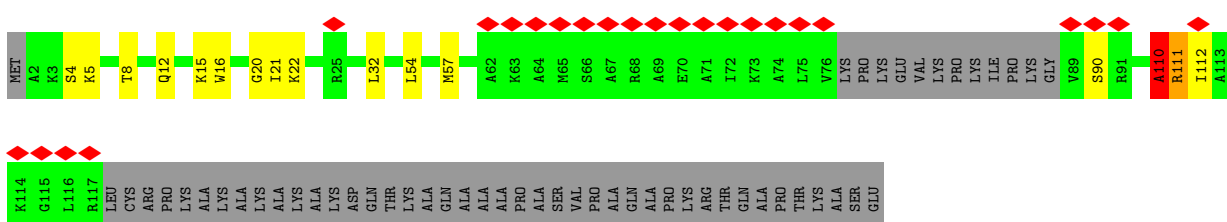
• Molecule 30: 60S ribosomal protein L27



• Molecule 31: 60S ribosomal protein L27a



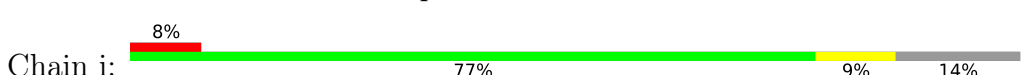
• Molecule 32: 60S ribosomal protein L29



• Molecule 33: 60S ribosomal protein L30

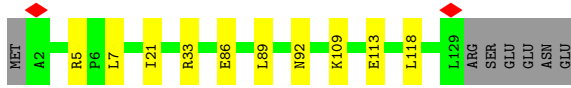
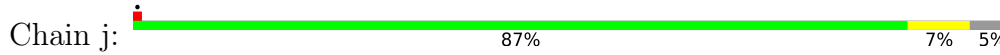


• Molecule 34: 60S ribosomal protein L31

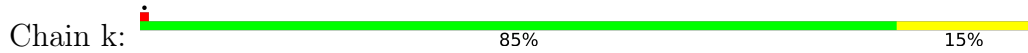




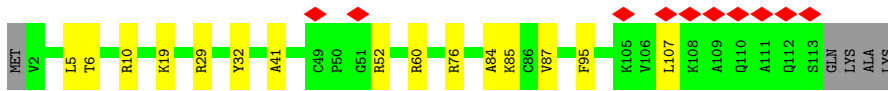
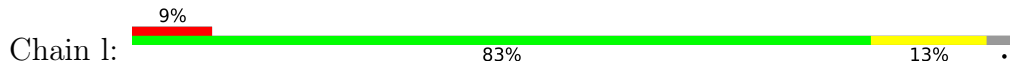
- Molecule 35: 60S ribosomal protein L32



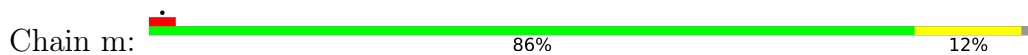
- Molecule 36: 60S ribosomal protein L35a



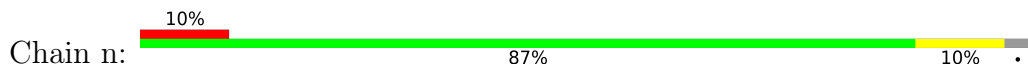
- Molecule 37: 60S ribosomal protein L34



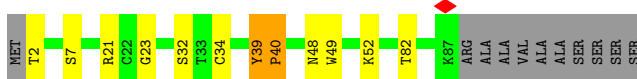
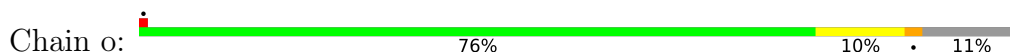
- Molecule 38: 60S ribosomal protein L35



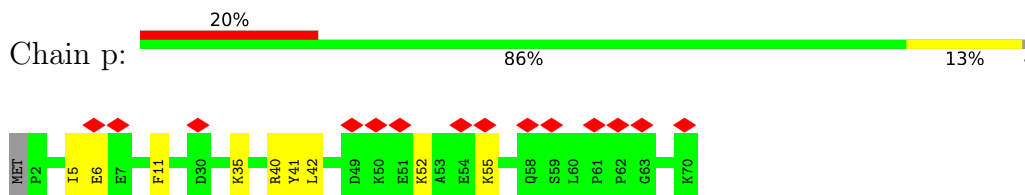
- Molecule 39: 60S ribosomal protein L36



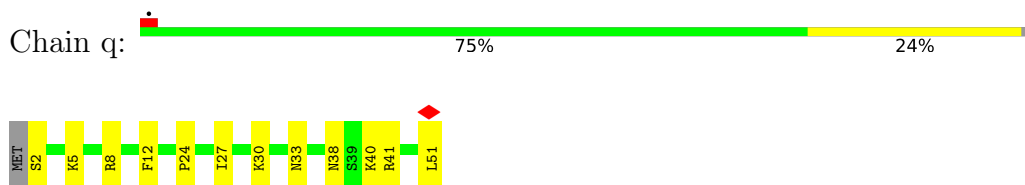
- Molecule 40: 60S ribosomal protein L37



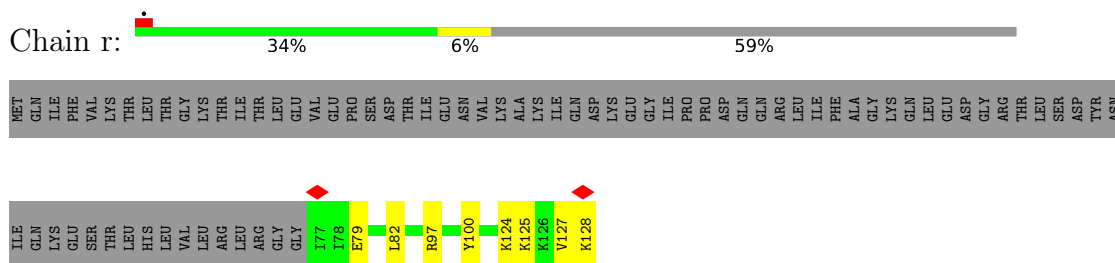
- Molecule 41: 60S ribosomal protein L38



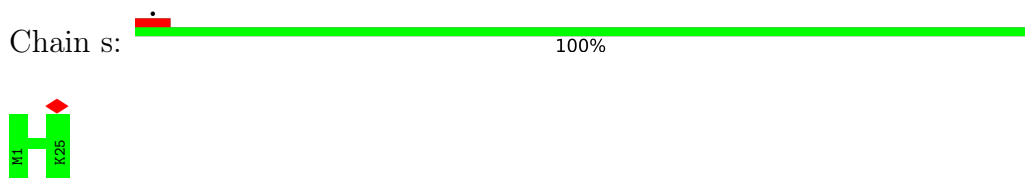
• Molecule 42: 60S ribosomal protein L39



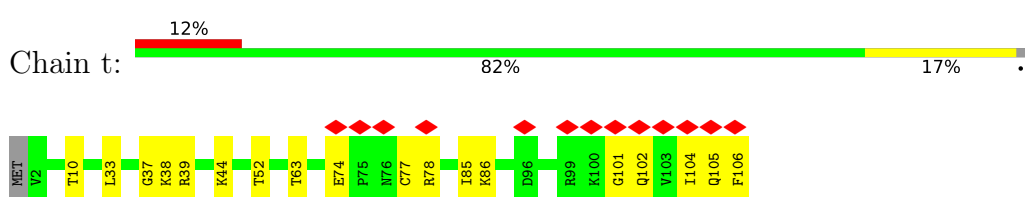
• Molecule 43: Ubiquitin-60S ribosomal protein L40



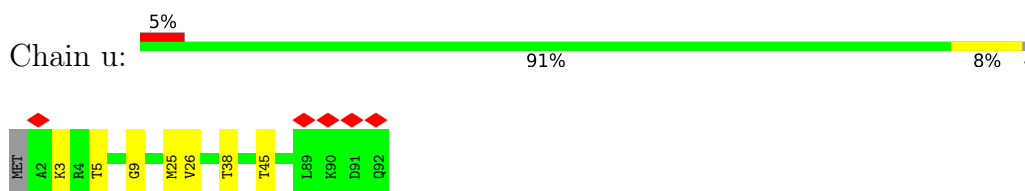
• Molecule 44: 60S ribosomal protein L41



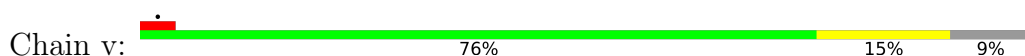
• Molecule 45: 60S ribosomal protein L36a

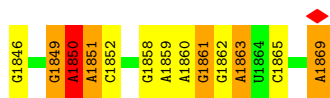


• Molecule 46: 60S ribosomal protein L37a

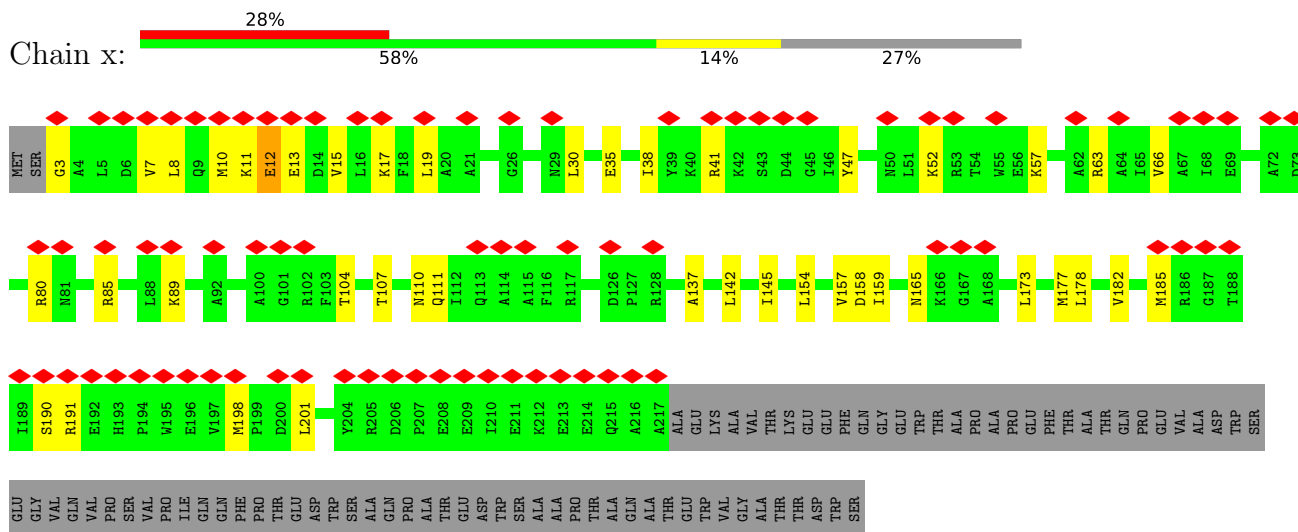


• Molecule 47: 60S ribosomal protein L28

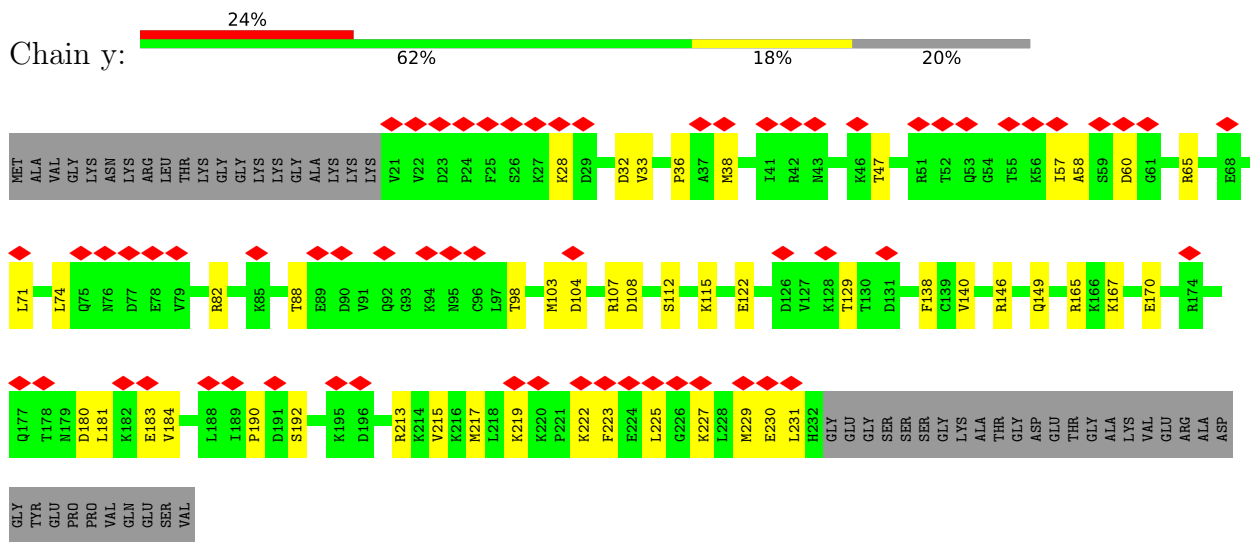




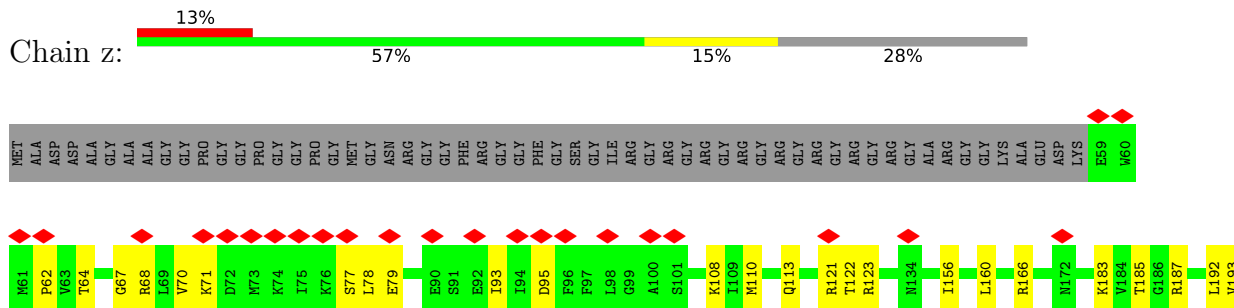
• Molecule 49: 40S ribosomal protein SA

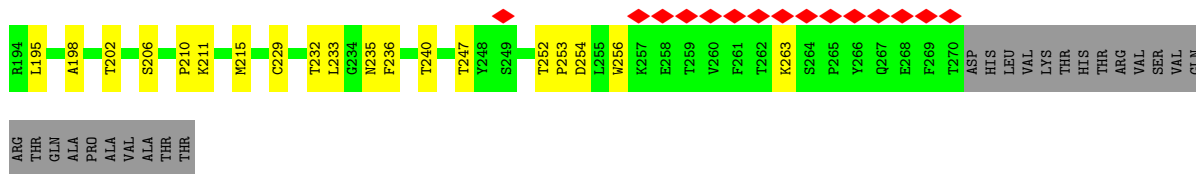


• Molecule 50: 40S ribosomal protein S3a

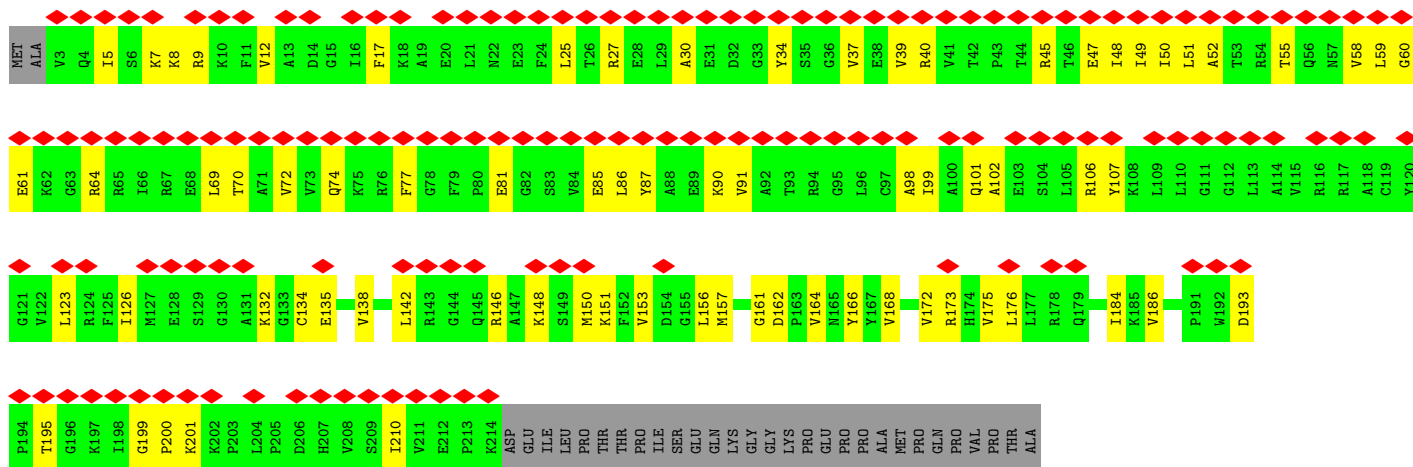


• Molecule 51: 40S ribosomal protein S2

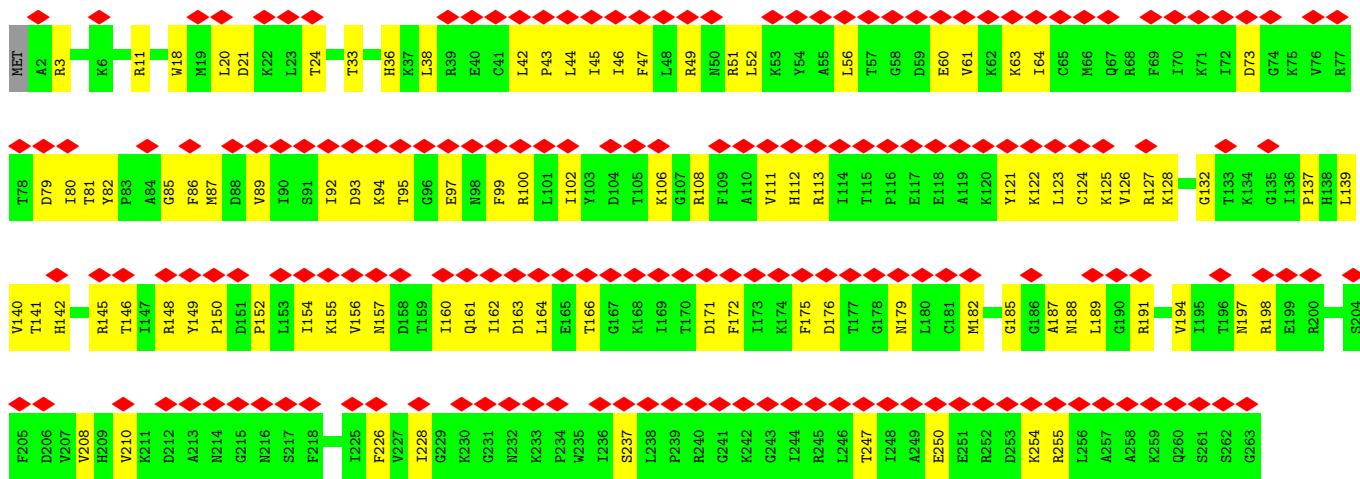




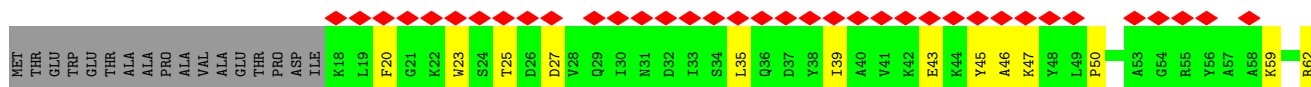
• Molecule 52: 40S ribosomal protein S3

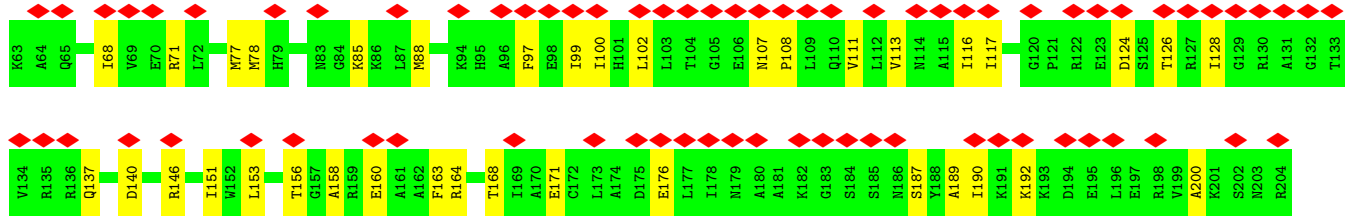


• Molecule 53: 40S ribosomal protein S4, X isoform

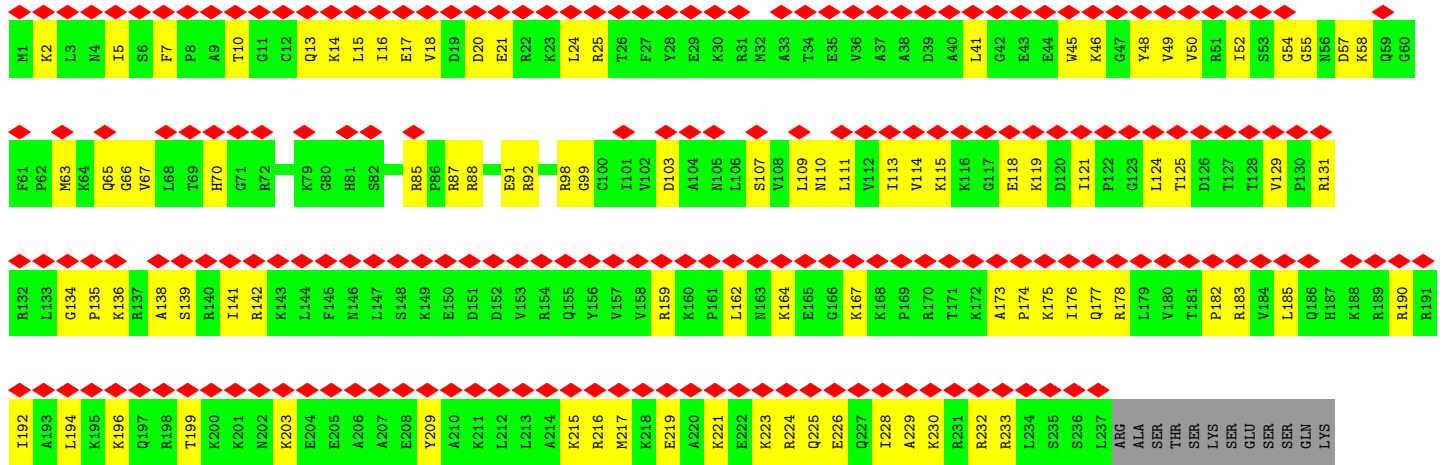
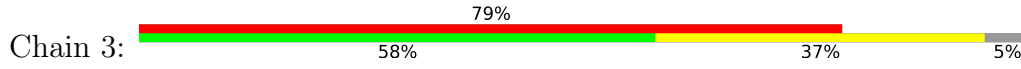


• Molecule 54: 40S ribosomal protein S5

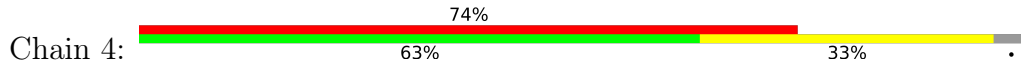




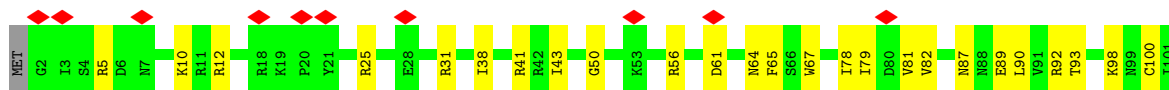
• Molecule 55: 40S ribosomal protein S6

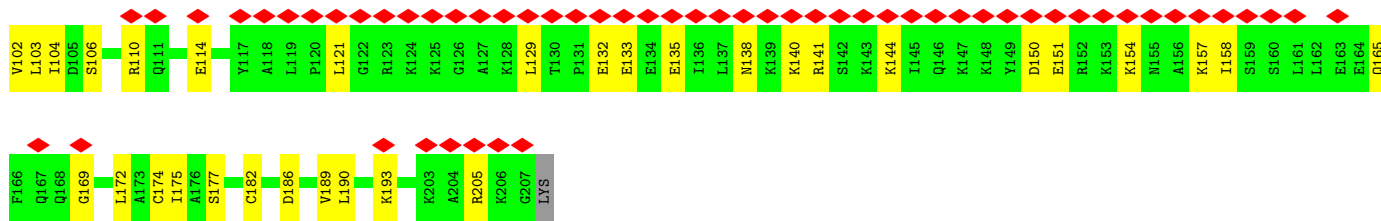


• Molecule 56: 40S ribosomal protein S7

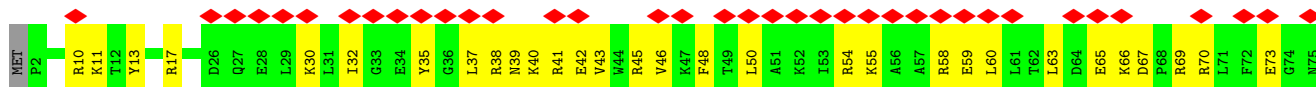
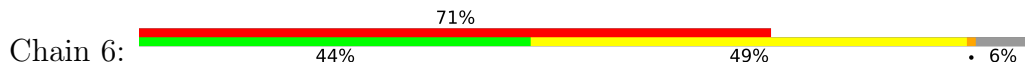


• Molecule 57: 40S ribosomal protein S8

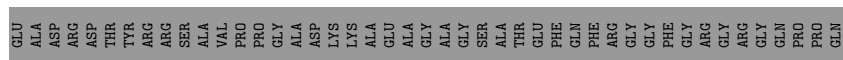
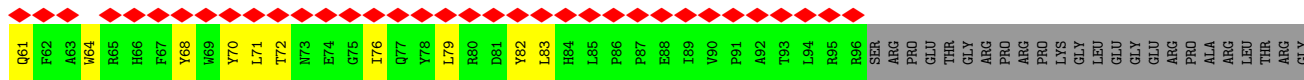
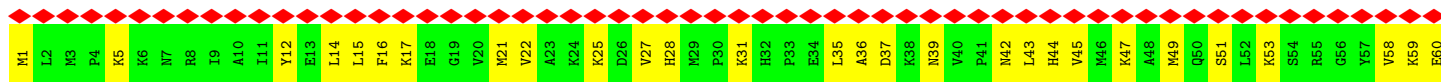
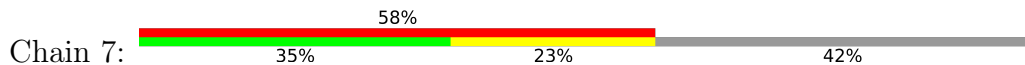




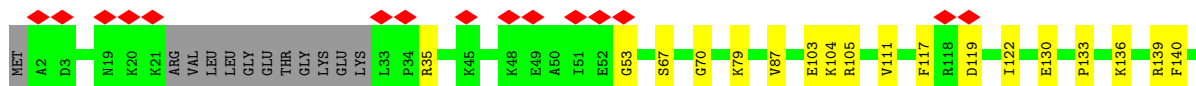
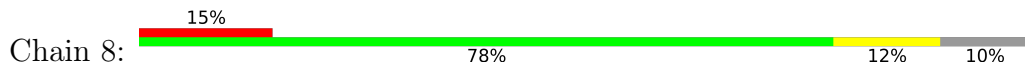
• Molecule 58: 40S ribosomal protein S9



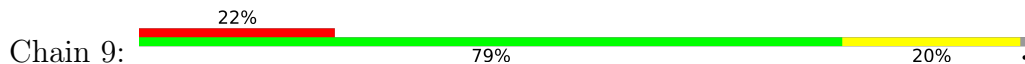
• Molecule 59: 40S ribosomal protein S10

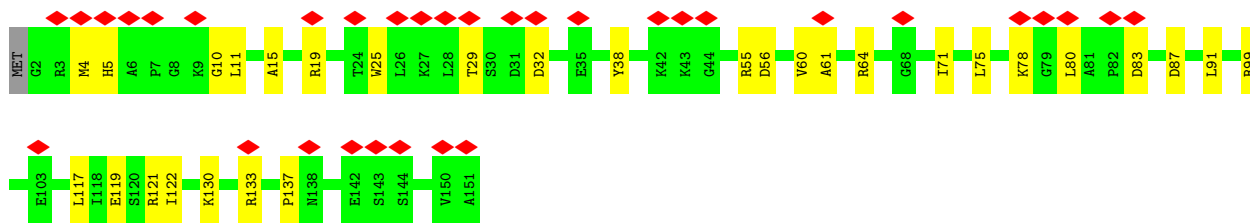


• Molecule 60: 40S ribosomal protein S11



• Molecule 61: 40S ribosomal protein S13

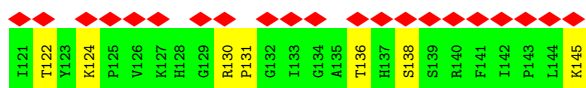
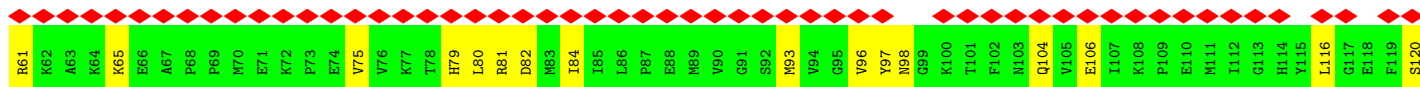
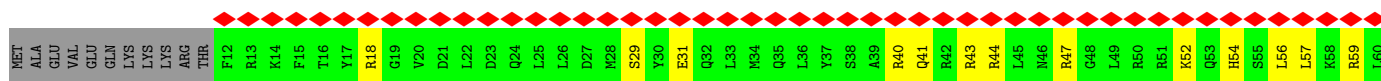




• Molecule 62: 40S ribosomal protein S14



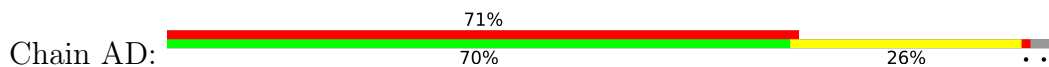
• Molecule 63: 40S ribosomal protein S15

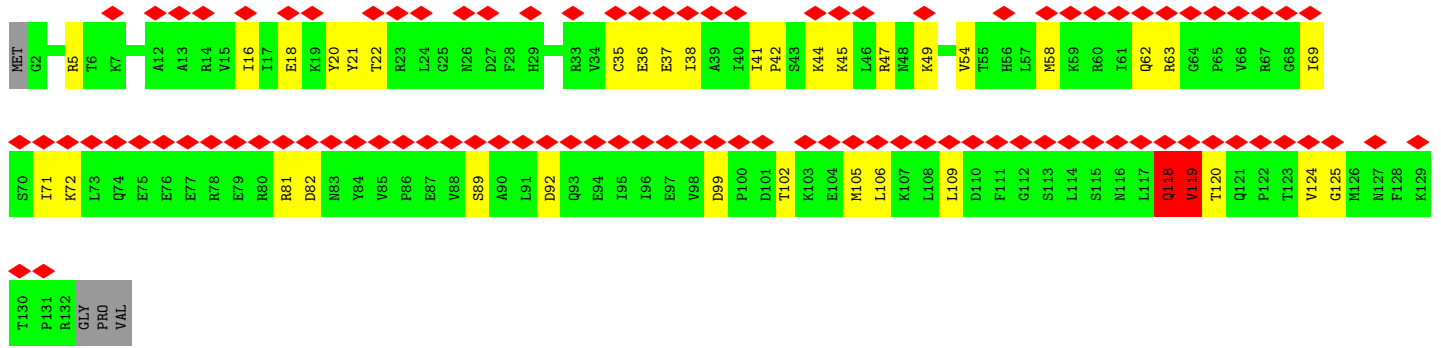


• Molecule 64: 40S ribosomal protein S16

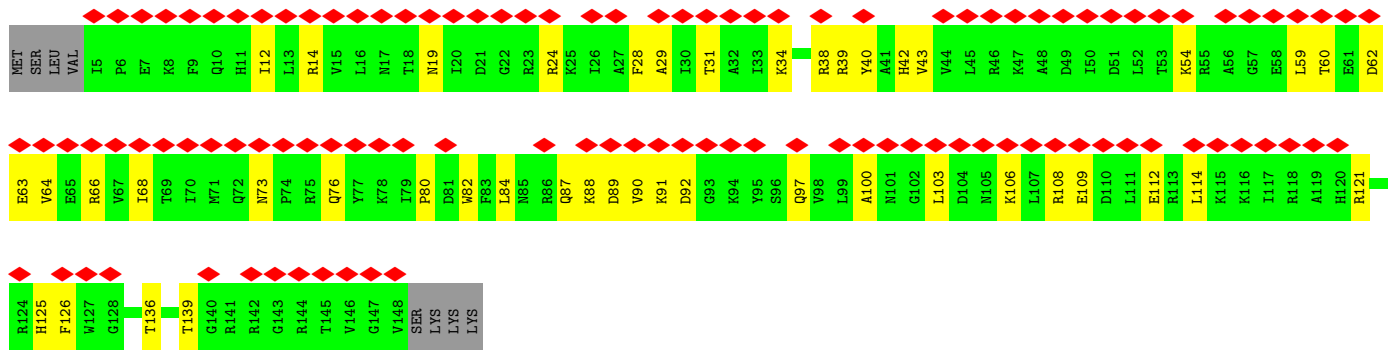
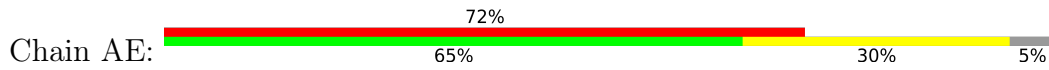


• Molecule 65: 40S ribosomal protein S17

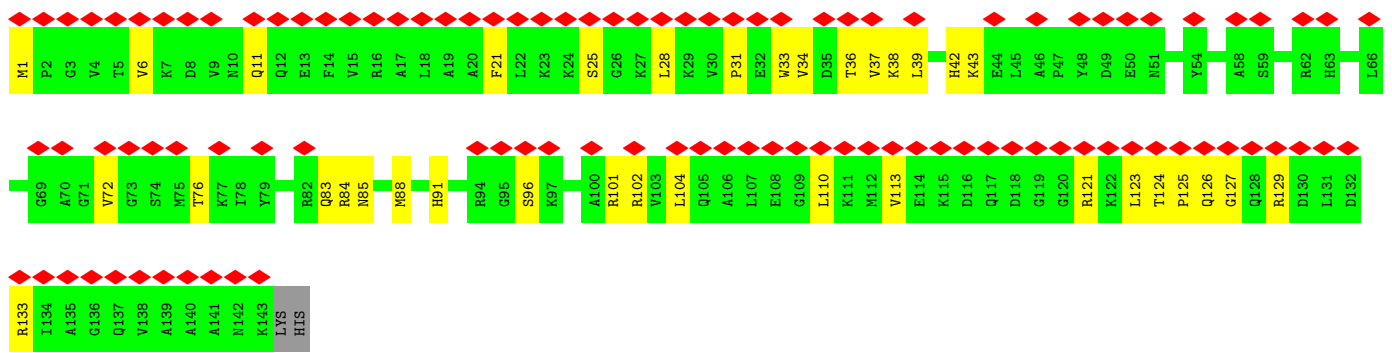
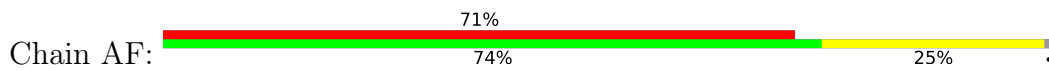




• Molecule 66: 40S ribosomal protein S18



• Molecule 67: 40S ribosomal protein S19

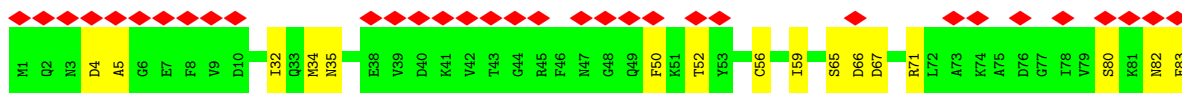
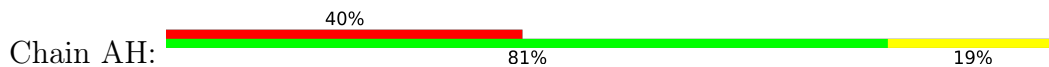


• Molecule 68: 40S ribosomal protein S20

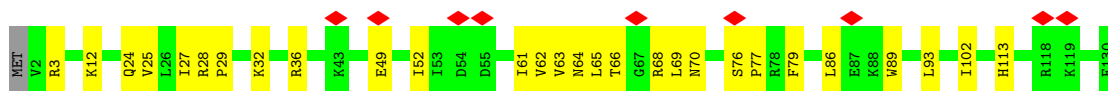
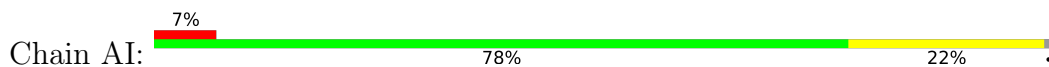




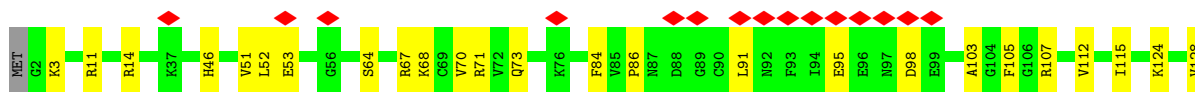
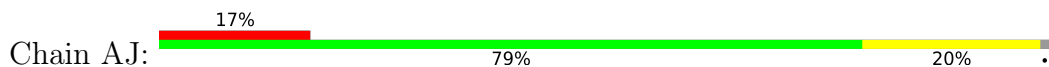
• Molecule 69: 40S ribosomal protein S21



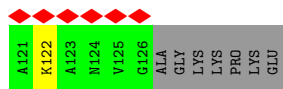
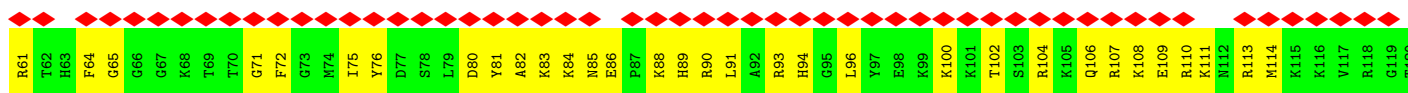
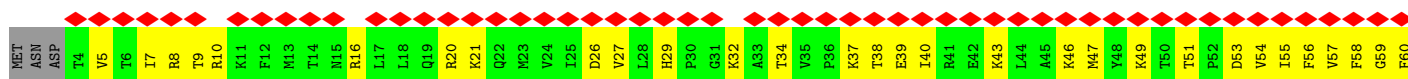
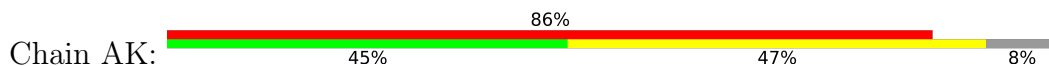
• Molecule 70: 40S ribosomal protein S15a



• Molecule 71: 40S ribosomal protein S23

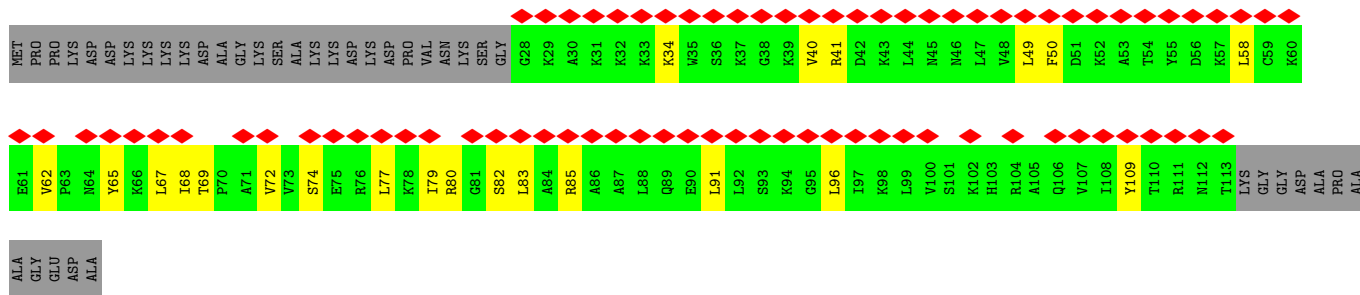


• Molecule 72: 40S ribosomal protein S24

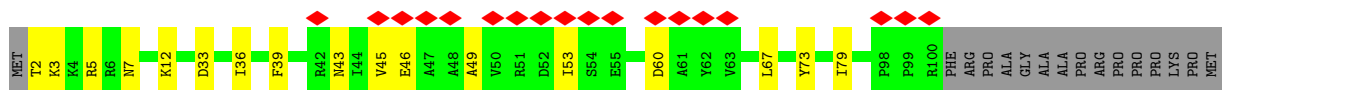
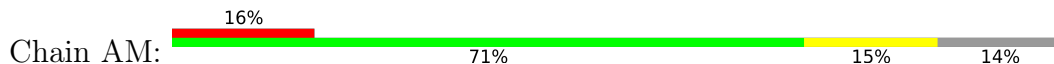


• Molecule 73: 40S ribosomal protein S25

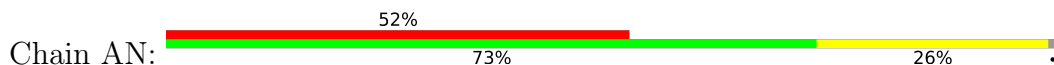




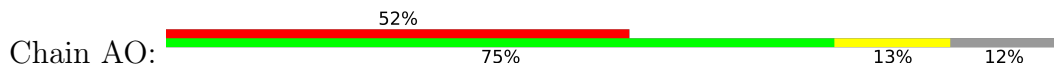
• Molecule 74: 40S ribosomal protein S26



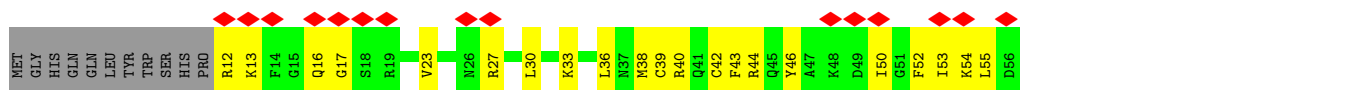
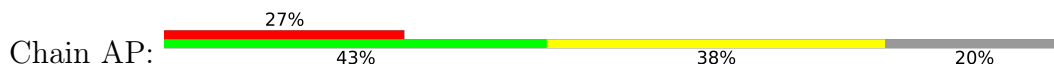
• Molecule 75: 40S ribosomal protein S27



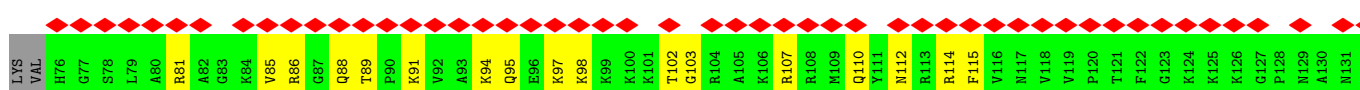
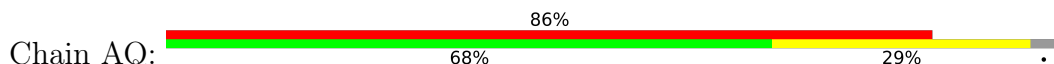
• Molecule 76: 40S ribosomal protein S28



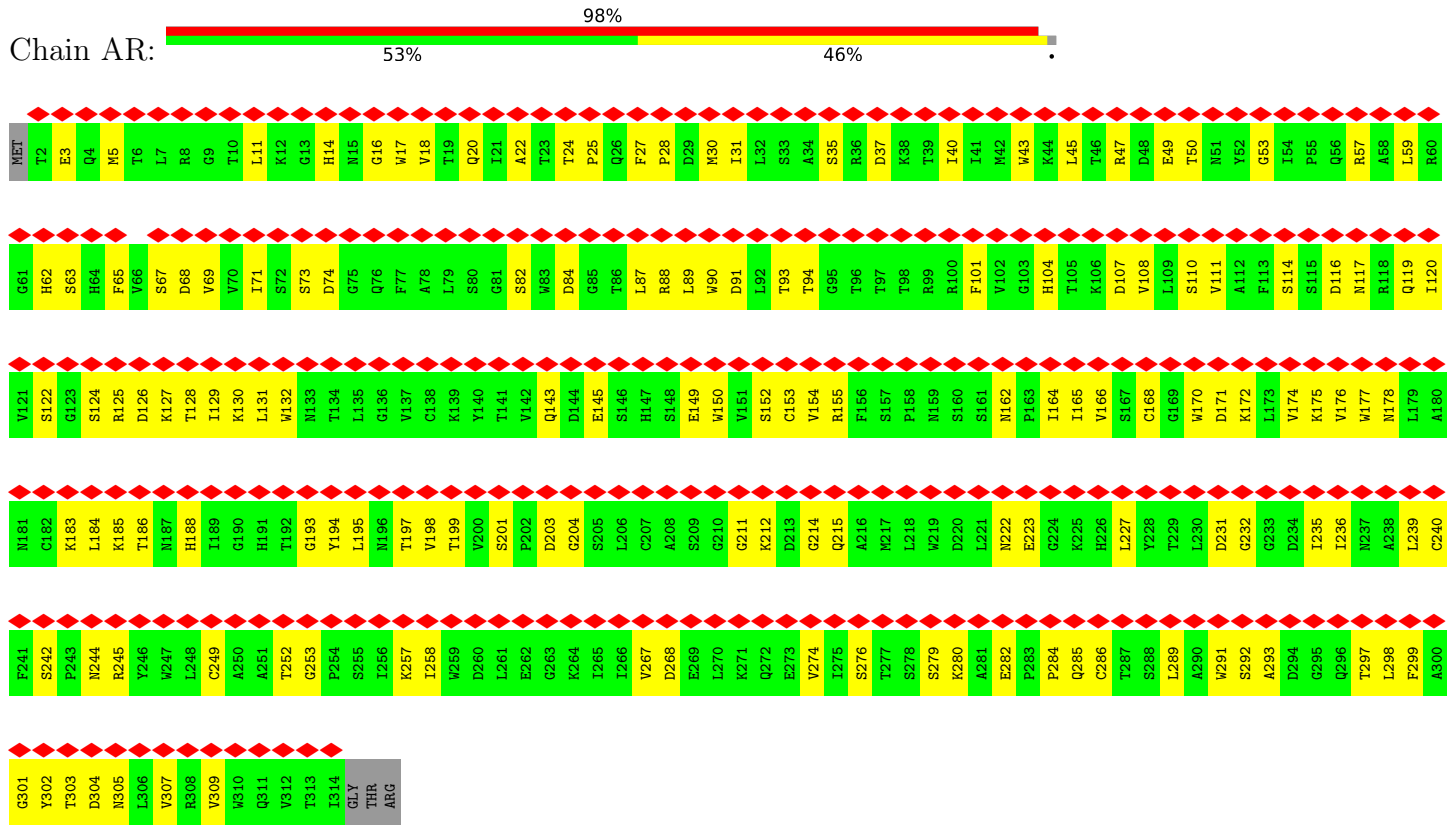
• Molecule 77: 40S ribosomal protein S29



• Molecule 78: 40S ribosomal protein S30



• Molecule 79: Receptor of activated protein C kinase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	148464	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0191	Depositor
Map size (Å)	439.9, 439.9, 439.9	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M2G, 2MG, 4AC, 1MG, ZN, OMG, OMC, 5MU, 6MZ, OMU, MG, UY1, 56B, GAL, B8N, MA6, 3AU, 1MA, H2U, PSU, G7M, A2M, 5MC, UR3

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	A	0.13	0/250	0.20	0/385
2	B	0.17	0/1402	0.27	0/2179
3	D	0.27	2/81567 (0.0%)	0.31	6/127232 (0.0%)
4	E	0.25	0/2858	0.27	0/4455
5	F	0.25	0/3675	0.29	0/5725
6	G	0.27	0/1929	0.48	0/2586
7	H	0.25	0/3279	0.44	0/4388
8	I	0.26	0/2938	0.44	0/3946
9	J	0.21	0/2425	0.42	0/3248
10	K	0.22	0/1785	0.46	0/2394
11	L	0.27	0/1905	0.47	0/2539
12	M	0.21	0/1863	0.45	1/2510 (0.0%)
13	N	0.23	0/1537	0.44	0/2066
14	O	0.22	0/1699	0.43	0/2270
15	P	0.19	0/1385	0.43	0/1852
16	Q	0.23	0/1713	0.43	0/2293
17	R	0.23	0/1142	0.44	0/1527
18	S	0.28	0/1746	0.44	0/2338
19	T	0.27	0/1673	0.44	0/2238
20	U	0.26	0/1300	0.45	0/1746
21	V	0.27	0/1537	0.45	0/2052
22	W	0.23	0/1524	0.42	0/2013
23	X	0.26	0/1493	0.41	0/2003
24	Y	0.24	0/1326	0.41	0/1770
25	Z	0.18	0/835	0.44	0/1122
26	a	0.24	0/993	0.41	0/1332
27	b	0.21	0/541	0.37	0/720
28	c	0.22	0/998	0.41	0/1340
29	d	0.23	0/1132	0.41	0/1504
30	e	0.22	0/1130	0.41	0/1507
31	f	0.26	0/1191	0.39	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.22	0/844	0.50	0/1115
33	h	0.22	0/765	0.37	0/1027
34	i	0.24	0/903	0.44	0/1216
35	j	0.25	0/1071	0.37	0/1429
36	k	0.28	0/895	0.53	0/1198
37	l	0.25	0/898	0.49	0/1197
38	m	0.20	0/1018	0.38	0/1344
39	n	0.18	0/843	0.36	0/1115
40	o	0.26	0/720	0.48	0/952
41	p	0.21	0/575	0.44	0/761
42	q	0.24	0/454	0.37	0/599
43	r	0.22	0/435	0.40	0/575
44	s	0.24	0/240	0.48	0/305
45	t	0.24	0/876	0.48	0/1156
46	u	0.24	0/718	0.39	0/953
47	v	0.26	0/1017	0.45	0/1364
48	w	0.21	0/37158	0.30	0/57908
49	x	0.16	0/1732	0.42	0/2355
50	y	0.15	0/1752	0.37	0/2345
51	z	0.17	0/1668	0.39	0/2254
52	0	0.16	0/1672	0.40	0/2250
53	1	0.17	0/2112	0.42	0/2842
54	2	0.15	0/1485	0.43	0/1998
55	3	0.18	0/1940	0.43	0/2583
56	4	0.15	0/1533	0.45	0/2053
57	5	0.17	0/1703	0.40	0/2275
58	6	0.21	0/1531	0.50	0/2045
59	7	0.15	0/834	0.40	0/1125
60	8	0.17	0/1170	0.38	0/1568
61	9	0.17	0/1232	0.37	0/1656
62	AA	0.20	0/1015	0.49	0/1361
63	AB	0.14	0/1126	0.40	0/1505
64	AC	0.16	0/1146	0.44	0/1534
65	AD	0.17	0/1071	0.52	3/1438 (0.2%)
66	AE	0.17	0/1187	0.49	0/1593
67	AF	0.15	0/1130	0.39	0/1515
68	AG	0.15	0/809	0.44	0/1087
69	AH	0.16	0/643	0.35	0/860
70	AI	0.18	0/1051	0.40	0/1406
71	AJ	0.16	0/1116	0.38	0/1490
72	AK	0.17	0/1019	0.48	0/1355
73	AL	0.15	0/688	0.40	0/921
74	AM	0.20	0/805	0.43	0/1079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	AN	0.17	0/657	0.41	0/883
76	AO	0.17	0/481	0.48	0/643
77	AP	0.18	0/375	0.49	0/492
78	AQ	0.18	0/458	0.54	0/602
79	AR	0.14	0/2493	0.46	0/3394
All	All	0.23	2/217835 (0.0%)	0.36	10/319592 (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
6	G	0	2
7	H	0	1
8	I	0	2
10	K	0	1
11	L	0	1
16	Q	0	1
20	U	0	1
21	V	0	1
22	W	0	1
24	Y	0	1
29	d	0	1
32	g	0	1
40	o	0	1
58	6	0	1
65	AD	0	1
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2415	OMU	O3'-P	5.14	1.61	1.56
3	D	3785	A2M	O3'-P	5.09	1.61	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2101	C	OP1-P-OP2	-13.30	79.71	119.60
3	D	2100	A	OP2-P-O3'	-12.50	70.50	108.00
3	D	2101	C	O5'-P-OP1	-9.67	78.98	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2100	A	OP1-P-O3'	9.52	136.56	108.00
3	D	2101	C	O5'-P-OP2	7.16	129.49	108.00
65	AD	118	GLN	CA-C-N	5.87	132.53	121.97
65	AD	118	GLN	C-N-CA	5.87	132.53	121.97
3	D	2100	A	O3'-P-O5'	-5.30	96.05	104.00
12	M	165	GLU	N-CA-C	-5.26	101.44	108.34
65	AD	119	VAL	CG1-CB-CG2	-5.07	99.64	110.80

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
58	6	101	LYS	Peptide
65	AD	118	GLN	Peptide
6	G	123	ARG	Peptide
6	G	239	ALA	Peptide
7	H	258	HIS	Peptide
8	I	110	ARG	Peptide
8	I	91	ALA	Peptide
10	K	130	LYS	Peptide
11	L	163	ASN	Peptide
16	Q	47	ALA	Peptide
20	U	131	ARG	Peptide
21	V	159	PRO	Peptide
22	W	102	LEU	Peptide
24	Y	80	VAL	Peptide
29	d	108	ARG	Peptide
32	g	110	ALA	Peptide
40	o	39	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	226	0	114	3	0
2	B	1647	0	832	20	0
3	D	75336	0	38155	798	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	2558	0	1296	23	0
5	F	3315	0	1685	41	0
6	G	1891	0	1986	31	0
7	H	3211	0	3356	49	0
8	I	2884	0	3060	43	0
9	J	2379	0	2408	35	0
10	K	1751	0	1905	35	0
11	L	1870	0	1996	22	0
12	M	1832	0	1962	33	0
13	N	1518	0	1601	32	0
14	O	1660	0	1692	22	0
15	P	1362	0	1399	33	0
16	Q	1682	0	1792	34	0
17	R	1120	0	1187	24	0
18	S	1701	0	1749	21	0
19	T	1641	0	1788	22	0
20	U	1273	0	1304	16	0
21	V	1513	0	1628	16	0
22	W	1508	0	1664	14	0
23	X	1453	0	1490	15	0
24	Y	1298	0	1366	11	0
25	Z	821	0	839	13	0
26	a	979	0	1039	10	0
27	b	528	0	541	2	0
28	c	981	0	1062	13	0
29	d	1115	0	1205	19	0
30	e	1107	0	1182	23	0
31	f	1162	0	1213	23	0
32	g	832	0	883	13	0
33	h	755	0	791	9	0
34	i	888	0	930	8	0
35	j	1053	0	1147	7	0
36	k	876	0	912	12	0
37	l	888	0	981	14	0
38	m	1010	0	1143	11	0
39	n	832	0	917	12	0
40	o	705	0	737	8	0
41	p	569	0	637	5	0
42	q	444	0	483	8	0
43	r	429	0	466	7	0
44	s	239	0	289	0	0
45	t	862	0	930	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	u	708	0	756	5	0
47	v	1002	0	1068	16	0
48	w	34933	0	17694	668	0
49	x	1695	0	1690	35	0
50	y	1725	0	1800	32	0
51	z	1633	0	1716	29	0
52	0	1646	0	1734	54	0
53	1	2070	0	2166	78	0
54	2	1464	0	1505	42	0
55	3	1917	0	2078	77	0
56	4	1510	0	1606	52	0
57	5	1674	0	1739	46	0
58	6	1506	0	1618	104	0
59	7	810	0	836	27	0
60	8	1150	0	1199	15	0
61	9	1208	0	1294	25	0
62	AA	1002	0	1023	28	0
63	AB	1103	0	1156	30	0
64	AC	1128	0	1195	36	0
65	AD	1057	0	1110	33	0
66	AE	1169	0	1198	37	0
67	AF	1111	0	1144	27	0
68	AG	799	0	850	41	0
69	AH	636	0	637	11	0
70	AI	1034	0	1080	24	0
71	AJ	1098	0	1167	21	0
72	AK	1002	0	1067	67	0
73	AL	680	0	744	18	0
74	AM	792	0	842	13	0
75	AN	643	0	650	15	0
76	AO	479	0	507	6	0
77	AP	370	0	373	18	0
78	AQ	452	0	494	18	0
79	AR	2436	0	2393	107	0
80	8	1	0	0	0	0
80	A	1	0	0	0	0
80	AA	1	0	0	0	0
80	AF	1	0	0	0	0
80	AJ	1	0	0	0	0
80	AM	1	0	0	0	0
80	D	401	0	0	0	0
80	E	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	F	5	0	0	0	0
80	G	2	0	0	0	0
80	H	1	0	0	0	0
80	I	1	0	0	0	0
80	N	1	0	0	0	0
80	O	1	0	0	0	0
80	S	1	0	0	0	0
80	U	2	0	0	0	0
80	V	2	0	0	0	0
80	X	1	0	0	0	0
80	a	1	0	0	0	0
80	g	1	0	0	0	0
80	j	1	0	0	0	0
80	k	1	0	0	0	0
80	l	1	0	0	0	0
80	w	100	0	0	0	0
81	B	11	0	10	0	0
82	AM	1	0	0	0	0
82	AP	1	0	0	0	0
82	o	1	0	0	0	0
82	r	1	0	0	0	0
82	t	1	0	0	0	0
82	u	1	0	0	0	0
All	All	207902	0	153881	3001	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 (3001) 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)
3:D:4745:G:H1	3:D:4955:A:N6	1.41	1.16
3:D:1:C:N4	5:F:156:U:H3	1.48	1.09
48:w:1471:C:N4	48:w:1476:A:H62	1.63	0.97
48:w:1471:C:H42	48:w:1476:A:H62	1.14	0.96
48:w:39:A:H62	48:w:515:G:H21	1.10	0.95
48:w:1748:G:H1	48:w:1786:U:H3	1.06	0.95
48:w:1471:C:H42	48:w:1476:A:N6	1.65	0.95
3:D:3751:G:H21	3:D:3775:A:H8	1.14	0.92
3:D:4946:U:HO2'	36:k:2:SER:N	1.67	0.92
3:D:1303:A:N6	3:D:2316:G:N7	2.17	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4092:G:H21	3:D:4093:G:H1	1.16	0.91
3:D:1095:A:H2	3:D:1200:G:H1	1.18	0.89
3:D:4095:G:H1	3:D:4113:U:H3	0.93	0.89
3:D:4993:G:H1	3:D:5058:A:H61	1.21	0.88
48:w:153:G:N3	55:3:13:GLN:NE2	2.22	0.87
59:7:21:MET:HG3	59:7:49:MET:HE1	1.58	0.85
3:D:1171:G:N2	3:D:1190:C:O2	2.06	0.85
58:6:150:ARG:O	58:6:154:GLN:HB2	1.76	0.85
3:D:740:G:N1	3:D:924:C:N3	2.25	0.85
70:AI:25:VAL:HG13	70:AI:65:LEU:HD21	1.58	0.84
3:D:1093:C:N3	3:D:1203:G:N1	2.26	0.84
79:AR:244:ASN:HB3	79:AR:245:ARG:HE	1.43	0.84
8:I:110:ARG:O	8:I:113:ARG:NH1	2.11	0.83
48:w:490:C:O2'	48:w:574:A:N1	2.11	0.83
3:D:1656:U:OP2	31:f:26:ARG:NH2	2.12	0.83
48:w:320:G:N2	48:w:331:C:O2	2.11	0.82
3:D:505:G:H1	3:D:653:U:H3	0.85	0.82
13:N:63:ASN:O	13:N:67:LEU:HB2	1.79	0.80
3:D:1100:U:H3	3:D:1194:G:H1	1.28	0.80
53:1:176:ASP:OD1	53:1:179:ASN:ND2	2.14	0.80
6:G:117:GLU:HB2	6:G:162:ASN:HB2	1.64	0.80
3:D:740:G:N2	3:D:924:C:O2	2.14	0.80
48:w:39:A:H62	48:w:515:G:N2	1.80	0.80
32:g:110:ALA:O	32:g:112:ILE:N	2.14	0.79
48:w:69:C:N3	48:w:80:G:N1	2.27	0.79
48:w:320:G:N1	48:w:331:C:N3	2.28	0.79
6:G:30:ARG:O	6:G:163:ARG:NH2	2.15	0.79
27:b:3:VAL:HG11	27:b:12:LYS:HE3	1.63	0.79
3:D:513:U:C4	3:D:646:G:O6	2.37	0.78
48:w:526:A:O2'	58:6:125:HIS:ND1	2.16	0.78
53:1:99:PHE:HE1	53:1:113:ARG:HD3	1.48	0.78
72:AK:43:LYS:HE2	72:AK:47:MET:HE3	1.66	0.78
3:D:989:U:H3	3:D:1064:G:H1	0.81	0.78
3:D:2557:G:H1	3:D:2570:U:H3	1.31	0.78
48:w:1497:G:N7	59:7:25:LYS:NZ	2.32	0.77
3:D:2487:G:H22	3:D:2492:C:H1'	1.48	0.77
48:w:643:A:OP1	58:6:39:ASN:ND2	2.18	0.77
48:w:1488:C:O2'	48:w:1490:OMG:OP2	2.01	0.76
64:AC:43:GLU:HG2	64:AC:44:PRO:HD3	1.67	0.76
50:y:107:ARG:NH2	62:AA:133:THR:O	2.18	0.76
48:w:952:G:H21	62:AA:52:THR:HG21	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:73:ASP:HA	53:1:164:LEU:HD13	1.68	0.76
17:R:96:GLU:HA	17:R:99:GLU:HG2	1.68	0.76
48:w:562:U:H1'	48:w:563:G:C8	2.21	0.76
57:5:165:GLN:HE22	57:5:172:LEU:H	1.32	0.75
3:D:3937:C:H1'	18:S:125:SER:HB2	1.66	0.75
50:y:71:LEU:HA	50:y:74:LEU:HB2	1.66	0.75
3:D:505:G:O6	3:D:653:U:O4	2.03	0.75
3:D:1171:G:N1	3:D:1190:C:N3	2.31	0.75
54:2:35:LEU:HD12	54:2:117:ILE:HD13	1.69	0.75
52:0:101:GLN:HG3	52:0:126:ILE:HD11	1.69	0.75
3:D:4906:C:O2	3:D:4915:G:N2	2.15	0.74
48:w:1858:G:OP2	62:AA:146:ARG:NH2	2.20	0.74
79:AR:62:HIS:HD2	79:AR:88:ARG:HG3	1.51	0.74
3:D:4894:A:H3'	3:D:4895:C:H5'	1.69	0.74
58:6:97:ILE:HA	58:6:100:LEU:HB2	1.69	0.74
31:f:17:HIS:O	31:f:19:HIS:N	2.18	0.74
48:w:69:C:O2	48:w:80:G:N2	2.16	0.74
48:w:534:G:N2	48:w:549:C:O2	2.19	0.74
56:4:100:ILE:HG12	56:4:125:VAL:HG21	1.70	0.74
3:D:2658:G:N2	3:D:2676:A:OP2	2.19	0.74
48:w:168:C:H5'	55:3:131:ARG:HH11	1.52	0.74
58:6:109:ARG:HH22	58:6:127:ARG:HH12	1.34	0.74
48:w:1745:A:H1'	55:3:66:GLY:HA2	1.70	0.74
49:x:38:ILE:HD11	49:x:47:TYR:HB3	1.70	0.74
35:j:21:ILE:HD12	35:j:33:ARG:HD2	1.70	0.74
50:y:88:THR:HG22	50:y:98:THR:HG22	1.69	0.73
71:AJ:138:LYS:NZ	71:AJ:139:GLU:O	2.21	0.73
3:D:481:G:N1	3:D:673:C:N3	2.31	0.73
58:6:32:ILE:HG23	58:6:37:LEU:HB2	1.69	0.73
3:D:4635:A:H2	3:D:4663:G:H21	1.36	0.73
3:D:4884:G:N7	10:K:272:ARG:NH2	2.37	0.73
5:F:82:A:N7	29:d:50:ARG:NH2	2.36	0.73
14:O:79:SER:OG	14:O:147:HIS:ND1	2.21	0.73
3:D:1095:A:N1	3:D:1200:G:O6	2.20	0.73
50:y:222:LYS:HG3	50:y:223:PHE:H	1.53	0.73
46:u:5:THR:HG21	46:u:9:GLY:H	1.54	0.73
65:AD:118:GLN:O	65:AD:119:VAL:HG23	1.89	0.73
48:w:462:OMC:HM22	48:w:463:C:H5'	1.68	0.73
55:3:2:LYS:HG2	55:3:17:GLU:HG3	1.69	0.73
79:AR:82:SER:OG	79:AR:84:ASP:OD1	2.07	0.72
11:L:105:VAL:HG13	11:L:136:VAL:HG12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1388:A:H61	52:0:161:GLY:HA3	1.54	0.72
48:w:1520:G:O2'	48:w:1521:C:OP1	2.06	0.72
48:w:120:U:H2'	48:w:121:OMU:H6	1.70	0.72
48:w:568:C:H2'	48:w:569:A:H8	1.54	0.72
3:D:4875:G:H2'	23:X:169:THR:HG22	1.70	0.72
74:AM:43:ASN:HB2	74:AM:46:GLU:HG3	1.69	0.72
6:G:27:ALA:O	6:G:128:ARG:NH2	2.22	0.72
48:w:334:C:OP2	55:3:190:ARG:NH2	2.22	0.72
48:w:575:A:OP1	72:AK:93:ARG:NE	2.22	0.71
55:3:55:GLY:H	55:3:63:MET:HE2	1.55	0.71
3:D:181:C:N4	3:D:254:G:O6	2.24	0.71
58:6:60:LEU:HA	58:6:63:LEU:HD12	1.71	0.71
48:w:492:C:O2	48:w:494:C:N4	2.23	0.71
3:D:4717:A:OP2	7:H:30:LYS:NZ	2.24	0.71
48:w:289:G:OP1	53:1:155:LYS:NZ	2.24	0.71
62:AA:103:ASN:HD21	62:AA:142:ARG:HA	1.55	0.71
51:z:210:PRO:HD3	51:z:236:PHE:HE2	1.55	0.71
79:AR:279:SER:HB2	79:AR:282:GLU:HB2	1.73	0.71
3:D:450:G:H1	3:D:1297:U:H3	1.38	0.71
48:w:885:U:H3	48:w:901:G:H1	1.39	0.71
3:D:478:G:OP1	47:v:66:ARG:NH2	2.23	0.71
3:D:1179:U:H3'	3:D:1180:C:H5''	1.71	0.71
48:w:894:G:H3'	48:w:895:G:H5''	1.73	0.71
3:D:1093:C:N4	3:D:1203:G:O6	2.22	0.70
58:6:137:VAL:HG22	58:6:157:ILE:HG13	1.74	0.70
3:D:963:G:O6	3:D:2095:A:N6	2.25	0.70
3:D:4093:G:H3'	3:D:4094:G:H8	1.57	0.70
12:M:105:GLU:HB2	12:M:109:GLU:HB2	1.74	0.70
25:Z:28:PRO:HB2	25:Z:34:MET:HG2	1.73	0.70
48:w:1834:A:H2	48:w:1837:G:H1	1.39	0.70
64:AC:58:LEU:HB3	64:AC:62:ARG:HD2	1.73	0.70
72:AK:20:ARG:NH1	72:AK:85:ASN:O	2.24	0.70
3:D:4742:G:H2'	3:D:4743:G:H8	1.55	0.70
3:D:740:G:O6	3:D:924:C:N4	2.23	0.70
48:w:925:G:H1	48:w:1017:U:H3	1.40	0.70
48:w:1222:G:H5''	54:2:78:MET:HE3	1.73	0.70
53:1:95:THR:HG21	72:AK:16:ARG:HE	1.56	0.70
8:I:212:ASN:HD22	8:I:255:SER:HB3	1.57	0.70
48:w:928:G:H1	48:w:1013:U:H3	1.40	0.70
64:AC:118:THR:HG23	64:AC:119:LEU:H	1.56	0.70
8:I:293:LEU:HA	8:I:298:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1271:G:O2'	11:L:34:ARG:NH2	2.26	0.69
48:w:820:U:O2	48:w:828:G:N2	2.24	0.69
48:w:1403:C:H2'	48:w:1433:C:H42	1.57	0.69
3:D:3689:G:O2'	3:D:3818:UY1:OP2	2.11	0.69
25:Z:62:THR:OG1	25:Z:73:THR:OG1	2.11	0.69
48:w:124:U:OP1	53:1:148:ARG:NH2	2.25	0.69
48:w:1597:C:OP2	73:AL:85:ARG:NH2	2.23	0.69
79:AR:128:THR:HB	79:AR:130:LYS:HZ1	1.58	0.69
48:w:522:A:N6	48:w:644:OMG:OP1	2.23	0.69
56:4:12:ASN:ND2	56:4:14:GLU:O	2.26	0.69
48:w:1734:G:H21	48:w:1800:A:H2	1.40	0.69
72:AK:37:LYS:HD2	72:AK:60:PHE:CE2	2.27	0.69
3:D:1274:A:HO2'	3:D:1275:G:H8	1.41	0.69
3:D:2623:A:OP1	25:Z:101:ARG:NH1	2.25	0.69
48:w:434:G:H21	48:w:473:A:H8	1.41	0.69
48:w:522:A:OP1	58:6:146:SER:OG	2.05	0.69
48:w:568:C:H2'	48:w:569:A:C8	2.28	0.69
51:z:113:GLN:HE21	51:z:122:THR:HG22	1.58	0.69
65:AD:18:GLU:OE2	65:AD:69:ILE:N	2.26	0.69
3:D:4741:C:H4'	3:D:4742:G:H5'	1.74	0.69
71:AJ:68:LYS:HB3	71:AJ:91:LEU:HD13	1.73	0.69
48:w:611:G:H2'	48:w:612:U:C6	2.28	0.69
62:AA:92:ALA:HB2	62:AA:125:LYS:HB2	1.75	0.69
3:D:1364:U:OP2	16:Q:36:ARG:NH2	2.26	0.68
48:w:114:G:O2'	48:w:382:C:O2'	2.11	0.68
49:x:80:ARG:NH2	49:x:165:ASN:O	2.26	0.68
79:AR:111:VAL:HG12	79:AR:122:SER:HA	1.74	0.68
3:D:1391:A:OP1	21:V:181:ARG:NH1	2.23	0.68
55:3:5:ILE:HD13	55:3:16:ILE:HD13	1.75	0.68
64:AC:103:ALA:HA	64:AC:106:LYS:HE2	1.75	0.68
48:w:1417:C:O2'	67:AF:1:MET:O	2.09	0.68
3:D:1094:G:O6	3:D:1201:U:O2	2.12	0.68
48:w:192:C:H5''	57:5:141:ARG:HH21	1.58	0.68
48:w:616:A:OP1	78:AQ:81:ARG:NH1	2.27	0.68
58:6:171:GLY:H	58:6:174:LYS:HD3	1.59	0.68
53:1:99:PHE:CE1	53:1:113:ARG:HD3	2.28	0.68
5:F:96:C:OP1	38:m:70:ARG:NH1	2.26	0.68
3:D:5022:U:O2'	3:D:5024:C:OP2	2.11	0.68
48:w:96:C:O2	48:w:473:A:O2'	2.11	0.68
58:6:130:ILE:HG12	58:6:135:ILE:HD11	1.76	0.68
12:M:61:ILE:HA	12:M:64:GLN:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2:20:PHE:HD2	54:2:23:TRP:HD1	1.42	0.68
41:p:40:ARG:NH1	41:p:41:TYR:OH	2.27	0.68
68:AG:95:SER:HA	68:AG:98:VAL:HG22	1.75	0.68
3:D:268:G:H2'	3:D:269:G:H8	1.59	0.68
3:D:661:C:H2'	3:D:662:C:C6	2.29	0.68
3:D:3711:A:H2	3:D:3712:A:H62	1.42	0.68
3:D:4092:G:N3	3:D:4093:G:N2	2.37	0.68
79:AR:67:SER:H	79:AR:82:SER:HA	1.59	0.68
3:D:481:G:O6	3:D:673:C:N4	2.19	0.67
3:D:1414:C:H2'	3:D:1415:G:H8	1.59	0.67
16:Q:64:VAL:HA	16:Q:67:HIS:CD2	2.29	0.67
51:z:210:PRO:HD3	51:z:236:PHE:CE2	2.29	0.67
55:3:57:ASP:OD1	55:3:58:LYS:N	2.27	0.67
3:D:4743:G:H2'	3:D:4744:A:C8	2.30	0.67
48:w:1748:G:O6	48:w:1786:U:O4	2.13	0.67
61:9:55:ARG:NE	61:9:56:ASP:OD1	2.21	0.67
79:AR:166:VAL:HG12	79:AR:176:VAL:HG12	1.75	0.67
3:D:1351:G:OP1	8:I:33:ARG:NH1	2.27	0.67
16:Q:64:VAL:HA	16:Q:67:HIS:HD2	1.58	0.67
26:a:111:GLU:HG3	26:a:131:ARG:HD3	1.76	0.67
52:0:106:ARG:HG3	52:0:175:VAL:HG12	1.75	0.67
3:D:739:G:O2'	3:D:740:G:O5'	2.10	0.67
49:x:173:LEU:HD21	49:x:177:MET:HE3	1.75	0.67
50:y:112:SER:O	50:y:115:LYS:NZ	2.28	0.67
79:AR:87:LEU:HB2	79:AR:101:PHE:HB2	1.76	0.67
48:w:1535:U:O2'	54:2:88:MET:SD	2.52	0.67
52:0:47:GLU:HG2	52:0:85:GLU:HB2	1.77	0.67
3:D:1819:G:O4'	9:J:142:PHE:HB3	1.94	0.67
48:w:1271:C:H42	48:w:1511:U:H3	1.41	0.67
28:c:37:LYS:HG3	28:c:38:LYS:HG2	1.76	0.67
48:w:881:G:N2	48:w:906:U:O2	2.27	0.67
52:0:69:LEU:HA	52:0:72:VAL:HG12	1.77	0.67
72:AK:91:LEU:HD22	72:AK:96:LEU:HD11	1.77	0.67
48:w:642:U:OP1	58:6:41:ARG:N	2.28	0.66
53:1:126:VAL:HA	53:1:141:THR:HA	1.76	0.66
48:w:570:C:O2'	72:AK:34:THR:O	2.12	0.66
78:AQ:94:LYS:NZ	78:AQ:95:GLN:O	2.25	0.66
3:D:1093:C:O2	3:D:1203:G:N2	2.19	0.66
8:I:298:ILE:HG22	21:V:131:PRO:HB3	1.78	0.66
3:D:1082:C:O2'	3:D:1083:U:O5'	2.13	0.66
3:D:3681:G:OP2	6:G:128:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:222:VAL:O	7:H:343:ARG:NH1	2.28	0.66
65:AD:36:GLU:OE2	65:AD:47:ARG:NH1	2.29	0.66
3:D:989:U:O2	3:D:1064:G:N2	2.22	0.66
3:D:4742:G:H2'	3:D:4743:G:C8	2.30	0.66
5:F:14:U:H5''	20:U:123:PRO:HD3	1.77	0.66
48:w:495:U:O3'	53:1:49:ARG:NH1	2.28	0.66
49:x:66:VAL:HG21	49:x:185:MET:HB3	1.78	0.66
63:AB:18:ARG:HD3	66:AE:90:VAL:HA	1.77	0.66
48:w:511:U:H2'	48:w:512:A2M:H8	1.78	0.66
3:D:691:C:H2'	3:D:692:A:C8	2.30	0.66
48:w:534:G:N1	48:w:549:C:N3	2.44	0.66
48:w:1605:G:OP1	67:AF:84:ARG:NH1	2.24	0.66
53:1:92:ILE:HG22	53:1:97:GLU:H	1.60	0.66
60:8:103:GLU:OE2	60:8:105:ARG:NH2	2.29	0.66
3:D:3717:A:H2'	3:D:3718:A2M:H8	1.78	0.66
3:D:4739:C:H2'	3:D:4740:G:H5'	1.77	0.66
61:9:99:ARG:NH2	61:9:119:GLU:OE2	2.28	0.66
50:y:57:ILE:HG13	50:y:58:ALA:H	1.60	0.65
68:AG:80:PHE:HB3	77:AP:52:PHE:HB3	1.79	0.65
48:w:317:C:OP2	55:3:183:ARG:NH2	2.29	0.65
49:x:85:ARG:NH1	65:AD:81:ARG:O	2.29	0.65
3:D:4093:G:H3'	3:D:4094:G:C8	2.31	0.65
3:D:4936:G:N7	10:K:183:ARG:NH2	2.44	0.65
7:H:254:ILE:HG23	7:H:266:VAL:HG11	1.76	0.65
48:w:508:A:H3'	48:w:509:OMG:H8	1.61	0.65
56:4:25:GLN:HA	56:4:28:LEU:HD22	1.77	0.65
72:AK:51:THR:HG22	72:AK:53:ASP:H	1.62	0.65
56:4:73:GLN:NE2	56:4:76:GLN:OE1	2.29	0.65
48:w:573:U:O2'	48:w:576:A2M:N6	2.20	0.65
6:G:36:GLU:HG3	6:G:91:GLY:HA2	1.78	0.65
15:P:15:LEU:HD12	15:P:134:LEU:HD13	1.79	0.65
48:w:831:G:H2'	48:w:832:G:H8	1.62	0.65
48:w:1568:C:OP1	67:AF:96:SER:OG	2.14	0.65
72:AK:76:TYR:OH	72:AK:86:GLU:OE1	2.12	0.65
3:D:1439:C:H2'	3:D:1440:U:H6	1.62	0.65
48:w:572:PSU:H5''	72:AK:60:PHE:H	1.62	0.65
3:D:2591:A:N6	3:D:2754:G:O2'	2.30	0.65
3:D:387:G:O2'	3:D:412:G:O6	2.09	0.65
48:w:1452:A:C2	48:w:1476:A:H1'	2.31	0.65
59:7:14:LEU:HD22	59:7:35:LEU:HD11	1.78	0.65
66:AE:38:ARG:O	66:AE:42:HIS:ND1	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3614:G:O2'	3:D:3615:G:OP1	2.13	0.65
48:w:39:A:N6	48:w:515:G:H21	1.90	0.65
48:w:807:G:H1	48:w:856:C:H5	1.42	0.65
48:w:819:G:H5'	53:1:255:ARG:HH22	1.59	0.65
55:3:21:GLU:HB2	55:3:25:ARG:NH1	2.12	0.65
58:6:86:VAL:HB	58:6:108:ARG:HD3	1.79	0.65
23:X:127:MET:HB3	24:Y:153:PRO:HG2	1.80	0.64
3:D:1097:C:H2'	3:D:1098:G:H8	1.61	0.64
3:D:4940:C:OP2	10:K:219:LYS:NZ	2.26	0.64
48:w:177:G:H22	48:w:313:A:H5'	1.62	0.64
53:1:112:HIS:NE2	53:1:237:SER:OG	2.26	0.64
58:6:103:GLU:HA	58:6:106:LEU:HB2	1.79	0.64
19:T:37:ARG:HD2	19:T:108:ILE:HD11	1.78	0.64
48:w:579:C:O2	72:AK:61:ARG:NH2	2.28	0.64
79:AR:175:LYS:HD3	79:AR:184:LEU:HD11	1.80	0.64
45:t:74:GLU:O	45:t:78:ARG:NH1	2.29	0.64
3:D:1447:C:H2'	3:D:1448:G:H8	1.62	0.64
42:q:30:LYS:HB2	42:q:33:ASN:HB2	1.79	0.64
48:w:494:C:N4	48:w:495:U:O4	2.31	0.64
48:w:639:C:OP1	78:AQ:114:ARG:NE	2.31	0.64
73:AL:40:VAL:HG23	73:AL:41:ARG:H	1.61	0.64
14:O:35:ASP:OD1	14:O:88:ARG:HG2	1.98	0.64
48:w:1536:G:H2'	48:w:1537:A:C8	2.33	0.64
3:D:760:G:H21	3:D:904:C:H42	1.44	0.64
48:w:1693:G:H21	48:w:1834:A:H8	1.46	0.64
64:AC:99:TYR:O	79:AR:57:ARG:NH1	2.30	0.64
71:AJ:68:LYS:HD2	71:AJ:91:LEU:HD22	1.78	0.64
48:w:1286:G:N2	48:w:1312:G:O2'	2.30	0.64
58:6:84:ILE:HA	58:6:150:ARG:HA	1.78	0.64
3:D:4141:G:H5''	3:D:4142:C:H5'	1.80	0.64
3:D:4734:A:H1'	3:D:4735:G:C8	2.32	0.64
13:N:106:GLN:HE21	13:N:111:LEU:HD23	1.63	0.64
48:w:526:A:H2'	48:w:527:C:C6	2.32	0.64
48:w:851:C:H5''	48:w:852:G:H5'	1.80	0.64
48:w:1302:G:O6	48:w:1307:U:O4	2.16	0.64
54:2:100:ILE:HG21	54:2:111:VAL:HG11	1.80	0.64
70:AI:27:ILE:HB	70:AI:61:ILE:HG23	1.80	0.64
3:D:2469:C:H5	3:D:2471:G:H1	1.46	0.64
19:T:47:PHE:HZ	19:T:144:GLU:HG3	1.62	0.64
58:6:65:GLU:O	58:6:66:LYS:HG2	1.98	0.64
3:D:662:C:H2'	3:D:663:G:C4	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:56:THR:HG23	15:P:63:ARG:HA	1.79	0.63
48:w:59:U:H2'	48:w:60:A:H2'	1.80	0.63
48:w:145:G:H2'	48:w:146:G:C8	2.33	0.63
53:1:152:PRO:HD2	55:3:216:ARG:HG3	1.79	0.63
59:7:15:LEU:HD22	59:7:49:MET:HE2	1.80	0.63
3:D:3717:A:H2'	3:D:3718:A2M:C8	2.28	0.63
66:AE:12:ILE:HD11	66:AE:19:ASN:HB3	1.78	0.63
5:F:55:U:H3	5:F:62:A:H2	1.45	0.63
26:a:45:ILE:HG21	26:a:53:PRO:HB3	1.80	0.63
48:w:523:A:H4'	58:6:131:ARG:HE	1.63	0.63
59:7:64:TRP:CD2	77:AP:23:VAL:HG12	2.33	0.63
48:w:186:C:H2'	48:w:187:G:C8	2.34	0.63
53:1:94:LYS:NZ	72:AK:16:ARG:O	2.29	0.63
68:AG:63:ILE:HD11	77:AP:43:PHE:CZ	2.33	0.63
3:D:2475:G:O6	28:c:48:ARG:NH2	2.32	0.63
48:w:1277:C:H2'	48:w:1278:A:H8	1.62	0.63
48:w:1550:G:H3'	48:w:1579:A:H61	1.62	0.63
55:3:70:HIS:HA	55:3:98:ARG:HH12	1.63	0.63
3:D:190:G:H2'	3:D:191:G:H8	1.64	0.63
48:w:583:C:H2'	48:w:584:G:H8	1.64	0.63
48:w:831:G:H2'	48:w:832:G:C8	2.33	0.63
48:w:918:U:OP2	61:9:64:ARG:NH1	2.24	0.63
3:D:730:G:OP2	11:L:76:ARG:NE	2.31	0.63
3:D:4537:C:H2'	3:D:4538:G:C8	2.34	0.63
59:7:27:VAL:HB	59:7:43:LEU:HD12	1.79	0.63
67:AF:113:VAL:HA	67:AF:123:LEU:HA	1.80	0.63
71:AJ:52:LEU:HD11	71:AJ:73:GLN:HB2	1.79	0.63
5:F:75:OMG:OP2	29:d:74:TYR:OH	2.17	0.63
48:w:198:U:O2'	48:w:202:G:O6	2.17	0.63
48:w:817:G:N2	48:w:847:A:N7	2.47	0.63
48:w:1734:G:O2'	48:w:1800:A:N6	2.27	0.63
49:x:11:LYS:HA	49:x:11:LYS:HE3	1.80	0.63
56:4:158:LEU:HD21	56:4:187:PHE:HD2	1.63	0.63
3:D:4988:U:H1'	3:D:4991:U:O2	1.99	0.63
3:D:4993:G:N2	3:D:5058:A:N1	2.39	0.63
5:F:110:U:H5''	42:q:8:ARG:HH22	1.62	0.63
58:6:152:ASP:O	58:6:155:LYS:NZ	2.31	0.63
3:D:3720:G:H22	3:D:3733:A:H2	1.46	0.62
48:w:837:A:H62	72:AK:8:ARG:HB3	1.63	0.62
49:x:89:LYS:NZ	65:AD:82:ASP:OD1	2.32	0.62
48:w:1743:G:H21	48:w:1791:A:H62	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:79:ASP:HB3	53:1:82:TYR:HB2	1.80	0.62
54:2:85:LYS:HB2	54:2:88:MET:HE2	1.81	0.62
73:AL:62:VAL:HA	73:AL:65:TYR:CD2	2.33	0.62
3:D:4882:U:OP1	17:R:117:LYS:NZ	2.31	0.62
23:X:128:LYS:NZ	23:X:130:GLU:OE2	2.33	0.62
48:w:1010:G:H2'	48:w:1011:A:H8	1.65	0.62
48:w:1427:C:O2'	48:w:1429:G:OP2	2.16	0.62
54:2:168:THR:OG1	54:2:171:GLU:OE1	2.16	0.62
58:6:136:ARG:NH1	58:6:159:PHE:O	2.32	0.62
3:D:2899:C:OP1	22:W:108:ARG:NH2	2.32	0.62
2:B:69:A:H2'	2:B:70:A:H8	1.63	0.62
3:D:2579:G:N2	3:D:2582:A:OP2	2.29	0.62
6:G:142:GLU:O	6:G:143:THR:OG1	2.17	0.62
33:h:47:ILE:HD12	33:h:94:LEU:HD11	1.80	0.62
56:4:122:LEU:HA	56:4:125:VAL:HG22	1.80	0.62
3:D:2262:G:OP2	47:v:98:ARG:NH2	2.29	0.62
31:f:148:ALA:HB2	39:n:6:PRO:HB2	1.82	0.62
48:w:1434:C:H5'	48:w:1437:C:H42	1.64	0.62
58:6:35:TYR:HE2	58:6:103:GLU:HB2	1.64	0.62
66:AE:54:LYS:HE2	66:AE:59:LEU:HB3	1.81	0.62
48:w:1217:A:H2'	48:w:1218:C:C6	2.35	0.62
3:D:257:C:H2'	3:D:258:G:C8	2.35	0.62
7:H:394:LYS:HA	7:H:397:ILE:HG12	1.80	0.62
9:J:59:ASP:OD2	9:J:81:HIS:ND1	2.28	0.62
33:h:21:VAL:HG11	33:h:96:ILE:HD12	1.81	0.62
48:w:1533:A:OP2	54:2:164:ARG:NH2	2.32	0.62
65:AD:16:ILE:HD11	65:AD:54:VAL:HG21	1.80	0.62
3:D:184:U:O2	3:D:254:G:N2	2.32	0.62
3:D:4594:U:H2'	3:D:4595:G:H8	1.64	0.62
16:Q:47:ALA:O	16:Q:49:ARG:N	2.32	0.62
48:w:844:U:H2'	48:w:845:G:C8	2.34	0.62
54:2:153:LEU:HD21	54:2:192:LYS:HB2	1.81	0.62
58:6:113:GLN:HA	58:6:116:LYS:HG2	1.80	0.62
3:D:1268:G:N7	32:g:111:ARG:NH1	2.48	0.61
48:w:981:A:H2'	48:w:982:G:C8	2.35	0.61
55:3:230:LYS:HA	55:3:233:ARG:HG2	1.80	0.61
3:D:1295:C:H4'	3:D:1296:G:C8	2.35	0.61
3:D:2263:A:OP1	47:v:107:ARG:NH2	2.33	0.61
48:w:550:C:H2'	48:w:551:U:C6	2.35	0.61
48:w:1464:C:OP1	65:AD:63:ARG:NH2	2.30	0.61
58:6:134:HIS:HE1	58:6:164:PRO:HG2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:7:1:MET:HE3	59:7:44:HIS:HD2	1.66	0.61
60:8:151:THR:HA	61:9:133:ARG:HH12	1.66	0.61
66:AE:108:ARG:O	66:AE:112:GLU:HG2	2.00	0.61
79:AR:201:SER:OG	79:AR:203:ASP:OD1	2.16	0.61
3:D:1518:A:OP1	31:f:27:LYS:NZ	2.25	0.61
10:K:110:ARG:HG3	10:K:110:ARG:O	1.99	0.61
48:w:1459:G:OP2	79:AR:280:LYS:NZ	2.30	0.61
52:0:40:ARG:HH22	68:AG:109:GLY:HA2	1.64	0.61
55:3:199:THR:O	55:3:203:LYS:HG2	2.00	0.61
3:D:1339:U:H2'	3:D:1340:OMC:C6	2.35	0.61
3:D:3651:A:OP2	6:G:200:ARG:NH1	2.34	0.61
6:G:101:VAL:HG22	6:G:165:VAL:HG22	1.81	0.61
48:w:581:U:O2'	72:AK:32:LYS:O	2.18	0.61
48:w:1545:A:H2'	48:w:1546:G:C8	2.36	0.61
3:D:4893:A:OP1	19:T:188:LYS:NZ	2.33	0.61
57:5:129:LEU:HG	57:5:132:GLU:HB2	1.82	0.61
79:AR:108:VAL:HA	79:AR:124:SER:HA	1.82	0.61
3:D:3612:C:H1'	3:D:5016:A:C8	2.35	0.61
8:I:7:LEU:HG	8:I:21:ASN:HB3	1.82	0.61
48:w:158:A:H2'	48:w:159:A2M:H8	1.81	0.61
48:w:1228:A:H2'	48:w:1229:G:C8	2.36	0.61
53:1:45:ILE:HD12	53:1:80:ILE:HD12	1.80	0.61
53:1:185:GLY:H	53:1:189:LEU:HD13	1.65	0.61
3:D:1214:C:N4	32:g:90:SER:OG	2.34	0.61
3:D:4623:OMG:OP1	7:H:19:ARG:NH2	2.34	0.61
17:R:95:ILE:O	17:R:96:GLU:HG3	2.01	0.61
48:w:1228:A:H2'	48:w:1229:G:H8	1.65	0.61
48:w:1619:A:O2'	63:AB:82:ASP:OD2	2.18	0.61
57:5:87:ASN:HB3	57:5:90:LEU:HG	1.81	0.61
74:AM:49:ALA:O	74:AM:53:ILE:HG12	1.99	0.61
3:D:253:G:O2'	3:D:254:G:O4'	2.13	0.61
3:D:684:G:OP2	3:D:685:C:N4	2.33	0.61
3:D:4993:G:H1	3:D:5058:A:N6	1.94	0.61
8:I:262:GLU:HB3	8:I:273:LEU:HD13	1.83	0.61
61:9:19:ARG:NH1	75:AN:84:HIS:OXT	2.31	0.61
71:AJ:128:VAL:HG11	71:AJ:138:LYS:HG2	1.81	0.61
48:w:574:A:H3'	48:w:575:A:H8	1.65	0.61
53:1:247:THR:OG1	53:1:250:GLU:OE1	2.19	0.61
8:I:46:LYS:HD2	8:I:113:ARG:HD3	1.83	0.60
48:w:577:U:H2'	48:w:578:C:H6	1.64	0.60
48:w:1532:C:O2	48:w:1635:C:O2'	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4:31:GLU:HA	56:4:36:LEU:HB3	1.83	0.60
3:D:977:C:OP2	10:K:59:ARG:NH1	2.34	0.60
55:3:139:SER:HA	55:3:142:ARG:HE	1.65	0.60
3:D:262:G:H2'	3:D:263:G:C8	2.37	0.60
3:D:664:G:H2'	3:D:666:G:C8	2.35	0.60
3:D:4145:C:H2'	3:D:4146:G:C8	2.36	0.60
14:O:190:LEU:HB3	14:O:197:VAL:HG22	1.83	0.60
48:w:522:A:H5'	58:6:145:PRO:HD2	1.82	0.60
48:w:1647:A:OP1	64:AC:138:ARG:NH1	2.35	0.60
52:0:58:VAL:HG13	52:0:59:LEU:HD12	1.81	0.60
72:AK:90:ARG:HA	72:AK:93:ARG:HD2	1.82	0.60
3:D:1097:C:H2'	3:D:1098:G:C8	2.36	0.60
3:D:2520:C:O2	3:D:2640:G:N2	2.35	0.60
47:v:97:ILE:HG21	47:v:107:ARG:HB3	1.83	0.60
79:AR:199:THR:HG21	79:AR:240:CYS:HA	1.82	0.60
48:w:69:C:N4	48:w:80:G:O6	2.22	0.60
48:w:81:U:H3'	48:w:82:G:H8	1.65	0.60
48:w:124:U:H3	48:w:340:C:H42	1.50	0.60
48:w:612:U:H2'	48:w:613:G:O4'	1.99	0.60
52:0:74:GLN:NE2	52:0:81:GLU:HA	2.17	0.60
58:6:84:ILE:O	58:6:108:ARG:NH2	2.31	0.60
64:AC:107:GLU:O	64:AC:111:ILE:HG12	2.00	0.60
3:D:4092:G:O2'	3:D:4094:G:O6	2.19	0.60
11:L:182:TYR:HB3	11:L:200:ARG:HG3	1.84	0.60
18:S:138:PHE:HA	18:S:143:ARG:HD2	1.82	0.60
30:e:101:PHE:O	30:e:102:ARG:HD3	2.01	0.60
48:w:889:U:OP2	48:w:896:U:N3	2.31	0.60
62:AA:56:VAL:HG23	62:AA:77:ALA:HB1	1.83	0.60
79:AR:110:SER:OG	79:AR:155:ARG:NH2	2.32	0.60
3:D:4474:A:H5''	43:r:125:LYS:HD2	1.83	0.60
34:i:64:ILE:HG23	34:i:68:LEU:HD23	1.83	0.60
3:D:184:U:O2'	3:D:189:G:O4'	2.17	0.60
3:D:2485:U:H2'	3:D:2486:G:H8	1.66	0.60
7:H:199:GLU:OE2	7:H:200:ARG:NH1	2.34	0.60
14:O:29:ALA:O	14:O:32:ARG:NH2	2.35	0.60
48:w:1639:G7M:H2'	48:w:1640:A:C8	2.37	0.60
57:5:157:LYS:NZ	57:5:158:ILE:O	2.34	0.60
65:AD:22:THR:O	79:AR:212:LYS:NZ	2.35	0.60
11:L:222:LYS:HB3	11:L:231:GLY:HA2	1.84	0.60
32:g:12:GLN:HB3	32:g:16:TRP:CZ3	2.36	0.60
55:3:14:LYS:HB2	55:3:124:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:418:A:N6	5:F:16:G:H1'	2.17	0.60
3:D:4694:G:O2'	13:N:71:ARG:NH2	2.35	0.60
16:Q:42:LYS:O	16:Q:46:ILE:HG12	2.02	0.60
49:x:198:MET:HE2	65:AD:89:SER:HB3	1.84	0.60
63:AB:96:VAL:HG11	63:AB:116:LEU:HG	1.82	0.60
79:AR:236:ILE:HG22	79:AR:252:THR:HG22	1.84	0.60
48:w:145:G:H2'	48:w:146:G:H8	1.67	0.59
48:w:453:C:O2'	55:3:92:ARG:O	2.18	0.59
48:w:1161:U:O4	71:AJ:3:LYS:NZ	2.35	0.59
58:6:136:ARG:HD2	58:6:139:LYS:HA	1.85	0.59
2:B:73:A:H5''	2:B:74:C:H5'	1.83	0.59
34:i:24:GLU:OE2	34:i:87:ARG:NH2	2.34	0.59
48:w:1354:G:N2	48:w:1357:A:OP2	2.32	0.59
3:D:703:G:H1'	35:j:5:ARG:HH22	1.67	0.59
3:D:2351:OMC:HM22	3:D:2352:U:H5'	1.84	0.59
3:D:2621:A:OP1	25:Z:80:LYS:NZ	2.34	0.59
53:1:43:PRO:HD2	53:1:46:ILE:HD11	1.83	0.59
53:1:122:LYS:HE3	53:1:162:ILE:HD11	1.83	0.59
3:D:711:A:H2'	3:D:712:C:C6	2.36	0.59
53:1:125:LYS:O	53:1:142:HIS:N	2.35	0.59
57:5:81:VAL:HG22	57:5:102:VAL:HG12	1.84	0.59
66:AE:106:LYS:HA	66:AE:109:GLU:HG2	1.85	0.59
79:AR:62:HIS:CD2	79:AR:88:ARG:HG3	2.34	0.59
8:I:195:LYS:HB2	8:I:200:ARG:HD2	1.83	0.59
10:K:101:ASN:OD1	10:K:105:ARG:NH2	2.36	0.59
3:D:515:C:H4'	3:D:516:C:OP1	2.02	0.59
3:D:1326:A2M:OP2	3:D:4445:U:O2'	2.20	0.59
12:M:187:LYS:HG3	12:M:198:THR:HB	1.83	0.59
36:k:63:LYS:HA	36:k:63:LYS:HE3	1.85	0.59
48:w:1597:C:O2'	48:w:1598:G:O4'	2.21	0.59
60:8:104:LYS:O	71:AJ:11:ARG:NH2	2.33	0.59
73:AL:58:LEU:HG	73:AL:62:VAL:HG21	1.84	0.59
32:g:110:ALA:C	32:g:112:ILE:H	2.09	0.59
53:1:106:LYS:HG3	53:1:108:ARG:H	1.67	0.59
64:AC:43:GLU:HG2	64:AC:44:PRO:CD	2.33	0.59
3:D:2083:C:OP2	21:V:14:ARG:NH1	2.36	0.59
48:w:67:C:H5	55:3:162:LEU:HB3	1.68	0.59
48:w:974:C:O2	62:AA:55:ARG:NH1	2.35	0.59
48:w:1236:G:O2'	63:AB:131:PRO:O	2.21	0.59
64:AC:118:THR:C	64:AC:120:LEU:H	2.11	0.59
75:AN:67:THR:HG22	75:AN:68:GLY:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:651:C:H2'	3:D:652:G:C8	2.37	0.59
3:D:1701:A:N7	3:D:2095:A:O2'	2.34	0.59
3:D:3811:G:O2'	3:D:3814:U:OP2	2.21	0.59
4:E:23:A:N3	4:E:118:C:O2'	2.31	0.59
16:Q:207:VAL:HG23	16:Q:208:GLU:HG3	1.85	0.59
58:6:70:ARG:HH22	58:6:94:LEU:HD21	1.67	0.59
72:AK:5:VAL:HG12	72:AK:29:HIS:HB3	1.85	0.59
79:AR:27:PHE:HB3	79:AR:30:MET:HB3	1.85	0.59
79:AR:107:ASP:OD2	79:AR:125:ARG:NH1	2.36	0.59
3:D:1332:C:H2'	3:D:1333:A:H8	1.68	0.58
13:N:187:VAL:HG12	13:N:188:GLN:H	1.67	0.58
14:O:38:ARG:HD3	14:O:83:ASP:HB2	1.85	0.58
18:S:68:ARG:NH1	18:S:124:ASP:O	2.33	0.58
30:e:66:SER:HB2	30:e:122:TYR:HE2	1.68	0.58
48:w:498:C:N4	48:w:499:G:O6	2.36	0.58
56:4:144:ILE:HG22	56:4:154:ILE:HG12	1.85	0.58
68:AG:22:ILE:HG22	68:AG:114:VAL:HG12	1.84	0.58
48:w:383:G:O2'	60:8:133:PRO:O	2.16	0.58
48:w:1628:C:OP1	67:AF:38:LYS:NZ	2.37	0.58
63:AB:61:ARG:HB3	63:AB:65:LYS:HZ1	1.68	0.58
67:AF:124:THR:HG23	67:AF:127:GLY:H	1.68	0.58
3:D:173:C:H5''	16:Q:129:ARG:HH21	1.68	0.58
3:D:1837:A:OP2	24:Y:130:ARG:NH2	2.31	0.58
3:D:2089:G:O2'	8:I:307:LYS:NZ	2.27	0.58
3:D:2626:U:O4	25:Z:97:ARG:NH1	2.36	0.58
4:E:23:A:HO2'	4:E:24:C:H6	1.51	0.58
8:I:204:ARG:NH2	8:I:205:ARG:O	2.36	0.58
12:M:150:LYS:HE3	12:M:177:MET:HE3	1.86	0.58
48:w:1004:PSU:H2'	48:w:1005:G:H8	1.68	0.58
52:0:25:LEU:HB3	52:0:34:TYR:CE1	2.38	0.58
3:D:4084:G:O6	6:G:72:ARG:NH2	2.33	0.58
21:V:16:LYS:O	21:V:33:ARG:NH2	2.36	0.58
21:V:157:GLY:O	21:V:188:ASN:ND2	2.36	0.58
48:w:379:C:O2	57:5:5:ARG:NE	2.36	0.58
48:w:493:A:N6	48:w:510:G:N3	2.50	0.58
48:w:1434:C:H4'	48:w:1435:C:O5'	2.02	0.58
52:0:135:GLU:HG2	52:0:153:VAL:HG12	1.85	0.58
3:D:690:C:OP2	10:K:111:LYS:NZ	2.37	0.58
3:D:3873:G:H2'	3:D:3874:G:C8	2.39	0.58
3:D:4377:G:O6	31:f:42:ARG:NH2	2.37	0.58
58:6:69:ARG:O	58:6:73:GLU:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1186:U:H2'	3:D:1187:G:N3	2.18	0.58
11:L:30:ILE:O	11:L:34:ARG:HG2	2.04	0.58
28:c:64:SER:HB2	38:m:69:LEU:HD13	1.86	0.58
37:l:5:LEU:HD11	37:l:32:TYR:CE1	2.38	0.58
54:2:187:SER:HB3	54:2:190:ILE:HG12	1.84	0.58
79:AR:174:VAL:HG22	79:AR:188:HIS:HB2	1.86	0.58
3:D:4635:A:H8	3:D:5048:A:H61	1.51	0.58
14:O:54:SER:HB2	14:O:135:ILE:HD11	1.86	0.58
56:4:61:ILE:HD11	56:4:176:VAL:HG22	1.84	0.58
67:AF:28:LEU:HA	67:AF:110:LEU:HD11	1.86	0.58
6:G:28:ARG:HB2	6:G:123:ARG:HB3	1.86	0.58
48:w:928:G:H2'	48:w:929:G:C8	2.38	0.58
7:H:107:ALA:HB2	7:H:201:LEU:HD22	1.85	0.58
25:Z:40:GLU:O	25:Z:44:GLN:HG2	2.04	0.58
48:w:1566:G:N7	67:AF:101:ARG:NH2	2.49	0.58
51:z:121:ARG:HH12	51:z:123:ARG:HH21	1.51	0.58
52:0:37:VAL:HG12	52:0:50:ILE:HA	1.85	0.58
55:3:192:ILE:O	55:3:196:LYS:HG3	2.04	0.58
57:5:41:ARG:HD3	57:5:43:ILE:HD12	1.86	0.58
79:AR:68:ASP:OD1	79:AR:69:VAL:N	2.37	0.58
3:D:173:C:H5''	16:Q:129:ARG:NH2	2.19	0.58
13:N:104:VAL:HG23	13:N:113:GLU:HB2	1.85	0.58
33:h:34:THR:HG23	33:h:95:ALA:HB2	1.85	0.58
48:w:1610:G:OP1	66:AE:125:HIS:NE2	2.29	0.58
72:AK:59:GLY:HA3	72:AK:71:GLY:HA3	1.84	0.58
9:J:33:ARG:O	9:J:37:VAL:HG12	2.03	0.57
16:Q:150:LEU:HD23	16:Q:154:VAL:HG12	1.85	0.57
48:w:1736:G:H2'	48:w:1737:G:C8	2.39	0.57
58:6:40:LYS:HA	58:6:43:VAL:HG12	1.86	0.57
58:6:46:VAL:HG23	58:6:102:ILE:HD11	1.85	0.57
3:D:1399:G:H2'	3:D:1400:G:C8	2.39	0.57
3:D:2578:G:N7	30:e:17:ARG:NH1	2.52	0.57
3:D:4459:U:H2'	3:D:4460:U:C6	2.39	0.57
17:R:70:GLN:HA	17:R:73:VAL:HG22	1.86	0.57
53:1:52:LEU:HD11	53:1:99:PHE:HE2	1.68	0.57
56:4:60:ILE:HD11	56:4:92:VAL:HG12	1.86	0.57
58:6:35:TYR:CE2	58:6:103:GLU:HB2	2.38	0.57
59:7:5:LYS:NZ	59:7:82:TYR:OH	2.35	0.57
3:D:2472:A:H1'	28:c:48:ARG:HB3	1.85	0.57
3:D:2474:G:H2'	3:D:2502:G:N2	2.19	0.57
3:D:4537:C:H2'	3:D:4538:G:H8	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:85:U:H4'	5:F:86:U:H5'	1.86	0.57
8:I:76:ILE:HD12	8:I:77:PRO:HD2	1.84	0.57
11:L:29:LYS:HA	11:L:32:ARG:HH21	1.68	0.57
48:w:35:C:H5'	48:w:579:C:H4'	1.87	0.57
48:w:107:A:H2'	48:w:108:G:C8	2.38	0.57
48:w:344:U:O2'	48:w:345:U:H5'	2.03	0.57
48:w:1849:G:O2'	48:w:1850:MA6:H8	2.05	0.57
70:AI:28:ARG:HB3	70:AI:29:PRO:HD3	1.85	0.57
3:D:739:G:O2'	3:D:740:G:H8	1.86	0.57
3:D:1194:G:H2'	3:D:1195:G:H8	1.69	0.57
69:AH:80:SER:O	69:AH:83:PHE:N	2.35	0.57
3:D:4946:U:O2'	36:k:2:SER:N	2.36	0.57
54:2:20:PHE:HE1	54:2:50:PRO:HD3	1.69	0.57
59:7:31:LYS:NZ	59:7:39:ASN:OD1	2.28	0.57
3:D:1771:U:H2'	3:D:1772:C:C6	2.39	0.57
3:D:4472:G:O2'	43:r:100:TYR:O	2.22	0.57
3:D:4918:C:H2'	3:D:4919:G:C8	2.39	0.57
47:v:26:SER:OG	47:v:28:GLU:OE1	2.12	0.57
48:w:1158:G:H5''	70:AI:76:SER:HB2	1.86	0.57
52:0:61:GLU:H	52:0:64:ARG:HG2	1.69	0.57
52:0:138:VAL:HG13	52:0:150:MET:HE2	1.86	0.57
54:2:140:ASP:HB2	76:AO:46:VAL:HG12	1.86	0.57
55:3:221:LYS:O	55:3:224:ARG:HG3	2.05	0.57
3:D:4076:G:OP1	12:M:73:ARG:NE	2.29	0.57
3:D:4494:OMG:HM21	26:a:22:VAL:HG11	1.87	0.57
48:w:921:G:C6	70:AI:28:ARG:HD2	2.39	0.57
48:w:1616:U:OP2	63:AB:43:ARG:NH2	2.38	0.57
48:w:1693:G:N2	48:w:1834:A:H8	2.02	0.57
53:1:250:GLU:O	53:1:254:LYS:HG2	2.04	0.57
3:D:1194:G:H2'	3:D:1195:G:C8	2.40	0.57
3:D:1676:C:O2'	3:D:3914:U:N3	2.38	0.57
23:X:15:ARG:HB3	23:X:27:LEU:HD23	1.87	0.57
48:w:839:C:H41	72:AK:9:THR:HG23	1.70	0.57
48:w:1155:U:OP1	51:z:185:THR:OG1	2.23	0.57
59:7:59:LYS:HG2	59:7:70:TYR:HB2	1.84	0.57
3:D:1296:G:H2'	3:D:1297:U:H6	1.68	0.57
3:D:4754:G:N7	10:K:279:ASN:HB2	2.19	0.57
36:k:78:HIS:HB3	36:k:83:MET:O	2.05	0.57
48:w:1261:C:O2	77:AP:12:ARG:NH1	2.38	0.57
54:2:108:PRO:HA	54:2:111:VAL:HG12	1.86	0.57
74:AM:12:LYS:HB2	74:AM:33:ASP:OD2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:254:G:O2'	3:D:255:C:O4'	2.20	0.57
3:D:1077:C:H4'	3:D:1215:C:N4	2.19	0.57
3:D:1414:C:H2'	3:D:1415:G:C8	2.39	0.57
3:D:2565:A:H3'	3:D:2566:G:C8	2.40	0.57
3:D:4745:G:N2	3:D:4955:A:N1	2.40	0.57
4:E:117:G:OP1	9:J:253:TYR:OH	2.22	0.57
20:U:22:LEU:HD13	20:U:90:PHE:CD2	2.40	0.57
21:V:66:MET:HE3	21:V:98:LEU:HD13	1.86	0.57
48:w:156:G:H2'	48:w:157:U:C6	2.40	0.57
48:w:380:G:OP1	57:5:31:ARG:NH1	2.34	0.57
48:w:1217:A:H2'	48:w:1218:C:H6	1.70	0.57
52:0:55:THR:HA	52:0:58:VAL:HG12	1.86	0.57
55:3:136:LYS:HA	55:3:176:ILE:HG22	1.86	0.57
56:4:36:LEU:HD21	56:4:40:LEU:HD13	1.87	0.57
75:AN:83:GLN:NE2	75:AN:84:HIS:OXT	2.37	0.57
79:AR:176:VAL:HG23	79:AR:185:LYS:HB3	1.86	0.57
3:D:189:G:H2'	3:D:190:G:H8	1.70	0.56
3:D:217:C:H5''	3:D:218:A:H4'	1.87	0.56
3:D:1442:C:O2'	3:D:1443:A:H5'	2.04	0.56
30:e:50:PRO:HD3	30:e:68:ILE:HG12	1.87	0.56
48:w:179:C:H3'	48:w:180:G:H8	1.70	0.56
48:w:562:U:H1'	48:w:563:G:H8	1.70	0.56
58:6:32:ILE:HD12	58:6:40:LYS:HG2	1.87	0.56
61:9:75:LEU:HD22	61:9:80:LEU:HD11	1.87	0.56
64:AC:80:GLN:O	64:AC:84:ILE:HG12	2.05	0.56
3:D:492:U:N3	3:D:493:G:O6	2.38	0.56
3:D:4110:C:H2'	3:D:4111:U:C6	2.39	0.56
41:p:35:LYS:HB3	41:p:42:LEU:HD21	1.87	0.56
56:4:10:LYS:HE3	56:4:20:GLU:HG3	1.86	0.56
3:D:276:C:H2'	39:n:29:ARG:NH2	2.21	0.56
3:D:498:C:H42	3:D:656:C:N4	2.04	0.56
10:K:46:ARG:HG3	10:K:62:MET:HE1	1.88	0.56
12:M:131:LYS:NZ	12:M:132:ARG:O	2.38	0.56
16:Q:178:ALA:N	31:f:134:GLU:OE1	2.34	0.56
48:w:317:C:H2'	48:w:318:A:H5''	1.87	0.56
48:w:525:A:H2'	48:w:526:A:H8	1.71	0.56
48:w:1500:G:H5'	52:0:176:LEU:HD11	1.88	0.56
48:w:1514:G:O2'	63:AB:79:HIS:ND1	2.35	0.56
79:AR:249:CYS:HA	79:AR:258:ILE:HA	1.88	0.56
48:w:26:U:H2'	48:w:27:A2M:H8	1.86	0.56
48:w:168:C:H5'	55:3:131:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:9:5:HIS:HB3	61:9:117:LEU:HD21	1.88	0.56
61:9:130:LYS:NZ	61:9:137:PRO:O	2.39	0.56
3:D:1820:C:O2'	3:D:1821:G:N7	2.36	0.56
9:J:3:PHE:CD2	9:J:4:VAL:HG22	2.39	0.56
9:J:204:VAL:O	9:J:208:MET:HG3	2.06	0.56
15:P:35:ARG:HD2	15:P:123:ILE:HA	1.86	0.56
22:W:105:LEU:HD23	22:W:138:LEU:HD23	1.87	0.56
48:w:1670:C:H2'	48:w:1671:G:C8	2.40	0.56
63:AB:81:ARG:NH1	63:AB:120:SER:OG	2.37	0.56
79:AR:120:ILE:HB	79:AR:132:TRP:HB2	1.87	0.56
7:H:80:GLU:OE1	7:H:323:TYR:OH	2.23	0.56
48:w:81:U:H3'	48:w:82:G:C8	2.40	0.56
48:w:125:C:OP1	48:w:127:C:N4	2.39	0.56
52:0:162:ASP:O	52:0:164:VAL:N	2.35	0.56
58:6:114:VAL:HG21	58:6:135:ILE:HD13	1.88	0.56
3:D:2487:G:N1	3:D:2492:C:O2	2.26	0.56
12:M:158:ALA:HB2	12:M:190:LEU:HD12	1.87	0.56
14:O:31:ILE:HD12	14:O:65:LEU:HB3	1.86	0.56
48:w:574:A:H4'	72:AK:89:HIS:CG	2.41	0.56
48:w:830:A:OP2	48:w:846:G:N2	2.24	0.56
49:x:13:GLU:OE1	49:x:17:LYS:NZ	2.39	0.56
56:4:69:LEU:O	56:4:73:GLN:HG2	2.05	0.56
58:6:111:GLN:HG2	58:6:123:ILE:HD11	1.88	0.56
30:e:123:LYS:O	30:e:124:THR:OG1	2.21	0.56
53:1:161:GLN:HB3	53:1:171:ASP:HB3	1.87	0.56
77:AP:17:GLY:O	77:AP:27:ARG:NH2	2.38	0.56
3:D:5016:A:H2	3:D:5033:G:H21	1.54	0.56
7:H:231:VAL:HG11	7:H:251:VAL:HG23	1.86	0.56
48:w:130:G:H2'	48:w:130:G:N3	2.21	0.56
48:w:1396:A:O2'	48:w:1398:G:N7	2.38	0.56
58:6:32:ILE:HG12	58:6:37:LEU:HD12	1.88	0.56
58:6:111:GLN:HA	58:6:130:ILE:HD11	1.86	0.56
78:AQ:107:ARG:HD3	78:AQ:110:GLN:HE21	1.71	0.56
79:AR:282:GLU:O	79:AR:284:PRO:HD3	2.06	0.56
3:D:1177:U:HO2'	9:J:286:SER:HG	1.54	0.56
3:D:1604:G:H2'	3:D:1605:G:C8	2.41	0.56
48:w:36:PSU:HN3	48:w:519:A:H61	1.52	0.56
48:w:1568:C:H2'	48:w:1569:A:C8	2.41	0.55
57:5:67:TRP:HA	57:5:189:VAL:HG12	1.86	0.55
66:AE:84:LEU:HD22	66:AE:97:GLN:HB2	1.86	0.55
75:AN:36:LYS:HE2	75:AN:41:TYR:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2464:C:O2'	3:D:2465:C:H6	1.89	0.55
3:D:3906:A:H2'	8:I:69:THR:HG23	1.89	0.55
48:w:845:G:H3'	48:w:846:G:H8	1.71	0.55
68:AG:17:ILE:HG23	68:AG:92:HIS:HB2	1.87	0.55
78:AQ:85:VAL:HA	78:AQ:88:GLN:HG2	1.87	0.55
3:D:4274:A:H2'	3:D:4275:G:C8	2.42	0.55
10:K:162:VAL:HG22	10:K:175:VAL:HG22	1.89	0.55
48:w:169:U:H4'	55:3:135:PRO:HA	1.89	0.55
48:w:820:U:OP2	58:6:83:ARG:NH1	2.40	0.55
68:AG:20:ILE:HD13	68:AG:98:VAL:HG21	1.88	0.55
3:D:2400:G:H21	37:l:6:THR:HG22	1.72	0.55
48:w:913:A:N6	56:4:98:ARG:O	2.36	0.55
48:w:1115:U:H3	48:w:1117:C:H41	1.53	0.55
52:0:193:ASP:HB3	52:0:199:GLY:HA3	1.88	0.55
63:AB:93:MET:SD	63:AB:104:GLN:NE2	2.80	0.55
68:AG:22:ILE:HA	68:AG:113:GLU:O	2.06	0.55
8:I:38:ASN:O	8:I:42:THR:HG23	2.06	0.55
67:AF:6:VAL:O	67:AF:11:GLN:NE2	2.39	0.55
79:AR:28:PRO:O	79:AR:47:ARG:NH2	2.40	0.55
3:D:1172:C:O2'	3:D:1189:G:N2	2.34	0.55
3:D:1173:G:N2	3:D:1188:C:N3	2.54	0.55
3:D:2101:C:O2'	3:D:2102:G:OP1	2.25	0.55
14:O:19:LYS:HA	14:O:23:CYS:SG	2.46	0.55
48:w:1263:U:O2	77:AP:16:GLN:NE2	2.39	0.55
48:w:1277:C:H2'	48:w:1278:A:C8	2.41	0.55
48:w:1630:A:OP1	66:AE:40:TYR:HB2	2.06	0.55
69:AH:67:ASP:OD2	69:AH:71:ARG:NH1	2.40	0.55
79:AR:286:CYS:HA	79:AR:302:TYR:HD1	1.71	0.55
3:D:3598:C:H2'	3:D:3599:A:H8	1.71	0.55
48:w:1405:A:H2'	48:w:1406:G:O4'	2.07	0.55
58:6:85:GLY:HA3	58:6:151:LEU:HB2	1.89	0.55
3:D:1372:A:OP1	18:S:202:ARG:NH2	2.38	0.55
48:w:1528:G:O2'	48:w:1666:C:OP1	2.24	0.55
53:1:160:ILE:HD13	53:1:172:PHE:HB2	1.88	0.55
64:AC:55:VAL:HG23	64:AC:56:LEU:HD12	1.88	0.55
72:AK:111:LYS:O	72:AK:114:MET:HG3	2.07	0.55
15:P:99:PHE:O	15:P:159:LYS:NZ	2.40	0.55
25:Z:24:ASP:OD1	25:Z:111:GLU:HA	2.07	0.55
28:c:38:LYS:O	28:c:40:ILE:HG12	2.07	0.55
48:w:565:G:H2'	48:w:566:U:C6	2.41	0.55
49:x:17:LYS:HB3	49:x:173:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:112:HIS:NE2	53:1:237:SER:O	2.40	0.55
55:3:49:VAL:HG13	55:3:114:VAL:HB	1.89	0.55
3:D:1100:U:O3'	3:D:1167:C:N4	2.40	0.54
3:D:3641:U:H5	3:D:3646:A:N7	2.05	0.54
3:D:3718:A2M:H2	3:D:3934:G:O4'	2.07	0.54
3:D:3910:C:H2'	3:D:3911:C:C6	2.41	0.54
13:N:106:GLN:NE2	13:N:113:GLU:OE2	2.39	0.54
20:U:22:LEU:HD13	20:U:90:PHE:HD2	1.72	0.54
50:y:71:LEU:HD22	50:y:82:ARG:HB3	1.89	0.54
53:1:125:LYS:HB2	53:1:226:PHE:CD1	2.42	0.54
62:AA:61:LYS:HB3	62:AA:76:LEU:HD11	1.87	0.54
3:D:62:A:N3	3:D:77:U:O2'	2.36	0.54
3:D:2414:G:H2'	3:D:2415:OMU:H6	1.89	0.54
12:M:50:ASP:HB2	28:c:40:ILE:HD12	1.88	0.54
38:m:107:GLN:O	38:m:111:GLU:HG3	2.07	0.54
48:w:156:G:OP1	55:3:2:LYS:NZ	2.40	0.54
48:w:575:A:OP1	72:AK:89:HIS:ND1	2.34	0.54
48:w:799:OMU:H2'	48:w:800:U:O4'	2.08	0.54
48:w:841:G:O6	72:AK:10:ARG:HG3	2.07	0.54
58:6:174:LYS:HE2	58:6:175:ARG:HH12	1.72	0.54
78:AQ:85:VAL:O	78:AQ:89:THR:HG23	2.07	0.54
48:w:126:G:N2	48:w:181:A:O4'	2.40	0.54
48:w:1562:C:H2'	48:w:1563:G:H8	1.72	0.54
51:z:108:LYS:HE3	51:z:110:MET:HB3	1.89	0.54
52:0:30:ALA:O	52:0:107:TYR:OH	2.23	0.54
58:6:107:GLU:O	58:6:113:GLN:NE2	2.36	0.54
64:AC:31:LEU:HD21	64:AC:33:LYS:HE2	1.89	0.54
3:D:1179:U:O2'	3:D:1180:C:OP1	2.21	0.54
3:D:2403:A:OP1	37:l:10:ARG:HD2	2.07	0.54
9:J:211:LEU:HB3	9:J:219:TYR:HB2	1.89	0.54
18:S:184:ILE:HG23	18:S:194:ARG:HH12	1.72	0.54
48:w:530:U:H2'	48:w:531:A:C8	2.43	0.54
48:w:656:G:H5'	48:w:662:G:N2	2.21	0.54
48:w:1417:C:N4	48:w:1422:G:OP2	2.40	0.54
48:w:1588:A:H2'	48:w:1589:A:C8	2.42	0.54
55:3:199:THR:O	55:3:203:LYS:NZ	2.40	0.54
72:AK:102:THR:O	72:AK:107:ARG:NH1	2.40	0.54
79:AR:203:ASP:OD1	79:AR:204:GLY:N	2.41	0.54
3:D:1697:G:H22	3:D:2084:C:P	2.31	0.54
35:j:89:LEU:HD13	35:j:118:LEU:HD22	1.88	0.54
48:w:429:C:O2'	48:w:811:A:N1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AE:34:LYS:HB3	66:AE:103:LEU:HD23	1.90	0.54
72:AK:106:GLN:NE2	72:AK:109:GLU:OE2	2.38	0.54
79:AR:129:ILE:HD13	79:AR:154:VAL:HG11	1.89	0.54
3:D:1857:C:H2'	3:D:1858:A:H8	1.72	0.54
3:D:3710:G:N2	3:D:3740:G:N7	2.56	0.54
3:D:4919:G:H2'	3:D:4920:C:C6	2.43	0.54
48:w:1606:G:O2'	48:w:1607:A:O5'	2.25	0.54
49:x:85:ARG:HD2	65:AD:81:ARG:HD2	1.89	0.54
72:AK:104:ARG:HA	72:AK:107:ARG:HG2	1.90	0.54
3:D:1942:A:H2'	3:D:1943:A:C8	2.43	0.54
3:D:4942:C:H5''	10:K:155:GLY:HA2	1.89	0.54
17:R:31:ILE:HD11	17:R:37:LEU:HB2	1.88	0.54
48:w:678:U:OP2	48:w:1026:C:N4	2.39	0.54
48:w:1283:C:O2'	48:w:1313:A:N1	2.30	0.54
55:3:135:PRO:HG2	55:3:141:ILE:HD12	1.90	0.54
3:D:1670:G:OP1	32:g:15:LYS:NZ	2.41	0.54
22:W:176:ARG:NH2	48:w:909:G:O5'	2.37	0.54
48:w:560:A:HO2'	58:6:165:TYR:HH	1.56	0.54
55:3:98:ARG:NH2	55:3:103:ASP:OD1	2.41	0.54
55:3:136:LYS:HG2	55:3:176:ILE:HA	1.88	0.54
64:AC:9:SER:HB2	64:AC:24:HIS:NE2	2.23	0.54
77:AP:46:TYR:O	77:AP:50:ILE:HG12	2.07	0.54
3:D:280:G:H5''	18:S:14:LYS:HE2	1.89	0.54
45:t:33:LEU:HA	45:t:38:LYS:HG2	1.90	0.54
48:w:67:C:C2	55:3:164:LYS:HD3	2.43	0.54
48:w:70:G:OP2	55:3:167:LYS:NZ	2.31	0.54
48:w:588:G:H5''	48:w:590:A2M:H4'	1.89	0.54
48:w:594:A:H4'	48:w:595:U:OP1	2.07	0.54
48:w:1667:U:H2'	48:w:1668:U:C6	2.43	0.54
51:z:193:VAL:HG11	51:z:240:THR:HA	1.89	0.54
3:D:1:C:N4	5:F:156:U:N3	2.27	0.54
3:D:4135:G:H2'	3:D:4136:G:H8	1.73	0.54
29:d:74:TYR:HD2	29:d:77:LYS:HB2	1.72	0.54
48:w:96:C:H1'	48:w:474:G:H5'	1.89	0.54
48:w:355:G:OP1	60:8:105:ARG:NH1	2.34	0.54
48:w:523:A:H3'	48:w:524:U:C6	2.43	0.54
48:w:532:C:O2'	48:w:533:A:H8	1.91	0.54
48:w:567:C:N3	48:w:568:C:N4	2.56	0.54
48:w:874:G:H2'	48:w:875:A:H8	1.72	0.54
53:1:45:ILE:HG13	53:1:61:VAL:HG11	1.90	0.54
53:1:100:ARG:NH2	53:1:121:TYR:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:3:221:LYS:HE2	55:3:224:ARG:HH21	1.72	0.54
62:AA:42:VAL:HG23	62:AA:43:HIS:H	1.73	0.54
79:AR:114:SER:OG	79:AR:116:ASP:OD1	2.26	0.54
79:AR:162:ASN:O	79:AR:164:ILE:N	2.41	0.54
3:D:375:G:OP2	40:o:52:LYS:NZ	2.38	0.53
3:D:1591:U:OP2	3:D:2856:C:O2'	2.22	0.53
3:D:2848:G:O2'	3:D:3838:U:O4	2.19	0.53
3:D:3732:A:H2'	3:D:3733:A:C8	2.43	0.53
5:F:127:U:O2'	5:F:128:C:H6	1.91	0.53
31:f:117:LEU:HD12	31:f:118:PRO:HD2	1.90	0.53
53:1:163:ASP:HB3	53:1:166:THR:HG22	1.90	0.53
56:4:144:ILE:HG13	70:AI:52:ILE:HB	1.90	0.53
57:5:151:GLU:HA	57:5:154:LYS:HD3	1.89	0.53
65:AD:58:MET:O	65:AD:62:GLN:HG2	2.08	0.53
79:AR:93:THR:HG23	79:AR:94:THR:HG23	1.90	0.53
2:B:30:G:OP1	48:w:1524:G:O2'	2.26	0.53
3:D:498:C:H42	3:D:656:C:H42	1.56	0.53
7:H:147:GLU:OE2	7:H:198:ARG:NH2	2.41	0.53
68:AG:93:SER:HB3	68:AG:97:ILE:HD11	1.91	0.53
79:AR:299:PHE:HD1	79:AR:309:VAL:HG12	1.73	0.53
3:D:3896:C:O2'	7:H:268:ARG:NH1	2.39	0.53
3:D:4967:A:H2'	3:D:4968:A:C8	2.43	0.53
9:J:107:ARG:NH2	9:J:116:ASP:OD1	2.41	0.53
48:w:184:G:H2'	48:w:185:G:C8	2.43	0.53
48:w:1144:A:H5'	48:w:1355:C:H41	1.73	0.53
48:w:1395:C:O2'	48:w:1396:A:OP1	2.24	0.53
79:AR:73:SER:HB3	79:AR:117:ASN:HD21	1.73	0.53
3:D:2755:A:OP1	30:e:65:ARG:NH1	2.41	0.53
3:D:4146:G:H2'	3:D:4147:G:C8	2.44	0.53
48:w:837:A:N6	72:AK:9:THR:H	2.06	0.53
48:w:1753:C:H2'	48:w:1754:G:O4'	2.08	0.53
52:0:48:ILE:HG13	52:0:86:LEU:HG	1.89	0.53
52:0:172:VAL:HA	52:0:184:ILE:O	2.09	0.53
54:2:20:PHE:HD2	54:2:23:TRP:CD1	2.25	0.53
66:AE:114:LEU:HD22	66:AE:126:PHE:HB2	1.91	0.53
3:D:969:C:O2'	10:K:123:ARG:NH1	2.38	0.53
3:D:3607:U:H2'	3:D:3608:A:C8	2.43	0.53
3:D:4691:A:H5'	13:N:71:ARG:HH11	1.72	0.53
3:D:4992:G:H2'	3:D:4993:G:C8	2.44	0.53
48:w:116:OMU:O5'	48:w:116:OMU:H6	2.08	0.53
48:w:291:G:N2	48:w:293:C:OP2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:x:110:ASN:O	49:x:111:GLN:HG3	2.08	0.53
55:3:228:ILE:HG23	55:3:232:ARG:NH2	2.23	0.53
3:D:651:C:H2'	3:D:652:G:H8	1.71	0.53
3:D:2758:G:O2'	3:D:2765:A:N3	2.35	0.53
3:D:4088:C:OP1	6:G:37:ARG:NH2	2.38	0.53
48:w:1030:A:H2'	48:w:1031:A2M:H8	1.90	0.53
48:w:1674:G:H4'	54:2:77:MET:HE1	1.91	0.53
53:1:36:HIS:ND1	53:1:85:GLY:HA3	2.24	0.53
53:1:188:ASN:HA	53:1:191:ARG:HH21	1.74	0.53
54:2:97:PHE:HD1	54:2:108:PRO:HB2	1.73	0.53
3:D:2493:G:H1'	5:F:127:U:OP1	2.09	0.53
5:F:141:C:H2'	5:F:142:U:C6	2.43	0.53
15:P:18:ARG:H	15:P:134:LEU:HA	1.74	0.53
48:w:874:G:H2'	48:w:875:A:C8	2.44	0.53
48:w:1274:G:H22	59:7:28:HIS:CE1	2.25	0.53
53:1:197:ASN:OD1	53:1:198:ARG:N	2.42	0.53
57:5:132:GLU:HA	57:5:135:GLU:HB2	1.91	0.53
3:D:1445:U:H2'	3:D:1446:C:C6	2.44	0.53
3:D:4910:G:H22	19:T:107:GLY:HA3	1.73	0.53
5:F:155:C:OP2	12:M:89:ARG:NH1	2.41	0.53
12:M:159:HIS:ND1	12:M:185:LYS:HA	2.23	0.53
29:d:88:GLU:N	29:d:88:GLU:OE1	2.41	0.53
48:w:57:U:O2'	48:w:499:G:N3	2.39	0.53
49:x:19:LEU:HD21	65:AD:106:LEU:HD11	1.91	0.53
63:AB:130:ARG:HE	63:AB:131:PRO:HD2	1.74	0.53
65:AD:45:LYS:O	65:AD:49:LYS:HG2	2.09	0.53
72:AK:110:ARG:HA	72:AK:113:ARG:HG2	1.90	0.53
3:D:4239:A:H2'	3:D:4240:G:C8	2.44	0.53
3:D:4924:C:O2	3:D:4926:C:N4	2.42	0.53
31:f:85:GLN:HA	31:f:88:VAL:HG22	1.90	0.53
48:w:1098:C:H2'	48:w:1099:G:C8	2.44	0.53
48:w:1677:U:OP1	54:2:71:ARG:NH1	2.42	0.53
51:z:108:LYS:HD3	51:z:233:LEU:HD13	1.90	0.53
67:AF:42:HIS:HB2	67:AF:83:GLN:HB2	1.89	0.53
76:AO:12:ALA:HB1	76:AO:32:VAL:HB	1.90	0.53
5:F:8:U:H2'	5:F:9:A:H8	1.74	0.53
6:G:137:ILE:HD11	6:G:149:LYS:HB2	1.91	0.53
12:M:108:GLN:O	12:M:112:GLN:HG2	2.09	0.53
16:Q:167:ARG:O	31:f:98:ALA:N	2.41	0.53
48:w:196:C:O2'	48:w:203:G:N2	2.41	0.53
48:w:523:A:H3'	48:w:524:U:H6	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1834:A:H2	48:w:1837:G:N1	2.05	0.53
3:D:462:G:H2'	3:D:463:A:C8	2.45	0.52
3:D:1332:C:H2'	3:D:1333:A:C8	2.44	0.52
3:D:4700:A:N1	13:N:72:THR:HG21	2.24	0.52
48:w:551:U:H5'	78:AQ:112:ASN:ND2	2.24	0.52
48:w:942:G:H2'	48:w:943:U:C6	2.44	0.52
56:4:38:ALA:H	56:4:41:ARG:HH12	1.56	0.52
68:AG:20:ILE:HD11	68:AG:91:LEU:HB2	1.90	0.52
79:AR:11:LEU:HD13	79:AR:307:VAL:HG23	1.91	0.52
2:B:10:2MG:O2'	2:B:11:C:OP1	2.27	0.52
3:D:965:G:N2	3:D:2092:G:H1'	2.24	0.52
3:D:4591:U:H2'	3:D:4592:C:C6	2.44	0.52
3:D:4635:A:O2'	3:D:4637:OMG:OP1	2.24	0.52
4:E:12:U:O3'	4:E:109:U:O2'	2.28	0.52
18:S:3:ALA:O	18:S:7:ILE:HD12	2.10	0.52
31:f:72:THR:HG22	31:f:110:LYS:HB3	1.91	0.52
48:w:345:U:O2	53:1:33:THR:OG1	2.25	0.52
48:w:844:U:H2'	48:w:845:G:H8	1.73	0.52
48:w:1648:G:N7	64:AC:17:LYS:HD3	2.24	0.52
51:z:198:ALA:HB1	51:z:202:THR:HG21	1.91	0.52
55:3:46:LYS:HB2	55:3:118:GLU:CD	2.34	0.52
55:3:49:VAL:HG12	55:3:115:LYS:HB3	1.91	0.52
57:5:61:ASP:N	57:5:61:ASP:OD1	2.42	0.52
68:AG:66:ARG:HG3	68:AG:68:THR:HG22	1.92	0.52
79:AR:244:ASN:HB3	79:AR:245:ARG:NE	2.20	0.52
3:D:3861:A:H2'	3:D:3862:A:C8	2.44	0.52
4:E:119:U:O4	9:J:258:LYS:NZ	2.42	0.52
48:w:1736:G:H2'	48:w:1737:G:H8	1.74	0.52
48:w:1797:U:H2'	48:w:1798:C:C6	2.44	0.52
51:z:252:THR:HG22	51:z:254:ASP:H	1.74	0.52
52:0:25:LEU:HB3	52:0:34:TYR:HE1	1.74	0.52
52:0:39:VAL:HG22	52:0:48:ILE:HG22	1.92	0.52
55:3:88:ARG:HB3	55:3:91:GLU:HB2	1.91	0.52
55:3:121:ILE:N	55:3:125:THR:OG1	2.43	0.52
56:4:39:GLN:O	56:4:43:LEU:HD13	2.10	0.52
56:4:50:GLU:HA	56:4:60:ILE:HG22	1.91	0.52
66:AE:40:TYR:CZ	66:AE:97:GLN:HG2	2.44	0.52
66:AE:136:THR:HA	66:AE:139:THR:HG23	1.90	0.52
68:AG:68:THR:O	77:AP:40:ARG:NH1	2.41	0.52
3:D:4378:A:O2'	3:D:4379:A:H2'	2.09	0.52
9:J:208:MET:O	9:J:212:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:576:A2M:H5''	48:w:576:A2M:H8	1.90	0.52
48:w:912:C:H3'	48:w:913:A:H5''	1.89	0.52
48:w:1010:G:H2'	48:w:1011:A:C8	2.45	0.52
48:w:1424:G:H2'	48:w:1425:G:H8	1.73	0.52
48:w:1519:U:O2'	48:w:1520:G:H5'	2.10	0.52
54:2:168:THR:N	54:2:171:GLU:OE2	2.27	0.52
58:6:30:LYS:NZ	78:AQ:115:PHE:HB3	2.24	0.52
72:AK:27:VAL:HG12	72:AK:29:HIS:HD2	1.75	0.52
3:D:914:U:O2'	3:D:915:A:OP2	2.24	0.52
3:D:1852:U:H5''	31:f:22:ILE:HD11	1.92	0.52
3:D:4140:C:O2'	3:D:4143:G:O6	2.20	0.52
3:D:4322:G:N2	3:D:4325:A:OP2	2.36	0.52
3:D:4460:U:H2'	3:D:4461:C:H6	1.75	0.52
47:v:117:ILE:O	47:v:121:GLN:HG2	2.09	0.52
48:w:830:A:P	48:w:846:G:H21	2.32	0.52
48:w:901:G:H2'	48:w:902:G:C8	2.45	0.52
48:w:1144:A:H2'	48:w:1145:A:C8	2.44	0.52
49:x:157:VAL:O	69:AH:65:SER:OG	2.27	0.52
2:B:23:A:H2'	2:B:24:G:C8	2.45	0.52
3:D:989:U:O4	3:D:1064:G:O6	2.27	0.52
3:D:2744:A:H2'	3:D:2745:A:C8	2.44	0.52
14:O:179:ASP:OD1	14:O:180:GLU:N	2.42	0.52
15:P:146:ARG:HG2	15:P:147:ARG:HG2	1.92	0.52
16:Q:19:GLN:HA	16:Q:22:VAL:HG13	1.92	0.52
36:k:78:HIS:HB2	36:k:85:ARG:HG3	1.92	0.52
48:w:181:A:H2'	48:w:182:C:C4	2.45	0.52
48:w:573:U:OP2	72:AK:93:ARG:NH1	2.36	0.52
48:w:893:U:H2'	48:w:894:G:C8	2.45	0.52
50:y:180:ASP:OD1	50:y:183:GLU:HG2	2.09	0.52
55:3:225:GLN:HA	55:3:228:ILE:HG22	1.91	0.52
67:AF:42:HIS:NE2	67:AF:43:LYS:HE3	2.25	0.52
79:AR:35:SER:OG	79:AR:37:ASP:OD1	2.17	0.52
2:B:69:A:H2'	2:B:70:A:C8	2.44	0.52
3:D:924:C:H2'	3:D:925:C:C6	2.45	0.52
3:D:4913:G:H4'	3:D:4914:C:O5'	2.10	0.52
7:H:218:ASP:OD2	7:H:348:ARG:NH1	2.43	0.52
9:J:124:GLU:O	9:J:126:THR:HG23	2.10	0.52
12:M:230:TYR:HA	12:M:233:ILE:HG12	1.92	0.52
48:w:839:C:N4	72:AK:9:THR:HG23	2.24	0.52
3:D:2415:OMU:H3'	3:D:2416:G:N2	2.24	0.52
3:D:2491:C:H2'	3:D:2492:C:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2539:C:H2'	3:D:2540:C:C6	2.45	0.52
48:w:523:A:O2'	58:6:131:ARG:NH2	2.43	0.52
48:w:1543:U:H4'	64:AC:43:GLU:CD	2.35	0.52
3:D:1870:C:H2'	3:D:1871:A2M:H8	1.91	0.52
4:E:24:C:H2'	4:E:25:G:O4'	2.10	0.52
13:N:92:MET:SD	13:N:161:ILE:HD11	2.50	0.52
48:w:122:G:H21	53:1:146:THR:HG21	1.75	0.52
53:1:102:ILE:HG13	53:1:182:MET:HE1	1.92	0.52
64:AC:72:VAL:HB	64:AC:84:ILE:HD11	1.92	0.52
2:B:70:A:H2'	2:B:71:G:H8	1.75	0.52
3:D:189:G:C2	3:D:253:G:N2	2.78	0.52
3:D:256:G:H2'	3:D:257:C:C6	2.44	0.52
5:F:83:C:O2'	5:F:84:A:H5''	2.09	0.52
9:J:155:THR:OG1	9:J:179:ARG:NH2	2.43	0.52
16:Q:4:SER:O	31:f:44:ASN:ND2	2.40	0.52
52:0:45:ARG:NH1	52:0:47:GLU:OE2	2.43	0.52
62:AA:76:LEU:HA	62:AA:79:GLN:HG2	1.92	0.52
66:AE:34:LYS:HB2	66:AE:100:ALA:HA	1.92	0.52
3:D:67:C:OP2	3:D:312:G:N2	2.43	0.51
3:D:1447:C:C2	3:D:1448:G:C8	2.99	0.51
3:D:3598:C:H2'	3:D:3599:A:C8	2.44	0.51
12:M:58:PRO:HD2	12:M:61:ILE:HD11	1.92	0.51
30:e:9:LYS:NZ	30:e:83:THR:O	2.29	0.51
48:w:144:U:H2'	48:w:145:G:H8	1.74	0.51
48:w:561:A:H61	48:w:590:A2M:C2	2.23	0.51
48:w:1321:G:H2'	48:w:1322:G:H8	1.75	0.51
67:AF:104:LEU:HD22	67:AF:121:ARG:HG3	1.92	0.51
72:AK:7:ILE:HD13	72:AK:43:LYS:HG2	1.91	0.51
3:D:1479:G:H2'	3:D:1480:C:C6	2.45	0.51
48:w:156:G:O2'	48:w:157:U:O4'	2.19	0.51
48:w:523:A:H4'	58:6:131:ARG:NE	2.25	0.51
48:w:614:C:H4'	48:w:615:C:H5''	1.91	0.51
48:w:897:U:H2'	48:w:898:U:O4'	2.10	0.51
48:w:1617:G:O6	63:AB:43:ARG:NH1	2.44	0.51
48:w:1752:C:H2'	48:w:1753:C:C5	2.45	0.51
54:2:20:PHE:CE1	54:2:50:PRO:HD3	2.45	0.51
58:6:55:LYS:NZ	58:6:59:GLU:OE2	2.26	0.51
79:AR:231:ASP:OD1	79:AR:232:GLY:N	2.43	0.51
3:D:5:A:H4'	12:M:192:ARG:HH21	1.76	0.51
3:D:71:C:H1'	16:Q:62:PRO:O	2.09	0.51
3:D:2803:U:H2'	3:D:2804:OMC:H6	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4146:G:H2'	3:D:4147:G:H8	1.75	0.51
9:J:83:LEU:N	9:J:84:PRO:HD2	2.25	0.51
14:O:152:LEU:HB3	14:O:165:ILE:HD12	1.92	0.51
16:Q:163:LYS:HB2	31:f:105:ARG:HH12	1.75	0.51
42:q:2:SER:O	42:q:5:LYS:NZ	2.39	0.51
48:w:146:G:H2'	48:w:147:A:O4'	2.10	0.51
48:w:581:U:OP1	72:AK:65:GLY:N	2.30	0.51
48:w:985:G:H4'	62:AA:138:ASP:OD2	2.11	0.51
48:w:1636:G:H21	54:2:164:ARG:NH1	2.09	0.51
48:w:1673:U:H2'	48:w:1674:G:O4'	2.10	0.51
58:6:67:ASP:HB3	58:6:70:ARG:HB3	1.91	0.51
62:AA:95:ILE:HD11	62:AA:129:ILE:HG12	1.90	0.51
3:D:937:U:OP1	17:R:46:ARG:NH1	2.42	0.51
3:D:2640:G:H2'	3:D:2641:A:C8	2.46	0.51
3:D:4117:U:O4'	12:M:43:GLN:NE2	2.44	0.51
22:W:99:MET:O	22:W:103:ARG:HG3	2.10	0.51
48:w:103:A:H5'	57:5:12:ARG:HH12	1.75	0.51
48:w:578:C:H2'	48:w:579:C:O4'	2.09	0.51
48:w:1201:U:H2'	48:w:1202:U:C6	2.45	0.51
54:2:68:ILE:HD11	54:2:151:ILE:HD11	1.93	0.51
58:6:128:VAL:O	58:6:132:GLN:HG2	2.10	0.51
70:AI:102:ILE:HG13	70:AI:113:HIS:HB3	1.92	0.51
71:AJ:53:GLU:HB3	71:AJ:71:ARG:HB2	1.92	0.51
72:AK:10:ARG:NH1	72:AK:26:ASP:OD1	2.42	0.51
3:D:1081:C:O2'	3:D:1082:C:H2'	2.11	0.51
3:D:1202:C:N3	3:D:1203:G:O2'	2.40	0.51
3:D:2485:U:H2'	3:D:2486:G:C8	2.44	0.51
3:D:3656:A:H2'	3:D:3657:U:H6	1.75	0.51
3:D:3669:G:H21	3:D:3672:G:N2	2.09	0.51
3:D:4238:G:H2'	3:D:4239:A:H8	1.75	0.51
3:D:4934:A:H2'	3:D:4935:C:H6	1.76	0.51
3:D:4935:C:H2'	3:D:4936:G:C8	2.46	0.51
48:w:186:C:H2'	48:w:187:G:H8	1.74	0.51
48:w:582:C:H4'	72:AK:32:LYS:HD3	1.93	0.51
51:z:166:ARG:HB3	51:z:247:THR:HG22	1.93	0.51
55:3:48:TYR:OH	55:3:119:LYS:O	2.28	0.51
72:AK:106:GLN:O	72:AK:109:GLU:HG3	2.11	0.51
79:AR:74:ASP:OD1	79:AR:74:ASP:N	2.43	0.51
79:AR:91:ASP:OD2	79:AR:94:THR:OG1	2.26	0.51
3:D:987:C:H2'	3:D:988:C:H6	1.76	0.51
3:D:1333:A:H2'	3:D:1334:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1821:G:N3	3:D:1821:G:H2'	2.25	0.51
3:D:4136:G:H2'	3:D:4137:C:C6	2.45	0.51
15:P:15:LEU:HD23	15:P:15:LEU:H	1.76	0.51
48:w:28:U:H2'	48:w:29:G:H8	1.76	0.51
53:1:125:LYS:HB2	53:1:226:PHE:HD1	1.76	0.51
58:6:78:LEU:HD22	58:6:87:LEU:HD22	1.93	0.51
68:AG:67:LYS:HA	77:AP:44:ARG:HD2	1.92	0.51
3:D:659:G:H2'	3:D:660:A:C8	2.45	0.51
3:D:1705:G:H2'	3:D:1706:A:O4'	2.11	0.51
3:D:4325:A:N3	9:J:36:LEU:HB3	2.26	0.51
8:I:228:THR:HG23	8:I:248:ARG:HH22	1.75	0.51
13:N:120:GLU:OE1	13:N:124:ARG:NH2	2.35	0.51
14:O:191:ILE:O	14:O:198:LYS:HB3	2.11	0.51
18:S:120:TRP:HE1	18:S:123:GLU:HG3	1.76	0.51
29:d:50:ARG:HD2	29:d:115:ARG:HH11	1.74	0.51
48:w:1101:U:H2'	48:w:1102:G:C8	2.45	0.51
53:1:51:ARG:HD2	53:1:111:VAL:HB	1.91	0.51
64:AC:34:VAL:N	64:AC:37:ARG:O	2.41	0.51
65:AD:37:GLU:HG2	79:AR:150:TRP:HZ3	1.76	0.51
3:D:189:G:H2'	3:D:190:G:C8	2.46	0.51
3:D:3612:C:H1'	3:D:5016:A:H8	1.76	0.51
3:D:3707:U:H2'	3:D:3708:C:C6	2.46	0.51
3:D:3946:G:H1	3:D:4067:U:H3	1.59	0.51
5:F:102:G:OP2	5:F:104:A:O2'	2.27	0.51
48:w:22:A:H4'	58:6:17:ARG:HA	1.93	0.51
48:w:505:G:O2'	48:w:506:G:O5'	2.29	0.51
48:w:561:A:H61	48:w:590:A2M:H2	1.76	0.51
48:w:678:U:H2'	48:w:679:A:H8	1.76	0.51
62:AA:85:CYS:HB3	62:AA:90:ILE:HB	1.93	0.51
79:AR:59:LEU:HD13	79:AR:90:TRP:CG	2.46	0.51
3:D:1296:G:H2'	3:D:1297:U:C6	2.46	0.51
9:J:3:PHE:HD2	9:J:4:VAL:HG22	1.76	0.51
16:Q:136:LYS:HG3	16:Q:136:LYS:O	2.10	0.51
57:5:64:ASN:HB3	57:5:186:ASP:HB3	1.91	0.51
58:6:114:VAL:HG11	58:6:130:ILE:HD11	1.93	0.51
62:AA:93:LEU:HD22	62:AA:124:MET:HG2	1.93	0.51
68:AG:94:PRO:HD2	68:AG:97:ILE:HD11	1.91	0.51
79:AR:11:LEU:HB2	79:AR:307:VAL:HG22	1.92	0.51
79:AR:274:VAL:HG23	79:AR:276:SER:H	1.75	0.51
9:J:62:CYS:HB3	9:J:105:LEU:HD22	1.92	0.51
10:K:190:HIS:HB3	10:K:193:PHE:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:73:HIS:HB3	28:c:116:LEU:HD23	1.93	0.51
31:f:37:GLY:H	31:f:41:HIS:HB2	1.76	0.51
48:w:185:G:H2'	48:w:186:C:H6	1.76	0.51
48:w:611:G:H2'	48:w:612:U:H6	1.75	0.51
48:w:815:PSU:O2	48:w:816:A:N6	2.44	0.51
57:5:177:SER:OG	57:5:182:CYS:SG	2.69	0.51
58:6:174:LYS:HE2	58:6:175:ARG:NH1	2.26	0.51
65:AD:99:ASP:OD1	65:AD:102:THR:OG1	2.18	0.51
73:AL:50:PHE:CE2	73:AL:83:LEU:HD21	2.46	0.51
3:D:76:A:N7	16:Q:74:ARG:NH2	2.59	0.50
3:D:457:G:H2'	3:D:458:C:C6	2.46	0.50
3:D:1071:C:N4	10:K:65:ARG:O	2.45	0.50
7:H:29:VAL:HG12	7:H:31:SER:H	1.75	0.50
10:K:111:LYS:O	10:K:112:MET:HG2	2.11	0.50
10:K:153:LEU:HD11	10:K:195:ILE:HG13	1.93	0.50
11:L:220:MET:O	11:L:221:LYS:HG2	2.11	0.50
43:r:127:VAL:HG13	43:r:128:LYS:HG2	1.92	0.50
48:w:1449:G:O2'	48:w:1450:G:H8	1.94	0.50
58:6:54:ARG:HD3	58:6:58:ARG:CZ	2.41	0.50
64:AC:97:GLN:HB2	64:AC:105:LYS:HD2	1.93	0.50
78:AQ:107:ARG:HD3	78:AQ:110:GLN:NE2	2.26	0.50
3:D:2899:C:P	22:W:108:ARG:HH22	2.34	0.50
9:J:121:GLY:HA3	9:J:168:ASP:O	2.11	0.50
13:N:41:ILE:HG22	13:N:43:VAL:HG13	1.93	0.50
18:S:183:THR:HG22	18:S:188:ARG:HG3	1.92	0.50
48:w:1088:U:H4'	48:w:1089:G:OP2	2.11	0.50
48:w:1272:C:H2'	48:w:1273:C:C6	2.46	0.50
54:2:156:THR:O	54:2:160:GLU:HG2	2.11	0.50
57:5:82:VAL:O	57:5:205:ARG:NH1	2.44	0.50
3:D:1095:A:N1	3:D:1200:G:C6	2.79	0.50
3:D:4895:C:H3'	3:D:4895:C:OP2	2.11	0.50
24:Y:51:GLY:HA3	24:Y:92:ARG:HG3	1.94	0.50
38:m:22:ASP:OD1	38:m:23:ASP:N	2.44	0.50
48:w:525:A:H2'	48:w:526:A:C8	2.46	0.50
48:w:559:G:O2'	48:w:560:A:H8	1.95	0.50
48:w:919:A:O2'	48:w:1020:A:N1	2.33	0.50
49:x:10:MET:HE2	49:x:15:VAL:HG12	1.93	0.50
52:0:164:VAL:O	52:0:168:VAL:HG22	2.11	0.50
53:1:44:LEU:HA	53:1:47:PHE:HB3	1.93	0.50
65:AD:124:VAL:HG13	65:AD:125:GLY:H	1.75	0.50
3:D:491:G:H4'	8:I:268:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:759:G:O2'	3:D:760:G:O4'	2.29	0.50
3:D:1695:U:H2'	3:D:1696:C:C6	2.46	0.50
3:D:3910:C:H2'	3:D:3911:C:H6	1.76	0.50
3:D:4578:G:H2'	3:D:4579:PSU:C6	2.46	0.50
21:V:161:SER:O	21:V:161:SER:OG	2.29	0.50
33:h:38:ILE:HD11	33:h:46:VAL:HG21	1.93	0.50
45:t:101:GLY:HA2	45:t:102:GLN:HB2	1.93	0.50
48:w:367:U:H4'	48:w:371:A:C8	2.46	0.50
48:w:909:G:H2'	48:w:910:G:C8	2.46	0.50
48:w:1462:U:H2'	48:w:1464:C:C4	2.46	0.50
48:w:1533:A:H2	48:w:1536:G:N3	2.10	0.50
48:w:1845:A:H2'	48:w:1846:G:C8	2.46	0.50
59:7:58:VAL:HG12	59:7:71:LEU:HA	1.92	0.50
66:AE:40:TYR:HA	66:AE:43:VAL:HG12	1.93	0.50
66:AE:62:ASP:N	66:AE:62:ASP:OD1	2.43	0.50
66:AE:73:ASN:HB3	66:AE:76:GLN:HE22	1.75	0.50
3:D:4145:C:H2'	3:D:4146:G:H8	1.77	0.50
5:F:96:C:H5''	38:m:66:LYS:HD2	1.93	0.50
7:H:17:LEU:O	7:H:19:ARG:N	2.45	0.50
20:U:111:SER:HB3	20:U:156:ILE:HD13	1.94	0.50
48:w:674:C:H2'	48:w:675:U:C6	2.47	0.50
48:w:1158:G:O3'	70:AI:76:SER:OG	2.25	0.50
48:w:1798:C:H2'	48:w:1799:G:O4'	2.10	0.50
71:AJ:46:HIS:CD2	71:AJ:103:ALA:HB2	2.46	0.50
74:AM:45:VAL:HG23	74:AM:46:GLU:H	1.75	0.50
2:B:4:U:HO2'	2:B:5:C:H6	1.59	0.50
3:D:43:U:OP1	18:S:85:VAL:HG23	2.11	0.50
3:D:93:G:H2'	3:D:94:A:C8	2.46	0.50
3:D:1308:C:H2'	3:D:1309:C:C6	2.47	0.50
3:D:1633:G:H5'	3:D:1634:A:OP1	2.12	0.50
3:D:2611:A:H5'	3:D:2688:G:H4'	1.94	0.50
3:D:2667:C:O4'	22:W:96:MET:HG3	2.11	0.50
5:F:8:U:H2'	5:F:9:A:C8	2.45	0.50
48:w:821:G:H1'	48:w:824:C:H5'	1.93	0.50
48:w:1627:C:C2	48:w:1628:C:C5	2.99	0.50
52:0:25:LEU:HD13	52:0:37:VAL:HG11	1.92	0.50
53:1:122:LYS:HE2	53:1:164:LEU:HD21	1.93	0.50
56:4:69:LEU:HD13	56:4:96:ALA:HB2	1.94	0.50
79:AR:292:SER:HB2	79:AR:297:THR:HB	1.93	0.50
2:B:4:U:O2'	2:B:5:C:O5'	2.30	0.50
3:D:369:G:N2	3:D:372:A:OP2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3599:A:H2'	3:D:3600:G:C8	2.46	0.50
3:D:4594:U:H2'	3:D:4595:G:C8	2.46	0.50
16:Q:65:ARG:HD2	16:Q:66:TYR:CE2	2.47	0.50
19:T:61:ARG:HA	19:T:70:PRO:HD2	1.94	0.50
31:f:9:ARG:NH1	31:f:12:ARG:HH21	2.10	0.50
48:w:380:G:P	57:5:56:ARG:HH22	2.35	0.50
48:w:574:A:H5''	72:AK:89:HIS:CE1	2.47	0.50
48:w:952:G:H2'	48:w:953:C:C6	2.47	0.50
48:w:1403:C:N4	48:w:1434:C:OP2	2.45	0.50
48:w:1673:U:H5''	64:AC:78:VAL:HG12	1.94	0.50
48:w:1678:A2M:H2'	48:w:1679:A:C8	2.47	0.50
62:AA:103:ASN:ND2	62:AA:142:ARG:HA	2.25	0.50
67:AF:113:VAL:HG12	67:AF:123:LEU:HB3	1.94	0.50
78:AQ:86:ARG:O	78:AQ:91:LYS:NZ	2.45	0.50
3:D:1846:G:H2'	3:D:1847:C:C6	2.47	0.50
48:w:529:A:H2'	48:w:530:U:O4'	2.12	0.50
48:w:1321:G:H2'	48:w:1322:G:C8	2.47	0.50
48:w:1323:U:H2'	48:w:1324:G:C8	2.47	0.50
66:AE:64:VAL:O	66:AE:68:ILE:HG12	2.12	0.50
3:D:325:U:H2'	3:D:326:C:C6	2.46	0.50
3:D:966:A:H5''	3:D:2092:G:H22	1.77	0.50
3:D:1503:A:H4'	3:D:1504:G:H5'	1.93	0.50
3:D:1720:C:H2'	3:D:1721:G:O4'	2.12	0.50
48:w:106:C:H2'	48:w:107:A:H8	1.76	0.50
48:w:300:U:H2'	48:w:301:A:H8	1.77	0.50
48:w:640:A:H2'	48:w:641:A:C8	2.47	0.50
48:w:1552:G:OP1	48:w:1557:C:H1'	2.12	0.50
72:AK:90:ARG:HG3	72:AK:93:ARG:HD2	1.94	0.50
3:D:192:G:H2'	3:D:193:G:H8	1.76	0.49
3:D:717:U:H2'	3:D:718:C:C6	2.47	0.49
16:Q:65:ARG:HD2	16:Q:66:TYR:CZ	2.47	0.49
23:X:85:ASP:OD1	23:X:123:SER:HB2	2.12	0.49
48:w:841:G:HO2'	48:w:842:C:H5	1.60	0.49
48:w:1452:A:H2	48:w:1476:A:H1'	1.75	0.49
48:w:1536:G:H2'	48:w:1537:A:H8	1.75	0.49
53:1:100:ARG:O	53:1:112:HIS:HB3	2.12	0.49
54:2:35:LEU:HD21	54:2:146:ARG:HD3	1.94	0.49
58:6:81:LEU:HD23	58:6:87:LEU:HD22	1.93	0.49
64:AC:40:GLU:H	64:AC:40:GLU:CD	2.19	0.49
3:D:1662:C:H2'	3:D:1663:C:C6	2.47	0.49
3:D:4546:A:N7	6:G:215:ASN:ND2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4733:C:H1'	3:D:4734:A:H2'	1.95	0.49
10:K:101:ASN:OD1	10:K:102:GLY:N	2.45	0.49
48:w:580:U:O3'	72:AK:64:PHE:HA	2.12	0.49
57:5:135:GLU:O	57:5:138:ASN:ND2	2.45	0.49
79:AR:289:LEU:HD22	79:AR:298:LEU:HD21	1.93	0.49
3:D:2563:C:H3'	3:D:2564:G:C8	2.47	0.49
3:D:2814:C:H5'	3:D:2815:A2M:OP2	2.12	0.49
3:D:4479:A:OP1	13:N:170:LYS:NZ	2.45	0.49
48:w:577:U:H2'	48:w:578:C:C6	2.45	0.49
48:w:629:A:C6	48:w:632:C:C2	2.99	0.49
48:w:1543:U:OP1	64:AC:37:ARG:NH1	2.45	0.49
48:w:1839:U:H2'	48:w:1840:U:C6	2.48	0.49
55:3:50:VAL:HG21	55:3:111:LEU:HB3	1.94	0.49
65:AD:35:CYS:HA	65:AD:38:ILE:HG12	1.94	0.49
79:AR:170:TRP:HA	79:AR:194:TYR:HB2	1.94	0.49
3:D:1773:OMU:H2'	3:D:1774:C:C6	2.47	0.49
3:D:3723:A:H2'	3:D:3724:A2M:H8	1.93	0.49
8:I:64:ALA:HB3	8:I:92:PHE:CE2	2.48	0.49
8:I:111:TRP:HD1	8:I:112:HIS:ND1	2.10	0.49
18:S:45:PRO:O	18:S:49:ARG:HG3	2.13	0.49
48:w:112:U:H4'	48:w:113:G:H5'	1.94	0.49
48:w:1263:U:H1'	77:AP:16:GLN:HE21	1.76	0.49
55:3:54:GLY:O	55:3:110:ASN:ND2	2.34	0.49
56:4:27:LEU:HA	56:4:30:LEU:HD23	1.95	0.49
61:9:38:TYR:CE1	61:9:78:LYS:HG3	2.48	0.49
65:AD:124:VAL:HG13	65:AD:125:GLY:N	2.27	0.49
79:AR:49:GLU:O	79:AR:50:THR:OG1	2.29	0.49
79:AR:242:SER:HB2	79:AR:291:TRP:NE1	2.27	0.49
3:D:1402:C:H2'	3:D:1403:G:H5''	1.95	0.49
3:D:1919:G:H1'	23:X:164:LYS:NZ	2.27	0.49
3:D:4740:G:C4	3:D:4742:G:C8	3.00	0.49
3:D:4991:U:H2'	3:D:4992:G:C8	2.48	0.49
48:w:65:C:H42	55:3:134:GLY:HA3	1.78	0.49
48:w:563:G:H5''	58:6:133:ARG:NH1	2.27	0.49
48:w:1255:G:OP1	48:w:1256:G:O2'	2.20	0.49
48:w:1740:C:H2'	48:w:1741:U:C6	2.47	0.49
63:AB:41:GLN:OE1	63:AB:84:ILE:HD12	2.13	0.49
79:AR:11:LEU:HD23	79:AR:43:TRP:CE3	2.47	0.49
79:AR:126:ASP:OD1	79:AR:128:THR:OG1	2.29	0.49
3:D:433:A:C2	3:D:3867:A:H4'	2.47	0.49
3:D:3897:G:H4'	7:H:254:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4114:C:O2'	3:D:4115:G:OP2	2.30	0.49
36:k:106:TYR:HB2	36:k:107:PRO:HD3	1.93	0.49
48:w:632:C:C2	48:w:633:C:C5	3.00	0.49
48:w:1551:U:O2'	48:w:1578:U:O4	2.25	0.49
66:AE:59:LEU:HD13	66:AE:63:GLU:HG3	1.94	0.49
72:AK:51:THR:O	72:AK:54:VAL:HG12	2.13	0.49
79:AR:127:LYS:HD2	79:AR:149:GLU:HA	1.94	0.49
3:D:490:C:H2'	3:D:491:G:C8	2.47	0.49
3:D:1244:G:H2'	3:D:1245:C:H6	1.78	0.49
3:D:1399:G:H2'	3:D:1400:G:H8	1.78	0.49
7:H:396:ARG:HA	7:H:399:LYS:HE2	1.95	0.49
18:S:159:ARG:HB2	18:S:164:LEU:HB2	1.94	0.49
30:e:25:ILE:HA	30:e:43:VAL:HG12	1.94	0.49
45:t:44:LYS:HE3	45:t:52:THR:HB	1.94	0.49
48:w:12:U:H2'	48:w:13:C:C6	2.47	0.49
48:w:604:A:H2'	48:w:605:A:C8	2.48	0.49
48:w:881:G:H1	48:w:906:U:H3	1.58	0.49
62:AA:27:VAL:HG13	62:AA:91:THR:H	1.77	0.49
64:AC:96:TYR:HA	64:AC:100:VAL:HG22	1.94	0.49
64:AC:123:ASP:OD2	64:AC:125:ARG:HG2	2.12	0.49
67:AF:85:ASN:HB2	67:AF:88:MET:HB2	1.95	0.49
68:AG:47:ASN:HB3	68:AG:91:LEU:HD22	1.93	0.49
72:AK:7:ILE:HA	72:AK:26:ASP:O	2.13	0.49
3:D:1570:G:N7	46:u:3:LYS:NZ	2.61	0.49
5:F:19:C:H2'	5:F:20:A:C8	2.48	0.49
29:d:51:LYS:O	29:d:70:VAL:HG13	2.12	0.49
47:v:68:SER:OG	47:v:69:GLY:N	2.44	0.49
48:w:953:C:O2	62:AA:55:ARG:NH2	2.46	0.49
48:w:1259:A:N6	48:w:1519:U:O5'	2.45	0.49
48:w:1446:A:HO2'	48:w:1447:G:H8	1.61	0.49
48:w:1629:C:H5''	66:AE:39:ARG:HG2	1.94	0.49
50:y:47:THR:OG1	50:y:65:ARG:NH1	2.45	0.49
59:7:42:ASN:HA	59:7:45:VAL:HG12	1.94	0.49
13:N:89:ARG:NH2	13:N:147:GLU:OE1	2.45	0.49
15:P:84:GLU:HA	15:P:170:TYR:OH	2.12	0.49
48:w:1:U:H5''	58:6:54:ARG:HH12	1.78	0.49
48:w:454:U:H2'	48:w:455:A:H8	1.78	0.49
48:w:827:A:C5	48:w:828:G:C5	3.00	0.49
48:w:1533:A:N3	48:w:1533:A:H2'	2.28	0.49
51:z:229:CYS:O	51:z:232:THR:HG22	2.13	0.49
54:2:99:ILE:HD11	54:2:171:GLU:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:AK:82:ALA:O	72:AK:86:GLU:CB	2.61	0.49
3:D:1933:G:H2'	3:D:1934:A:C8	2.47	0.49
3:D:4137:C:H2'	3:D:4138:C:C6	2.48	0.49
3:D:4524:G:C2	7:H:252:ALA:HB1	2.47	0.49
8:I:66:SER:O	8:I:66:SER:OG	2.23	0.49
13:N:91:LYS:HG2	13:N:145:ILE:HG12	1.94	0.49
16:Q:126:LEU:N	16:Q:138:ASP:OD2	2.46	0.49
48:w:29:G:H2'	48:w:30:C:H6	1.78	0.49
48:w:69:C:H3'	48:w:70:G:H8	1.78	0.49
48:w:551:U:H4'	78:AQ:112:ASN:HB3	1.95	0.49
49:x:137:ALA:HB1	49:x:142:LEU:HB3	1.94	0.49
2:B:6:2MG:H2'	2:B:7:A:C8	2.48	0.48
3:D:958:G:H21	10:K:125:LEU:H	1.61	0.48
3:D:1760:OMG:H2'	3:D:1761:G:C8	2.48	0.48
3:D:4745:G:H1	3:D:4955:A:H61	0.63	0.48
7:H:370:THR:O	7:H:370:THR:HG22	2.13	0.48
8:I:74:ALA:O	8:I:76:ILE:N	2.46	0.48
12:M:57:TRP:HB3	12:M:61:ILE:HD11	1.93	0.48
12:M:99:ALA:HB1	12:M:136:LEU:HD11	1.94	0.48
26:a:13:LYS:HD2	26:a:128:LEU:HD11	1.94	0.48
27:b:2:LYS:NZ	27:b:4:GLU:OE2	2.43	0.48
30:e:22:LYS:NZ	30:e:132:GLN:O	2.34	0.48
48:w:191:A:H2'	48:w:192:C:O4'	2.13	0.48
48:w:521:A:H4'	48:w:824:C:O2	2.13	0.48
48:w:1276:A:O2'	59:7:51:SER:HA	2.13	0.48
48:w:1457:U:H2'	48:w:1458:G:H8	1.77	0.48
48:w:1636:G:OP1	48:w:1636:G:H3'	2.13	0.48
49:x:3:GLY:HA2	49:x:63:ARG:HH21	1.77	0.48
52:0:142:LEU:HG	52:0:150:MET:HE1	1.95	0.48
57:5:129:LEU:O	57:5:133:GLU:HG2	2.13	0.48
67:AF:33:TRP:CE3	67:AF:37:VAL:HG12	2.47	0.48
79:AR:143:GLN:NE2	79:AR:145:GLU:OE2	2.46	0.48
3:D:399:G:OP1	20:U:20:SER:OG	2.19	0.48
3:D:2258:C:O2	10:K:91:THR:OG1	2.31	0.48
3:D:3680:U:OP1	6:G:54:ARG:NH2	2.47	0.48
3:D:4260:U:H2'	3:D:4261:C:C6	2.49	0.48
16:Q:46:ILE:HD11	16:Q:51:ALA:HA	1.95	0.48
31:f:90:ALA:HB3	31:f:120:GLN:HE21	1.77	0.48
48:w:1520:G:HO2'	48:w:1521:C:P	2.36	0.48
55:3:159:ARG:HB3	55:3:173:ALA:HB2	1.95	0.48
59:7:1:MET:HE3	59:7:44:HIS:CD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AG:62:ARG:HH21	68:AG:79:ARG:HD2	1.77	0.48
3:D:121:A:H62	3:D:152:U:H3	1.61	0.48
3:D:967:C:O2'	3:D:969:C:OP2	2.30	0.48
3:D:1818:G:O2'	3:D:1820:C:OP2	2.24	0.48
3:D:1824:G:H2'	3:D:1825:A:C8	2.49	0.48
3:D:2745:A:H2'	3:D:2746:A:C8	2.48	0.48
4:E:111:C:H2'	4:E:112:U:O4'	2.13	0.48
24:Y:115:LYS:HG2	24:Y:126:VAL:HG11	1.93	0.48
48:w:526:A:N6	48:w:588:G:O6	2.46	0.48
48:w:1302:G:N2	48:w:1305:C:OP2	2.45	0.48
49:x:41:ARG:HD3	49:x:47:TYR:CZ	2.47	0.48
52:0:151:LYS:O	52:0:153:VAL:HG13	2.13	0.48
72:AK:55:ILE:HG22	72:AK:75:ILE:HG23	1.95	0.48
3:D:485:C:H3'	3:D:486:C:H5''	1.96	0.48
3:D:968:C:H4'	10:K:110:ARG:NH1	2.28	0.48
3:D:1942:A:H2'	3:D:1943:A:H8	1.78	0.48
3:D:2527:A:P	22:W:38:ARG:HH22	2.36	0.48
3:D:2545:U:H2'	3:D:2546:G:C6	2.48	0.48
3:D:2565:A:H3'	3:D:2566:G:H8	1.78	0.48
3:D:4229:U:OP1	45:t:63:THR:OG1	2.32	0.48
3:D:4473:A:OP1	43:r:124:LYS:NZ	2.47	0.48
48:w:632:C:N3	48:w:633:C:N4	2.61	0.48
48:w:1025:U:H2'	48:w:1026:C:O4'	2.14	0.48
48:w:1636:G:H21	54:2:164:ARG:CZ	2.26	0.48
55:3:190:ARG:O	55:3:194:LEU:HG	2.12	0.48
69:AH:4:ASP:OD1	69:AH:5:ALA:N	2.45	0.48
69:AH:35:ASN:OD1	69:AH:52:THR:HG22	2.13	0.48
70:AI:32:LYS:O	70:AI:36:ARG:HG2	2.14	0.48
3:D:450:G:O6	3:D:1297:U:O4	2.32	0.48
3:D:1696:C:H2'	3:D:1697:G:C8	2.48	0.48
3:D:2561:C:H2'	3:D:2562:G:O4'	2.13	0.48
3:D:2730:U:H2'	3:D:2731:C:C6	2.48	0.48
3:D:3720:G:OP1	39:n:75:LYS:NZ	2.45	0.48
3:D:4745:G:N1	3:D:4955:A:N6	2.22	0.48
5:F:86:U:H4'	5:F:87:G:OP1	2.11	0.48
15:P:23:ASN:HB3	15:P:129:ASP:OD1	2.14	0.48
17:R:96:GLU:HA	17:R:99:GLU:CG	2.41	0.48
35:j:86:GLU:OE1	35:j:86:GLU:N	2.47	0.48
48:w:316:G:H2'	48:w:317:C:C6	2.48	0.48
48:w:612:U:H3'	48:w:613:G:C8	2.48	0.48
50:y:167:LYS:HA	50:y:170:GLU:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:0:98:ALA:HB1	52:0:186:VAL:HG23	1.95	0.48
57:5:89:GLU:OE1	57:5:92:ARG:NH1	2.47	0.48
58:6:175:ARG:HH21	58:6:178:ALA:HB2	1.77	0.48
63:AB:93:MET:HE1	63:AB:106:GLU:HB2	1.95	0.48
78:AQ:97:LYS:HG2	78:AQ:98:LYS:H	1.79	0.48
79:AR:3:GLU:HB3	79:AR:267:VAL:HG13	1.95	0.48
3:D:2601:A:N6	3:D:2744:A:OP2	2.43	0.48
8:I:109:ARG:HB3	8:I:111:TRP:CZ3	2.48	0.48
29:d:31:SER:HA	29:d:48:PRO:HA	1.95	0.48
52:0:195:THR:H	52:0:201:LYS:HD2	1.77	0.48
60:8:130:GLU:HB3	60:8:140:PHE:CE2	2.48	0.48
66:AE:89:ASP:O	66:AE:91:LYS:N	2.47	0.48
3:D:385:A:N3	3:D:387:G:H5''	2.28	0.48
3:D:1307:A:H2'	3:D:1308:C:C6	2.49	0.48
3:D:1504:G:H2'	3:D:1505:C:C6	2.49	0.48
3:D:1646:A:O2'	40:o:49:TRP:O	2.28	0.48
3:D:2765:A:H2'	3:D:2766:A:C8	2.49	0.48
3:D:4274:A:H2'	3:D:4275:G:H8	1.79	0.48
3:D:4967:A:H2'	3:D:4968:A:H8	1.78	0.48
3:D:5016:A:N3	3:D:5016:A:H2'	2.29	0.48
50:y:190:PRO:O	50:y:192:SER:N	2.45	0.48
51:z:70:VAL:HG21	51:z:93:ILE:HG23	1.96	0.48
68:AG:32:LEU:HD12	68:AG:85:HIS:HB2	1.94	0.48
68:AG:62:ARG:NH1	68:AG:81:GLN:HE21	2.11	0.48
3:D:37:U:H4'	31:f:32:ARG:HD2	1.96	0.48
3:D:406:C:O2'	3:D:407:A:OP1	2.29	0.48
3:D:3848:U:H2'	3:D:3849:A:H8	1.79	0.48
3:D:4238:G:H2'	3:D:4239:A:C8	2.47	0.48
3:D:4935:C:H2'	3:D:4936:G:H8	1.78	0.48
10:K:161:ARG:NH1	17:R:106:ASP:OD2	2.46	0.48
13:N:77:VAL:O	13:N:80:MET:HG2	2.13	0.48
17:R:128:LYS:HB2	17:R:128:LYS:HE3	1.65	0.48
29:d:111:LEU:HD23	29:d:111:LEU:H	1.78	0.48
40:o:34:CYS:HB3	40:o:39:TYR:H	1.79	0.48
48:w:1189:A:H2'	48:w:1190:A:C8	2.49	0.48
61:9:25:TRP:CG	75:AN:82:LYS:HD3	2.49	0.48
3:D:10:A:H2'	3:D:11:G:C8	2.49	0.48
3:D:2542:G:H2'	3:D:2543:A:C8	2.49	0.48
3:D:4625:C:O2'	3:D:4626:A:H5'	2.14	0.48
17:R:8:GLU:HB3	23:X:151:LYS:HG3	1.96	0.48
41:p:52:LYS:HA	41:p:55:LYS:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:566:U:H2'	48:w:567:C:O4'	2.13	0.48
48:w:676:C:H5''	61:9:5:HIS:CD2	2.48	0.48
48:w:932:G:O2'	48:w:934:G:OP2	2.26	0.48
51:z:256:TRP:CD2	70:AI:68:ARG:HD3	2.49	0.48
68:AG:85:HIS:HB3	68:AG:87:ARG:HH22	1.78	0.48
79:AR:20:GLN:HG2	79:AR:68:ASP:OD1	2.14	0.48
79:AR:178:ASN:HB3	79:AR:183:LYS:H	1.79	0.48
3:D:3607:U:H2'	3:D:3608:A:H8	1.77	0.48
4:E:23:A:O2'	4:E:24:C:H6	1.96	0.48
6:G:178:PRO:HG2	46:u:26:VAL:HG13	1.95	0.48
9:J:125:VAL:HG23	9:J:126:THR:H	1.78	0.48
21:V:43:PHE:O	21:V:47:VAL:HG12	2.14	0.48
48:w:64:A:H2	48:w:83:A:H62	1.62	0.48
48:w:455:A:H2'	48:w:456:C:C6	2.49	0.48
48:w:1299:A:OP1	63:AB:59:ARG:NH2	2.44	0.48
50:y:227:LYS:HA	50:y:230:GLU:HG3	1.96	0.48
56:4:36:LEU:HG	56:4:39:GLN:HB2	1.96	0.48
65:AD:92:ASP:N	65:AD:92:ASP:OD1	2.47	0.48
72:AK:58:PHE:CZ	72:AK:72:PHE:HB3	2.49	0.48
72:AK:83:LYS:HA	72:AK:91:LEU:HD11	1.95	0.48
1:A:27:U:O2'	48:w:626:G:O6	2.25	0.47
3:D:513:U:N3	3:D:646:G:C6	2.82	0.47
3:D:2448:G:H2'	3:D:2449:A:C8	2.49	0.47
3:D:2856:C:O2	7:H:242:ARG:NH2	2.44	0.47
3:D:3599:A:H2'	3:D:3600:G:H8	1.79	0.47
3:D:4116:C:N3	12:M:38:ASN:ND2	2.57	0.47
3:D:5024:C:N4	3:D:5029:C:O4'	2.46	0.47
8:I:106:LYS:HD3	8:I:108:TRP:CZ2	2.49	0.47
13:N:96:TYR:HA	13:N:177:ASP:OD1	2.14	0.47
29:d:56:GLN:NE2	29:d:65:GLN:O	2.47	0.47
48:w:160:U:O2'	48:w:162:C:OP2	2.31	0.47
48:w:921:G:C5	70:AI:28:ARG:HD2	2.49	0.47
48:w:996:A:H2'	48:w:997:A:C8	2.49	0.47
48:w:1390:U:H2'	48:w:1391:OMC:C6	2.49	0.47
53:1:11:ARG:NH2	53:1:20:LEU:HB3	2.29	0.47
53:1:61:VAL:HA	53:1:64:ILE:HG22	1.96	0.47
55:3:182:PRO:HA	55:3:185:LEU:HD12	1.96	0.47
3:D:1:C:N4	5:F:156:U:C4	2.81	0.47
3:D:1326:A2M:H2'	3:D:1327:C:C6	2.49	0.47
3:D:4578:G:H2'	3:D:4579:PSU:H6	1.78	0.47
19:T:54:TYR:OH	19:T:73:PHE:O	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:v:7:TRP:N	47:v:44:ILE:HD11	2.29	0.47
48:w:29:G:H2'	48:w:30:C:C6	2.49	0.47
48:w:29:G:OP1	71:AJ:124:LYS:NZ	2.42	0.47
48:w:1628:C:H2'	48:w:1629:C:H6	1.78	0.47
53:1:127:ARG:N	53:1:140:VAL:O	2.31	0.47
54:2:27:ASP:OD1	54:2:107:ASN:ND2	2.47	0.47
56:4:66:VAL:N	56:4:67:PRO:HD2	2.28	0.47
57:5:165:GLN:HE22	57:5:172:LEU:HD23	1.79	0.47
58:6:84:ILE:HD13	58:6:150:ARG:HG2	1.95	0.47
58:6:111:GLN:OE1	58:6:127:ARG:NH1	2.47	0.47
71:AJ:105:PHE:CD2	71:AJ:112:VAL:HB	2.49	0.47
72:AK:81:TYR:HA	72:AK:84:LYS:HB3	1.95	0.47
75:AN:50:ALA:H	75:AN:71:ALA:HB2	1.78	0.47
78:AQ:81:ARG:HD2	78:AQ:81:ARG:C	2.39	0.47
79:AR:14:HIS:CD2	79:AR:18:VAL:HG22	2.49	0.47
3:D:190:G:H2'	3:D:191:G:C8	2.46	0.47
3:D:1084:C:H2'	3:D:1085:C:H6	1.79	0.47
14:O:205:PRO:HG2	14:O:208:LYS:HG3	1.95	0.47
48:w:57:U:O3'	48:w:499:G:N2	2.41	0.47
48:w:803:C:H2'	48:w:804:U:C6	2.49	0.47
49:x:35:GLU:O	49:x:38:ILE:HG22	2.13	0.47
51:z:211:LYS:O	51:z:215:MET:HG3	2.14	0.47
51:z:232:THR:HG23	51:z:235:ASN:HB2	1.96	0.47
53:1:145:ARG:HH12	53:1:162:ILE:HG21	1.79	0.47
58:6:70:ARG:HH12	58:6:94:LEU:HD13	1.79	0.47
58:6:86:VAL:HG11	58:6:105:PHE:CD1	2.49	0.47
59:7:72:THR:O	59:7:76:ILE:HG13	2.15	0.47
79:AR:45:LEU:HA	79:AR:53:GLY:HA2	1.96	0.47
2:B:51:U:H2'	2:B:52:G:C8	2.48	0.47
3:D:262:G:H2'	3:D:263:G:H8	1.78	0.47
3:D:1260:G:H2'	3:D:1261:G:H8	1.80	0.47
3:D:4504:C:H2'	3:D:4505:C:C6	2.49	0.47
3:D:4731:G:N3	3:D:4732:G:H1'	2.29	0.47
3:D:4918:C:H2'	3:D:4919:G:H8	1.79	0.47
7:H:240:LEU:HB3	7:H:244:THR:HG21	1.96	0.47
17:R:36:ALA:HB2	17:R:52:PHE:CZ	2.49	0.47
28:c:127:LEU:O	28:c:134:LYS:HA	2.13	0.47
48:w:25:A:HO2'	48:w:26:U:H6	1.61	0.47
48:w:869:A:C5	56:4:114:GLN:HG3	2.49	0.47
48:w:1003:U:H5''	50:y:165:ARG:NH2	2.30	0.47
48:w:1113:A:O2'	48:w:1114:U:H5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1139:C:H2'	48:w:1140:G:O4'	2.14	0.47
48:w:1289:U:H2'	48:w:1290:G:C8	2.49	0.47
48:w:1746:U:H4'	55:3:65:GLN:HE22	1.80	0.47
52:0:102:ALA:HB2	52:0:186:VAL:HG21	1.95	0.47
55:3:58:LYS:HA	55:3:107:SER:OG	2.14	0.47
55:3:217:MET:O	55:3:221:LYS:HB2	2.14	0.47
56:4:42:GLU:N	56:4:42:GLU:OE1	2.47	0.47
58:6:142:VAL:HG12	58:6:144:ILE:H	1.80	0.47
79:AR:301:GLY:HA2	79:AR:307:VAL:HG12	1.96	0.47
3:D:2415:OMU:H4'	3:D:2416:G:OP1	2.14	0.47
3:D:3722:G:H2'	3:D:3723:A:H8	1.79	0.47
3:D:4239:A:H2'	3:D:4240:G:H8	1.79	0.47
3:D:4584:A:H2'	3:D:4585:U:O4'	2.14	0.47
3:D:4601:U:H2'	3:D:4602:A:H8	1.79	0.47
3:D:4699:U:H1'	3:D:4700:A:H5''	1.96	0.47
3:D:4934:A:H2'	3:D:4935:C:C6	2.49	0.47
3:D:4991:U:H2'	3:D:4992:G:H8	1.79	0.47
7:H:294:LYS:HG3	7:H:294:LYS:O	2.15	0.47
29:d:50:ARG:HD2	29:d:115:ARG:NH1	2.29	0.47
36:k:33:VAL:HG23	36:k:38:GLU:HB2	1.96	0.47
48:w:841:G:N3	48:w:842:C:C5	2.82	0.47
48:w:1239:U:H5''	63:AB:124:LYS:HD2	1.97	0.47
48:w:1615:U:O4	63:AB:40:ARG:NH2	2.48	0.47
49:x:104:THR:O	49:x:107:THR:OG1	2.30	0.47
55:3:228:ILE:HG23	55:3:232:ARG:HH21	1.80	0.47
63:AB:29:SER:OG	63:AB:31:GLU:OE1	2.31	0.47
71:AJ:95:GLU:OE1	71:AJ:140:ARG:NH2	2.48	0.47
74:AM:60:ASP:N	74:AM:60:ASP:OD1	2.48	0.47
75:AN:38:PRO:O	75:AN:40:CYS:N	2.46	0.47
3:D:1177:U:O2'	9:J:286:SER:OG	2.24	0.47
3:D:4291:G:OP2	45:t:10:THR:HG22	2.15	0.47
17:R:25:VAL:HB	17:R:38:VAL:HG22	1.94	0.47
17:R:34:ASN:O	17:R:51:PRO:HA	2.14	0.47
33:h:11:LEU:HD23	33:h:11:LEU:H	1.79	0.47
48:w:568:C:H42	48:w:582:C:H42	1.62	0.47
48:w:1692:PSU:H2'	48:w:1693:G:C8	2.50	0.47
51:z:253:PRO:HA	51:z:256:TRP:CD1	2.50	0.47
52:0:17:PHE:HD1	52:0:77:PHE:CE2	2.32	0.47
74:AM:45:VAL:HG23	74:AM:46:GLU:N	2.30	0.47
79:AR:107:ASP:O	79:AR:125:ARG:N	2.40	0.47
3:D:23:C:H2'	3:D:24:G:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:192:G:H2'	3:D:193:G:C8	2.48	0.47
3:D:1174:G:H1	3:D:1186:U:H3	1.62	0.47
3:D:1202:C:H3'	3:D:1203:G:C5'	2.45	0.47
3:D:1617:G:H1'	3:D:2513:A:N6	2.29	0.47
3:D:4580:U:O2'	7:H:182:GLU:OE2	2.25	0.47
9:J:41:LYS:HB2	24:Y:68:THR:O	2.14	0.47
13:N:173:ARG:HB3	43:r:127:VAL:HB	1.95	0.47
15:P:151:ILE:HG13	15:P:152:GLY:H	1.80	0.47
48:w:85:A:H2'	48:w:86:C:C6	2.50	0.47
48:w:561:A:O2'	58:6:132:GLN:HG3	2.15	0.47
48:w:591:U:H4'	48:w:592:C:O5'	2.13	0.47
48:w:1102:G:H22	48:w:1130:G:N2	2.12	0.47
48:w:1351:G:H4'	49:x:110:ASN:HA	1.96	0.47
48:w:1424:G:H2'	48:w:1425:G:C8	2.49	0.47
48:w:1433:C:H4'	48:w:1435:C:H1'	1.97	0.47
48:w:1442:OMU:HM23	48:w:1442:OMU:H1'	1.56	0.47
48:w:1601:A:N6	48:w:1635:C:OP2	2.47	0.47
48:w:1665:G:OP1	67:AF:91:HIS:NE2	2.40	0.47
50:y:71:LEU:CD2	50:y:82:ARG:HB3	2.45	0.47
51:z:183:LYS:HA	51:z:195:LEU:O	2.14	0.47
57:5:150:ASP:OD1	57:5:150:ASP:N	2.47	0.47
58:6:42:GLU:O	58:6:46:VAL:HG22	2.14	0.47
67:AF:72:VAL:O	67:AF:76:THR:HG23	2.13	0.47
71:AJ:84:PHE:CE2	71:AJ:86:PRO:HA	2.50	0.47
3:D:460:C:H2'	3:D:461:G:H8	1.79	0.47
3:D:922:C:H2'	3:D:923:C:H6	1.80	0.47
3:D:2362:U:H2'	3:D:2363:A2M:H8	1.96	0.47
3:D:5006:U:H4'	3:D:5007:A:H5'	1.96	0.47
13:N:12:ILE:HG21	13:N:18:ILE:HD12	1.95	0.47
48:w:1208:A:OP2	48:w:1835:A:O2'	2.26	0.47
49:x:158:ASP:OD2	69:AH:32:ILE:HD13	2.14	0.47
53:1:139:LEU:O	53:1:146:THR:HA	2.15	0.47
53:1:198:ARG:HB2	53:1:208:VAL:HG22	1.96	0.47
58:6:109:ARG:HB2	58:6:112:THR:HG23	1.97	0.47
61:9:11:LEU:HD12	61:9:11:LEU:O	2.15	0.47
64:AC:118:THR:C	64:AC:120:LEU:N	2.72	0.47
1:A:25:U:H4'	63:AB:145:LYS:HE2	1.96	0.47
3:D:1317:U:H2'	3:D:1318:C:C6	2.50	0.47
3:D:2095:A:H4'	3:D:2096:G:N7	2.30	0.47
3:D:4092:G:H1'	3:D:4093:G:H21	1.79	0.47
15:P:20:LEU:HD13	15:P:132:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1007:C:H2'	48:w:1008:A:C8	2.50	0.47
48:w:1408:U:H4'	64:AC:24:HIS:HE1	1.79	0.47
51:z:206:SER:OG	51:z:210:PRO:HG2	2.15	0.47
56:4:38:ALA:H	56:4:41:ARG:NH1	2.13	0.47
56:4:165:ASN:HB3	56:4:169:LYS:NZ	2.30	0.47
68:AG:94:PRO:O	68:AG:98:VAL:HG13	2.15	0.47
79:AR:89:LEU:HD13	79:AR:101:PHE:HE1	1.79	0.47
3:D:44:A:OP2	18:S:85:VAL:HG21	2.15	0.47
3:D:737:C:C5	3:D:739:G:H5''	2.50	0.47
3:D:959:G:N7	10:K:123:ARG:HG3	2.30	0.47
3:D:1716:G:H4'	24:Y:125:TRP:CH2	2.49	0.47
3:D:1932:A:OP1	19:T:49:ARG:NH2	2.41	0.47
13:N:63:ASN:OD1	13:N:66:GLU:HG3	2.14	0.47
48:w:191:A:H5''	57:5:140:LYS:HE2	1.96	0.47
48:w:201:C:H3'	48:w:202:G:C8	2.50	0.47
48:w:564:A:H2'	48:w:565:G:O4'	2.15	0.47
48:w:1869:A:H2'	74:AM:39:PHE:CD2	2.50	0.47
53:1:47:PHE:O	53:1:51:ARG:HB3	2.14	0.47
54:2:153:LEU:HG	54:2:189:ALA:HA	1.95	0.47
58:6:13:TYR:HA	58:6:48:PHE:HB3	1.97	0.47
58:6:109:ARG:NH2	58:6:127:ARG:HH12	2.08	0.47
59:7:12:TYR:HB3	59:7:83:LEU:HD11	1.97	0.47
3:D:505:G:H2'	3:D:506:C:C6	2.50	0.46
3:D:665:C:H4'	3:D:666:G:O5'	2.14	0.46
3:D:1084:C:H2'	3:D:1085:C:C6	2.50	0.46
3:D:3880:G:H2'	3:D:3881:G:C8	2.50	0.46
5:F:128:C:H2'	5:F:129:C:C6	2.49	0.46
48:w:1785:C:H2'	48:w:1786:U:O4'	2.15	0.46
49:x:30:LEU:HD22	49:x:47:TYR:CZ	2.49	0.46
53:1:157:ASN:O	53:1:175:PHE:HB2	2.15	0.46
55:3:223:LYS:HA	55:3:223:LYS:HD2	1.71	0.46
58:6:130:ILE:HG12	58:6:135:ILE:CD1	2.44	0.46
62:AA:56:VAL:HG22	62:AA:81:VAL:HG13	1.97	0.46
66:AE:28:PHE:O	66:AE:31:THR:OG1	2.24	0.46
76:AO:34:PHE:HE1	76:AO:42:ILE:HG12	1.80	0.46
3:D:1719:A:P	3:D:1719:A:H8	2.38	0.46
3:D:4135:G:H2'	3:D:4136:G:C8	2.50	0.46
3:D:4173:G:H2'	3:D:4174:U:C6	2.51	0.46
48:w:1004:PSU:H2'	48:w:1005:G:C8	2.48	0.46
48:w:1597:C:H4'	48:w:1603:G:C6	2.50	0.46
48:w:1705:C:H2'	48:w:1706:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:185:GLY:N	53:1:189:LEU:HD13	2.30	0.46
57:5:141:ARG:HG3	57:5:144:LYS:HB3	1.96	0.46
62:AA:72:TYR:O	62:AA:75:MET:HG3	2.15	0.46
72:AK:46:LYS:HD3	72:AK:46:LYS:HA	1.72	0.46
3:D:654:C:H4'	8:I:269:LYS:HG2	1.96	0.46
3:D:919:C:H2'	3:D:920:C:H6	1.80	0.46
3:D:1703:C:H6	11:L:39:GLN:HE22	1.61	0.46
3:D:1857:C:H2'	3:D:1858:A:C8	2.50	0.46
3:D:2639:U:O2'	3:D:2694:G:O6	2.33	0.46
3:D:2824:OMC:H1'	3:D:2824:OMC:HM23	1.61	0.46
3:D:3861:A:H2'	3:D:3862:A:H8	1.80	0.46
4:E:46:C:O2'	4:E:47:G:H8	1.98	0.46
13:N:12:ILE:HG12	13:N:53:LYS:O	2.15	0.46
39:n:76:ARG:HD2	39:n:76:ARG:HA	1.77	0.46
48:w:572:PSU:H2'	48:w:573:U:O4'	2.15	0.46
48:w:845:G:H3'	48:w:846:G:C8	2.49	0.46
48:w:1845:A:H2'	48:w:1846:G:H8	1.80	0.46
55:3:2:LYS:HD3	55:3:15:LEU:HD13	1.97	0.46
56:4:42:GLU:HG2	56:4:43:LEU:HD12	1.98	0.46
57:5:78:ILE:HD13	57:5:104:ILE:HG22	1.96	0.46
58:6:175:ARG:NE	58:6:175:ARG:HA	2.30	0.46
68:AG:24:LEU:HD13	68:AG:112:VAL:HG22	1.97	0.46
3:D:3669:G:H21	3:D:3672:G:H21	1.63	0.46
3:D:4734:A:O2'	3:D:4735:G:OP2	2.32	0.46
16:Q:121:ARG:HA	16:Q:121:ARG:HD2	1.73	0.46
47:v:107:ARG:O	47:v:111:ILE:HG12	2.16	0.46
48:w:1681:U:H2'	48:w:1682:C:C6	2.50	0.46
50:y:181:LEU:HA	50:y:184:VAL:HG22	1.98	0.46
55:3:18:VAL:HG21	55:3:24:LEU:HD21	1.97	0.46
56:4:145:ARG:O	56:4:152:ARG:HA	2.16	0.46
60:8:111:VAL:HG12	60:8:140:PHE:HB2	1.97	0.46
3:D:1431:C:H2'	3:D:1432:G:O4'	2.16	0.46
3:D:1577:G:O2'	3:D:1612:G:H4'	2.15	0.46
3:D:1751:A:H2'	3:D:1752:G:C8	2.50	0.46
5:F:16:G:O2'	5:F:17:A:H8	1.98	0.46
7:H:10:ARG:HG2	7:H:11:HIS:N	2.30	0.46
11:L:31:LYS:HD3	11:L:31:LYS:HA	1.76	0.46
24:Y:105:PHE:O	24:Y:109:VAL:HG13	2.15	0.46
30:e:51:ARG:HB2	30:e:65:ARG:HG2	1.96	0.46
50:y:108:ASP:N	50:y:108:ASP:OD1	2.49	0.46
62:AA:96:LYS:HE2	62:AA:132:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AE:63:GLU:HB3	66:AE:66:ARG:HH21	1.79	0.46
72:AK:80:ASP:OD1	72:AK:81:TYR:N	2.47	0.46
3:D:1247:U:H2'	3:D:1248:C:C6	2.50	0.46
3:D:1445:U:H2'	3:D:1446:C:H6	1.79	0.46
3:D:2477:A:H2'	3:D:2478:C:C6	2.51	0.46
7:H:153:MET:HB3	7:H:194:LEU:HD11	1.98	0.46
7:H:214:ASP:HA	7:H:284:ILE:O	2.15	0.46
9:J:236:MET:HA	9:J:239:MET:HB3	1.97	0.46
17:R:25:VAL:HG12	17:R:45:VAL:HG21	1.96	0.46
48:w:440:G:O2'	48:w:1737:G:H1'	2.15	0.46
48:w:1221:G:H2'	48:w:1222:G:C8	2.51	0.46
48:w:1447:G:OP1	68:AG:87:ARG:NH1	2.46	0.46
79:AR:5:MET:N	79:AR:268:ASP:OD2	2.48	0.46
79:AR:143:GLN:HE21	79:AR:145:GLU:HG2	1.80	0.46
3:D:188:G:N2	3:D:190:G:O6	2.48	0.46
3:D:1345:A:H2'	3:D:1346:C:C6	2.51	0.46
3:D:1413:C:H2'	3:D:1414:C:C2	2.49	0.46
3:D:2580:U:O2'	30:e:79:HIS:ND1	2.43	0.46
3:D:3654:G:O2'	3:D:3693:U:OP1	2.30	0.46
3:D:4458:C:H2'	3:D:4459:U:C6	2.50	0.46
4:E:13:A:OP1	4:E:109:U:O2'	2.34	0.46
10:K:177:GLY:O	10:K:178:PRO:C	2.59	0.46
19:T:140:ARG:O	19:T:144:GLU:HG2	2.16	0.46
26:a:107:ASN:OD1	26:a:108:ASN:N	2.48	0.46
48:w:11:A:H8	48:w:1357:A:O2'	1.99	0.46
48:w:445:A:H2'	48:w:446:G:C8	2.50	0.46
48:w:574:A:N3	48:w:574:A:H2'	2.31	0.46
48:w:1804:OMU:HM23	48:w:1804:OMU:H1'	1.62	0.46
50:y:28:LYS:HE2	50:y:28:LYS:HB3	1.71	0.46
55:3:50:VAL:CG2	55:3:111:LEU:HB3	2.45	0.46
58:6:162:ARG:NH2	58:6:169:ARG:HD2	2.31	0.46
64:AC:53:GLU:HB2	64:AC:54:PRO:HD3	1.98	0.46
79:AR:172:LYS:HG3	79:AR:193:GLY:C	2.40	0.46
3:D:1401:C:H2'	3:D:1402:C:C6	2.51	0.46
3:D:2755:A:OP2	30:e:51:ARG:NH1	2.48	0.46
3:D:3844:U:OP2	7:H:239:LYS:HG2	2.15	0.46
3:D:3848:U:H2'	3:D:3849:A:C8	2.51	0.46
3:D:4136:G:H2'	3:D:4137:C:H6	1.81	0.46
3:D:4957:C:H2'	3:D:4958:C:C6	2.51	0.46
6:G:116:LEU:HD23	6:G:164:ALA:HB2	1.98	0.46
8:I:154:VAL:HG11	8:I:174:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:99:GLU:O	17:R:103:LYS:HG2	2.16	0.46
29:d:2:LYS:HB3	29:d:2:LYS:HE3	1.78	0.46
29:d:50:ARG:HG2	29:d:51:LYS:H	1.81	0.46
48:w:346:C:OP1	53:1:38:LEU:N	2.39	0.46
48:w:526:A:H2'	48:w:527:C:H6	1.78	0.46
54:2:128:ILE:HD12	54:2:137:GLN:HB3	1.98	0.46
57:5:110:ARG:HA	57:5:121:LEU:HD23	1.98	0.46
59:7:31:LYS:NZ	59:7:36:ALA:O	2.49	0.46
60:8:117:PHE:C	60:8:119:ASP:H	2.24	0.46
65:AD:41:ILE:HA	65:AD:42:PRO:HD3	1.83	0.46
67:AF:126:GLN:HG3	67:AF:129:ARG:HH11	1.81	0.46
72:AK:16:ARG:H	72:AK:16:ARG:HD3	1.80	0.46
77:AP:53:ILE:HG13	77:AP:53:ILE:O	2.16	0.46
79:AR:40:ILE:HB	79:AR:59:LEU:HD12	1.97	0.46
3:D:458:C:H2'	3:D:459:C:H6	1.81	0.46
3:D:691:C:H2'	3:D:692:A:H8	1.76	0.46
3:D:1380:G:N2	3:D:1381:U:O4	2.42	0.46
3:D:2520:C:H2'	3:D:2521:G:H8	1.81	0.46
3:D:2809:G:O2'	3:D:4644:G:OP1	2.32	0.46
3:D:4188:U:H2'	3:D:4189:U:C6	2.50	0.46
3:D:4415:A:H4'	14:O:74:LYS:HE2	1.98	0.46
12:M:165:GLU:O	12:M:166:LEU:HB2	2.16	0.46
13:N:150:ASP:OD2	13:N:153:LEU:HG	2.15	0.46
33:h:31:TYR:OH	33:h:59:GLU:OE2	2.29	0.46
38:m:89:ARG:O	38:m:93:ARG:HG2	2.16	0.46
42:q:12:PHE:HE2	42:q:51:LEU:HD22	1.80	0.46
48:w:377:G:H5'	57:5:98:LYS:HB3	1.97	0.46
48:w:1136:U:H2'	48:w:1137:U:C6	2.51	0.46
49:x:85:ARG:O	49:x:89:LYS:HG2	2.15	0.46
67:AF:129:ARG:O	67:AF:133:ARG:HG3	2.15	0.46
75:AN:67:THR:HG22	75:AN:68:GLY:N	2.31	0.46
3:D:151:G:OP2	18:S:4:TYR:OH	2.28	0.46
3:D:1415:G:H2'	3:D:1416:G:C8	2.51	0.46
3:D:1439:C:H2'	3:D:1440:U:C6	2.47	0.46
5:F:89:U:H2'	5:F:90:C:C6	2.51	0.46
47:v:65:LYS:O	47:v:102:TYR:OH	2.22	0.46
48:w:520:A:O5'	58:6:11:LYS:HD2	2.16	0.46
48:w:1256:G:H8	68:AG:66:ARG:HB2	1.80	0.46
48:w:1298:G:H1'	63:AB:79:HIS:H	1.80	0.46
48:w:1398:G:H1'	79:AR:63:SER:OG	2.16	0.46
48:w:1446:A:N3	48:w:1447:G:C8	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:5:193:LYS:HD3	57:5:193:LYS:HA	1.78	0.46
2:B:8:U:O2'	2:B:21:A:N1	2.45	0.45
3:D:106:A:H2'	3:D:107:G:O4'	2.16	0.45
3:D:457:G:H2'	3:D:458:C:H6	1.79	0.45
3:D:515:C:O2'	3:D:646:G:N2	2.50	0.45
3:D:1447:C:H2'	3:D:1448:G:C8	2.46	0.45
3:D:2562:G:O2'	3:D:2565:A:N6	2.49	0.45
3:D:3923:A:H2'	3:D:3924:C:C6	2.51	0.45
3:D:4775:C:N3	3:D:4859:C:N4	2.63	0.45
7:H:285:TYR:CD1	7:H:363:ILE:HD13	2.51	0.45
14:O:69:ARG:HG3	14:O:70:ILE:N	2.31	0.45
48:w:913:A:OP1	56:4:99:ARG:NH2	2.49	0.45
48:w:1013:U:C2	48:w:1014:G:C8	3.04	0.45
48:w:1119:A:O3'	75:AN:72:ARG:NH1	2.46	0.45
50:y:138:PHE:O	50:y:213:ARG:N	2.49	0.45
58:6:107:GLU:HA	58:6:112:THR:HG21	1.98	0.45
61:9:60:VAL:HG12	61:9:61:ALA:O	2.15	0.45
66:AE:59:LEU:HB2	66:AE:63:GLU:OE2	2.16	0.45
70:AI:49:GLU:O	70:AI:64:ASN:ND2	2.48	0.45
3:D:2296:G:O2'	8:I:242:PRO:O	2.30	0.45
3:D:2431:A:OP1	42:q:41:ARG:NH1	2.42	0.45
3:D:3712:A:H2'	3:D:3713:U:O4'	2.16	0.45
3:D:4619:U:H2'	3:D:4620:OMU:H6	1.97	0.45
4:E:7:G:H4'	9:J:33:ARG:NH1	2.31	0.45
25:Z:25:CYS:SG	25:Z:112:LEU:HD22	2.56	0.45
26:a:43:LYS:HE3	26:a:43:LYS:HB3	1.69	0.45
48:w:30:C:O2'	48:w:596:U:OP1	2.34	0.45
48:w:191:A:OP2	57:5:140:LYS:NZ	2.35	0.45
48:w:562:U:H5''	58:6:132:GLN:HB2	1.99	0.45
48:w:676:C:H5''	61:9:5:HIS:HD2	1.81	0.45
48:w:1612:G:H5''	66:AE:88:LYS:HD3	1.97	0.45
48:w:1628:C:H2'	48:w:1629:C:C6	2.51	0.45
48:w:1863:A:H8	74:AM:79:ILE:HG21	1.81	0.45
55:3:177:GLN:HG3	55:3:178:ARG:N	2.31	0.45
58:6:111:GLN:NE2	58:6:127:ARG:HB2	2.31	0.45
58:6:162:ARG:NH1	58:6:169:ARG:HB2	2.30	0.45
61:9:15:ALA:HB2	75:AN:20:LYS:HD3	1.97	0.45
79:AR:104:HIS:HE1	79:AR:122:SER:HB3	1.81	0.45
3:D:496:G:H2'	3:D:497:G:C8	2.51	0.45
3:D:911:U:H2'	3:D:912:G:O4'	2.16	0.45
3:D:1400:G:H2'	3:D:1401:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2566:G:H2'	3:D:2567:G:H8	1.80	0.45
3:D:4112:C:O2	3:D:4112:C:H2'	2.15	0.45
3:D:4457:PSU:H1'	7:H:252:ALA:HB3	1.98	0.45
4:E:49:A:OP2	9:J:225:GLN:HB2	2.15	0.45
5:F:140:C:H2'	5:F:141:C:C6	2.51	0.45
8:I:150:LEU:O	8:I:152:LEU:N	2.49	0.45
16:Q:42:LYS:HE3	16:Q:46:ILE:HD13	1.97	0.45
47:v:97:ILE:CG2	47:v:107:ARG:HB3	2.45	0.45
48:w:434:G:N2	48:w:473:A:H8	2.11	0.45
48:w:924:G:H21	61:9:87:ASP:CG	2.24	0.45
48:w:1653:U:H3	48:w:1671:G:H1	1.63	0.45
56:4:78:ARG:O	56:4:82:GLU:HG2	2.16	0.45
59:7:14:LEU:HA	59:7:17:LYS:HE2	1.97	0.45
67:AF:31:PRO:HD2	67:AF:34:VAL:HG13	1.98	0.45
69:AH:56:CYS:SG	69:AH:59:ILE:HG12	2.57	0.45
79:AR:165:ILE:HG13	79:AR:177:TRP:HB2	1.96	0.45
2:B:70:A:H2'	2:B:71:G:C8	2.51	0.45
3:D:75:G:O2'	16:Q:101:ARG:NH1	2.43	0.45
3:D:2097:U:OP1	11:L:35:LYS:NZ	2.42	0.45
3:D:2745:A:H2'	3:D:2746:A:H8	1.80	0.45
3:D:4178:A:H2'	3:D:4179:G:C8	2.52	0.45
11:L:137:GLU:N	11:L:138:PRO:HD2	2.31	0.45
12:M:165:GLU:C	12:M:167:VAL:H	2.23	0.45
15:P:113:ILE:HD11	66:AE:14:ARG:HD3	1.97	0.45
25:Z:38:ASN:ND2	25:Z:90:TYR:OH	2.50	0.45
38:m:81:LEU:HA	38:m:84:ARG:HG2	1.98	0.45
48:w:49:C:N4	48:w:472:C:O2'	2.49	0.45
48:w:1189:A:H2'	48:w:1190:A:H8	1.81	0.45
48:w:1493:C:O2'	48:w:1499:U:O4	2.23	0.45
52:0:146:ARG:O	52:0:148:LYS:HD3	2.16	0.45
57:5:38:ILE:HD11	57:5:81:VAL:HG23	1.99	0.45
60:8:136:LYS:O	60:8:139:ARG:NH1	2.48	0.45
65:AD:37:GLU:HG2	79:AR:150:TRP:CZ3	2.51	0.45
3:D:257:C:H2'	3:D:258:G:H8	1.81	0.45
3:D:1095:A:C2	3:D:1200:G:N1	2.65	0.45
3:D:3925:OMU:HM23	3:D:3925:OMU:H1'	1.74	0.45
4:E:48:G:O2'	4:E:49:A:O5'	2.35	0.45
14:O:55:ASP:OD1	14:O:162:ARG:HG3	2.16	0.45
21:V:148:VAL:HG12	21:V:152:PHE:CZ	2.52	0.45
48:w:181:A:H2'	48:w:182:C:C5	2.51	0.45
48:w:320:G:O6	48:w:331:C:N4	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1221:G:H2'	48:w:1222:G:H8	1.80	0.45
48:w:1520:G:OP1	66:AE:136:THR:N	2.34	0.45
50:y:60:ASP:OD1	50:y:60:ASP:N	2.50	0.45
53:1:124:CYS:HA	53:1:142:HIS:CE1	2.52	0.45
67:AF:37:VAL:HG23	67:AF:38:LYS:N	2.31	0.45
73:AL:40:VAL:HG23	73:AL:41:ARG:N	2.29	0.45
78:AQ:81:ARG:HD2	78:AQ:81:ARG:O	2.16	0.45
3:D:131:C:H3'	3:D:132:G:H8	1.81	0.45
3:D:668:C:H4'	8:I:6:PRO:HB3	1.99	0.45
3:D:4069:U:H2'	3:D:4070:U:C6	2.52	0.45
3:D:4600:G:O2'	3:D:4601:U:P	2.75	0.45
3:D:4749:C:H2'	3:D:4750:G:O4'	2.17	0.45
3:D:4769:G:H5''	19:T:176:ARG:HD3	1.97	0.45
6:G:205:ASN:HB2	6:G:206:PRO:HD2	1.98	0.45
17:R:119:ARG:HG3	19:T:189:ILE:HG23	1.97	0.45
19:T:80:PHE:HA	19:T:83:THR:HG22	1.99	0.45
48:w:334:C:H5	55:3:190:ARG:CZ	2.30	0.45
48:w:876:C:H2'	48:w:877:C:C6	2.52	0.45
48:w:1330:G:H4'	48:w:1331:C:H3'	1.99	0.45
48:w:1648:G:H5''	64:AC:125:ARG:HB2	1.97	0.45
50:y:217:MET:HE2	50:y:217:MET:HB2	1.83	0.45
53:1:87:MET:SD	53:1:123:LEU:HB2	2.57	0.45
55:3:18:VAL:HG12	55:3:20:ASP:H	1.82	0.45
58:6:77:LEU:HD23	58:6:80:ARG:HH11	1.82	0.45
61:9:38:TYR:CZ	61:9:78:LYS:HG3	2.52	0.45
3:D:1078:A:H1'	3:D:1234:G:N2	2.31	0.45
3:D:1198:G:H2'	3:D:1199:G:C8	2.52	0.45
3:D:1867:A:H2'	3:D:1868:A:C8	2.52	0.45
3:D:1927:U:OP1	3:D:1949:U:O2'	2.31	0.45
3:D:4460:U:H2'	3:D:4461:C:C6	2.51	0.45
7:H:228:TYR:CE1	7:H:270:GLY:HA2	2.52	0.45
15:P:19:LYS:HG2	15:P:133:VAL:HG12	1.99	0.45
23:X:15:ARG:HG3	23:X:16:CYS:O	2.17	0.45
48:w:363:A:H61	48:w:400:C:H1'	1.82	0.45
48:w:363:A:N6	48:w:400:C:H1'	2.31	0.45
48:w:867:G:H2'	48:w:868:G:C8	2.52	0.45
48:w:945:U:H2'	48:w:946:U:C6	2.51	0.45
48:w:1230:C:H5'	48:w:1607:A:O2'	2.17	0.45
49:x:89:LYS:HE2	49:x:201:LEU:HD21	1.99	0.45
58:6:60:LEU:HB3	58:6:70:ARG:NH1	2.32	0.45
58:6:82:VAL:HG12	58:6:87:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:AK:104:ARG:HH21	72:AK:108:LYS:NZ	2.14	0.45
3:D:183:C:H1'	3:D:184:U:H5	1.82	0.45
3:D:4744:A:H2'	3:D:4745:G:O4'	2.16	0.45
3:D:4761:G:OP2	19:T:37:ARG:NH1	2.50	0.45
6:G:120:PRO:HA	6:G:162:ASN:HB3	1.97	0.45
6:G:142:GLU:OE2	6:G:143:THR:N	2.49	0.45
7:H:61:ASP:O	7:H:63:PRO:HD3	2.16	0.45
11:L:87:PRO:HG2	11:L:144:TYR:CD2	2.52	0.45
11:L:96:ARG:HD2	11:L:139:TYR:CE2	2.51	0.45
13:N:133:ALA:O	13:N:146:LEU:HA	2.16	0.45
15:P:128:LEU:HD11	15:P:130:PHE:HE1	1.81	0.45
25:Z:106:SER:O	25:Z:109:SER:HB3	2.17	0.45
26:a:92:ASP:OD1	26:a:94:VAL:HG22	2.17	0.45
30:e:17:ARG:NH2	30:e:18:TYR:OH	2.50	0.45
36:k:50:VAL:HG22	36:k:69:VAL:HG12	1.99	0.45
45:t:85:ILE:HG22	45:t:86:LYS:N	2.31	0.45
48:w:113:G:O2'	60:8:67:SER:OG	2.28	0.45
48:w:300:U:H2'	48:w:301:A:C8	2.52	0.45
52:0:123:LEU:HG	52:0:134:CYS:SG	2.57	0.45
58:6:37:LEU:HB3	58:6:42:GLU:OE2	2.16	0.45
58:6:83:ARG:HG2	58:6:150:ARG:HD3	1.99	0.45
67:AF:102:ARG:HD3	67:AF:102:ARG:HA	1.83	0.45
72:AK:100:LYS:HE2	72:AK:102:THR:HB	1.99	0.45
3:D:1448:G:H2'	3:D:1449:C:H6	1.82	0.45
3:D:1759:G:H1	3:D:1773:OMU:C2	2.29	0.45
3:D:2602:G:H2'	3:D:2603:C:C6	2.52	0.45
3:D:3656:A:H2'	3:D:3657:U:C6	2.52	0.45
3:D:4737:G:H2'	3:D:4738:C:C6	2.51	0.45
13:N:21:LYS:HB3	13:N:21:LYS:HE3	1.80	0.45
20:U:4:TYR:CZ	20:U:18:ARG:HG3	2.51	0.45
22:W:90:PRO:HB2	22:W:93:VAL:HG12	1.98	0.45
48:w:96:C:H2'	48:w:97:U:C6	2.52	0.45
48:w:116:OMU:HM23	48:w:116:OMU:H1'	1.68	0.45
48:w:166:A2M:N6	48:w:167:G:O6	2.50	0.45
48:w:420:G:O2'	48:w:660:C:N3	2.43	0.45
48:w:498:C:H5'	48:w:499:G:OP2	2.16	0.45
48:w:1164:G:O2'	48:w:1165:G:H5'	2.17	0.45
52:0:7:LYS:HD3	52:0:7:LYS:HA	1.81	0.45
53:1:42:LEU:HD22	53:1:47:PHE:HB2	1.99	0.45
56:4:145:ARG:NE	70:AI:49:GLU:OE2	2.44	0.45
64:AC:15:ARG:HA	64:AC:19:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AG:24:LEU:HB2	68:AG:87:ARG:HB2	1.99	0.45
2:B:63:G:H2'	2:B:64:G:H8	1.82	0.45
3:D:175:C:H2'	3:D:176:G:C8	2.52	0.45
3:D:271:C:H2'	3:D:272:U:C6	2.52	0.45
3:D:1400:G:H2'	3:D:1401:C:C6	2.52	0.45
3:D:1818:G:O2'	3:D:1819:G:H5''	2.18	0.45
3:D:2632:PSU:H2'	3:D:2633:U:C6	2.51	0.45
3:D:3710:G:H5'	3:D:3711:A:OP1	2.16	0.45
7:H:28:LYS:HG3	7:H:30:LYS:HG3	1.99	0.45
12:M:205:THR:C	12:M:206:GLN:HG3	2.42	0.45
25:Z:35:ASP:HB3	25:Z:38:ASN:OD1	2.16	0.45
48:w:65:C:C6	55:3:174:PRO:HB3	2.52	0.45
48:w:77:A:C8	55:3:175:LYS:HA	2.52	0.45
48:w:168:C:OP1	55:3:131:ARG:NH1	2.50	0.45
48:w:213:G:H2'	48:w:214:U:O4'	2.16	0.45
48:w:563:G:H2'	48:w:564:A:C8	2.52	0.45
49:x:7:VAL:HG13	49:x:8:LEU:HG	1.99	0.45
53:1:194:VAL:O	53:1:210:VAL:HA	2.16	0.45
63:AB:98:ASN:OD1	63:AB:122:THR:HA	2.16	0.45
65:AD:49:LYS:HB3	65:AD:49:LYS:HE2	1.75	0.45
68:AG:20:ILE:HG22	68:AG:116:ILE:HD13	1.99	0.45
68:AG:22:ILE:CG1	68:AG:89:ILE:HB	2.47	0.45
79:AR:25:PRO:HA	79:AR:293:ALA:HB1	2.00	0.45
79:AR:222:ASN:OD1	79:AR:223:GLU:N	2.49	0.45
3:D:493:G:H2'	3:D:494:U:O4'	2.17	0.44
3:D:1662:C:H2'	3:D:1663:C:H6	1.82	0.44
3:D:4095:G:N2	3:D:4113:U:O2	2.30	0.44
3:D:5004:C:H2'	3:D:5005:G:O4'	2.17	0.44
5:F:144:U:H2'	5:F:145:C:C6	2.52	0.44
9:J:289:ARG:O	9:J:292:GLU:HG3	2.17	0.44
13:N:8:GLN:HG2	13:N:74:CYS:SG	2.57	0.44
48:w:418:A:H2'	48:w:419:G:C8	2.52	0.44
48:w:1113:A:C6	48:w:1121:G:C6	3.06	0.44
48:w:1514:G:H21	63:AB:97:TYR:HE1	1.64	0.44
48:w:1678:A2M:HM'3	48:w:1678:A2M:H1'	1.47	0.44
49:x:57:LYS:NZ	69:AH:66:ASP:OD1	2.51	0.44
50:y:103:MET:HG2	50:y:104:ASP:N	2.31	0.44
51:z:156:ILE:O	51:z:160:LEU:HD23	2.16	0.44
51:z:263:LYS:HD3	69:AH:50:PHE:HZ	1.82	0.44
52:0:8:LYS:HB3	68:AG:61:LEU:HD21	1.99	0.44
52:0:210:ILE:HD13	65:AD:16:ILE:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:86:PHE:CE2	53:1:87:MET:HE3	2.52	0.44
54:2:35:LEU:O	54:2:39:ILE:HG12	2.17	0.44
79:AR:14:HIS:CE1	79:AR:35:SER:HB2	2.51	0.44
3:D:252:C:N4	3:D:253:G:O6	2.50	0.44
3:D:1274:A:O2'	3:D:1275:G:H8	1.97	0.44
3:D:1405:C:H42	3:D:1413:C:H42	1.64	0.44
3:D:1893:C:H1'	3:D:1937:C:O2	2.17	0.44
3:D:2458:C:H5''	18:S:67:ARG:HD2	1.99	0.44
3:D:2764:A:H2'	3:D:2765:A:H8	1.81	0.44
3:D:4174:U:H2'	3:D:4175:G:H8	1.82	0.44
3:D:4928:C:H2'	3:D:4929:C:C6	2.52	0.44
3:D:4945:G:H1'	10:K:158:ARG:HH22	1.83	0.44
10:K:205:ASN:OD1	10:K:260:LYS:NZ	2.31	0.44
15:P:41:GLU:HG2	15:P:48:PRO:HD3	1.98	0.44
16:Q:48:PRO:HB2	38:m:120:ALA:HB2	1.99	0.44
22:W:38:ARG:O	22:W:39:GLN:HB2	2.18	0.44
29:d:52:ASP:OD1	29:d:110:LYS:HG2	2.16	0.44
30:e:41:ALA:HB2	30:e:77:TYR:HE1	1.82	0.44
48:w:102:A:H4'	48:w:104:A:C8	2.52	0.44
48:w:103:A:H5'	57:5:12:ARG:NH1	2.32	0.44
48:w:111:A:H5'	60:8:70:GLY:HA2	2.00	0.44
48:w:917:U:H2'	48:w:918:U:C6	2.52	0.44
48:w:1328:OMG:HM23	48:w:1328:OMG:H1'	1.68	0.44
49:x:12:GLU:O	49:x:15:VAL:HG22	2.17	0.44
52:0:27:ARG:HG2	59:7:61:GLN:HE21	1.81	0.44
52:0:70:THR:HG23	52:0:86:LEU:HD13	1.99	0.44
54:2:43:GLU:C	54:2:45:TYR:H	2.24	0.44
54:2:158:ALA:N	54:2:176:GLU:OE2	2.50	0.44
56:4:71:SER:HA	56:4:74:LYS:HE2	1.98	0.44
58:6:142:VAL:HG11	58:6:147:PHE:CG	2.52	0.44
77:AP:33:LYS:O	77:AP:36:LEU:HD23	2.17	0.44
3:D:7:C:H2'	3:D:8:U:C6	2.52	0.44
3:D:124:C:OP1	18:S:144:ARG:HD2	2.17	0.44
3:D:1319:U:OP2	31:f:22:ILE:HG22	2.17	0.44
3:D:1763:C:N4	3:D:1769:G:H22	2.14	0.44
3:D:3944:OMG:HM23	3:D:3944:OMG:H1'	1.81	0.44
3:D:4620:OMU:OP2	3:D:4670:C:N4	2.37	0.44
14:O:34:PHE:HD2	14:O:89:VAL:HG23	1.83	0.44
31:f:125:LYS:HA	31:f:145:VAL:O	2.17	0.44
42:q:12:PHE:CE2	42:q:51:LEU:HD22	2.53	0.44
48:w:192:C:H2'	48:w:193:C:C6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:532:C:C2	48:w:533:A:C8	3.06	0.44
48:w:600:G:H1	48:w:622:C:H5	1.62	0.44
48:w:1441:U:O2	48:w:1443:C:N4	2.45	0.44
50:y:180:ASP:O	50:y:184:VAL:HG13	2.17	0.44
52:0:40:ARG:NH1	68:AG:107:GLU:O	2.50	0.44
63:AB:52:LYS:HG2	63:AB:80:LEU:HD11	1.98	0.44
71:AJ:67:ARG:HG3	71:AJ:115:ILE:HG12	1.99	0.44
3:D:1751:A:H2'	3:D:1752:G:H8	1.82	0.44
3:D:1881:C:H5'	3:D:2281:U:H1'	1.99	0.44
3:D:3607:U:OP1	22:W:88:ARG:NH1	2.50	0.44
3:D:4481:U:H2'	3:D:4482:U:H6	1.82	0.44
5:F:124:U:OP1	5:F:126:C:N4	2.49	0.44
15:P:32:ARG:NH1	15:P:126:TYR:HE1	2.16	0.44
24:Y:28:ALA:HA	24:Y:31:MET:HG2	1.98	0.44
36:k:93:PRO:O	36:k:95:LYS:N	2.51	0.44
41:p:5:ILE:HD11	41:p:11:PHE:HD1	1.82	0.44
47:v:47:LYS:HB2	47:v:102:TYR:CZ	2.52	0.44
48:w:185:G:H2'	48:w:186:C:C6	2.52	0.44
48:w:907:G:H2'	48:w:908:A:C8	2.53	0.44
48:w:909:G:H2'	48:w:910:G:H8	1.83	0.44
48:w:918:U:P	61:9:64:ARG:HH22	2.41	0.44
48:w:963:A:H2'	48:w:964:A:C8	2.53	0.44
48:w:1520:G:N3	48:w:1520:G:H2'	2.33	0.44
55:3:229:ALA:O	55:3:232:ARG:HG2	2.16	0.44
56:4:52:GLU:HG3	56:4:53:VAL:O	2.17	0.44
60:8:103:GLU:OE1	71:AJ:14:ARG:NH2	2.50	0.44
70:AI:69:LEU:HG	70:AI:70:ASN:O	2.17	0.44
1:A:19:U:O4	1:A:20:A:N6	2.49	0.44
3:D:458:C:H2'	3:D:459:C:C6	2.52	0.44
3:D:1743:A:O4'	9:J:15:ARG:HD2	2.17	0.44
3:D:3943:A:H5'	3:D:3944:OMG:OP2	2.18	0.44
3:D:4088:C:H2'	3:D:4089:G:C8	2.53	0.44
3:D:4254:G:H2'	3:D:4254:G:N3	2.33	0.44
4:E:58:A:H2'	4:E:59:G:H8	1.82	0.44
5:F:94:G:H21	40:o:82:THR:HB	1.83	0.44
19:T:193:THR:O	19:T:197:LYS:HG2	2.17	0.44
29:d:47:MET:HE1	29:d:118:ILE:HD11	2.00	0.44
48:w:297:A:H4'	53:1:132:GLY:O	2.17	0.44
48:w:1199:A:H2'	48:w:1200:A:C8	2.53	0.44
55:3:215:LYS:O	55:3:219:GLU:HG2	2.18	0.44
79:AR:31:ILE:HG22	79:AR:43:TRP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2583:C:OP2	37:I:76:ARG:NH1	2.45	0.44
3:D:2864:A:H2'	3:D:2865:U:C6	2.53	0.44
3:D:3746:A:H5''	6:G:244:GLY:HA3	2.00	0.44
3:D:3756:A:C2'	3:D:3757:G:H5'	2.48	0.44
7:H:229:LYS:HG3	7:H:272:LYS:HD3	1.98	0.44
12:M:166:LEU:HD23	18:S:7:ILE:HG12	2.00	0.44
12:M:250:ILE:O	12:M:254:GLU:HG2	2.18	0.44
19:T:47:PHE:CZ	19:T:144:GLU:HG3	2.49	0.44
22:W:136:ARG:O	22:W:140:GLU:HG3	2.18	0.44
37:I:84:ALA:O	37:I:87:VAL:HG12	2.17	0.44
47:v:28:GLU:OE2	47:v:31:ASN:ND2	2.51	0.44
48:w:68:A:H8	48:w:68:A:OP1	2.00	0.44
48:w:556:U:O4	48:w:560:A:N6	2.51	0.44
48:w:656:G:N2	48:w:663:C:H5''	2.33	0.44
48:w:819:G:H4'	53:1:255:ARG:HH12	1.82	0.44
48:w:1067:C:H2'	48:w:1068:G:O4'	2.17	0.44
76:AO:46:VAL:HG11	76:AO:56:LEU:HD13	1.98	0.44
76:AO:62:GLU:O	76:AO:62:GLU:HG2	2.17	0.44
79:AR:194:TYR:O	79:AR:212:LYS:N	2.48	0.44
79:AR:195:LEU:HA	79:AR:211:GLY:HA3	1.99	0.44
3:D:1:C:H2'	3:D:2:G:C8	2.52	0.44
3:D:302:C:OP1	18:S:68:ARG:HB2	2.17	0.44
3:D:1175:A:H2	3:D:1185:G:H22	1.64	0.44
3:D:3734:PSU:H2'	3:D:3735:G:O4'	2.17	0.44
3:D:3736:A:H2'	3:D:3737:A:C8	2.52	0.44
3:D:4219:A:C6	3:D:4220:6MZ:H9	2.53	0.44
7:H:103:LYS:HB2	7:H:103:LYS:HE2	1.83	0.44
8:I:150:LEU:HB3	8:I:151:PRO:HD3	1.99	0.44
9:J:125:VAL:O	9:J:126:THR:OG1	2.33	0.44
15:P:31:ASP:O	15:P:35:ARG:HG3	2.18	0.44
20:U:54:GLN:HA	20:U:83:TRP:CD1	2.52	0.44
48:w:1365:G:H2'	48:w:1366:G:H8	1.82	0.44
53:1:11:ARG:HH21	53:1:20:LEU:HB3	1.82	0.44
53:1:149:TYR:HB3	55:3:209:TYR:CG	2.52	0.44
53:1:226:PHE:CE2	53:1:228:ILE:HD13	2.53	0.44
58:6:126:ALA:O	58:6:130:ILE:HG13	2.18	0.44
67:AF:37:VAL:C	67:AF:39:LEU:H	2.26	0.44
79:AR:212:LYS:HD2	79:AR:235:ILE:HD12	2.00	0.44
79:AR:215:GLN:HB3	79:AR:231:ASP:CG	2.43	0.44
3:D:2529:A:O2'	3:D:2531:C:OP2	2.36	0.44
3:D:3911:C:H2'	3:D:3912:U:H6	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4860:G:H2'	3:D:4861:G:H8	1.83	0.44
14:O:53:VAL:HG12	14:O:134:VAL:HG22	1.99	0.44
20:U:35:ALA:HB2	20:U:58:VAL:HG23	1.98	0.44
29:d:67:ILE:HD13	29:d:107:THR:HG21	1.99	0.44
48:w:523:A:H2'	48:w:524:U:O4'	2.18	0.44
48:w:1323:U:H2'	48:w:1324:G:H8	1.83	0.44
48:w:1425:G:H2'	48:w:1426:U:C6	2.53	0.44
53:1:80:ILE:HG13	53:1:81:THR:HG23	2.00	0.44
75:AN:19:HIS:HB3	75:AN:21:LYS:O	2.17	0.44
3:D:411:G:H4'	3:D:412:G:H5''	1.98	0.44
3:D:1186:U:H2'	3:D:1187:G:C2	2.51	0.44
3:D:1406:G:H2'	3:D:1407:C:C5	2.52	0.44
5:F:92:U:H2'	5:F:93:C:O4'	2.17	0.44
8:I:235:LEU:HD23	8:I:240:LEU:HD11	2.00	0.44
10:K:99:ASP:OD1	10:K:99:ASP:N	2.50	0.44
23:X:128:LYS:HZ2	23:X:128:LYS:HB3	1.82	0.44
24:Y:80:VAL:HG22	24:Y:81:LYS:H	1.82	0.44
34:i:106:VAL:O	34:i:106:VAL:HG12	2.18	0.44
48:w:144:U:H2'	48:w:145:G:C8	2.52	0.44
48:w:475:C:C2	48:w:476:A:C8	3.05	0.44
48:w:579:C:H2'	48:w:580:U:C6	2.53	0.44
48:w:644:OMG:HM23	48:w:644:OMG:H1'	1.73	0.44
48:w:827:A:C6	48:w:828:G:C4	3.06	0.44
48:w:1227:G:C2	48:w:1228:A:C8	3.06	0.44
48:w:1457:U:H2'	48:w:1458:G:C8	2.52	0.44
48:w:1743:G:N2	48:w:1791:A:H62	2.15	0.44
50:y:103:MET:HB3	50:y:215:VAL:HG22	2.00	0.44
55:3:5:ILE:HG21	55:3:45:TRP:HH2	1.83	0.44
55:3:5:ILE:O	55:3:13:GLN:HA	2.18	0.44
57:5:110:ARG:O	57:5:114:GLU:HG3	2.18	0.44
58:6:110:LEU:HD11	58:6:135:ILE:HD12	2.00	0.44
78:AQ:102:THR:OG1	78:AQ:103:GLY:N	2.50	0.44
79:AR:212:LYS:HA	79:AR:235:ILE:HD11	2.00	0.44
3:D:168:C:H2'	3:D:169:G:C8	2.53	0.43
3:D:208:A:H2	3:D:233:U:H5''	1.83	0.43
3:D:958:G:O2'	10:K:123:ARG:O	2.27	0.43
3:D:1092:G:H2'	3:D:1093:C:C6	2.53	0.43
3:D:4910:G:H4'	7:H:95:THR:HG22	2.00	0.43
8:I:178:ASN:HA	8:I:181:LYS:HG2	2.00	0.43
48:w:106:C:H2'	48:w:107:A:C8	2.53	0.43
48:w:454:U:H2'	48:w:455:A:C8	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:900:C:H3'	48:w:901:G:C8	2.53	0.43
48:w:1378:A:H4'	48:w:1379:A:O5'	2.18	0.43
52:0:60:GLY:HA3	52:0:64:ARG:HG2	2.00	0.43
53:1:63:LYS:NZ	72:AK:84:LYS:O	2.49	0.43
54:2:47:LYS:NZ	64:AC:115:TYR:O	2.45	0.43
65:AD:54:VAL:O	65:AD:58:MET:HG2	2.16	0.43
69:AH:80:SER:O	69:AH:82:ASN:N	2.51	0.43
79:AR:252:THR:HG21	79:AR:257:LYS:HE3	1.99	0.43
3:D:68:U:OP1	18:S:178:HIS:ND1	2.35	0.43
3:D:662:C:H2'	3:D:663:G:N9	2.31	0.43
3:D:1577:G:H5'	3:D:1578:U:H5''	2.01	0.43
3:D:2479:G:H2'	3:D:2480:G:H8	1.83	0.43
3:D:2520:C:H2'	3:D:2521:G:C8	2.53	0.43
5:F:141:C:H2'	5:F:142:U:H6	1.83	0.43
7:H:29:VAL:HG13	7:H:348:ARG:HD3	2.00	0.43
8:I:67:TRP:HB2	8:I:71:ARG:HH11	1.83	0.43
14:O:32:ARG:HD3	14:O:32:ARG:HA	1.75	0.43
14:O:36:LEU:HD11	14:O:69:ARG:HD2	1.99	0.43
15:P:94:LEU:O	15:P:174:ILE:HA	2.17	0.43
16:Q:65:ARG:HG3	31:f:69:PHE:CG	2.52	0.43
48:w:92:A:H1'	53:1:3:ARG:HB3	2.00	0.43
48:w:448:A:H5''	57:5:25:ARG:HA	1.99	0.43
48:w:458:A:H2'	48:w:459:C:C6	2.53	0.43
48:w:1476:A:H5'	48:w:1477:U:OP1	2.18	0.43
51:z:67:GLY:HA2	51:z:93:ILE:HD11	1.99	0.43
52:0:132:LYS:HD3	52:0:156:LEU:HD12	2.00	0.43
53:1:95:THR:HG21	72:AK:16:ARG:NE	2.30	0.43
57:5:157:LYS:HE2	57:5:157:LYS:HB2	1.83	0.43
66:AE:82:TRP:CD1	66:AE:82:TRP:H	2.35	0.43
68:AG:96:GLU:HG2	68:AG:97:ILE:HG23	1.99	0.43
3:D:6:C:H2'	3:D:7:C:C6	2.53	0.43
3:D:1244:G:H2'	3:D:1245:C:C6	2.52	0.43
3:D:1443:A:C6	3:D:2103:G:C6	3.06	0.43
3:D:3684:G:H2'	3:D:3685:C:C6	2.54	0.43
3:D:3868:G:H22	3:D:3900:G:H1'	1.83	0.43
3:D:4541:G:N2	3:D:4544:A:OP2	2.41	0.43
3:D:5001:PSU:H2'	3:D:5002:U:O4'	2.17	0.43
9:J:79:TYR:O	9:J:82:GLU:HG2	2.18	0.43
10:K:118:THR:HG21	35:j:92:ASN:OD1	2.18	0.43
13:N:61:TRP:CZ3	17:R:33:GLN:HG3	2.53	0.43
14:O:208:LYS:HA	14:O:211:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:75:VAL:HG21	18:S:80:THR:HG22	1.99	0.43
33:h:56:ARG:O	33:h:60:ILE:HG12	2.19	0.43
36:k:106:TYR:O	36:k:108:SER:N	2.51	0.43
39:n:64:SER:O	39:n:64:SER:OG	2.28	0.43
48:w:641:A:H2'	48:w:642:U:O4'	2.18	0.43
48:w:816:A:OP2	58:6:10:ARG:NH2	2.51	0.43
48:w:1278:A:H2'	48:w:1279:C:C6	2.54	0.43
52:0:51:LEU:HD12	52:0:91:VAL:HG12	2.00	0.43
56:4:80:VAL:HG22	56:4:92:VAL:HG23	1.99	0.43
57:5:174:CYS:HB2	57:5:190:LEU:HD21	2.00	0.43
63:AB:136:THR:HG22	63:AB:138:SER:N	2.33	0.43
70:AI:25:VAL:HG22	70:AI:63:VAL:HB	2.00	0.43
3:D:268:G:H2'	3:D:269:G:C8	2.46	0.43
3:D:1077:C:H4'	3:D:1215:C:C4	2.52	0.43
3:D:2083:C:P	21:V:14:ARG:HH12	2.40	0.43
3:D:2422:OMC:HM23	3:D:2422:OMC:H1'	1.88	0.43
3:D:4968:A:H2'	3:D:4969:C:C6	2.53	0.43
15:P:114:ASP:OD2	66:AE:14:ARG:NH2	2.51	0.43
17:R:118:MET:HE3	17:R:122:ILE:HG13	2.01	0.43
39:n:16:LYS:HD3	39:n:16:LYS:HA	1.78	0.43
42:q:24:PRO:HG2	42:q:27:ILE:HG12	1.99	0.43
48:w:830:A:N1	48:w:831:G:C4	2.86	0.43
48:w:1134:G:H2'	48:w:1135:C:C6	2.54	0.43
48:w:1407:U:H4'	64:AC:71:ARG:NH2	2.33	0.43
48:w:1437:C:H5''	48:w:1438:A:OP2	2.18	0.43
50:y:32:ASP:OD1	50:y:33:VAL:N	2.51	0.43
52:0:49:ILE:HA	52:0:87:TYR:O	2.18	0.43
55:3:177:GLN:HG3	55:3:178:ARG:H	1.83	0.43
58:6:97:ILE:H	58:6:97:ILE:HD12	1.83	0.43
58:6:176:LYS:HA	58:6:179:LYS:HG2	2.01	0.43
59:7:79:LEU:HG	59:7:83:LEU:HD12	1.99	0.43
62:AA:71:PRO:HB3	62:AA:114:SER:OG	2.18	0.43
73:AL:68:ILE:HB	73:AL:109:TYR:HB2	1.99	0.43
73:AL:91:LEU:HD11	73:AL:96:LEU:HD22	2.00	0.43
79:AR:114:SER:HB3	79:AR:119:GLN:H	1.83	0.43
3:D:1732:C:O2'	3:D:1733:G:H5'	2.18	0.43
3:D:2543:A:H2'	3:D:2544:G:O4'	2.18	0.43
4:E:58:A:H2'	4:E:59:G:C8	2.54	0.43
19:T:81:TRP:HB2	19:T:104:VAL:HG11	2.01	0.43
39:n:75:LYS:HA	39:n:75:LYS:HD2	1.84	0.43
48:w:561:A:N3	58:6:132:GLN:NE2	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1349:G:H2'	48:w:1350:U:C6	2.53	0.43
48:w:1372:U:OP1	48:w:1385:G:N2	2.42	0.43
52:0:99:ILE:HG23	52:0:173:ARG:HH21	1.84	0.43
52:0:210:ILE:HD11	65:AD:20:TYR:CE1	2.54	0.43
56:4:101:LEU:HD22	56:4:116:ARG:HD3	2.00	0.43
58:6:54:ARG:HG2	58:6:58:ARG:NH1	2.33	0.43
68:AG:107:GLU:HG2	68:AG:108:PRO:HD3	2.01	0.43
76:AO:31:ARG:HH22	76:AO:43:ILE:HD11	1.83	0.43
79:AR:253:GLY:O	79:AR:286:CYS:N	2.51	0.43
3:D:151:G:O6	12:M:142:THR:HG23	2.19	0.43
3:D:920:C:H2'	3:D:921:C:H6	1.83	0.43
3:D:2490:U:H3'	3:D:2491:C:O4'	2.16	0.43
3:D:3860:A:N3	20:U:131:ARG:NH1	2.59	0.43
5:F:23:C:OP2	29:d:15:ARG:NE	2.39	0.43
13:N:115:ARG:O	13:N:116:ASN:C	2.62	0.43
37:l:19:LYS:HA	37:l:19:LYS:HD3	1.76	0.43
38:m:4:ILE:O	38:m:4:ILE:HG13	2.17	0.43
48:w:173:A:H2'	48:w:174:OMC:O4'	2.18	0.43
48:w:1311:C:H2'	48:w:1312:G:C8	2.53	0.43
48:w:1408:U:H4'	64:AC:24:HIS:CE1	2.54	0.43
49:x:145:ILE:HG13	49:x:159:ILE:HB	2.00	0.43
52:0:156:LEU:O	52:0:157:MET:HE2	2.19	0.43
53:1:52:LEU:CD1	53:1:99:PHE:HE2	2.31	0.43
54:2:102:LEU:HD11	73:AL:67:LEU:HD13	2.01	0.43
54:2:113:VAL:HA	54:2:116:ILE:HG12	1.99	0.43
56:4:10:LYS:HE2	56:4:46:THR:O	2.19	0.43
56:4:134:VAL:HG12	56:4:173:PHE:CE2	2.54	0.43
65:AD:71:ILE:HG13	65:AD:72:LYS:N	2.34	0.43
72:AK:56:PHE:HD1	72:AK:94:HIS:CD2	2.37	0.43
75:AN:56:CYS:SG	75:AN:59:CYS:HB2	2.59	0.43
3:D:277:G:N7	39:n:29:ARG:NH2	2.63	0.43
3:D:424:U:H2'	3:D:425:U:C6	2.53	0.43
3:D:1294:A:H1'	3:D:1296:G:N1	2.33	0.43
3:D:1375:C:O2'	3:D:1376:C:H5'	2.17	0.43
3:D:1401:C:H2'	3:D:1402:C:H6	1.84	0.43
3:D:3641:U:OP2	3:D:3646:A:N6	2.48	0.43
3:D:3877:A:N3	3:D:4401:G:O2'	2.39	0.43
3:D:4095:G:O6	3:D:4113:U:O4	2.36	0.43
10:K:50:LEU:HD23	10:K:50:LEU:H	1.84	0.43
15:P:144:LYS:HE2	15:P:146:ARG:O	2.19	0.43
34:i:36:VAL:HG11	34:i:44:ARG:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:t:104:ILE:HA	45:t:105:GLN:HA	1.69	0.43
45:t:105:GLN:HG3	45:t:106:PHE:H	1.83	0.43
48:w:811:A:HO2'	48:w:812:A:P	2.42	0.43
48:w:830:A:H3'	48:w:830:A:N3	2.33	0.43
48:w:1199:A:OP1	74:AM:2:THR:N	2.52	0.43
48:w:1413:G:H2'	48:w:1414:A:H8	1.83	0.43
50:y:225:LEU:O	50:y:229:MET:HG2	2.19	0.43
79:AR:249:CYS:SG	79:AR:291:TRP:NE1	2.88	0.43
3:D:406:C:HO2'	3:D:407:A:P	2.41	0.43
3:D:674:G:H2'	3:D:675:C:C6	2.54	0.43
3:D:1196:G:H2'	3:D:1197:C:C6	2.54	0.43
3:D:1480:C:O2'	3:D:1482:G:OP2	2.36	0.43
3:D:2264:C:H2'	3:D:2265:G:O4'	2.18	0.43
3:D:3688:U:OP2	6:G:198:ARG:NH1	2.51	0.43
3:D:4137:C:H2'	3:D:4138:C:H6	1.83	0.43
12:M:156:VAL:O	12:M:156:VAL:HG12	2.19	0.43
15:P:35:ARG:HB2	15:P:126:TYR:OH	2.19	0.43
15:P:111:GLU:OE1	66:AE:14:ARG:NH2	2.51	0.43
26:a:65:VAL:HG23	26:a:73:ARG:HA	2.01	0.43
30:e:83:THR:HG23	37:l:95:PHE:CZ	2.54	0.43
48:w:95:G:N2	48:w:474:G:OP2	2.51	0.43
48:w:291:G:H1'	48:w:292:A:H2'	2.01	0.43
48:w:371:A:OP2	57:5:10:LYS:HB2	2.19	0.43
48:w:1491:G:H2'	48:w:1492:U:C6	2.54	0.43
48:w:1747:C:H2'	48:w:1748:G:O4'	2.19	0.43
53:1:145:ARG:NH1	53:1:162:ILE:HG21	2.34	0.43
58:6:135:ILE:O	58:6:141:VAL:HG23	2.18	0.43
62:AA:42:VAL:HG23	62:AA:43:HIS:N	2.33	0.43
62:AA:56:VAL:HA	62:AA:60:MET:HE2	2.00	0.43
65:AD:119:VAL:HG12	65:AD:120:THR:N	2.34	0.43
75:AN:33:MET:HE3	75:AN:73:LEU:HD21	2.01	0.43
3:D:2351:OMC:HM23	8:I:95:MET:HG3	2.00	0.43
3:D:3724:A2M:HM'3	3:D:3724:A2M:H1'	1.60	0.43
3:D:3732:A:H2'	3:D:3733:A:H8	1.83	0.43
3:D:4459:U:H2'	3:D:4460:U:H6	1.81	0.43
5:F:66:A:H2'	5:F:67:U:C6	2.54	0.43
6:G:116:LEU:HB2	6:G:126:LEU:HB2	2.01	0.43
9:J:179:ARG:HA	9:J:179:ARG:HD3	1.83	0.43
9:J:211:LEU:HD23	9:J:211:LEU:HA	1.88	0.43
22:W:16:ARG:NH1	37:l:29:ARG:HH12	2.16	0.43
32:g:16:TRP:CD1	32:g:21:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:352:U:H2'	48:w:353:C:C6	2.54	0.43
48:w:504:G:H2'	48:w:504:G:N3	2.33	0.43
48:w:561:A:C3'	58:6:134:HIS:HE2	2.32	0.43
56:4:8:ILE:H	56:4:8:ILE:HD12	1.84	0.43
57:5:165:GLN:NE2	57:5:172:LEU:HD23	2.33	0.43
70:AI:25:VAL:O	70:AI:62:VAL:HA	2.19	0.43
72:AK:114:MET:HE2	72:AK:122:LYS:HD3	2.00	0.43
79:AR:104:HIS:CE1	79:AR:122:SER:HB3	2.54	0.43
3:D:10:A:H2'	3:D:11:G:H8	1.83	0.43
3:D:658:C:C4	3:D:659:G:C8	3.07	0.43
3:D:741:C:H42	3:D:923:C:H42	1.66	0.43
3:D:1464:C:H5''	32:g:32:LEU:HD12	2.00	0.43
3:D:1778:C:H4'	9:J:4:VAL:O	2.19	0.43
3:D:2415:OMU:HM23	3:D:2415:OMU:H1'	1.51	0.43
4:E:11:A:O2'	4:E:13:A:OP2	2.27	0.43
6:G:206:PRO:HD3	6:G:213:GLY:CA	2.48	0.43
15:P:44:THR:HG21	15:P:72:CYS:SG	2.59	0.43
15:P:169:LYS:HD3	15:P:170:TYR:HB2	2.01	0.43
26:a:87:SER:HA	26:a:97:TYR:HB3	2.01	0.43
29:d:65:GLN:O	29:d:65:GLN:HG3	2.19	0.43
30:e:101:PHE:C	30:e:102:ARG:HD3	2.44	0.43
39:n:44:ILE:HD13	39:n:44:ILE:HA	1.86	0.43
48:w:179:C:C2	48:w:180:G:C8	3.07	0.43
50:y:146:ARG:HB2	50:y:149:GLN:HB2	2.01	0.43
51:z:64:THR:O	51:z:68:ARG:HG3	2.18	0.43
52:0:9:ARG:HA	52:0:12:VAL:HG12	2.01	0.43
53:1:18:TRP:N	53:1:18:TRP:CD1	2.86	0.43
55:3:67:VAL:CG2	55:3:99:GLY:HA2	2.49	0.43
56:4:31:GLU:HB3	56:4:41:ARG:NH2	2.34	0.43
58:6:94:LEU:HD23	58:6:94:LEU:H	1.83	0.43
62:AA:28:PHE:HA	62:AA:92:ALA:O	2.18	0.43
67:AF:21:PHE:O	67:AF:25:SER:OG	2.29	0.43
72:AK:54:VAL:HG22	72:AK:76:TYR:HB2	2.01	0.43
73:AL:49:LEU:HD12	73:AL:49:LEU:HA	1.90	0.43
79:AR:68:ASP:HB2	79:AR:110:SER:HA	2.00	0.43
3:D:1:C:H42	5:F:156:U:H3	0.63	0.42
3:D:126:C:H2'	3:D:127:G:H8	1.83	0.42
3:D:683:C:H2'	3:D:684:G:O4'	2.18	0.42
3:D:987:C:H2'	3:D:988:C:C6	2.53	0.42
3:D:1306:C:H2'	3:D:1307:A:H8	1.83	0.42
3:D:2079:G:H2'	3:D:2080:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2484:A:H3'	3:D:2485:U:O4'	2.19	0.42
3:D:3664:G:H2'	3:D:3665:G:H8	1.84	0.42
3:D:3744:OMG:HM23	3:D:3744:OMG:H1'	1.78	0.42
5:F:67:U:H2'	5:F:68:G:H8	1.84	0.42
15:P:35:ARG:O	15:P:39:VAL:HG23	2.19	0.42
30:e:83:THR:HG22	30:e:85:TYR:HD1	1.83	0.42
48:w:590:A2M:H1'	48:w:590:A2M:HM'3	1.70	0.42
48:w:616:A:H1'	78:AQ:85:VAL:CG2	2.49	0.42
48:w:633:C:O2'	78:AQ:89:THR:HG21	2.19	0.42
48:w:1380:C:H2'	48:w:1381:G:O4'	2.18	0.42
48:w:1859:A:O2'	48:w:1860:A:H5'	2.19	0.42
51:z:121:ARG:HH12	51:z:123:ARG:NH2	2.16	0.42
58:6:55:LYS:O	58:6:59:GLU:OE1	2.37	0.42
68:AG:46:LYS:NZ	68:AG:100:GLN:OE1	2.43	0.42
74:AM:67:LEU:HD12	74:AM:67:LEU:HA	1.91	0.42
79:AR:168:CYS:HB3	79:AR:198:VAL:HG13	2.00	0.42
3:D:1095:A:H2'	3:D:1096:C:H6	1.84	0.42
3:D:2101:C:H3'	3:D:2102:G:C2	2.54	0.42
3:D:4968:A:H2'	3:D:4969:C:H6	1.83	0.42
4:E:39:C:N3	15:P:73:THR:HG22	2.33	0.42
7:H:238:LYS:HE2	7:H:238:LYS:HB2	1.84	0.42
28:c:129:ARG:HD3	28:c:135:LYS:HD2	2.00	0.42
32:g:16:TRP:HD1	32:g:21:ILE:HD11	1.83	0.42
48:w:89:C:O2'	48:w:499:G:H5''	2.18	0.42
48:w:801:PSU:C4	48:w:802:A:C8	3.07	0.42
48:w:890:U:P	48:w:897:U:H3	2.42	0.42
48:w:1748:G:H2'	48:w:1749:G:H8	1.84	0.42
48:w:1778:C:H2'	48:w:1779:G:C8	2.55	0.42
48:w:1861:G:H5''	74:AM:3:LYS:HA	2.02	0.42
54:2:25:THR:HG21	54:2:46:ALA:HB1	2.00	0.42
61:9:4:MET:HE3	61:9:121:ARG:HE	1.85	0.42
61:9:83:ASP:OD1	61:9:83:ASP:N	2.51	0.42
79:AR:214:GLY:HA2	79:AR:236:ILE:HG12	2.00	0.42
2:B:23:A:H2'	2:B:24:G:H8	1.82	0.42
3:D:4635:A:H8	3:D:5048:A:N6	2.16	0.42
7:H:36:ASP:HA	7:H:37:PRO:HD3	1.88	0.42
7:H:214:ASP:N	7:H:214:ASP:OD1	2.52	0.42
13:N:37:ASP:OD1	13:N:39:ASN:ND2	2.52	0.42
20:U:32:THR:HA	20:U:58:VAL:HG21	2.01	0.42
48:w:164:A:H2'	48:w:165:G:C4	2.55	0.42
48:w:468:A2M:HM'3	48:w:468:A2M:H1'	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:554:A:H2'	48:w:555:A:C8	2.54	0.42
48:w:656:G:H21	48:w:663:C:H5''	1.84	0.42
48:w:1018:U:H5''	61:9:71:ILE:HD12	2.02	0.42
48:w:1700:C:C2	48:w:1834:A:N6	2.87	0.42
49:x:41:ARG:HB2	49:x:47:TYR:CD1	2.54	0.42
54:2:126:THR:HG23	54:2:128:ILE:HG13	2.01	0.42
55:3:10:THR:HB	55:3:129:VAL:H	1.83	0.42
55:3:41:LEU:HD23	55:3:41:LEU:H	1.84	0.42
57:5:89:GLU:O	57:5:93:THR:HG22	2.19	0.42
63:AB:54:HIS:HA	63:AB:57:LEU:HD23	2.01	0.42
64:AC:128:GLU:OE2	64:AC:138:ARG:NH2	2.52	0.42
72:AK:37:LYS:HE3	72:AK:58:PHE:HA	2.02	0.42
79:AR:284:PRO:O	79:AR:285:GLN:NE2	2.50	0.42
2:B:4:U:O2'	2:B:5:C:H6	2.02	0.42
3:D:171:U:H2'	3:D:172:C:H4'	2.01	0.42
3:D:1601:A:O2'	40:o:2:THR:HG21	2.19	0.42
3:D:1677:PSU:H4'	3:D:1680:G:C2	2.55	0.42
3:D:1777:C:H2'	3:D:1778:C:C6	2.55	0.42
3:D:3896:C:H1'	7:H:268:ARG:NH1	2.34	0.42
3:D:4503:A:H2'	3:D:4504:C:C6	2.55	0.42
3:D:4730:C:H1'	3:D:4731:G:C2	2.54	0.42
13:N:21:LYS:HB2	13:N:24:THR:OG1	2.20	0.42
17:R:50:MET:HE3	17:R:50:MET:HB2	1.96	0.42
48:w:159:A2M:H1'	48:w:159:A2M:HM'3	1.57	0.42
48:w:678:U:H2'	48:w:679:A:C8	2.53	0.42
52:0:135:GLU:HG2	52:0:153:VAL:CG1	2.49	0.42
55:3:85:ARG:O	55:3:87:ARG:NH1	2.53	0.42
3:D:137:G:H2'	3:D:138:G:H8	1.84	0.42
3:D:1437:C:H2'	3:D:1438:U:C2	2.55	0.42
3:D:1443:A:N6	3:D:2103:G:C6	2.87	0.42
3:D:2333:G:N7	8:I:189:MET:HE3	2.34	0.42
3:D:3713:U:H2'	3:D:3714:G:H8	1.84	0.42
8:I:334:THR:HG21	11:L:51:TYR:OH	2.20	0.42
11:L:80:ASN:HB3	24:Y:141:VAL:O	2.19	0.42
15:P:113:ILE:HG21	15:P:119:TYR:HD1	1.84	0.42
16:Q:65:ARG:HG3	31:f:69:PHE:CD2	2.54	0.42
17:R:32:ASP:HA	23:X:145:PHE:CZ	2.54	0.42
32:g:54:LEU:HA	32:g:57:MET:HE3	2.02	0.42
36:k:93:PRO:C	36:k:95:LYS:H	2.27	0.42
48:w:179:C:C4	48:w:180:G:C5	3.07	0.42
48:w:1114:U:O2'	48:w:1115:U:H2'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2:97:PHE:HD1	54:2:108:PRO:CB	2.33	0.42
58:6:17:ARG:H	58:6:17:ARG:HG2	1.70	0.42
59:7:37:ASP:OD1	59:7:37:ASP:N	2.52	0.42
68:AG:26:SER:HB3	68:AG:32:LEU:HG	2.01	0.42
79:AR:65:PHE:O	79:AR:82:SER:HB2	2.20	0.42
79:AR:152:SER:HB2	79:AR:168:CYS:SG	2.59	0.42
3:D:659:G:C6	3:D:660:A:N6	2.87	0.42
3:D:1246:G:H2'	3:D:1247:U:C6	2.54	0.42
3:D:1248:C:H2'	3:D:1249:C:C6	2.54	0.42
3:D:1301:C:H2'	3:D:1302:U:H4'	2.00	0.42
3:D:4173:G:H2'	3:D:4174:U:H6	1.83	0.42
3:D:4192:A:H2'	3:D:4193:C:H6	1.84	0.42
3:D:4768:G:OP1	19:T:168:TYR:OH	2.35	0.42
4:E:3:C:H2'	4:E:4:U:C6	2.54	0.42
6:G:181:LYS:HB2	6:G:184:ARG:HG3	2.01	0.42
8:I:218:ILE:HA	8:I:229:LEU:HD22	2.01	0.42
12:M:102:TYR:OH	12:M:208:ASN:HB2	2.20	0.42
13:N:46:SER:O	13:N:55:LEU:HD12	2.19	0.42
16:Q:200:LYS:O	16:Q:204:GLU:HG2	2.19	0.42
37:l:60:ARG:HA	37:l:60:ARG:HD2	1.91	0.42
48:w:112:U:H2'	48:w:115:U:H5	1.85	0.42
48:w:1215:C:O2'	48:w:1645:C:OP2	2.38	0.42
48:w:1471:C:N4	48:w:1476:A:N6	2.35	0.42
48:w:1842:4AC:O7	48:w:1842:4AC:H5	2.20	0.42
55:3:167:LYS:HB3	55:3:167:LYS:HE3	1.69	0.42
60:8:122:ILE:HD12	60:8:122:ILE:H	1.84	0.42
63:AB:136:THR:HG22	63:AB:138:SER:H	1.85	0.42
71:AJ:51:VAL:HG13	71:AJ:70:VAL:HG13	2.01	0.42
75:AN:20:LYS:HG3	75:AN:21:LYS:N	2.35	0.42
79:AR:176:VAL:HG23	79:AR:185:LYS:CB	2.49	0.42
3:D:1095:A:H2'	3:D:1096:C:C6	2.55	0.42
3:D:1207:C:C2	3:D:1208:G:C8	3.07	0.42
3:D:4196:OMG:H1'	3:D:4196:OMG:HM23	1.73	0.42
5:F:16:G:O2'	5:F:17:A:O5'	2.34	0.42
8:I:318:PRO:C	8:I:320:LYS:H	2.28	0.42
11:L:87:PRO:HG2	11:L:144:TYR:CE2	2.55	0.42
17:R:104:MET:O	17:R:109:ARG:NH2	2.52	0.42
19:T:151:ALA:O	19:T:155:THR:HG23	2.20	0.42
19:T:181:ALA:O	19:T:185:VAL:HG22	2.20	0.42
48:w:154:U:H2'	48:w:155:G:C1'	2.49	0.42
48:w:1203:G:H2'	48:w:1204:A:N3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1540:G:C6	48:w:1594:A:C6	3.08	0.42
48:w:1598:G:N7	73:AL:82:SER:N	2.67	0.42
48:w:1619:A:OP2	63:AB:47:ARG:NH2	2.53	0.42
51:z:95:ASP:OD2	51:z:95:ASP:N	2.52	0.42
59:7:16:PHE:HB2	59:7:79:LEU:HD21	2.01	0.42
70:AI:77:PRO:HG2	70:AI:79:PHE:CE2	2.54	0.42
71:AJ:138:LYS:HD2	71:AJ:139:GLU:H	1.85	0.42
73:AL:69:THR:H	73:AL:72:VAL:HG12	1.85	0.42
3:D:295:A:OP2	45:t:39:ARG:NH1	2.52	0.42
3:D:449:C:H4'	3:D:450:G:OP2	2.20	0.42
3:D:646:G:H3'	3:D:647:G:H8	1.85	0.42
3:D:660:A:H2'	3:D:661:C:O4'	2.20	0.42
3:D:1098:G:H2'	3:D:1099:C:C6	2.54	0.42
3:D:1407:C:O2	3:D:1409:C:H1'	2.20	0.42
3:D:1693:U:H2'	3:D:1694:C:O4'	2.20	0.42
3:D:1855:G:OP1	32:g:4:SER:HB2	2.18	0.42
3:D:2364:OMG:H1'	3:D:2364:OMG:HM23	1.68	0.42
3:D:2469:C:H5'	3:D:2470:C:OP2	2.19	0.42
3:D:2477:A:H2'	3:D:2478:C:H6	1.84	0.42
3:D:4127:A:N1	12:M:37:LYS:HG2	2.35	0.42
3:D:4906:C:H2'	3:D:4907:G:C8	2.55	0.42
3:D:4980:C:N3	20:U:69:ARG:NH2	2.68	0.42
5:F:82:A:H5''	5:F:85:U:O2	2.19	0.42
7:H:297:LYS:HD2	7:H:297:LYS:C	2.45	0.42
20:U:21:ASN:HB3	20:U:145:HIS:CE1	2.54	0.42
25:Z:80:LYS:HE3	25:Z:108:GLU:HA	2.02	0.42
45:t:85:ILE:HG22	45:t:86:LYS:H	1.83	0.42
46:u:38:THR:HA	46:u:45:THR:HA	2.01	0.42
48:w:360:A:N6	48:w:400:C:O2'	2.53	0.42
48:w:615:C:OP2	71:AJ:64:SER:OG	2.28	0.42
48:w:1472:C:H2'	48:w:1473:G:O4'	2.19	0.42
48:w:1501:C:H2'	48:w:1502:C:H6	1.85	0.42
49:x:178:LEU:O	49:x:182:VAL:HG13	2.20	0.42
50:y:122:GLU:HG2	50:y:140:VAL:HG12	2.02	0.42
52:0:5:ILE:HD11	52:0:9:ARG:HD2	2.02	0.42
53:1:93:ASP:OD1	53:1:94:LYS:N	2.52	0.42
65:AD:44:LYS:HG3	65:AD:47:ARG:NH2	2.33	0.42
72:AK:88:LYS:HD3	72:AK:91:LEU:HD12	2.01	0.42
73:AL:74:SER:OG	73:AL:79:ILE:O	2.29	0.42
77:AP:30:LEU:HA	77:AP:39:CYS:HA	2.01	0.42
3:D:187:U:O2'	3:D:189:G:OP2	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1443:A:H2'	3:D:1444:G:O4'	2.19	0.42
3:D:2348:G:OP1	3:D:2351:OMC:N4	2.49	0.42
3:D:2724:G:O2'	3:D:2726:G:OP2	2.38	0.42
3:D:4065:G:H2'	3:D:4066:U:C6	2.55	0.42
3:D:4070:U:H2'	3:D:4071:U:C6	2.55	0.42
3:D:4097:G:O2'	3:D:4098:A:O5'	2.36	0.42
7:H:14:LEU:O	7:H:17:LEU:HB2	2.20	0.42
9:J:166:ALA:HB1	9:J:171:LEU:HD12	2.02	0.42
28:c:112:ALA:O	28:c:116:LEU:HG	2.19	0.42
48:w:519:A:O3'	58:6:11:LYS:HG3	2.20	0.42
48:w:803:C:H2'	48:w:804:U:H6	1.84	0.42
48:w:910:G:H2'	48:w:911:C:C6	2.55	0.42
48:w:980:A:H2'	48:w:981:A:C8	2.54	0.42
48:w:1809:A:H2'	48:w:1810:U:C6	2.55	0.42
52:0:61:GLU:N	52:0:64:ARG:HG2	2.34	0.42
58:6:88:ASP:OD1	58:6:91:LYS:HG2	2.19	0.42
79:AR:120:ILE:O	79:AR:131:LEU:HA	2.20	0.42
79:AR:149:GLU:N	79:AR:171:ASP:OD2	2.46	0.42
3:D:75:G:N7	16:Q:102:ARG:HG2	2.35	0.42
3:D:271:C:H2'	3:D:272:U:H6	1.85	0.42
3:D:462:G:H2'	3:D:463:A:H8	1.82	0.42
3:D:1087:A:H2'	3:D:1088:C:C6	2.55	0.42
3:D:1309:C:H2'	3:D:1310:C:C6	2.55	0.42
3:D:2486:G:N1	3:D:2493:G:N7	2.67	0.42
3:D:2611:A:H2'	3:D:2612:G:C8	2.55	0.42
3:D:3825:A2M:HM'3	3:D:3825:A2M:HI1'	1.85	0.42
3:D:4115:G:O2'	3:D:4116:C:P	2.78	0.42
3:D:4996:C:H4'	34:i:26:THR:HG23	2.01	0.42
4:E:4:U:H2'	4:E:5:A:H8	1.85	0.42
7:H:219:VAL:HG11	7:H:337:VAL:CG2	2.49	0.42
7:H:295:ASP:HA	7:H:296:GLY:HA2	1.77	0.42
15:P:39:VAL:HG22	15:P:123:ILE:HD12	2.02	0.42
15:P:151:ILE:HG13	15:P:152:GLY:N	2.35	0.42
19:T:74:ARG:HD3	19:T:146:GLY:O	2.19	0.42
30:e:87:VAL:HG12	30:e:127:ASN:ND2	2.34	0.42
34:i:68:LEU:HD22	34:i:106:VAL:O	2.19	0.42
35:j:109:LYS:O	35:j:113:GLU:HG2	2.20	0.42
43:r:79:GLU:OE2	43:r:82:LEU:HG	2.20	0.42
48:w:78:C:HI1'	55:3:175:LYS:HG3	2.02	0.42
48:w:551:U:H2'	48:w:552:G:C1'	2.50	0.42
48:w:573:U:N3	48:w:576:A2M:OP2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:835:C:N4	72:AK:9:THR:O	2.53	0.42
48:w:1101:U:H2'	48:w:1102:G:H8	1.84	0.42
48:w:1374:C:H2'	48:w:1375:G:O4'	2.19	0.42
56:4:130:LEU:HD21	56:4:156:VAL:HG21	2.01	0.42
57:5:100:CYS:HB3	57:5:175:ILE:HD12	2.02	0.42
58:6:101:LYS:HZ3	58:6:103:GLU:CD	2.27	0.42
60:8:79:LYS:HB2	60:8:87:VAL:HG12	2.02	0.42
65:AD:105:MET:HE2	65:AD:105:MET:HB3	1.90	0.42
66:AE:80:PRO:HG2	67:AF:36:THR:HG21	2.02	0.42
66:AE:89:ASP:O	66:AE:92:ASP:N	2.52	0.42
72:AK:20:ARG:HG3	72:AK:76:TYR:CE2	2.55	0.42
72:AK:114:MET:CE	72:AK:122:LYS:HD3	2.49	0.42
74:AM:36:ILE:HB	74:AM:73:TYR:HB2	2.01	0.42
3:D:1412:G:C6	3:D:1413:C:N4	2.87	0.41
3:D:2461:G:H2'	3:D:2462:C:C6	2.55	0.41
3:D:4424:A:OP2	43:r:97:ARG:NH2	2.53	0.41
4:E:3:C:H2'	4:E:4:U:H6	1.85	0.41
33:h:37:MET:HG3	33:h:97:ILE:HD11	2.00	0.41
48:w:551:U:H2'	48:w:552:G:O4'	2.20	0.41
48:w:597:G:H2'	48:w:598:G:O4'	2.20	0.41
48:w:1274:G:H4'	59:7:47:LYS:NZ	2.35	0.41
48:w:1288:OMU:H2'	48:w:1289:U:C6	2.55	0.41
48:w:1320:G:H2'	48:w:1321:G:O4'	2.21	0.41
48:w:1436:C:H1'	48:w:1438:A:H5'	2.02	0.41
49:x:154:LEU:HD22	49:x:157:VAL:HG11	2.02	0.41
59:7:53:LYS:HE2	59:7:60:GLU:OE1	2.19	0.41
64:AC:12:VAL:HG22	64:AC:23:ALA:HB3	2.02	0.41
66:AE:73:ASN:HB3	66:AE:76:GLN:NE2	2.35	0.41
67:AF:124:THR:OG1	67:AF:125:PRO:HD2	2.20	0.41
71:AJ:98:ASP:OD1	71:AJ:140:ARG:NH1	2.51	0.41
77:AP:38:MET:HG2	77:AP:42:CYS:SG	2.59	0.41
79:AR:16:GLY:H	79:AR:305:ASN:CB	2.33	0.41
79:AR:17:TRP:HB2	79:AR:303:THR:HA	2.01	0.41
79:AR:199:THR:OG1	79:AR:239:LEU:O	2.29	0.41
79:AR:304:ASP:OD1	79:AR:304:ASP:N	2.44	0.41
3:D:650:C:H2'	3:D:651:C:H6	1.84	0.41
3:D:1314:C:C2	3:D:1315:C:C5	3.08	0.41
3:D:1727:U:H2'	3:D:1728:U:C6	2.55	0.41
3:D:2566:G:C4	3:D:2567:G:C8	3.08	0.41
3:D:4281:A:O2'	3:D:4282:A:H2'	2.20	0.41
3:D:4773:C:O2'	3:D:4774:C:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:119:U:H5''	4:E:120:U:H5''	2.01	0.41
7:H:224:LYS:HG2	7:H:340:THR:HG22	2.01	0.41
7:H:359:ALA:C	7:H:360:LEU:HD23	2.45	0.41
21:V:88:ASP:HB3	21:V:109:ALA:HB2	2.00	0.41
32:g:5:LYS:HE3	32:g:8:THR:HB	2.02	0.41
40:o:32:SER:O	40:o:40:PRO:HG3	2.20	0.41
48:w:1204:A:H2'	48:w:1205:C:O4'	2.20	0.41
48:w:1466:G:OP1	65:AD:5:ARG:HG2	2.21	0.41
48:w:1639:G7M:O2'	48:w:1640:A:OP1	2.36	0.41
50:y:36:PRO:HD3	50:y:98:THR:OG1	2.20	0.41
53:l:56:LEU:N	53:l:60:GLU:OE2	2.46	0.41
63:AB:56:LEU:HD22	63:AB:80:LEU:HD12	2.03	0.41
68:AG:32:LEU:HA	68:AG:32:LEU:HD23	1.67	0.41
71:AJ:51:VAL:HG22	71:AJ:70:VAL:HG11	2.01	0.41
72:AK:49:LYS:HE2	72:AK:49:LYS:HB2	1.93	0.41
79:AR:194:TYR:CE2	79:AR:212:LYS:HD3	2.55	0.41
3:D:138:G:H2'	3:D:139:G:H8	1.85	0.41
3:D:175:C:H2'	3:D:176:G:H8	1.86	0.41
3:D:407:A:O2'	3:D:410:A:OP1	2.34	0.41
3:D:505:G:H2'	3:D:506:C:H6	1.85	0.41
3:D:967:C:H2'	10:K:110:ARG:NH2	2.35	0.41
3:D:1590:C:H5''	3:D:1591:U:O5'	2.19	0.41
3:D:2096:G:N3	3:D:2096:G:H2'	2.35	0.41
3:D:2096:G:O2'	3:D:2098:G:O2'	2.38	0.41
3:D:2465:C:H2'	3:D:2466:G:O4'	2.20	0.41
3:D:2764:A:H2'	3:D:2765:A:C8	2.56	0.41
3:D:4092:G:H1'	3:D:4093:G:N2	2.35	0.41
3:D:4260:U:H2'	3:D:4261:C:H6	1.84	0.41
3:D:4536:OMC:HM22	3:D:4537:C:O4'	2.20	0.41
3:D:4761:G:P	19:T:37:ARG:HH12	2.43	0.41
3:D:5024:C:H5'	3:D:5025:C:H6	1.86	0.41
6:G:125:LYS:HA	6:G:128:ARG:HD2	2.02	0.41
8:I:51:PRO:HB3	8:I:111:TRP:CZ2	2.55	0.41
8:I:330:PRO:HG3	11:L:47:ARG:NH2	2.35	0.41
14:O:32:ARG:O	14:O:33:ILE:C	2.62	0.41
20:U:4:TYR:OH	20:U:18:ARG:HG3	2.21	0.41
21:V:63:LEU:HB2	21:V:88:ASP:HA	2.02	0.41
33:h:17:ARG:HB3	33:h:101:ASP:OD2	2.21	0.41
37:l:5:LEU:HD11	37:l:32:TYR:CZ	2.55	0.41
37:l:41:ALA:O	37:l:52:ARG:HD2	2.20	0.41
48:w:940:U:H3	48:w:1002:U:H3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1482:C:P	77:AP:54:LYS:HZ3	2.44	0.41
50:y:129:THR:HB	50:y:180:ASP:HA	2.02	0.41
56:4:61:ILE:HG13	56:4:93:VAL:CG2	2.50	0.41
58:6:50:LEU:HD11	58:6:101:LYS:HA	2.02	0.41
59:7:22:VAL:HG22	59:7:68:TYR:HD1	1.84	0.41
66:AE:24:ARG:HB2	66:AE:29:ALA:HB2	2.02	0.41
3:D:256:G:H2'	3:D:257:C:H6	1.83	0.41
3:D:734:G:C2	3:D:735:G:C8	3.09	0.41
3:D:963:G:H3'	11:L:29:LYS:NZ	2.36	0.41
3:D:1078:A:H5'	3:D:1079:C:OP2	2.21	0.41
3:D:1278:C:H2'	3:D:1279:A:O4'	2.20	0.41
3:D:1534:A2M:HM'3	3:D:1534:A2M:H1'	1.93	0.41
3:D:2415:OMU:H3'	3:D:2416:G:H21	1.85	0.41
3:D:2690:C:H2'	3:D:2691:U:O4'	2.21	0.41
3:D:3652:A:H2'	3:D:3653:A:C8	2.55	0.41
3:D:3722:G:H2'	3:D:3723:A:C8	2.54	0.41
9:J:123:VAL:HG12	9:J:248:ARG:CZ	2.51	0.41
10:K:69:TYR:O	10:K:70:LYS:HB3	2.20	0.41
10:K:250:GLN:NE2	10:K:254:ASP:OD2	2.33	0.41
13:N:4:ILE:HG12	13:N:61:TRP:CH2	2.55	0.41
16:Q:172:GLU:HG2	39:n:2:ALA:HB3	2.01	0.41
17:R:86:TRP:C	17:R:88:ALA:H	2.29	0.41
39:n:59:GLU:O	39:n:62:LYS:HG2	2.21	0.41
47:v:32:LEU:O	47:v:33:LYS:HB2	2.20	0.41
48:w:154:U:H2'	48:w:155:G:H1'	2.02	0.41
48:w:155:G:C6	48:w:156:G:C6	3.08	0.41
48:w:346:C:H2'	48:w:347:G:O4'	2.21	0.41
48:w:380:G:OP1	57:5:56:ARG:NH2	2.53	0.41
48:w:868:G:H21	56:4:111:LYS:HD2	1.86	0.41
48:w:1139:C:H5	48:w:1149:A:H62	1.69	0.41
48:w:1223:A:H2'	48:w:1224:G:O4'	2.20	0.41
51:z:77:SER:C	51:z:79:GLU:N	2.78	0.41
61:9:91:LEU:HG	61:9:122:ILE:HG13	2.03	0.41
63:AB:75:VAL:HG12	63:AB:93:MET:HB3	2.01	0.41
71:AJ:107:ARG:CG	71:AJ:112:VAL:HG22	2.50	0.41
77:AP:13:LYS:HD2	77:AP:13:LYS:HA	1.85	0.41
79:AR:24:THR:CG2	79:AR:27:PHE:HB2	2.51	0.41
3:D:6:C:H5''	12:M:197:LYS:HG2	2.01	0.41
3:D:150:U:H3	12:M:162:ASP:HB2	1.85	0.41
3:D:922:C:O2'	3:D:923:C:O5'	2.31	0.41
3:D:1355:G:OP1	21:V:108:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1846:G:H2'	3:D:1847:C:H6	1.86	0.41
3:D:2318:G:N2	3:D:2321:G:OP2	2.40	0.41
3:D:4273:A:H2'	3:D:4274:A:C8	2.56	0.41
6:G:117:GLU:HA	6:G:124:GLY:HA2	2.03	0.41
7:H:155:LYS:HD3	7:H:156:TYR:CE2	2.55	0.41
48:w:154:U:H2'	48:w:155:G:O4'	2.20	0.41
48:w:190:G:O2'	48:w:208:G:N2	2.47	0.41
48:w:519:A:O2'	58:6:11:LYS:HE2	2.21	0.41
48:w:567:C:H2'	48:w:568:C:C6	2.55	0.41
48:w:896:U:H2'	48:w:897:U:C5	2.55	0.41
48:w:1340:U:OP2	48:w:1341:C:O2'	2.37	0.41
48:w:1407:U:H2'	48:w:1408:U:C6	2.56	0.41
48:w:1617:G:N2	48:w:1619:A:H3'	2.35	0.41
55:3:216:ARG:HD3	55:3:216:ARG:HA	1.86	0.41
56:4:143:ARG:HB2	56:4:155:LYS:HB2	2.03	0.41
56:4:165:ASN:O	56:4:169:LYS:HG2	2.21	0.41
62:AA:151:LEU:H	62:AA:151:LEU:HD23	1.85	0.41
79:AR:22:ALA:HB1	79:AR:71:ILE:HG13	2.02	0.41
2:B:65:C:H2'	2:B:66:U:H5'	2.03	0.41
3:D:461:G:H2'	3:D:462:G:H8	1.84	0.41
3:D:2423:A:H2'	3:D:2424:OMG:C8	2.55	0.41
3:D:2539:C:H2'	3:D:2540:C:H6	1.84	0.41
3:D:2634:C:H2'	3:D:2635:U:H6	1.86	0.41
3:D:2846:G:O2'	26:a:19:GLY:O	2.29	0.41
3:D:2864:A:H2'	3:D:2865:U:H6	1.85	0.41
3:D:4928:C:H2'	3:D:4929:C:H6	1.86	0.41
4:E:55:A:H4'	15:P:155:HIS:HB2	2.02	0.41
8:I:281:MET:HE3	8:I:281:MET:HB3	1.93	0.41
11:L:220:MET:C	11:L:222:LYS:H	2.28	0.41
16:Q:51:ALA:HB2	16:Q:149:GLN:NE2	2.35	0.41
20:U:94:MET:HE3	20:U:94:MET:HB2	1.85	0.41
23:X:81:TRP:HE3	23:X:128:LYS:O	2.03	0.41
41:p:6:GLU:N	41:p:6:GLU:OE2	2.53	0.41
42:q:38:ASN:C	42:q:40:LYS:H	2.29	0.41
48:w:613:G:C2	48:w:627:OMU:H4'	2.56	0.41
48:w:1142:G:N2	48:w:1145:A:OP2	2.48	0.41
48:w:1391:OMC:O4'	77:AP:55:LEU:HD11	2.20	0.41
48:w:1435:C:H42	68:AG:49:LYS:NZ	2.18	0.41
48:w:1621:U:H5'	48:w:1623:A:O2'	2.21	0.41
53:1:139:LEU:HD21	53:1:154:ILE:HG21	2.02	0.41
55:3:7:PHE:HD1	55:3:113:ILE:HB	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4:10:LYS:HE3	56:4:20:GLU:CG	2.50	0.41
56:4:25:GLN:CA	56:4:28:LEU:HD22	2.47	0.41
58:6:38:ARG:HG2	58:6:38:ARG:HH21	1.84	0.41
64:AC:28:GLY:HA3	64:AC:67:ASP:OD2	2.21	0.41
70:AI:24:GLN:HA	70:AI:63:VAL:O	2.20	0.41
72:AK:82:ALA:O	72:AK:86:GLU:HB2	2.19	0.41
3:D:174:C:H2'	3:D:175:C:H6	1.86	0.41
3:D:233:U:O2'	3:D:234:G:H5''	2.20	0.41
3:D:1327:C:H2'	3:D:1328:G:C8	2.55	0.41
3:D:1362:G:OP1	16:Q:39:ARG:NH2	2.53	0.41
3:D:2411:C:H2'	3:D:2412:A:C8	2.55	0.41
3:D:2685:C:H2'	3:D:2686:G:O4'	2.20	0.41
3:D:4320:G:H2'	3:D:4321:U:C6	2.55	0.41
3:D:4670:C:O2'	3:D:4672:A:OP2	2.29	0.41
3:D:4739:C:C2'	3:D:4740:G:H5'	2.50	0.41
3:D:5048:A:OP1	34:i:31:LYS:HD2	2.20	0.41
5:F:93:C:O2'	5:F:94:G:H8	2.04	0.41
6:G:47:ASP:OD1	6:G:47:ASP:N	2.50	0.41
25:Z:42:PHE:CE1	25:Z:46:ARG:HG3	2.55	0.41
30:e:10:VAL:HG13	30:e:83:THR:HB	2.03	0.41
30:e:135:ARG:HD3	30:e:135:ARG:HA	1.93	0.41
48:w:1406:G:H2'	48:w:1407:U:C6	2.56	0.41
48:w:1452:A:H4'	48:w:1453:C:O5'	2.21	0.41
49:x:159:ILE:HD11	69:AH:34:MET:HE1	2.03	0.41
52:0:52:ALA:O	52:0:90:LYS:HA	2.21	0.41
52:0:74:GLN:HE22	52:0:81:GLU:HA	1.84	0.41
52:0:166:TYR:O	52:0:200:PRO:HG3	2.20	0.41
53:1:92:ILE:HG22	53:1:97:GLU:N	2.31	0.41
57:5:106:SER:OG	57:5:169:GLY:HA2	2.20	0.41
62:AA:47:LEU:HD23	62:AA:47:LEU:HA	1.87	0.41
70:AI:3:ARG:HH22	70:AI:28:ARG:NH2	2.19	0.41
70:AI:86:LEU:HD21	70:AI:113:HIS:HB2	2.02	0.41
72:AK:40:ILE:HG13	72:AK:60:PHE:CZ	2.55	0.41
75:AN:11:SER:HB3	75:AN:14:GLU:OE1	2.20	0.41
79:AR:40:ILE:HG21	79:AR:69:VAL:HG21	2.02	0.41
3:D:418:A:C2	5:F:17:A:H1'	2.55	0.41
3:D:978:G:H2'	3:D:979:C:C6	2.56	0.41
3:D:1086:C:H2'	3:D:1087:A:H8	1.85	0.41
3:D:1092:G:H2'	3:D:1093:C:H6	1.85	0.41
3:D:1448:G:H2'	3:D:1449:C:C6	2.56	0.41
3:D:4342:C:O3'	45:t:37:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4492:U:O2'	3:D:4512:U:O2	2.32	0.41
7:H:170:LEU:O	7:H:328:ASN:ND2	2.43	0.41
12:M:157:ILE:HG12	12:M:170:LEU:HD23	2.02	0.41
13:N:27:VAL:HG12	13:N:84:VAL:HG21	2.03	0.41
15:P:120:ASP:HB3	15:P:123:ILE:HG12	2.02	0.41
22:W:135:LYS:HG2	22:W:139:MET:HE2	2.03	0.41
23:X:43:ARG:HA	23:X:43:ARG:HD2	1.71	0.41
48:w:445:A:H4'	57:5:50:GLY:O	2.21	0.41
48:w:518:G:H2'	48:w:519:A:O4'	2.20	0.41
48:w:528:A:C6	48:w:558:G:C6	3.09	0.41
48:w:634:A:H3'	48:w:635:G:H8	1.86	0.41
48:w:686:PSU:O4	56:4:118:ARG:NH2	2.54	0.41
48:w:807:G:C2	48:w:808:A:C8	3.08	0.41
48:w:1102:G:N2	48:w:1130:G:N2	2.69	0.41
48:w:1365:G:H2'	48:w:1366:G:C8	2.55	0.41
48:w:1727:G:H2'	48:w:1728:U:C6	2.56	0.41
48:w:1728:U:H2'	48:w:1729:U:O4'	2.21	0.41
48:w:1839:U:H1'	48:w:1863:A:H2	1.86	0.41
53:1:137:PRO:HB2	53:1:150:PRO:CD	2.51	0.41
54:2:124:ASP:HA	54:2:200:ALA:HB2	2.03	0.41
55:3:226:GLU:O	55:3:230:LYS:HG3	2.20	0.41
56:4:134:VAL:O	56:4:134:VAL:HG23	2.21	0.41
58:6:82:VAL:HG12	58:6:87:LEU:HB3	2.03	0.41
68:AG:54:VAL:HG12	68:AG:56:MET:HE3	2.03	0.41
73:AL:58:LEU:HA	73:AL:62:VAL:HG23	2.02	0.41
73:AL:79:ILE:HG22	73:AL:80:ARG:O	2.21	0.41
2:B:16:H2U:H2'	2:B:18:G:OP1	2.20	0.41
3:D:37:U:H2'	3:D:38:A:O4'	2.21	0.41
3:D:75:G:H3'	16:Q:74:ARG:HD2	2.03	0.41
3:D:137:G:H2'	3:D:138:G:C8	2.55	0.41
3:D:678:C:H2'	3:D:679:C:C6	2.56	0.41
3:D:1776:A:H2'	3:D:1777:C:C6	2.55	0.41
3:D:2096:G:H4'	3:D:2099:G:O5'	2.21	0.41
3:D:2544:G:H5''	3:D:2545:U:H5''	2.02	0.41
3:D:3871:A:H2'	3:D:3872:A:C8	2.56	0.41
3:D:4082:G:H2'	3:D:4083:U:C6	2.56	0.41
3:D:4563:U:H2'	3:D:4564:A:H8	1.85	0.41
8:I:298:ILE:O	8:I:302:LEU:HG	2.21	0.41
9:J:264:LYS:HE3	9:J:266:TRP:CH2	2.56	0.41
10:K:119:GLU:HG3	35:j:7:LEU:HD22	2.03	0.41
11:L:35:LYS:O	11:L:39:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:140:VAL:HG21	12:M:166:LEU:O	2.20	0.41
17:R:108:ASP:HB2	19:T:199:HIS:NE2	2.35	0.41
20:U:10:ASN:HD21	20:U:13:LYS:NZ	2.18	0.41
22:W:180:LYS:HG2	22:W:181:LYS:HZ2	1.86	0.41
28:c:79:PHE:CD1	38:m:36:VAL:HG11	2.56	0.41
29:d:127:GLN:OE1	29:d:127:GLN:HA	2.20	0.41
30:e:10:VAL:HG11	30:e:85:TYR:HB2	2.03	0.41
32:g:20:GLY:O	32:g:22:LYS:HG2	2.21	0.41
40:o:2:THR:O	40:o:7:SER:OG	2.27	0.41
48:w:633:C:O2'	78:AQ:86:ARG:NH1	2.54	0.41
48:w:804:U:H2'	48:w:805:U:C6	2.56	0.41
48:w:818:A:H2'	48:w:819:G:C8	2.56	0.41
48:w:821:G:O2'	48:w:823:U:H4'	2.21	0.41
48:w:899:U:OP2	48:w:900:C:H5''	2.20	0.41
48:w:1016:U:H5'	61:9:15:ALA:O	2.21	0.41
48:w:1130:G:H4'	61:9:10:GLY:HA2	2.03	0.41
48:w:1398:G:H4'	79:AR:88:ARG:HH22	1.86	0.41
48:w:1447:G:O2'	48:w:1448:A:H5'	2.21	0.41
48:w:1481:G:O3'	77:AP:54:LYS:NZ	2.54	0.41
48:w:1638:G:H5''	73:AL:34:LYS:HD2	2.01	0.41
48:w:1670:C:H2'	48:w:1671:G:H8	1.84	0.41
48:w:1690:U:H2'	48:w:1691:U:C6	2.55	0.41
48:w:1702:G:H2'	48:w:1703:OMC:O4'	2.20	0.41
48:w:1804:OMU:H2'	48:w:1805:G:O4'	2.21	0.41
49:x:52:LYS:HB2	65:AD:109:LEU:HD21	2.02	0.41
50:y:219:LYS:HE2	50:y:219:LYS:HB2	1.98	0.41
50:y:222:LYS:HG3	50:y:223:PHE:N	2.27	0.41
51:z:62:PRO:HD3	51:z:71:LYS:HD2	2.03	0.41
52:0:8:LYS:HG2	68:AG:61:LEU:HD11	2.03	0.41
53:1:187:ALA:O	53:1:191:ARG:NH2	2.54	0.41
54:2:163:PHE:CE2	54:2:164:ARG:HG3	2.56	0.41
55:3:52:ILE:HG23	55:3:109:LEU:HD21	2.01	0.41
55:3:138:ALA:O	55:3:141:ILE:HG22	2.20	0.41
56:4:23:ILE:O	56:4:27:LEU:HD23	2.21	0.41
57:5:65:PHE:CE1	57:5:78:ILE:HD11	2.55	0.41
57:5:79:ILE:HG12	57:5:103:LEU:O	2.20	0.41
58:6:11:LYS:HD3	58:6:11:LYS:HA	1.41	0.41
60:8:35:ARG:NH1	60:8:53:GLY:O	2.54	0.41
61:9:29:THR:HG22	61:9:32:ASP:OD2	2.20	0.41
65:AD:21:TYR:CE1	65:AD:58:MET:HE1	2.56	0.41
68:AG:29:VAL:O	68:AG:33:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AG:96:GLU:HA	68:AG:99:LYS:HZ2	1.84	0.41
79:AR:176:VAL:HG22	79:AR:186:THR:O	2.21	0.41
2:B:18:G:O2'	2:B:57:G:N1	2.47	0.41
3:D:318:A:H2'	3:D:319:A:C8	2.56	0.41
3:D:1333:A:H2'	3:D:1334:A:H8	1.86	0.41
3:D:1397:A:H5''	31:f:113:GLY:O	2.21	0.41
3:D:1498:G:OP1	21:V:150:ARG:NH1	2.53	0.41
3:D:1699:A:H3'	3:D:1700:G:H5''	2.03	0.41
3:D:2478:C:H2'	3:D:2479:G:C8	2.55	0.41
3:D:2743:A:H2'	3:D:2744:A:C8	2.55	0.41
3:D:3668:C:H5'	6:G:8:GLN:O	2.21	0.41
3:D:3707:U:H2'	3:D:3708:C:H6	1.84	0.41
3:D:4252:C:OP2	3:D:4253:A:O2'	2.27	0.41
3:D:4637:OMG:HM23	3:D:4637:OMG:H1'	1.65	0.41
5:F:5:U:H2'	5:F:6:C:H6	1.85	0.41
9:J:65:ALA:HB2	9:J:74:ILE:HD13	2.03	0.41
11:L:154:ILE:HG22	11:L:187:MET:HE1	2.03	0.41
12:M:244:PRO:HA	12:M:247:VAL:HG12	2.01	0.41
19:T:10:ASP:OD1	19:T:37:ARG:HD3	2.21	0.41
23:X:155:PRO:O	23:X:156:HIS:C	2.64	0.41
37:l:85:LYS:HB2	37:l:85:LYS:HE3	1.77	0.41
48:w:96:C:H2'	48:w:97:U:H6	1.86	0.41
48:w:493:A:H62	48:w:509:OMG:HN21	1.68	0.41
48:w:1649:U:H3	48:w:1675:A:H2	1.68	0.41
51:z:256:TRP:CE2	70:AI:68:ARG:HD3	2.55	0.41
54:2:59:LYS:HD3	54:2:62:ARG:HH11	1.86	0.41
54:2:97:PHE:CD1	54:2:108:PRO:HB2	2.55	0.41
56:4:70:LYS:HB3	56:4:74:LYS:HZ3	1.85	0.41
58:6:113:GLN:OE1	58:6:116:LYS:HD3	2.20	0.41
63:AB:44:ARG:HG2	63:AB:84:ILE:HD11	2.03	0.41
63:AB:93:MET:HA	63:AB:93:MET:HE2	2.03	0.41
65:AD:109:LEU:HD23	65:AD:109:LEU:HA	1.85	0.41
68:AG:39:LEU:HD23	68:AG:39:LEU:HA	1.91	0.41
70:AI:12:LYS:HA	70:AI:12:LYS:HD3	1.92	0.41
3:D:189:G:C2	3:D:190:G:C5	3.09	0.40
3:D:1081:C:O2'	3:D:1082:C:O5'	2.27	0.40
3:D:1733:G:N3	3:D:4214:A:H2'	2.36	0.40
7:H:86:VAL:O	7:H:202:GLU:N	2.54	0.40
8:I:146:GLU:HB3	8:I:175:LYS:HG2	2.02	0.40
12:M:48:LYS:HB3	28:c:42:THR:HG23	2.03	0.40
20:U:16:LYS:HB3	20:U:149:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:72:ASP:O	28:c:76:ILE:HG12	2.21	0.40
34:i:37:GLY:O	34:i:41:ARG:HG3	2.21	0.40
38:m:15:GLU:H	38:m:15:GLU:CD	2.29	0.40
40:o:21:ARG:C	40:o:23:GLY:H	2.29	0.40
48:w:428:OMU:H6	48:w:428:OMU:H2'	1.84	0.40
48:w:475:C:H1'	48:w:507:G:H2'	2.03	0.40
48:w:591:U:OP2	48:w:593:C:H5'	2.21	0.40
48:w:1610:G:P	66:AE:121:ARG:HH21	2.43	0.40
59:7:16:PHE:HB2	59:7:79:LEU:HD11	2.02	0.40
64:AC:25:CYS:HB2	64:AC:91:ALA:HB1	2.03	0.40
68:AG:64:THR:HG22	68:AG:77:TRP:HE3	1.86	0.40
70:AI:65:LEU:O	70:AI:66:THR:OG1	2.33	0.40
79:AR:153:CYS:SG	79:AR:197:THR:HA	2.61	0.40
3:D:499:G:N1	3:D:500:G:N7	2.69	0.40
3:D:1183:C:O2	3:D:1183:C:H2'	2.21	0.40
3:D:1246:G:H2'	3:D:1247:U:H6	1.86	0.40
3:D:1297:U:N3	3:D:1298:C:C5	2.89	0.40
3:D:3702:A:C6	3:D:3703:G:C8	3.09	0.40
3:D:3928:A:H2'	3:D:3929:G:O4'	2.22	0.40
3:D:4892:A:H2'	3:D:4893:A:O4'	2.21	0.40
6:G:82:ILE:HD11	6:G:99:GLY:HA3	2.03	0.40
10:K:180:VAL:HG21	10:K:258:LEU:HD11	2.02	0.40
13:N:18:ILE:HG12	13:N:27:VAL:HG22	2.02	0.40
15:P:40:LEU:HD23	15:P:40:LEU:HA	1.84	0.40
18:S:146:PRO:O	18:S:147:ASP:HB2	2.20	0.40
37:l:107:LEU:HD23	37:l:107:LEU:HA	1.90	0.40
48:w:500:A:O2'	48:w:501:C:O4'	2.33	0.40
48:w:902:G:C6	48:w:903:A:H8	2.40	0.40
48:w:1408:U:H2'	48:w:1409:A:C8	2.57	0.40
48:w:1601:A:H1'	48:w:1604:G:O6	2.22	0.40
48:w:1643:PSU:H2'	48:w:1644:C:C6	2.56	0.40
48:w:1676:U:H2'	48:w:1677:U:O4'	2.22	0.40
48:w:1752:C:H5'	48:w:1754:G:OP2	2.21	0.40
51:z:187:ARG:HD3	51:z:192:LEU:HD12	2.02	0.40
56:4:116:ARG:CZ	56:4:121:THR:HG22	2.52	0.40
57:5:140:LYS:HB3	57:5:140:LYS:HE3	1.81	0.40
58:6:164:PRO:HB3	58:6:171:GLY:N	2.36	0.40
68:AG:61:LEU:HB2	68:AG:82:MET:HB3	2.03	0.40
3:D:184:U:N3	3:D:189:G:N7	2.70	0.40
3:D:327:U:O2'	39:n:30:ARG:NH1	2.46	0.40
3:D:921:C:H2'	3:D:922:C:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2306:G:H1'	3:D:2332:A:N6	2.36	0.40
3:D:3773:U:H1'	3:D:3775:A:H2	1.87	0.40
3:D:4966:A:H2'	3:D:4967:A:O4'	2.21	0.40
4:E:42:A:C5	4:E:43:U:C5	3.09	0.40
8:I:232:VAL:O	8:I:233:SER:OG	2.31	0.40
15:P:113:ILE:HD12	66:AE:14:ARG:HB2	2.03	0.40
45:t:77:CYS:O	45:t:78:ARG:NE	2.55	0.40
46:u:25:MET:HE3	46:u:25:MET:HB2	1.92	0.40
48:w:116:OMU:HN3	48:w:347:G:H1	1.69	0.40
48:w:144:U:C2	48:w:313:A:N6	2.90	0.40
48:w:867:G:H21	56:4:111:LYS:NZ	2.19	0.40
50:y:38:MET:HE2	50:y:231:LEU:HD11	2.02	0.40
53:1:21:ASP:OD1	53:1:24:THR:OG1	2.22	0.40
53:1:89:VAL:HB	53:1:100:ARG:NH2	2.36	0.40
54:2:20:PHE:CD2	54:2:23:TRP:HD1	2.30	0.40
55:3:46:LYS:HA	55:3:46:LYS:HD3	1.96	0.40
58:6:42:GLU:HA	58:6:45:ARG:HB3	2.04	0.40
72:AK:40:ILE:HG22	72:AK:57:VAL:HG21	2.03	0.40
73:AL:77:LEU:HB3	73:AL:79:ILE:HG12	2.04	0.40
74:AM:5:ARG:HG3	74:AM:7:ASN:O	2.22	0.40
2:B:62:C:H2'	2:B:63:G:C8	2.56	0.40
3:D:1094:G:O6	3:D:1201:U:C2	2.74	0.40
3:D:1354:A:OP2	21:V:106:THR:HG21	2.21	0.40
3:D:1719:A:H2'	3:D:1720:C:C6	2.56	0.40
3:D:2276:A:H2'	3:D:2277:C:O4'	2.22	0.40
3:D:2412:A:H2'	3:D:2413:U:C6	2.56	0.40
3:D:4688:C:H2'	3:D:4689:PSU:C6	2.56	0.40
3:D:4876:U:OP2	23:X:165:PRO:HG3	2.21	0.40
3:D:5026:U:H1'	3:D:5027:C:C5	2.57	0.40
5:F:16:G:HO2'	5:F:17:A:P	2.44	0.40
6:G:205:ASN:O	6:G:208:GLU:HG2	2.20	0.40
7:H:155:LYS:HD3	7:H:156:TYR:CZ	2.57	0.40
8:I:260:LEU:HD23	8:I:260:LEU:HA	1.96	0.40
10:K:209:PRO:HB2	10:K:211:HIS:CE1	2.56	0.40
16:Q:2:ALA:HA	16:Q:3:PRO:HD3	1.97	0.40
21:V:94:GLU:O	21:V:95:VAL:C	2.64	0.40
23:X:7:LEU:O	23:X:103:ALA:HB1	2.21	0.40
36:k:109:ARG:HG3	36:k:110:ILE:HD12	2.03	0.40
37:l:41:ALA:HB3	37:l:52:ARG:HG3	2.03	0.40
48:w:112:U:H2'	48:w:115:U:C5	2.56	0.40
48:w:520:A:P	58:6:11:LYS:HD2	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:571:U:O2'	72:AK:60:PHE:O	2.39	0.40
48:w:585:C:H2'	48:w:586:G:O4'	2.22	0.40
48:w:1265:A:O2'	48:w:1266:C:H6	2.04	0.40
48:w:1315:U:C2	48:w:1316:C:C6	3.10	0.40
48:w:1741:U:H2'	48:w:1742:C:O4'	2.22	0.40
49:x:190:SER:O	49:x:191:ARG:HB2	2.22	0.40
53:1:128:LYS:HA	53:1:156:VAL:HG23	2.03	0.40
72:AK:20:ARG:HG2	72:AK:21:LYS:N	2.36	0.40
72:AK:38:THR:OG1	72:AK:39:GLU:N	2.54	0.40
79:AR:168:CYS:HB3	79:AR:198:VAL:CG1	2.52	0.40
79:AR:227:LEU:HD12	79:AR:227:LEU:HA	1.91	0.40
3:D:266:C:H1'	3:D:267:G:C8	2.57	0.40
3:D:389:A:H1'	29:d:90:ALA:O	2.22	0.40
3:D:479:G:H1'	47:v:100:ASN:OD1	2.21	0.40
3:D:737:C:C6	3:D:739:G:H5''	2.57	0.40
3:D:1613:A:H5''	6:G:183:GLY:HA2	2.03	0.40
3:D:1660:U:H2'	31:f:12:ARG:O	2.22	0.40
3:D:2267:U:OP1	47:v:37:SER:OG	2.20	0.40
3:D:2683:C:H2'	3:D:2684:C:C6	2.57	0.40
3:D:2706:G:H2'	3:D:2708:U:C2	2.56	0.40
3:D:3765:G:O2'	3:D:3767:C:N4	2.54	0.40
3:D:4393:G:O4'	3:D:4447:5MC:HM53	2.22	0.40
3:D:4870:G:H5''	17:R:91:TRP:CD2	2.57	0.40
3:D:5057:C:H2'	3:D:5058:A:C8	2.56	0.40
14:O:212:LEU:HD23	14:O:213:HIS:N	2.36	0.40
24:Y:64:VAL:HG13	24:Y:72:VAL:HG13	2.04	0.40
30:e:88:ASP:OD2	30:e:121:ARG:NH2	2.54	0.40
30:e:103:ASP:OD2	30:e:106:LEU:HG	2.21	0.40
48:w:33:G:H2'	48:w:34:PSU:O4'	2.21	0.40
48:w:192:C:H2'	48:w:193:C:H6	1.87	0.40
48:w:943:U:O2'	62:AA:135:ILE:O	2.39	0.40
48:w:1103:C:H2'	48:w:1104:G:H8	1.86	0.40
48:w:1665:G:P	67:AF:91:HIS:HE2	2.42	0.40
58:6:77:LEU:HA	58:6:80:ARG:NH1	2.37	0.40
62:AA:131:ASP:OD2	62:AA:131:ASP:C	2.64	0.40
64:AC:24:HIS:O	64:AC:68:ILE:HA	2.20	0.40
66:AE:60:THR:O	66:AE:64:VAL:HG23	2.21	0.40
70:AI:89:TRP:O	70:AI:93:LEU:HB2	2.21	0.40
73:AL:41:ARG:HA	73:AL:41:ARG:HD2	1.83	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	
6	G	245/257 (95%)	228 (93%)	17 (7%)	0	100	100
7	H	396/403 (98%)	375 (95%)	21 (5%)	0	100	100
8	I	361/427 (84%)	338 (94%)	23 (6%)	0	100	100
9	J	291/297 (98%)	271 (93%)	20 (7%)	0	100	100
10	K	211/288 (73%)	189 (90%)	22 (10%)	0	100	100
11	L	223/248 (90%)	213 (96%)	10 (4%)	0	100	100
12	M	223/266 (84%)	208 (93%)	15 (7%)	0	100	100
13	N	188/192 (98%)	176 (94%)	12 (6%)	0	100	100
14	O	202/214 (94%)	187 (93%)	15 (7%)	0	100	100
15	P	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
16	Q	206/211 (98%)	189 (92%)	15 (7%)	2 (1%)	12	18
17	R	134/215 (62%)	122 (91%)	12 (9%)	0	100	100
18	S	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
19	T	198/203 (98%)	191 (96%)	7 (4%)	0	100	100
20	U	155/184 (84%)	143 (92%)	12 (8%)	0	100	100
21	V	185/188 (98%)	174 (94%)	11 (6%)	0	100	100
22	W	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
23	X	173/176 (98%)	160 (92%)	13 (8%)	0	100	100
24	Y	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
25	Z	99/128 (77%)	92 (93%)	6 (6%)	1 (1%)	12	18
26	a	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
27	b	61/157 (39%)	59 (97%)	2 (3%)	0	100	100
28	c	118/156 (76%)	110 (93%)	8 (7%)	0	100	100
29	d	132/145 (91%)	123 (93%)	9 (7%)	0	100	100
30	e	133/136 (98%)	126 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	f	145/148 (98%)	132 (91%)	13 (9%)	0	100	100
32	g	100/159 (63%)	92 (92%)	6 (6%)	2 (2%)	6	7
33	h	95/115 (83%)	94 (99%)	1 (1%)	0	100	100
34	i	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
35	j	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
36	k	107/110 (97%)	101 (94%)	6 (6%)	0	100	100
37	l	110/117 (94%)	104 (94%)	6 (6%)	0	100	100
38	m	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
39	n	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
40	o	84/97 (87%)	79 (94%)	4 (5%)	1 (1%)	10	15
41	p	67/70 (96%)	60 (90%)	7 (10%)	0	100	100
42	q	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	r	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
44	s	23/25 (92%)	23 (100%)	0	0	100	100
45	t	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
46	u	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
47	v	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
49	x	213/295 (72%)	205 (96%)	7 (3%)	1 (0%)	24	35
50	y	210/264 (80%)	196 (93%)	14 (7%)	0	100	100
51	z	210/293 (72%)	198 (94%)	11 (5%)	1 (0%)	24	35
52	0	210/243 (86%)	190 (90%)	20 (10%)	0	100	100
53	1	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
54	2	185/204 (91%)	169 (91%)	16 (9%)	0	100	100
55	3	235/249 (94%)	227 (97%)	8 (3%)	0	100	100
56	4	185/194 (95%)	168 (91%)	17 (9%)	0	100	100
57	5	204/208 (98%)	196 (96%)	8 (4%)	0	100	100
58	6	180/194 (93%)	166 (92%)	14 (8%)	0	100	100
59	7	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
60	8	138/158 (87%)	128 (93%)	10 (7%)	0	100	100
61	9	148/151 (98%)	140 (95%)	8 (5%)	0	100	100
62	AA	132/151 (87%)	120 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	AB	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
64	AC	140/146 (96%)	124 (89%)	15 (11%)	1 (1%)	18	27
65	AD	129/135 (96%)	108 (84%)	19 (15%)	2 (2%)	7	10
66	AE	142/152 (93%)	128 (90%)	14 (10%)	0	100	100
67	AF	141/145 (97%)	131 (93%)	10 (7%)	0	100	100
68	AG	100/119 (84%)	92 (92%)	8 (8%)	0	100	100
69	AH	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
70	AI	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
71	AJ	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
72	AK	121/133 (91%)	115 (95%)	6 (5%)	0	100	100
73	AL	84/125 (67%)	76 (90%)	8 (10%)	0	100	100
74	AM	97/115 (84%)	93 (96%)	4 (4%)	0	100	100
75	AN	81/84 (96%)	69 (85%)	11 (14%)	1 (1%)	10	15
76	AO	59/69 (86%)	53 (90%)	6 (10%)	0	100	100
77	AP	43/56 (77%)	43 (100%)	0	0	100	100
78	AQ	55/59 (93%)	48 (87%)	7 (13%)	0	100	100
79	AR	311/317 (98%)	268 (86%)	43 (14%)	0	100	100
All	All	10947/12400 (88%)	10216 (93%)	719 (7%)	12 (0%)	49	63

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	48	PRO
32	g	111	ARG
64	AC	119	LEU
65	AD	119	VAL
32	g	110	ALA
49	x	12	GLU
16	Q	47	ALA
65	AD	118	GLN
25	Z	55	ASN
51	z	78	LEU
75	AN	39	GLY
40	o	40	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	189/199 (95%)	189 (100%)	0	100	100
7	H	346/349 (99%)	346 (100%)	0	100	100
8	I	301/348 (86%)	301 (100%)	0	100	100
9	J	245/250 (98%)	245 (100%)	0	100	100
10	K	193/252 (77%)	193 (100%)	0	100	100
11	L	194/215 (90%)	194 (100%)	0	100	100
12	M	195/223 (87%)	195 (100%)	0	100	100
13	N	169/171 (99%)	169 (100%)	0	100	100
14	O	174/181 (96%)	174 (100%)	0	100	100
15	P	143/149 (96%)	143 (100%)	0	100	100
16	Q	174/177 (98%)	174 (100%)	0	100	100
17	R	116/161 (72%)	116 (100%)	0	100	100
18	S	171/172 (99%)	171 (100%)	0	100	100
19	T	172/174 (99%)	172 (100%)	0	100	100
20	U	138/163 (85%)	138 (100%)	0	100	100
21	V	164/165 (99%)	164 (100%)	0	100	100
22	W	159/175 (91%)	159 (100%)	0	100	100
23	X	156/157 (99%)	156 (100%)	0	100	100
24	Y	139/140 (99%)	139 (100%)	0	100	100
25	Z	90/115 (78%)	90 (100%)	0	100	100
26	a	101/107 (94%)	101 (100%)	0	100	100
27	b	55/126 (44%)	55 (100%)	0	100	100
28	c	107/133 (80%)	107 (100%)	0	100	100
29	d	124/135 (92%)	124 (100%)	0	100	100
30	e	117/118 (99%)	117 (100%)	0	100	100
31	f	120/121 (99%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	g	81/126 (64%)	81 (100%)	0	100	100
33	h	82/97 (84%)	82 (100%)	0	100	100
34	i	98/110 (89%)	98 (100%)	0	100	100
35	j	114/121 (94%)	114 (100%)	0	100	100
36	k	88/89 (99%)	88 (100%)	0	100	100
37	l	96/100 (96%)	96 (100%)	0	100	100
38	m	109/110 (99%)	109 (100%)	0	100	100
39	n	86/89 (97%)	86 (100%)	0	100	100
40	o	73/80 (91%)	72 (99%)	1 (1%)	59	77
41	p	64/65 (98%)	64 (100%)	0	100	100
42	q	47/48 (98%)	47 (100%)	0	100	100
43	r	48/116 (41%)	48 (100%)	0	100	100
44	s	24/24 (100%)	24 (100%)	0	100	100
45	t	93/94 (99%)	93 (100%)	0	100	100
46	u	74/75 (99%)	74 (100%)	0	100	100
47	v	109/121 (90%)	109 (100%)	0	100	100
49	x	178/243 (73%)	178 (100%)	0	100	100
50	y	194/231 (84%)	194 (100%)	0	100	100
51	z	176/225 (78%)	176 (100%)	0	100	100
52	0	175/202 (87%)	175 (100%)	0	100	100
53	1	223/225 (99%)	223 (100%)	0	100	100
54	2	154/170 (91%)	154 (100%)	0	100	100
55	3	206/218 (94%)	206 (100%)	0	100	100
56	4	168/174 (97%)	168 (100%)	0	100	100
57	5	175/180 (97%)	175 (100%)	0	100	100
58	6	160/168 (95%)	160 (100%)	0	100	100
59	7	87/136 (64%)	87 (100%)	0	100	100
60	8	125/142 (88%)	125 (100%)	0	100	100
61	9	130/131 (99%)	130 (100%)	0	100	100
62	AA	104/119 (87%)	104 (100%)	0	100	100
63	AB	120/130 (92%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	AC	117/121 (97%)	117 (100%)	0	100	100
65	AD	117/122 (96%)	117 (100%)	0	100	100
66	AE	119/132 (90%)	118 (99%)	1 (1%)	73	85
67	AF	113/115 (98%)	113 (100%)	0	100	100
68	AG	89/107 (83%)	89 (100%)	0	100	100
69	AH	67/67 (100%)	67 (100%)	0	100	100
70	AI	112/113 (99%)	112 (100%)	0	100	100
71	AJ	113/115 (98%)	113 (100%)	0	100	100
72	AK	106/115 (92%)	106 (100%)	0	100	100
73	AL	73/103 (71%)	73 (100%)	0	100	100
74	AM	86/98 (88%)	86 (100%)	0	100	100
75	AN	73/76 (96%)	73 (100%)	0	100	100
76	AO	54/62 (87%)	54 (100%)	0	100	100
77	AP	39/49 (80%)	39 (100%)	0	100	100
78	AQ	46/48 (96%)	46 (100%)	0	100	100
79	AR	272/275 (99%)	272 (100%)	0	100	100
All	All	9509/10553 (90%)	9507 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	o	48	ASN
66	AE	87	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
7	H	184	GLN
7	H	245	HIS
8	I	43	ASN
8	I	50	GLN
8	I	61	GLN
8	I	198	ASN
8	I	212	ASN
8	I	231	ASN

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Mol	Chain	Res	Type
8	I	329	ASN
9	J	198	HIS
9	J	202	GLN
9	J	229	ASN
9	J	267	ASN
11	L	39	GLN
11	L	80	ASN
11	L	206	ASN
11	L	235	ASN
11	L	239	GLN
12	M	94	GLN
12	M	153	GLN
13	N	39	ASN
13	N	98	HIS
13	N	102	ASN
13	N	106	GLN
14	O	177	ASN
16	Q	205	GLN
17	R	34	ASN
18	S	8	GLN
18	S	15	GLN
20	U	10	ASN
21	V	7	HIS
22	W	40	GLN
22	W	158	GLN
24	Y	54	HIS
24	Y	66	ASN
24	Y	144	ASN
25	Z	38	ASN
25	Z	41	GLN
29	d	14	ASN
29	d	20	ASN
29	d	96	HIS
31	f	60	HIS
32	g	6	ASN
34	i	121	ASN
35	j	107	ASN
37	l	73	HIS
39	n	15	HIS
40	o	66	HIS
42	q	17	GLN
47	v	4	HIS

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Mol	Chain	Res	Type
49	x	110	ASN
49	x	113	GLN
50	y	186	ASN
51	z	113	GLN
52	0	165	ASN
53	1	188	ASN
53	1	224	ASN
54	2	137	GLN
54	2	203	ASN
55	3	70	HIS
57	5	9	HIS
57	5	88	ASN
57	5	165	GLN
58	6	177	ASN
59	7	77	GLN
60	8	18	GLN
62	AA	38	ASN
62	AA	103	ASN
64	AC	80	GLN
65	AD	93	GLN
66	AE	87	GLN
66	AE	101	ASN
66	AE	135	HIS
67	AF	63	HIS
67	AF	142	ASN
69	AH	2	GLN
70	AI	120	HIS
71	AJ	16	HIS
71	AJ	23	HIS
71	AJ	39	ASN
73	AL	46	ASN
78	AQ	76	HIS
79	AR	14	HIS
79	AR	62	HIS
79	AR	104	HIS
79	AR	143	GLN
79	AR	196	ASN

5.3.3 RNA

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	10/14 (71%)	1 (10%)	0
2	B	75/76 (98%)	18 (24%)	3 (4%)
3	D	3496/5070 (68%)	616 (17%)	24 (0%)
4	E	119/120 (99%)	14 (11%)	0
48	w	1624/1869 (86%)	418 (25%)	0
5	F	155/156 (99%)	28 (18%)	2 (1%)
All	All	5479/7305 (75%)	1095 (19%)	29 (0%)

All (1095) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	21	U
2	B	4	U
2	B	5	C
2	B	6	2MG
2	B	11	C
2	B	16	H2U
2	B	17	H2U
2	B	18	G
2	B	21	A
2	B	42	U
2	B	46	G7M
2	B	47	H2U
2	B	48	5MC
2	B	56	C
2	B	57	G
2	B	66	U
2	B	74	C
2	B	75	C
2	B	76	A
3	D	2	G
3	D	25	A
3	D	39	A
3	D	42	A
3	D	48	G
3	D	56	A
3	D	59	A
3	D	64	A
3	D	65	A
3	D	69	A
3	D	91	G

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Mol	Chain	Res	Type
3	D	98	A
3	D	108	A
3	D	109	G
3	D	110	C
3	D	117	C
3	D	119	G
3	D	120	A
3	D	143	C
3	D	144	G
3	D	145	G
3	D	152	U
3	D	159	C
3	D	171	U
3	D	172	C
3	D	180	C
3	D	181	C
3	D	183	C
3	D	185	C
3	D	186	G
3	D	187	U
3	D	188	G
3	D	189	G
3	D	200	U
3	D	209	U
3	D	218	A
3	D	220	C
3	D	234	G
3	D	256	G
3	D	258	G
3	D	259	C
3	D	261	G
3	D	265	C
3	D	266	C
3	D	267	G
3	D	275	C
3	D	276	C
3	D	280	G
3	D	306	A
3	D	315	G
3	D	316	U
3	D	340	C
3	D	344	A

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Mol	Chain	Res	Type
3	D	345	C
3	D	350	C
3	D	387	G
3	D	396	A
3	D	407	A
3	D	408	A
3	D	410	A
3	D	412	G
3	D	413	G
3	D	449	C
3	D	450	G
3	D	452	A
3	D	453	G
3	D	454	U
3	D	465	G
3	D	467	U
3	D	468	U
3	D	484	U
3	D	485	C
3	D	486	C
3	D	491	G
3	D	494	U
3	D	495	C
3	D	498	C
3	D	499	G
3	D	509	A
3	D	510	U
3	D	513	U
3	D	514	U
3	D	515	C
3	D	516	C
3	D	517	C
3	D	645	G
3	D	654	C
3	D	657	C
3	D	658	C
3	D	659	G
3	D	661	C
3	D	662	C
3	D	665	C
3	D	667	A
3	D	668	C

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Mol	Chain	Res	Type
3	D	670	G
3	D	673	C
3	D	685	C
3	D	686	A
3	D	703	G
3	D	704	C
3	D	731	G
3	D	738	C
3	D	739	G
3	D	740	G
3	D	742	G
3	D	746	A
3	D	754	U
3	D	760	G
3	D	904	C
3	D	905	C
3	D	913	U
3	D	914	U
3	D	915	A
3	D	917	A
3	D	918	G
3	D	923	C
3	D	924	C
3	D	925	C
3	D	926	G
3	D	932	A
3	D	933	G
3	D	934	C
3	D	935	A
3	D	936	C
3	D	937	U
3	D	944	A
3	D	945	U
3	D	959	G
3	D	960	A
3	D	961	G
3	D	962	C
3	D	965	G
3	D	966	A
3	D	970	G
3	D	971	U
3	D	972	C

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Mol	Chain	Res	Type
3	D	977	C
3	D	982	U
3	D	984	C
3	D	988	C
3	D	989	U
3	D	1066	G
3	D	1069	G
3	D	1071	C
3	D	1075	G
3	D	1078	A
3	D	1082	C
3	D	1083	U
3	D	1094	G
3	D	1096	C
3	D	1168	G
3	D	1173	G
3	D	1178	G
3	D	1179	U
3	D	1180	C
3	D	1182	C
3	D	1183	C
3	D	1184	A
3	D	1193	C
3	D	1196	G
3	D	1200	G
3	D	1202	C
3	D	1203	G
3	D	1210	C
3	D	1211	G
3	D	1214	C
3	D	1219	G
3	D	1241	C
3	D	1262	G
3	D	1266	G
3	D	1269	G
3	D	1270	A
3	D	1271	G
3	D	1272	C
3	D	1273	G
3	D	1275	G
3	D	1277	G
3	D	1280	C

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Mol	Chain	Res	Type
3	D	1284	G
3	D	1285	U
3	D	1287	G
3	D	1294	A
3	D	1295	C
3	D	1296	G
3	D	1301	C
3	D	1302	U
3	D	1303	A
3	D	1304	C
3	D	1313	C
3	D	1326	A2M
3	D	1337	A
3	D	1354	A
3	D	1358	G
3	D	1359	G
3	D	1365	C
3	D	1366	G
3	D	1377	G
3	D	1379	C
3	D	1387	A
3	D	1394	G
3	D	1397	A
3	D	1398	A
3	D	1403	G
3	D	1404	G
3	D	1407	C
3	D	1408	G
3	D	1409	C
3	D	1410	U
3	D	1411	C
3	D	1412	G
3	D	1414	C
3	D	1415	G
3	D	1417	C
3	D	1420	A
3	D	1439	C
3	D	1441	C
3	D	1442	C
3	D	1443	A
3	D	1482	G
3	D	1483	C

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Mol	Chain	Res	Type
3	D	1498	G
3	D	1502	G
3	D	1514	U
3	D	1534	A2M
3	D	1535	C
3	D	1547	A
3	D	1564	A
3	D	1566	C
3	D	1578	U
3	D	1591	U
3	D	1596	U
3	D	1624	G
3	D	1625	OMG
3	D	1631	A
3	D	1633	G
3	D	1634	A
3	D	1640	C
3	D	1642	A
3	D	1654	G
3	D	1661	C
3	D	1676	C
3	D	1677	PSU
3	D	1678	C
3	D	1694	C
3	D	1698	C
3	D	1699	A
3	D	1700	G
3	D	1701	A
3	D	1702	C
3	D	1703	C
3	D	1705	G
3	D	1734	G
3	D	1740	C
3	D	1741	G
3	D	1742	A
3	D	1756	U
3	D	1757	U
3	D	1758	G
3	D	1760	OMG
3	D	1763	C
3	D	1787	A
3	D	1797	G

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Mol	Chain	Res	Type
3	D	1804	A
3	D	1810	G
3	D	1821	G
3	D	1822	U
3	D	1836	G
3	D	1837	A
3	D	1842	G
3	D	1843	A
3	D	1855	G
3	D	1869	G
3	D	1882	U
3	D	1897	A
3	D	1918	U
3	D	1919	G
3	D	1920	C
3	D	1921	C
3	D	1922	G
3	D	1925	G
3	D	1931	C
3	D	1932	A
3	D	1940	G
3	D	1948	G
3	D	1951	G
3	D	1959	U
3	D	1960	A
3	D	1961	G
3	D	1962	A
3	D	2024	G
3	D	2025	A
3	D	2026	A
3	D	2034	G
3	D	2046	G
3	D	2048	U
3	D	2055	G
3	D	2056	G
3	D	2069	A
3	D	2084	C
3	D	2085	G
3	D	2089	G
3	D	2092	G
3	D	2093	A
3	D	2096	G

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Mol	Chain	Res	Type
3	D	2097	U
3	D	2098	G
3	D	2099	G
3	D	2100	A
3	D	2102	G
3	D	2103	G
3	D	2104	G
3	D	2105	A
3	D	2257	C
3	D	2258	C
3	D	2259	G
3	D	2277	C
3	D	2289	C
3	D	2300	A
3	D	2301	G
3	D	2313	A
3	D	2333	G
3	D	2348	G
3	D	2351	OMC
3	D	2360	A
3	D	2397	G
3	D	2416	G
3	D	2421	G
3	D	2422	OMC
3	D	2424	OMG
3	D	2425	U
3	D	2450	G
3	D	2453	A
3	D	2465	C
3	D	2470	C
3	D	2474	G
3	D	2475	G
3	D	2483	G
3	D	2484	A
3	D	2485	U
3	D	2487	G
3	D	2488	C
3	D	2489	C
3	D	2491	C
3	D	2493	G
3	D	2494	U
3	D	2503	G

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Mol	Chain	Res	Type
3	D	2504	C
3	D	2505	C
3	D	2511	A
3	D	2513	A
3	D	2519	U
3	D	2529	A
3	D	2537	A
3	D	2545	U
3	D	2546	G
3	D	2547	G
3	D	2554	U
3	D	2555	G
3	D	2565	A
3	D	2573	A
3	D	2583	C
3	D	2587	A
3	D	2618	G
3	D	2627	C
3	D	2653	C
3	D	2662	G
3	D	2669	C
3	D	2676	A
3	D	2687	U
3	D	2694	G
3	D	2695	A
3	D	2696	A
3	D	2707	U
3	D	2708	U
3	D	2711	G
3	D	2712	G
3	D	2724	G
3	D	2726	G
3	D	2729	C
3	D	2739	C
3	D	2742	G
3	D	2743	A
3	D	2746	A
3	D	2754	G
3	D	2760	G
3	D	2761	U
3	D	2763	U
3	D	2764	A

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Mol	Chain	Res	Type
3	D	2769	U
3	D	2770	C
3	D	2788	U
3	D	2790	U
3	D	2814	C
3	D	2815	A2M
3	D	2826	U
3	D	2827	G
3	D	2855	G
3	D	2856	C
3	D	2867	C
3	D	2874	U
3	D	2877	G
3	D	2892	C
3	D	2900	U
3	D	3604	A
3	D	3605	C
3	D	3606	U
3	D	3615	G
3	D	3618	C
3	D	3626	G
3	D	3635	A
3	D	3644	U
3	D	3648	A
3	D	3662	A
3	D	3673	C
3	D	3674	G
3	D	3710	G
3	D	3711	A
3	D	3712	A
3	D	3727	A
3	D	3735	G
3	D	3736	A
3	D	3750	G
3	D	3753	G
3	D	3757	G
3	D	3758	PSU
3	D	3760	A2M
3	D	3763	A
3	D	3771	C
3	D	3776	G
3	D	3777	G

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Mol	Chain	Res	Type
3	D	3783	A
3	D	3784	A
3	D	3786	U
3	D	3802	U
3	D	3811	G
3	D	3812	C
3	D	3814	U
3	D	3817	A
3	D	3818	UY1
3	D	3819	G
3	D	3823	G
3	D	3838	U
3	D	3840	U
3	D	3867	A
3	D	3877	A
3	D	3878	C
3	D	3879	G
3	D	3885	G
3	D	3892	U
3	D	3897	G
3	D	3901	A
3	D	3906	A
3	D	3907	G
3	D	3908	A
3	D	3915	U
3	D	3938	G
3	D	3939	G
3	D	3943	A
3	D	3944	OMG
3	D	3946	G
3	D	4066	U
3	D	4076	G
3	D	4086	G
3	D	4093	G
3	D	4094	G
3	D	4097	G
3	D	4098	A
3	D	4111	U
3	D	4112	C
3	D	4113	U
3	D	4114	C
3	D	4115	G

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Mol	Chain	Res	Type
3	D	4116	C
3	D	4119	C
3	D	4122	G
3	D	4127	A
3	D	4133	C
3	D	4140	C
3	D	4142	C
3	D	4143	G
3	D	4144	C
3	D	4145	C
3	D	4150	G
3	D	4162	C
3	D	4163	U
3	D	4170	A
3	D	4183	G
3	D	4184	G
3	D	4191	G
3	D	4203	A
3	D	4229	U
3	D	4233	A
3	D	4251	A
3	D	4254	G
3	D	4257	A
3	D	4268	A
3	D	4273	A
3	D	4281	A
3	D	4291	G
3	D	4297	G
3	D	4305	G
3	D	4329	G
3	D	4330	G
3	D	4332	C
3	D	4339	A
3	D	4349	C
3	D	4373	G
3	D	4377	G
3	D	4378	A
3	D	4380	A
3	D	4387	C
3	D	4391	G
3	D	4394	A
3	D	4415	A

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Mol	Chain	Res	Type
3	D	4421	C
3	D	4422	A
3	D	4448	G
3	D	4449	A
3	D	4452	U
3	D	4453	C
3	D	4464	A
3	D	4466	C
3	D	4475	G
3	D	4500	PSU
3	D	4512	U
3	D	4513	A
3	D	4519	C
3	D	4524	G
3	D	4545	G
3	D	4548	A
3	D	4549	G
3	D	4554	G
3	D	4560	C
3	D	4567	G
3	D	4570	G
3	D	4573	G
3	D	4575	G
3	D	4584	A
3	D	4590	A
3	D	4600	G
3	D	4601	U
3	D	4617	G
3	D	4636	U
3	D	4637	OMG
3	D	4647	G
3	D	4656	A
3	D	4657	U
3	D	4670	C
3	D	4672	A
3	D	4679	G
3	D	4695	C
3	D	4700	A
3	D	4708	A
3	D	4709	U
3	D	4730	C
3	D	4731	G

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Mol	Chain	Res	Type
3	D	4733	C
3	D	4734	A
3	D	4740	G
3	D	4741	C
3	D	4742	G
3	D	4745	G
3	D	4754	G
3	D	4757	C
3	D	4759	C
3	D	4761	G
3	D	4765	G
3	D	4772	C
3	D	4774	C
3	D	4860	G
3	D	4870	G
3	D	4871	C
3	D	4875	G
3	D	4881	U
3	D	4882	U
3	D	4883	C
3	D	4889	G
3	D	4894	A
3	D	4895	C
3	D	4896	G
3	D	4900	C
3	D	4901	G
3	D	4910	G
3	D	4912	G
3	D	4914	C
3	D	4927	G
3	D	4928	C
3	D	4940	C
3	D	4941	G
3	D	4943	A
3	D	4955	A
3	D	4960	G
3	D	4966	A
3	D	4976	U
3	D	4985	U
3	D	4990	C
3	D	4991	U
3	D	5014	A

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Mol	Chain	Res	Type
3	D	5016	A
3	D	5017	G
3	D	5022	U
3	D	5023	C
3	D	5024	C
3	D	5025	C
3	D	5028	G
3	D	5030	U
3	D	5034	A
3	D	5041	G
3	D	5050	C
3	D	5054	C
3	D	5058	A
3	D	5060	A
3	D	5061	A
3	D	5062	G
3	D	5069	U
4	E	7	G
4	E	20	U
4	E	22	A
4	E	23	A
4	E	24	C
4	E	47	G
4	E	53	U
4	E	54	A
4	E	64	G
4	E	97	G
4	E	100	A
4	E	102	U
4	E	103	A
4	E	110	G
5	F	2	G
5	F	17	A
5	F	23	C
5	F	34	U
5	F	35	C
5	F	48	A
5	F	59	A
5	F	63	U
5	F	81	C
5	F	82	A
5	F	83	C

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Mol	Chain	Res	Type
5	F	84	A
5	F	85	U
5	F	86	U
5	F	87	G
5	F	103	A
5	F	105	C
5	F	110	U
5	F	114	G
5	F	123	U
5	F	124	U
5	F	125	C
5	F	126	C
5	F	127	U
5	F	128	C
5	F	150	C
5	F	151	G
5	F	153	C
48	w	2	A
48	w	11	A
48	w	17	C
48	w	21	U
48	w	22	A
48	w	26	U
48	w	33	G
48	w	34	PSU
48	w	41	G
48	w	42	A
48	w	43	U
48	w	44	U
48	w	46	A
48	w	49	C
48	w	54	A
48	w	60	A
48	w	61	A
48	w	62	G
48	w	63	U
48	w	66	G
48	w	67	C
48	w	68	A
48	w	69	C
48	w	70	G
48	w	78	C

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Mol	Chain	Res	Type
48	w	80	G
48	w	81	U
48	w	83	A
48	w	84	A
48	w	86	C
48	w	97	U
48	w	103	A
48	w	112	U
48	w	113	G
48	w	117	C
48	w	120	U
48	w	121	OMU
48	w	126	G
48	w	129	C
48	w	130	G
48	w	143	U
48	w	149	A
48	w	155	G
48	w	158	A
48	w	159	A2M
48	w	160	U
48	w	162	C
48	w	163	U
48	w	166	A2M
48	w	167	G
48	w	169	U
48	w	171	A
48	w	173	A
48	w	175	A
48	w	178	C
48	w	182	C
48	w	184	G
48	w	190	G
48	w	194	C
48	w	196	C
48	w	197	U
48	w	198	U
48	w	199	C
48	w	200	G
48	w	207	G
48	w	211	G
48	w	214	U

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Mol	Chain	Res	Type
48	w	215	G
48	w	216	C
48	w	226	A
48	w	291	G
48	w	292	A
48	w	293	C
48	w	295	C
48	w	310	C
48	w	311	C
48	w	312	G
48	w	313	A
48	w	314	U
48	w	316	G
48	w	318	A
48	w	319	C
48	w	332	G
48	w	335	G
48	w	345	U
48	w	346	C
48	w	351	G
48	w	362	C
48	w	364	A
48	w	370	G
48	w	380	G
48	w	381	C
48	w	385	G
48	w	386	C
48	w	398	A
48	w	400	C
48	w	401	A
48	w	407	G
48	w	408	A
48	w	409	C
48	w	413	G
48	w	418	A
48	w	421	G
48	w	428	OMU
48	w	438	G
48	w	441	C
48	w	448	A
48	w	449	A
48	w	450	C

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Mol	Chain	Res	Type
48	w	451	G
48	w	452	G
48	w	466	G
48	w	468	A2M
48	w	471	G
48	w	472	C
48	w	473	A
48	w	474	G
48	w	482	G
48	w	485	A
48	w	487	U
48	w	488	U
48	w	489	A
48	w	493	A
48	w	496	C
48	w	497	C
48	w	498	C
48	w	500	A
48	w	501	C
48	w	502	C
48	w	506	G
48	w	507	G
48	w	516	A
48	w	519	A
48	w	520	A
48	w	523	A
48	w	531	A
48	w	532	C
48	w	533	A
48	w	534	G
48	w	549	C
48	w	552	G
48	w	553	U
48	w	554	A
48	w	556	U
48	w	557	U
48	w	558	G
48	w	559	G
48	w	560	A
48	w	562	U
48	w	567	C
48	w	575	A

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Mol	Chain	Res	Type
48	w	576	A2M
48	w	583	C
48	w	587	A
48	w	588	G
48	w	589	G
48	w	590	A2M
48	w	592	C
48	w	593	C
48	w	594	A
48	w	595	U
48	w	597	G
48	w	604	A
48	w	605	A
48	w	606	G
48	w	608	C
48	w	610	G
48	w	614	C
48	w	617	G
48	w	622	C
48	w	623	G
48	w	627	OMU
48	w	634	A
48	w	638	C
48	w	643	A
48	w	644	OMG
48	w	655	A
48	w	659	G
48	w	660	C
48	w	664	A
48	w	668	A2M
48	w	669	A
48	w	671	A
48	w	672	A
48	w	688	U
48	w	810	A
48	w	811	A
48	w	812	A
48	w	818	A
48	w	819	G
48	w	821	G
48	w	822	PSU
48	w	823	U

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Mol	Chain	Res	Type
48	w	827	A
48	w	829	C
48	w	830	A
48	w	834	C
48	w	835	C
48	w	836	G
48	w	837	A
48	w	838	G
48	w	839	C
48	w	840	C
48	w	841	G
48	w	842	C
48	w	845	G
48	w	847	A
48	w	869	A
48	w	870	A
48	w	872	A
48	w	877	C
48	w	878	G
48	w	880	G
48	w	882	U
48	w	883	U
48	w	884	C
48	w	888	U
48	w	889	U
48	w	890	U
48	w	891	G
48	w	893	U
48	w	895	G
48	w	896	U
48	w	898	U
48	w	899	U
48	w	900	C
48	w	901	G
48	w	904	A
48	w	909	G
48	w	911	C
48	w	913	A
48	w	917	U
48	w	920	A
48	w	930	C
48	w	933	G

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Mol	Chain	Res	Type
48	w	934	G
48	w	958	G
48	w	963	A
48	w	972	A
48	w	990	A
48	w	992	A
48	w	999	G
48	w	1001	A
48	w	1017	U
48	w	1023	A
48	w	1027	A
48	w	1055	A
48	w	1061	U
48	w	1062	A
48	w	1083	A
48	w	1085	C
48	w	1109	C
48	w	1115	U
48	w	1116	C
48	w	1118	C
48	w	1119	A
48	w	1121	G
48	w	1123	C
48	w	1126	G
48	w	1133	A
48	w	1148	A
48	w	1149	A
48	w	1153	C
48	w	1154	U
48	w	1157	G
48	w	1181	A
48	w	1183	A
48	w	1195	A
48	w	1207	G
48	w	1208	A
48	w	1215	C
48	w	1217	A
48	w	1221	G
48	w	1224	G
48	w	1242	U
48	w	1243	U
48	w	1251	A

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Mol	Chain	Res	Type
48	w	1253	A
48	w	1256	G
48	w	1257	G
48	w	1259	A
48	w	1264	C
48	w	1265	A
48	w	1271	C
48	w	1274	G
48	w	1275	G
48	w	1284	A
48	w	1285	G
48	w	1286	G
48	w	1289	U
48	w	1293	A
48	w	1295	A
48	w	1298	G
48	w	1301	A
48	w	1302	G
48	w	1304	U
48	w	1307	U
48	w	1308	U
48	w	1309	C
48	w	1314	U
48	w	1331	C
48	w	1332	A
48	w	1342	U
48	w	1348	G
48	w	1371	U
48	w	1372	U
48	w	1373	C
48	w	1378	A
48	w	1396	A
48	w	1397	U
48	w	1401	A
48	w	1402	A
48	w	1403	C
48	w	1404	U
48	w	1406	G
48	w	1415	C
48	w	1417	C
48	w	1428	G
48	w	1429	G

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Mol	Chain	Res	Type
48	w	1430	C
48	w	1433	C
48	w	1434	C
48	w	1435	C
48	w	1436	C
48	w	1438	A
48	w	1440	C
48	w	1442	OMU
48	w	1449	G
48	w	1450	G
48	w	1452	A
48	w	1453	C
48	w	1454	A
48	w	1462	U
48	w	1463	U
48	w	1476	A
48	w	1477	U
48	w	1487	A
48	w	1489	A
48	w	1490	OMG
48	w	1495	G
48	w	1497	G
48	w	1498	A
48	w	1507	G
48	w	1508	A
48	w	1515	G
48	w	1521	C
48	w	1522	A
48	w	1526	G
48	w	1527	C
48	w	1528	G
48	w	1533	A
48	w	1543	U
48	w	1545	A
48	w	1546	G
48	w	1548	G
48	w	1552	G
48	w	1553	C
48	w	1556	A
48	w	1557	C
48	w	1569	A
48	w	1570	G

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Mol	Chain	Res	Type
48	w	1574	C
48	w	1575	G
48	w	1579	A
48	w	1580	A
48	w	1585	U
48	w	1586	U
48	w	1588	A
48	w	1599	U
48	w	1601	A
48	w	1602	U
48	w	1607	A
48	w	1621	U
48	w	1623	A
48	w	1624	U
48	w	1630	A
48	w	1632	G
48	w	1633	A
48	w	1635	C
48	w	1637	A
48	w	1638	G
48	w	1639	G7M
48	w	1640	A
48	w	1648	G
48	w	1654	G
48	w	1663	A
48	w	1665	G
48	w	1671	G
48	w	1698	C
48	w	1699	A
48	w	1721	U
48	w	1722	G
48	w	1743	G
48	w	1744	G
48	w	1745	A
48	w	1748	G
48	w	1751	C
48	w	1753	C
48	w	1754	G
48	w	1778	C
48	w	1779	G
48	w	1782	G
48	w	1783	C

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Mol	Chain	Res	Type
48	w	1784	G
48	w	1786	U
48	w	1813	A
48	w	1824	A
48	w	1829	G
48	w	1838	U
48	w	1849	G
48	w	1850	MA6
48	w	1851	MA6
48	w	1852	C
48	w	1861	G
48	w	1862	G
48	w	1863	A
48	w	1865	C
48	w	1869	A

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	5	C
2	B	10	2MG
2	B	16	H2U
3	D	1	C
3	D	406	C
3	D	515	C
3	D	914	U
3	D	922	C
3	D	987	C
3	D	1081	C
3	D	1590	C
3	D	1625	OMG
3	D	1633	G
3	D	1755	C
3	D	2101	C
3	D	2102	G
3	D	2675	G
3	D	2763	U
3	D	3614	G
3	D	3673	C
3	D	4113	U
3	D	4115	G
3	D	4600	G

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Mol	Chain	Res	Type
3	D	4678	G
3	D	4699	U
3	D	4913	G
3	D	5016	A
5	F	16	G
5	F	86	U

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

211 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
48	PSU	w	109	48	18,21,22	1.08	1 (5%)	22,30,33	1.84	5 (22%)
48	OMU	w	121	48	19,22,23	2.87	6 (31%)	26,31,34	1.60	5 (19%)
3	OMG	D	3792	3	23,26,27	2.56	8 (34%)	33,38,41	1.89	9 (27%)
3	6MZ	D	4220	3	22,25,26	2.84	4 (18%)	30,36,39	2.20	10 (33%)
3	UR3	D	4530	80,3	19,22,23	2.66	7 (36%)	26,32,35	1.30	2 (7%)
48	A2M	w	468	48	22,25,26	1.55	2 (9%)	31,36,39	1.02	2 (6%)
3	PSU	D	4361	3	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
3	1MA	D	1322	3	21,25,26	0.71	1 (4%)	31,37,40	0.79	1 (3%)
3	PSU	D	4471	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
3	A2M	D	400	3	22,25,26	1.41	1 (4%)	31,36,39	0.98	2 (6%)
3	A2M	D	1524	3	22,25,26	1.48	2 (9%)	31,36,39	1.04	3 (9%)
3	A2M	D	3825	3	22,25,26	1.37	1 (4%)	31,36,39	1.02	2 (6%)
48	PSU	w	1056	48	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
48	PSU	w	1625	48	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
2	PSU	B	35	2,1	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
48	PSU	w	863	48	18,21,22	1.07	1 (5%)	22,30,33	1.80	4 (18%)
3	A2M	D	3724	3	22,25,26	1.40	1 (4%)	31,36,39	0.97	3 (9%)
48	PSU	w	814	48	18,21,22	1.02	1 (5%)	22,30,33	1.70	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	A2M	w	1678	48	22,25,26	1.49	3 (13%)	31,36,39	1.04	3 (9%)
48	A2M	w	1031	48	22,25,26	1.39	1 (4%)	31,36,39	1.00	1 (3%)
48	MA6	w	1851	48	23,26,27	1.28	4 (17%)	34,38,41	2.29	11 (32%)
48	PSU	w	686	48	18,21,22	1.06	1 (5%)	22,30,33	1.82	4 (18%)
48	OMG	w	436	48	23,26,27	2.61	8 (34%)	33,38,41	1.97	9 (27%)
5	OMG	F	75	5	23,26,27	2.59	8 (34%)	33,38,41	1.91	9 (27%)
3	PSU	D	3762	3	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
48	A2M	w	159	48	22,25,26	1.62	4 (18%)	31,36,39	1.02	3 (9%)
48	PSU	w	649	48	18,21,22	1.07	1 (5%)	22,30,33	1.81	5 (22%)
3	PSU	D	4299	3	18,21,22	1.02	1 (5%)	22,30,33	1.74	4 (18%)
3	OMU	D	4498	80,3	19,22,23	2.79	6 (31%)	26,31,34	1.73	5 (19%)
48	PSU	w	822	48	18,21,22	1.10	1 (5%)	22,30,33	1.74	4 (18%)
2	56B	B	34	2,81	29,35,36	2.84	10 (34%)	36,52,55	2.30	7 (19%)
3	PSU	D	4403	80,3	18,21,22	1.07	1 (5%)	22,30,33	1.80	5 (22%)
3	OMG	D	2424	3	23,26,27	2.59	9 (39%)	33,38,41	1.92	10 (30%)
3	OMU	D	4620	3	19,22,23	2.79	6 (31%)	26,31,34	1.73	5 (19%)
3	OMC	D	4456	3	19,22,23	2.86	8 (42%)	26,31,34	0.77	0
3	PSU	D	1782	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
48	OMG	w	683	48	23,26,27	2.60	8 (34%)	33,38,41	1.92	9 (27%)
48	OMU	w	1442	80,48	19,22,23	2.93	8 (42%)	26,31,34	1.68	4 (15%)
3	PSU	D	3734	3	18,21,22	1.06	1 (5%)	22,30,33	1.85	5 (22%)
48	OMG	w	1490	80,48	23,26,27	2.61	8 (34%)	33,38,41	1.90	9 (27%)
3	OMG	D	3899	3	23,26,27	2.55	9 (39%)	33,38,41	1.96	10 (30%)
3	A2M	D	2815	3	22,25,26	1.51	1 (4%)	31,36,39	1.01	3 (9%)
3	A2M	D	3830	3	22,25,26	1.38	1 (4%)	31,36,39	1.07	2 (6%)
3	OMC	D	2351	80,3	19,22,23	2.85	8 (42%)	26,31,34	0.92	2 (7%)
3	OMG	D	3944	3	23,26,27	2.61	8 (34%)	33,38,41	1.96	9 (27%)
3	OMG	D	4494	3	23,26,27	2.58	9 (39%)	33,38,41	1.93	9 (27%)
3	5MC	D	4447	80,3	18,22,23	3.66	7 (38%)	26,32,35	1.14	1 (3%)
3	A2M	D	1326	3	22,25,26	1.36	1 (4%)	31,36,39	1.01	2 (6%)
48	PSU	w	105	48	18,21,22	1.04	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	4353	3	18,21,22	1.05	1 (5%)	22,30,33	1.85	4 (18%)
48	G7M	w	1639	2,48	23,26,27	2.82	8 (34%)	35,39,42	1.75	8 (22%)
48	OMU	w	116	48	19,22,23	2.90	7 (36%)	26,31,34	1.67	4 (15%)
48	PSU	w	1004	48	18,21,22	1.03	1 (5%)	22,30,33	1.77	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UY1	B	39	2	19,22,23	1.24	2 (10%)	22,31,34	0.97	1 (4%)
48	4AC	w	1842	48	21,24,25	0.57	0	29,34,37	1.19	4 (13%)
3	PSU	D	4457	3	18,21,22	1.02	1 (5%)	22,30,33	1.75	5 (22%)
3	OMC	D	4536	3	19,22,23	2.86	8 (42%)	26,31,34	0.75	0
3	PSU	D	5001	80,3	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
3	OMC	D	2365	80,3	19,22,23	2.85	8 (42%)	26,31,34	0.69	0
3	PSU	D	3637	80,3	18,21,22	1.01	1 (5%)	22,30,33	1.81	4 (18%)
3	OMC	D	3841	3	19,22,23	2.86	8 (42%)	26,31,34	0.70	0
3	PSU	D	4423	3	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
48	PSU	w	210	48	18,21,22	1.09	1 (5%)	22,30,33	1.76	4 (18%)
48	PSU	w	406	48	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	D	4228	3	23,26,27	2.55	9 (39%)	33,38,41	1.95	10 (30%)
48	PSU	w	801	48	18,21,22	1.09	1 (5%)	22,30,33	1.71	4 (18%)
48	OMU	w	1326	48	19,22,23	2.91	8 (42%)	26,31,34	1.70	4 (15%)
48	PSU	w	1445	48	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
48	A2M	w	512	48	22,25,26	1.50	1 (4%)	31,36,39	1.04	2 (6%)
48	OMG	w	601	48	23,26,27	2.60	8 (34%)	33,38,41	1.90	9 (27%)
3	OMG	D	4196	80,2,3	23,26,27	2.56	8 (34%)	33,38,41	1.90	9 (27%)
2	2MG	B	10	2	23,26,27	2.67	7 (30%)	32,38,41	2.18	10 (31%)
3	OMG	D	4499	3	23,26,27	2.58	9 (39%)	33,38,41	1.93	10 (30%)
2	H2U	B	16	2	18,21,22	1.00	2 (11%)	21,30,33	1.27	2 (9%)
3	PSU	D	3764	3	18,21,22	1.02	1 (5%)	22,30,33	1.73	4 (18%)
3	PSU	D	5010	3	18,21,22	1.03	1 (5%)	22,30,33	1.80	4 (18%)
48	PSU	w	651	48	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	1744	80,3	18,21,22	1.01	1 (5%)	22,30,33	1.85	4 (18%)
48	PSU	w	815	48	18,21,22	1.05	1 (5%)	22,30,33	1.84	5 (22%)
48	OMG	w	1328	48	23,26,27	2.61	8 (34%)	33,38,41	1.94	9 (27%)
48	OMU	w	627	48	19,22,23	2.96	8 (42%)	26,31,34	1.67	4 (15%)
2	1MA	B	58	2	21,25,26	0.96	2 (9%)	31,37,40	0.75	0
3	PSU	D	4576	3	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
3	OMG	D	4370	3	23,26,27	2.57	9 (39%)	33,38,41	1.95	10 (30%)
2	3AU	B	20	2	24,28,29	2.78	9 (37%)	33,40,43	1.40	5 (15%)
3	PSU	D	3639	3	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	3695	3	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
48	PSU	w	1046	48	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	w	93	48	18,21,22	1.04	1 (5%)	22,30,33	1.67	4 (18%)
48	B8N	w	1248	48	24,29,30	0.91	1 (4%)	29,42,45	1.05	1 (3%)
2	5MC	B	48	2	18,22,23	3.82	8 (44%)	26,32,35	1.02	2 (7%)
3	OMG	D	4392	3	23,26,27	2.56	9 (39%)	33,38,41	1.94	10 (30%)
3	A2M	D	2401	80,3	22,25,26	1.38	1 (4%)	31,36,39	0.99	2 (6%)
2	2MG	B	6	2	23,26,27	2.66	7 (30%)	32,38,41	2.12	9 (28%)
48	A2M	w	166	48	22,25,26	1.57	3 (13%)	31,36,39	1.05	4 (12%)
3	OMG	D	4623	3	23,26,27	2.55	9 (39%)	33,38,41	1.96	10 (30%)
48	OMG	w	509	48	23,26,27	2.61	8 (34%)	33,38,41	1.96	10 (30%)
48	PSU	w	34	48	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
2	M2G	B	26	2	24,27,28	1.09	2 (8%)	35,40,43	0.85	1 (2%)
48	OMU	w	1288	48	19,22,23	2.97	8 (42%)	26,31,34	1.66	4 (15%)
3	PSU	D	4296	3	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
3	OMG	D	1760	3	23,26,27	2.65	8 (34%)	33,38,41	1.94	9 (27%)
3	UY1	D	3818	80,3	19,22,23	1.14	1 (5%)	22,31,34	0.94	1 (4%)
3	PSU	D	1792	3	18,21,22	1.01	1 (5%)	22,30,33	1.73	4 (18%)
48	OMC	w	174	48	19,22,23	3.03	8 (42%)	26,31,34	0.69	0
3	PSU	D	1781	3	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
48	PSU	w	1177	48	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	1862	3	18,21,22	1.02	1 (5%)	22,30,33	1.83	4 (18%)
3	A2M	D	398	3	22,25,26	1.41	1 (4%)	31,36,39	1.03	3 (9%)
48	A2M	w	27	48	22,25,26	1.43	1 (4%)	31,36,39	0.98	1 (3%)
48	PSU	w	1081	48	18,21,22	1.02	1 (5%)	22,30,33	1.82	5 (22%)
3	PSU	D	1677	80,3	18,21,22	1.04	1 (5%)	22,30,33	1.76	3 (13%)
48	PSU	w	1045	48	18,21,22	1.02	1 (5%)	22,30,33	1.77	4 (18%)
3	OMU	D	1773	3	19,22,23	2.95	8 (42%)	26,31,34	1.64	4 (15%)
2	M2G	B	27	2	24,27,28	1.14	2 (8%)	35,40,43	0.86	1 (2%)
2	1MG	B	37	2	22,26,27	2.67	7 (31%)	33,39,42	1.75	8 (24%)
3	OMU	D	4227	3	19,22,23	2.82	6 (31%)	26,31,34	1.79	4 (15%)
3	PSU	D	4628	3	18,21,22	1.01	1 (5%)	22,30,33	1.77	4 (18%)
3	A2M	D	3718	3	22,25,26	1.37	1 (4%)	31,36,39	0.98	3 (9%)
3	A2M	D	2787	3	22,25,26	1.35	1 (4%)	31,36,39	1.00	2 (6%)
3	PSU	D	4312	3	18,21,22	1.02	1 (5%)	22,30,33	1.82	4 (18%)
48	OMC	w	1391	48	19,22,23	2.99	8 (42%)	26,31,34	0.68	0
3	PSU	D	4972	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	B	55	2	18,21,22	1.11	1 (5%)	22,30,33	1.74	4 (18%)
3	PSU	D	3758	3	18,21,22	0.97	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4500	3	18,21,22	1.04	1 (5%)	22,30,33	1.89	5 (22%)
3	PSU	D	4689	3	18,21,22	1.07	1 (5%)	22,30,33	1.81	4 (18%)
48	OMU	w	428	48	19,22,23	2.89	7 (36%)	26,31,34	1.72	4 (15%)
48	OMC	w	462	48	19,22,23	3.02	8 (42%)	26,31,34	0.78	0
48	OMG	w	644	48	23,26,27	2.61	8 (34%)	33,38,41	1.93	10 (30%)
3	PSU	D	4579	3	18,21,22	1.02	1 (5%)	22,30,33	1.81	4 (18%)
48	OMU	w	799	48	19,22,23	2.93	8 (42%)	26,31,34	1.69	5 (19%)
48	A2M	w	576	48	22,25,26	1.44	2 (9%)	31,36,39	1.10	4 (12%)
3	A2M	D	1871	80,3	22,25,26	1.42	2 (9%)	31,36,39	1.10	2 (6%)
48	PSU	w	1232	48	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
3	PSU	D	4552	3	18,21,22	1.06	1 (5%)	22,30,33	1.83	4 (18%)
3	OMG	D	2364	3	23,26,27	2.54	9 (39%)	33,38,41	1.93	9 (27%)
3	OMG	D	3744	3	23,26,27	2.57	9 (39%)	33,38,41	1.93	10 (30%)
48	PSU	w	1692	48	18,21,22	1.02	1 (5%)	22,30,33	1.77	4 (18%)
3	OMC	D	2422	80,3	19,22,23	2.90	8 (42%)	26,31,34	0.72	0
3	A2M	D	3785	80,3	22,25,26	1.41	1 (4%)	31,36,39	1.26	3 (9%)
3	OMU	D	3925	3	19,22,23	2.80	6 (31%)	26,31,34	1.74	4 (15%)
48	PSU	w	609	48	18,21,22	1.03	1 (5%)	22,30,33	1.89	5 (22%)
48	A2M	w	1383	48	22,25,26	1.43	1 (4%)	31,36,39	1.12	4 (12%)
3	PSU	D	3851	3	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	1536	3	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
48	4AC	w	1337	48	21,24,25	0.63	0	29,34,37	1.17	5 (17%)
2	5MU	B	54	2	19,22,23	4.74	5 (26%)	28,32,35	3.60	9 (32%)
3	PSU	D	4532	3	18,21,22	1.01	1 (5%)	22,30,33	1.72	4 (18%)
3	PSU	D	1860	3	18,21,22	1.04	1 (5%)	22,30,33	1.83	5 (22%)
48	6MZ	w	1832	80,48	22,25,26	2.80	4 (18%)	30,36,39	2.21	10 (33%)
3	PSU	D	4293	3	18,21,22	0.99	1 (5%)	22,30,33	1.65	4 (18%)
3	PSU	D	3920	80,3	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
3	OMC	D	3887	3	19,22,23	2.87	8 (42%)	26,31,34	0.76	0
3	PSU	D	4420	3	18,21,22	1.05	1 (5%)	22,30,33	1.67	4 (18%)
48	PSU	w	572	48	18,21,22	1.12	1 (5%)	22,30,33	1.78	4 (18%)
48	PSU	w	1643	80,48	18,21,22	1.08	1 (5%)	22,30,33	1.76	4 (18%)
3	PSU	D	4431	3	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	D	3730	3	18,21,22	1.03	1 (5%)	22,30,33	1.77	4 (18%)
3	A2M	D	1534	80,3	22,25,26	1.36	1 (4%)	31,36,39	1.29	6 (19%)
3	PSU	D	1683	80,3	18,21,22	1.08	1 (5%)	22,30,33	1.87	4 (18%)
3	OMU	D	4306	3	19,22,23	2.75	6 (31%)	26,31,34	1.72	5 (19%)
3	OMG	D	4618	3	23,26,27	2.57	9 (39%)	33,38,41	1.95	10 (30%)
3	PSU	D	3715	3	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
48	OMC	w	1703	80,48	19,22,23	2.94	8 (42%)	26,31,34	0.70	0
3	OMC	D	2824	3	19,22,23	2.89	8 (42%)	26,31,34	0.76	0
3	OMU	D	2415	3	19,22,23	2.83	6 (31%)	26,31,34	1.88	5 (19%)
48	PSU	w	1174	80,48	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
48	A2M	w	590	48	22,25,26	1.51	2 (9%)	31,36,39	1.01	1 (3%)
2	G7M	B	46	2	23,26,27	2.82	9 (39%)	35,39,42	1.68	8 (22%)
3	PSU	D	4442	3	18,21,22	1.04	2 (11%)	22,30,33	1.86	5 (22%)
3	OMG	D	3627	3	23,26,27	2.56	9 (39%)	33,38,41	1.98	10 (30%)
48	OMC	w	517	80,48	19,22,23	3.00	8 (42%)	26,31,34	0.76	0
3	OMU	D	2837	3	19,22,23	2.77	6 (31%)	26,31,34	1.83	5 (19%)
3	PSU	D	3768	3	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)
48	A2M	w	668	80,48	22,25,26	1.52	2 (9%)	31,36,39	0.98	1 (3%)
48	OMU	w	172	48	19,22,23	2.91	7 (36%)	26,31,34	1.72	5 (19%)
3	OMC	D	2861	3	19,22,23	2.89	8 (42%)	26,31,34	0.68	0
48	MA6	w	1850	48	23,26,27	1.36	4 (17%)	34,38,41	2.20	10 (29%)
3	OMG	D	1316	3	23,26,27	2.57	10 (43%)	33,38,41	1.95	9 (27%)
3	5MC	D	3782	80,3	18,22,23	3.64	8 (44%)	26,32,35	1.06	2 (7%)
2	H2U	B	47	2	18,21,22	1.03	2 (11%)	21,30,33	0.77	0
48	PSU	w	218	48	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
48	PSU	w	866	48	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
48	PSU	w	119	48	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
3	PSU	D	3770	3	18,21,22	1.07	1 (5%)	22,30,33	1.82	4 (18%)
48	PSU	w	1367	48	18,21,22	1.06	1 (5%)	22,30,33	1.80	5 (22%)
3	A2M	D	2363	80,3	22,25,26	1.37	2 (9%)	31,36,39	0.97	2 (6%)
2	H2U	B	17	2	18,21,22	1.01	2 (11%)	21,30,33	0.89	2 (9%)
3	OMG	D	1625	80,3	23,26,27	2.59	8 (34%)	33,38,41	1.91	9 (27%)
48	A2M	w	484	48	22,25,26	1.46	1 (4%)	31,36,39	1.00	2 (6%)
3	PSU	D	2508	3	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
48	PSU	w	966	48	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	w	1238	48	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
48	OMU	w	1804	48	19,22,23	2.89	8 (42%)	26,31,34	1.76	5 (19%)
48	PSU	w	36	48	18,21,22	1.06	1 (5%)	22,30,33	1.78	5 (22%)
3	PSU	D	4521	80,3	18,21,22	1.05	1 (5%)	22,30,33	1.86	4 (18%)
3	OMG	D	4637	3	23,26,27	2.56	9 (39%)	33,38,41	1.92	9 (27%)
48	PSU	w	1244	48	18,21,22	1.07	1 (5%)	22,30,33	1.79	5 (22%)
3	OMC	D	1340	3	19,22,23	2.84	8 (42%)	26,31,34	0.75	0
3	OMC	D	3808	3	19,22,23	2.86	8 (42%)	26,31,34	0.80	0
48	PSU	w	681	80,48	18,21,22	1.05	1 (5%)	22,30,33	1.79	4 (18%)
3	OMG	D	1522	3	23,26,27	2.57	9 (39%)	33,38,41	1.98	10 (30%)
3	OMC	D	3701	80,3	19,22,23	2.87	8 (42%)	26,31,34	0.73	0
48	PSU	w	1347	48	18,21,22	1.02	1 (5%)	22,30,33	1.78	4 (18%)
48	A2M	w	99	80,48	22,25,26	1.41	1 (4%)	31,36,39	1.03	2 (6%)
3	OMC	D	2804	3	19,22,23	2.86	8 (42%)	26,31,34	0.86	1 (3%)
3	PSU	D	2632	3	18,21,22	1.02	1 (5%)	22,30,33	1.71	4 (18%)
3	PSU	D	3853	80,3	18,21,22	0.99	1 (5%)	22,30,33	1.66	4 (18%)
3	A2M	D	3760	3	22,25,26	1.54	3 (13%)	31,36,39	1.09	3 (9%)
3	A2M	D	4523	80,3	22,25,26	1.42	1 (4%)	31,36,39	1.08	3 (9%)

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
48	PSU	w	109	48	-	0/7/25/26	0/2/2/2
48	OMU	w	121	48	-	0/9/27/28	0/2/2/2
3	OMG	D	3792	3	-	0/9/27/28	0/3/3/3
3	6MZ	D	4220	3	-	0/9/27/28	0/3/3/3
3	UR3	D	4530	80,3	-	0/7/25/26	0/2/2/2
48	A2M	w	468	48	-	3/9/27/28	0/3/3/3
3	PSU	D	4361	3	-	0/7/25/26	0/2/2/2
3	1MA	D	1322	3	-	2/7/25/26	0/3/3/3
3	PSU	D	4471	3	-	0/7/25/26	0/2/2/2
3	A2M	D	400	3	-	0/9/27/28	0/3/3/3
3	A2M	D	1524	3	-	3/9/27/28	0/3/3/3
3	A2M	D	3825	3	-	0/9/27/28	0/3/3/3
48	PSU	w	1056	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	w	1625	48	-	0/7/25/26	0/2/2/2
2	PSU	B	35	2,1	-	0/7/25/26	0/2/2/2
48	PSU	w	863	48	-	0/7/25/26	0/2/2/2
3	A2M	D	3724	3	-	1/9/27/28	0/3/3/3
48	PSU	w	814	48	-	0/7/25/26	0/2/2/2
48	A2M	w	1678	48	-	1/9/27/28	0/3/3/3
48	A2M	w	1031	48	-	0/9/27/28	0/3/3/3
48	MA6	w	1851	48	-	3/11/29/30	0/3/3/3
48	PSU	w	686	48	-	0/7/25/26	0/2/2/2
48	OMG	w	436	48	-	0/9/27/28	0/3/3/3
5	OMG	F	75	5	-	0/9/27/28	0/3/3/3
3	PSU	D	3762	3	-	0/7/25/26	0/2/2/2
48	A2M	w	159	48	-	4/9/27/28	0/3/3/3
48	PSU	w	649	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4299	3	-	0/7/25/26	0/2/2/2
3	OMU	D	4498	80,3	-	0/9/27/28	0/2/2/2
48	PSU	w	822	48	-	0/7/25/26	0/2/2/2
2	56B	B	34	2,81	-	2/12/43/44	0/4/4/4
3	PSU	D	4403	80,3	-	0/7/25/26	0/2/2/2
3	OMG	D	2424	3	-	2/9/27/28	0/3/3/3
3	OMU	D	4620	3	-	0/9/27/28	0/2/2/2
3	OMC	D	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	D	1782	3	-	0/7/25/26	0/2/2/2
48	OMG	w	683	48	-	0/9/27/28	0/3/3/3
48	OMU	w	1442	80,48	-	1/9/27/28	0/2/2/2
3	PSU	D	3734	3	-	0/7/25/26	0/2/2/2
48	OMG	w	1490	80,48	-	3/9/27/28	0/3/3/3
3	OMG	D	3899	3	-	0/9/27/28	0/3/3/3
3	A2M	D	2815	3	-	3/9/27/28	0/3/3/3
3	A2M	D	3830	3	-	0/9/27/28	0/3/3/3
3	OMC	D	2351	80,3	-	4/9/27/28	0/2/2/2
3	OMG	D	3944	3	-	3/9/27/28	0/3/3/3
3	OMG	D	4494	3	-	1/9/27/28	0/3/3/3
3	5MC	D	4447	80,3	-	4/7/25/26	0/2/2/2
3	A2M	D	1326	3	-	1/9/27/28	0/3/3/3
48	PSU	w	105	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4353	3	-	0/7/25/26	0/2/2/2
48	G7M	w	1639	2,48	-	2/7/25/26	0/3/3/3
48	OMU	w	116	48	-	1/9/27/28	0/2/2/2
48	PSU	w	1004	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UY1	B	39	2	-	1/9/27/28	0/2/2/2
48	4AC	w	1842	48	-	0/11/29/30	0/2/2/2
3	PSU	D	4457	3	-	0/7/25/26	0/2/2/2
3	OMC	D	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	D	5001	80,3	-	0/7/25/26	0/2/2/2
3	OMC	D	2365	80,3	-	0/9/27/28	0/2/2/2
3	PSU	D	3637	80,3	-	0/7/25/26	0/2/2/2
3	OMC	D	3841	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4423	3	-	0/7/25/26	0/2/2/2
48	PSU	w	210	48	-	0/7/25/26	0/2/2/2
48	PSU	w	406	48	-	0/7/25/26	0/2/2/2
3	OMG	D	4228	3	-	0/9/27/28	0/3/3/3
48	PSU	w	801	48	-	0/7/25/26	0/2/2/2
48	OMU	w	1326	48	-	4/9/27/28	0/2/2/2
48	PSU	w	1445	48	-	0/7/25/26	0/2/2/2
48	A2M	w	512	48	-	0/9/27/28	0/3/3/3
48	OMG	w	601	48	-	1/9/27/28	0/3/3/3
3	OMG	D	4196	80,2,3	-	1/9/27/28	0/3/3/3
2	2MG	B	10	2	-	0/9/27/28	0/3/3/3
3	OMG	D	4499	3	-	0/9/27/28	0/3/3/3
2	H2U	B	16	2	-	6/7/38/39	0/2/2/2
3	PSU	D	3764	3	-	0/7/25/26	0/2/2/2
3	PSU	D	5010	3	-	0/7/25/26	0/2/2/2
48	PSU	w	651	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1744	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	815	48	-	0/7/25/26	0/2/2/2
48	OMG	w	1328	48	-	1/9/27/28	0/3/3/3
48	OMU	w	627	48	-	0/9/27/28	0/2/2/2
2	1MA	B	58	2	-	0/7/25/26	0/3/3/3
3	PSU	D	4576	3	-	0/7/25/26	0/2/2/2
3	OMG	D	4370	3	-	2/9/27/28	0/3/3/3
2	3AU	B	20	2	-	8/16/34/35	0/2/2/2
3	PSU	D	3639	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3695	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1046	48	-	0/7/25/26	0/2/2/2
48	PSU	w	93	48	-	0/7/25/26	0/2/2/2
48	B8N	w	1248	48	-	2/16/34/35	0/2/2/2
2	5MC	B	48	2	-	0/7/25/26	0/2/2/2
3	OMG	D	4392	3	-	0/9/27/28	0/3/3/3
3	A2M	D	2401	80,3	-	1/9/27/28	0/3/3/3
2	2MG	B	6	2	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A2M	w	166	48	-	3/9/27/28	0/3/3/3
3	OMG	D	4623	3	-	0/9/27/28	0/3/3/3
48	OMG	w	509	48	-	0/9/27/28	0/3/3/3
48	PSU	w	34	48	-	3/7/25/26	0/2/2/2
2	M2G	B	26	2	-	0/11/29/30	0/3/3/3
48	OMU	w	1288	48	-	1/9/27/28	0/2/2/2
3	PSU	D	4296	3	-	0/7/25/26	0/2/2/2
3	OMG	D	1760	3	-	2/9/27/28	0/3/3/3
3	UY1	D	3818	80,3	-	4/9/27/28	0/2/2/2
3	PSU	D	1792	3	-	0/7/25/26	0/2/2/2
48	OMC	w	174	48	-	0/9/27/28	0/2/2/2
3	PSU	D	1781	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1177	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1862	3	-	0/7/25/26	0/2/2/2
3	A2M	D	398	3	-	1/9/27/28	0/3/3/3
48	A2M	w	27	48	-	0/9/27/28	0/3/3/3
48	PSU	w	1081	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1677	80,3	-	4/7/25/26	0/2/2/2
48	PSU	w	1045	48	-	0/7/25/26	0/2/2/2
3	OMU	D	1773	3	-	0/9/27/28	0/2/2/2
2	M2G	B	27	2	-	0/11/29/30	0/3/3/3
2	1MG	B	37	2	-	0/7/25/26	0/3/3/3
3	OMU	D	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4628	3	-	0/7/25/26	0/2/2/2
3	A2M	D	3718	3	-	0/9/27/28	0/3/3/3
3	A2M	D	2787	3	-	3/9/27/28	0/3/3/3
3	PSU	D	4312	3	-	0/7/25/26	0/2/2/2
48	OMC	w	1391	48	-	0/9/27/28	0/2/2/2
3	PSU	D	4972	3	-	0/7/25/26	0/2/2/2
2	PSU	B	55	2	-	1/7/25/26	0/2/2/2
3	PSU	D	3758	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4500	3	-	4/7/25/26	0/2/2/2
3	PSU	D	4689	3	-	0/7/25/26	0/2/2/2
48	OMU	w	428	48	-	7/9/27/28	0/2/2/2
48	OMC	w	462	48	-	1/9/27/28	0/2/2/2
48	OMG	w	644	48	-	3/9/27/28	0/3/3/3
3	PSU	D	4579	3	-	0/7/25/26	0/2/2/2
48	OMU	w	799	48	-	3/9/27/28	0/2/2/2
48	A2M	w	576	48	-	2/9/27/28	0/3/3/3
3	A2M	D	1871	80,3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	w	1232	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4552	3	-	0/7/25/26	0/2/2/2
3	OMG	D	2364	3	-	2/9/27/28	0/3/3/3
3	OMG	D	3744	3	-	1/9/27/28	0/3/3/3
48	PSU	w	1692	48	-	0/7/25/26	0/2/2/2
3	OMC	D	2422	80,3	-	1/9/27/28	0/2/2/2
3	A2M	D	3785	80,3	-	3/9/27/28	0/3/3/3
3	OMU	D	3925	3	-	1/9/27/28	0/2/2/2
48	PSU	w	609	48	-	0/7/25/26	0/2/2/2
48	A2M	w	1383	48	-	1/9/27/28	0/3/3/3
3	PSU	D	3851	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1536	3	-	0/7/25/26	0/2/2/2
48	4AC	w	1337	48	-	0/11/29/30	0/2/2/2
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2
3	PSU	D	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1860	3	-	0/7/25/26	0/2/2/2
48	6MZ	w	1832	80,48	-	2/9/27/28	0/3/3/3
3	PSU	D	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3920	80,3	-	0/7/25/26	0/2/2/2
3	OMC	D	3887	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4420	3	-	0/7/25/26	0/2/2/2
48	PSU	w	572	48	-	2/7/25/26	0/2/2/2
48	PSU	w	1643	80,48	-	0/7/25/26	0/2/2/2
3	PSU	D	4431	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3730	3	-	0/7/25/26	0/2/2/2
3	A2M	D	1534	80,3	-	3/9/27/28	0/3/3/3
3	PSU	D	1683	80,3	-	0/7/25/26	0/2/2/2
3	OMU	D	4306	3	-	0/9/27/28	0/2/2/2
3	OMG	D	4618	3	-	0/9/27/28	0/3/3/3
3	PSU	D	3715	3	-	0/7/25/26	0/2/2/2
48	OMC	w	1703	80,48	-	2/9/27/28	0/2/2/2
3	OMC	D	2824	3	-	1/9/27/28	0/2/2/2
3	OMU	D	2415	3	-	1/9/27/28	0/2/2/2
48	PSU	w	1174	80,48	-	0/7/25/26	0/2/2/2
48	A2M	w	590	48	-	4/9/27/28	0/3/3/3
2	G7M	B	46	2	-	3/7/25/26	0/3/3/3
3	PSU	D	4442	3	-	0/7/25/26	0/2/2/2
3	OMG	D	3627	3	-	0/9/27/28	0/3/3/3
48	OMC	w	517	80,48	-	0/9/27/28	0/2/2/2
3	OMU	D	2837	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	D	3768	3	-	0/7/25/26	0/2/2/2
48	A2M	w	668	80,48	-	2/9/27/28	0/3/3/3
48	OMU	w	172	48	-	0/9/27/28	0/2/2/2
3	OMC	D	2861	3	-	0/9/27/28	0/2/2/2
48	MA6	w	1850	48	-	0/11/29/30	0/3/3/3
3	OMG	D	1316	3	-	0/9/27/28	0/3/3/3
3	5MC	D	3782	80,3	-	0/7/25/26	0/2/2/2
2	H2U	B	47	2	-	2/7/38/39	0/2/2/2
48	PSU	w	218	48	-	0/7/25/26	0/2/2/2
48	PSU	w	866	48	-	0/7/25/26	0/2/2/2
48	PSU	w	119	48	-	0/7/25/26	0/2/2/2
3	PSU	D	3770	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1367	48	-	0/7/25/26	0/2/2/2
3	A2M	D	2363	80,3	-	0/9/27/28	0/3/3/3
2	H2U	B	17	2	-	1/7/38/39	0/2/2/2
3	OMG	D	1625	80,3	-	0/9/27/28	0/3/3/3
48	A2M	w	484	48	-	0/9/27/28	0/3/3/3
3	PSU	D	2508	3	-	0/7/25/26	0/2/2/2
48	PSU	w	966	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1238	48	-	2/7/25/26	0/2/2/2
48	OMU	w	1804	48	-	1/9/27/28	0/2/2/2
48	PSU	w	36	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4521	80,3	-	0/7/25/26	0/2/2/2
3	OMG	D	4637	3	-	1/9/27/28	0/3/3/3
48	PSU	w	1244	48	-	0/7/25/26	0/2/2/2
3	OMC	D	1340	3	-	0/9/27/28	0/2/2/2
3	OMC	D	3808	3	-	0/9/27/28	0/2/2/2
48	PSU	w	681	80,48	-	0/7/25/26	0/2/2/2
3	OMG	D	1522	3	-	0/9/27/28	0/3/3/3
3	OMC	D	3701	80,3	-	4/9/27/28	0/2/2/2
48	PSU	w	1347	48	-	0/7/25/26	0/2/2/2
48	A2M	w	99	80,48	-	1/9/27/28	0/3/3/3
3	OMC	D	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	D	2632	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3853	80,3	-	0/7/25/26	0/2/2/2
3	A2M	D	3760	3	-	2/9/27/28	0/3/3/3
3	A2M	D	4523	80,3	-	0/9/27/28	0/3/3/3

All (770) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4220	6MZ	C6-N6	12.21	1.47	1.34
48	w	1832	6MZ	C6-N6	12.03	1.47	1.34
2	B	54	5MU	C2-N1	10.87	1.55	1.38
2	B	54	5MU	C6-N1	10.82	1.56	1.38
3	D	4447	5MC	C6-C5	9.48	1.50	1.34
2	B	48	5MC	C6-C5	9.47	1.50	1.34
2	B	54	5MU	C4-C5	9.33	1.60	1.44
3	D	3782	5MC	C6-C5	9.17	1.49	1.34
2	B	10	2MG	C2-N3	7.79	1.46	1.31
2	B	6	2MG	C2-N3	7.69	1.46	1.31
2	B	48	5MC	C4-N3	7.49	1.46	1.34
3	D	1760	OMG	C4-N3	7.43	1.51	1.34
3	D	3944	OMG	C4-N3	7.39	1.51	1.34
48	w	1490	OMG	C4-N3	7.29	1.51	1.34
48	w	436	OMG	C4-N3	7.29	1.51	1.34
48	w	601	OMG	C4-N3	7.27	1.51	1.34
48	w	1328	OMG	C4-N3	7.26	1.51	1.34
48	w	1288	OMU	C2-N1	7.26	1.50	1.38
48	w	683	OMG	C4-N3	7.25	1.51	1.34
48	w	509	OMG	C4-N3	7.24	1.51	1.34
48	w	644	OMG	C4-N3	7.24	1.51	1.34
5	F	75	OMG	C4-N3	7.17	1.51	1.34
3	D	1773	OMU	C2-N1	7.17	1.49	1.38
3	D	4637	OMG	C4-N3	7.15	1.51	1.34
3	D	3744	OMG	C4-N3	7.15	1.51	1.34
2	B	54	5MU	C4-N3	-7.14	1.25	1.38
3	D	3792	OMG	C4-N3	7.14	1.51	1.34
3	D	4618	OMG	C4-N3	7.14	1.51	1.34
3	D	4196	OMG	C4-N3	7.12	1.51	1.34
3	D	1625	OMG	C4-N3	7.12	1.51	1.34
3	D	1522	OMG	C4-N3	7.12	1.51	1.34
3	D	4499	OMG	C4-N3	7.10	1.51	1.34
3	D	4494	OMG	C4-N3	7.09	1.51	1.34
3	D	4370	OMG	C4-N3	7.08	1.51	1.34
3	D	4228	OMG	C4-N3	7.08	1.51	1.34
3	D	3627	OMG	C4-N3	7.06	1.51	1.34
48	w	1442	OMU	C2-N1	7.06	1.49	1.38
3	D	2424	OMG	C4-N3	7.05	1.51	1.34
48	w	627	OMU	C2-N1	7.05	1.49	1.38
48	w	799	OMU	C2-N1	7.05	1.49	1.38
3	D	2364	OMG	C4-N3	7.05	1.51	1.34
3	D	4623	OMG	C4-N3	7.01	1.50	1.34
3	D	3899	OMG	C4-N3	7.01	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	116	OMU	C2-N1	7.01	1.49	1.38
3	D	4392	OMG	C4-N3	7.00	1.50	1.34
3	D	1316	OMG	C4-N3	7.00	1.50	1.34
48	w	172	OMU	C2-N1	6.98	1.49	1.38
48	w	1326	OMU	C2-N1	6.97	1.49	1.38
48	w	428	OMU	C2-N1	6.96	1.49	1.38
3	D	3782	5MC	C4-N3	6.92	1.45	1.34
48	w	1804	OMU	C2-N1	6.92	1.49	1.38
3	D	2415	OMU	C2-N1	6.88	1.49	1.38
2	B	34	56B	C14-C13	6.87	1.52	1.32
48	w	627	OMU	C2-N3	6.77	1.50	1.38
3	D	4227	OMU	C2-N1	6.76	1.49	1.38
48	w	121	OMU	C2-N1	6.76	1.49	1.38
3	D	3925	OMU	C2-N1	6.74	1.49	1.38
3	D	4530	UR3	C2-N1	6.71	1.48	1.38
2	B	10	2MG	C4-N3	6.66	1.50	1.34
3	D	4447	5MC	C4-N3	6.65	1.45	1.34
3	D	1773	OMU	C2-N3	6.65	1.49	1.38
48	w	1288	OMU	C2-N3	6.64	1.49	1.38
2	B	54	5MU	C6-C5	6.64	1.45	1.34
2	B	48	5MC	C2-N3	6.63	1.49	1.36
3	D	4620	OMU	C2-N1	6.60	1.49	1.38
48	w	1442	OMU	C2-N3	6.60	1.49	1.38
2	B	6	2MG	C4-N3	6.60	1.49	1.34
48	w	172	OMU	C2-N3	6.59	1.49	1.38
48	w	116	OMU	C2-N3	6.58	1.49	1.38
3	D	4498	OMU	C2-N1	6.58	1.49	1.38
48	w	799	OMU	C2-N3	6.57	1.49	1.38
48	w	1326	OMU	C2-N3	6.55	1.49	1.38
48	w	121	OMU	C2-N3	6.54	1.49	1.38
2	B	46	G7M	C2-N2	6.53	1.49	1.34
2	B	46	G7M	C4-N3	6.53	1.49	1.34
2	B	37	1MG	C2-N3	6.52	1.46	1.34
48	w	1639	G7M	C2-N2	6.51	1.49	1.34
48	w	428	OMU	C2-N3	6.51	1.49	1.38
2	B	20	3AU	C2-N1	6.49	1.47	1.38
48	w	1804	OMU	C2-N3	6.48	1.49	1.38
48	w	1639	G7M	C4-N3	6.46	1.49	1.34
3	D	2837	OMU	C2-N1	6.45	1.48	1.38
48	w	462	OMC	C2-N3	6.37	1.49	1.36
48	w	174	OMC	C2-N3	6.34	1.49	1.36
48	w	517	OMC	C2-N3	6.33	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	1MG	C4-N3	6.32	1.49	1.34
3	D	4306	OMU	C2-N1	6.29	1.48	1.38
48	w	1391	OMC	C2-N3	6.29	1.49	1.36
2	B	37	1MG	C2-N2	6.26	1.45	1.34
3	D	4227	OMU	C2-N3	6.25	1.49	1.38
2	B	34	56B	C4-N3	6.24	1.49	1.34
3	D	2837	OMU	C2-N3	6.23	1.49	1.38
3	D	4620	OMU	C2-N3	6.23	1.49	1.38
3	D	2415	OMU	C2-N3	6.22	1.49	1.38
3	D	3782	5MC	C2-N3	6.18	1.48	1.36
3	D	4306	OMU	C2-N3	6.18	1.49	1.38
3	D	4498	OMU	C2-N3	6.18	1.49	1.38
3	D	3925	OMU	C2-N3	6.17	1.49	1.38
48	w	1703	OMC	C2-N3	6.14	1.48	1.36
2	B	20	3AU	C2-N3	6.12	1.49	1.38
48	w	174	OMC	C6-C5	6.11	1.49	1.35
3	D	2824	OMC	C2-N3	6.09	1.48	1.36
3	D	2861	OMC	C2-N3	6.07	1.48	1.36
3	D	2422	OMC	C2-N3	6.06	1.48	1.36
3	D	3887	OMC	C2-N3	6.03	1.48	1.36
3	D	4530	UR3	C6-C5	6.02	1.49	1.35
2	B	20	3AU	C6-C5	6.01	1.49	1.35
3	D	1340	OMC	C2-N3	6.01	1.48	1.36
48	w	462	OMC	C6-C5	6.00	1.49	1.35
3	D	4456	OMC	C2-N3	5.99	1.48	1.36
48	w	1391	OMC	C6-C5	5.98	1.49	1.35
3	D	2804	OMC	C2-N3	5.97	1.48	1.36
3	D	3701	OMC	C6-C5	5.96	1.48	1.35
48	w	517	OMC	C6-C5	5.96	1.48	1.35
3	D	3841	OMC	C2-N3	5.96	1.48	1.36
3	D	4447	5MC	C2-N3	5.95	1.48	1.36
3	D	4536	OMC	C2-N3	5.95	1.48	1.36
3	D	3701	OMC	C2-N3	5.94	1.48	1.36
3	D	2351	OMC	C2-N3	5.93	1.48	1.36
3	D	2365	OMC	C2-N3	5.93	1.48	1.36
48	w	1703	OMC	C6-C5	5.92	1.48	1.35
2	B	34	56B	C11-C10	5.89	1.63	1.54
3	D	2861	OMC	C6-C5	5.89	1.48	1.35
3	D	1773	OMU	C6-C5	5.87	1.48	1.35
48	w	627	OMU	C6-C5	5.86	1.48	1.35
48	w	799	OMU	C6-C5	5.86	1.48	1.35
48	w	1442	OMU	C6-C5	5.86	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	1288	OMU	C6-C5	5.86	1.48	1.35
3	D	3808	OMC	C2-N3	5.86	1.48	1.36
3	D	4536	OMC	C6-C5	5.84	1.48	1.35
3	D	2365	OMC	C6-C5	5.84	1.48	1.35
3	D	2422	OMC	C6-C5	5.84	1.48	1.35
3	D	2804	OMC	C6-C5	5.83	1.48	1.35
3	D	3808	OMC	C6-C5	5.83	1.48	1.35
48	w	428	OMU	C6-C5	5.83	1.48	1.35
48	w	1326	OMU	C6-C5	5.82	1.48	1.35
3	D	3841	OMC	C6-C5	5.82	1.48	1.35
3	D	2824	OMC	C6-C5	5.81	1.48	1.35
3	D	4456	OMC	C6-C5	5.80	1.48	1.35
48	w	1639	G7M	C2-N3	5.80	1.47	1.33
48	w	172	OMU	C6-C5	5.79	1.48	1.35
48	w	1804	OMU	C6-C5	5.78	1.48	1.35
3	D	2351	OMC	C6-C5	5.77	1.48	1.35
3	D	3887	OMC	C6-C5	5.76	1.48	1.35
48	w	121	OMU	C6-C5	5.76	1.48	1.35
3	D	1340	OMC	C6-C5	5.75	1.48	1.35
2	B	46	G7M	C2-N3	5.72	1.47	1.33
48	w	116	OMU	C6-C5	5.72	1.48	1.35
3	D	4306	OMU	C6-C5	5.66	1.48	1.35
3	D	4620	OMU	C6-C5	5.64	1.48	1.35
3	D	4498	OMU	C6-C5	5.63	1.48	1.35
3	D	2415	OMU	C6-C5	5.63	1.48	1.35
3	D	4227	OMU	C6-C5	5.62	1.48	1.35
3	D	1760	OMG	C2-N3	5.61	1.46	1.33
2	B	34	56B	C2-N3	5.59	1.46	1.33
3	D	2837	OMU	C6-C5	5.56	1.48	1.35
3	D	3925	OMU	C6-C5	5.54	1.47	1.35
48	w	1328	OMG	C2-N3	5.54	1.46	1.33
48	w	644	OMG	C2-N3	5.49	1.46	1.33
3	D	1625	OMG	C2-N3	5.45	1.46	1.33
48	w	436	OMG	C2-N3	5.45	1.46	1.33
48	w	509	OMG	C2-N3	5.45	1.46	1.33
48	w	1490	OMG	C2-N3	5.45	1.46	1.33
48	w	601	OMG	C2-N3	5.43	1.46	1.33
5	F	75	OMG	C2-N3	5.43	1.46	1.33
3	D	3944	OMG	C2-N3	5.42	1.46	1.33
48	w	683	OMG	C2-N3	5.40	1.46	1.33
3	D	2424	OMG	C2-N3	5.38	1.46	1.33
3	D	4196	OMG	C2-N3	5.36	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4494	OMG	C2-N3	5.35	1.46	1.33
3	D	4370	OMG	C2-N3	5.35	1.46	1.33
3	D	4637	OMG	C2-N3	5.28	1.45	1.33
3	D	4499	OMG	C2-N3	5.27	1.45	1.33
3	D	2815	A2M	O5'-C5'	-5.27	1.31	1.44
3	D	3792	OMG	C2-N3	5.26	1.45	1.33
3	D	1760	OMG	C2-N2	5.26	1.46	1.34
3	D	3744	OMG	C2-N3	5.26	1.45	1.33
3	D	1522	OMG	C2-N3	5.22	1.45	1.33
3	D	4618	OMG	C2-N3	5.22	1.45	1.33
48	w	174	OMC	C4-N3	5.21	1.45	1.34
3	D	4392	OMG	C2-N3	5.21	1.45	1.33
3	D	1316	OMG	C2-N3	5.20	1.45	1.33
3	D	4228	OMG	C2-N3	5.19	1.45	1.33
48	w	462	OMC	C4-N3	5.19	1.45	1.34
3	D	3785	A2M	O5'-C5'	-5.19	1.32	1.44
3	D	3627	OMG	C2-N3	5.18	1.45	1.33
3	D	4623	OMG	C2-N3	5.18	1.45	1.33
2	B	6	2MG	C2-N1	5.17	1.45	1.36
48	w	601	OMG	C2-N2	5.16	1.46	1.34
2	B	48	5MC	C6-N1	5.15	1.46	1.38
3	D	2364	OMG	C2-N3	5.15	1.45	1.33
48	w	1490	OMG	C2-N2	5.14	1.46	1.34
3	D	3944	OMG	C2-N2	5.14	1.46	1.34
48	w	1328	OMG	C2-N2	5.14	1.46	1.34
48	w	517	OMC	C4-N3	5.13	1.44	1.34
48	w	1391	OMC	C4-N3	5.13	1.44	1.34
3	D	3899	OMG	C2-N3	5.13	1.45	1.33
48	w	644	OMG	C2-N2	5.12	1.46	1.34
3	D	2424	OMG	C2-N2	5.12	1.46	1.34
2	B	10	2MG	C2-N1	5.11	1.44	1.36
48	w	436	OMG	C2-N2	5.09	1.46	1.34
3	D	4447	5MC	C6-N1	5.09	1.46	1.38
48	w	509	OMG	C2-N2	5.08	1.46	1.34
48	w	683	OMG	C2-N2	5.07	1.46	1.34
48	w	668	A2M	O5'-C5'	-5.05	1.32	1.44
3	D	3825	A2M	O5'-C5'	-5.05	1.32	1.44
3	D	3744	OMG	C2-N2	5.04	1.46	1.34
3	D	4499	OMG	C2-N2	5.04	1.46	1.34
3	D	1625	OMG	C2-N2	5.03	1.46	1.34
5	F	75	OMG	C2-N2	5.03	1.46	1.34
3	D	4370	OMG	C2-N2	5.02	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	1703	OMC	C4-N3	5.01	1.44	1.34
3	D	1871	A2M	O5'-C5'	-5.00	1.32	1.44
3	D	4618	OMG	C2-N2	5.00	1.46	1.34
3	D	4494	OMG	C2-N2	5.00	1.46	1.34
3	D	4623	OMG	C2-N2	4.98	1.46	1.34
3	D	1524	A2M	O5'-C5'	-4.98	1.32	1.44
48	w	512	A2M	O5'-C5'	-4.98	1.32	1.44
3	D	3792	OMG	C2-N2	4.97	1.46	1.34
3	D	3830	A2M	O5'-C5'	-4.96	1.32	1.44
3	D	3627	OMG	C2-N2	4.96	1.46	1.34
3	D	3899	OMG	C2-N2	4.96	1.46	1.34
3	D	1316	OMG	C2-N2	4.95	1.46	1.34
48	w	468	A2M	O5'-C5'	-4.95	1.32	1.44
3	D	3782	5MC	C6-N1	4.94	1.46	1.38
3	D	1522	OMG	C2-N2	4.94	1.45	1.34
3	D	400	A2M	O5'-C5'	-4.93	1.32	1.44
3	D	2364	OMG	C2-N2	4.92	1.45	1.34
3	D	4637	OMG	C2-N2	4.92	1.45	1.34
3	D	4392	OMG	C2-N2	4.92	1.45	1.34
48	w	174	OMC	C4-N4	4.92	1.45	1.33
3	D	4196	OMG	C2-N2	4.92	1.45	1.34
3	D	2401	A2M	O5'-C5'	-4.91	1.32	1.44
3	D	4228	OMG	C2-N2	4.90	1.45	1.34
48	w	462	OMC	C4-N4	4.89	1.45	1.33
48	w	1391	OMC	C4-N4	4.89	1.45	1.33
3	D	1326	A2M	O5'-C5'	-4.88	1.32	1.44
3	D	398	A2M	O5'-C5'	-4.88	1.32	1.44
3	D	4530	UR3	C2-N3	4.88	1.48	1.39
3	D	2787	A2M	O5'-C5'	-4.87	1.32	1.44
48	w	99	A2M	O5'-C5'	-4.85	1.32	1.44
3	D	3760	A2M	O5'-C5'	-4.84	1.32	1.44
48	w	517	OMC	C4-N4	4.84	1.45	1.33
3	D	2422	OMC	C4-N3	4.83	1.44	1.34
48	w	1703	OMC	C4-N4	4.81	1.45	1.33
3	D	2824	OMC	C4-N3	4.81	1.44	1.34
3	D	4523	A2M	O5'-C5'	-4.81	1.33	1.44
48	w	27	A2M	O5'-C5'	-4.81	1.33	1.44
3	D	3887	OMC	C4-N3	4.80	1.44	1.34
48	w	159	A2M	O5'-C5'	-4.79	1.33	1.44
3	D	2422	OMC	C4-N4	4.77	1.45	1.33
3	D	2861	OMC	C4-N3	4.77	1.44	1.34
3	D	3701	OMC	C4-N3	4.77	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1340	OMC	C4-N3	4.76	1.44	1.34
3	D	3701	OMC	C4-N4	4.76	1.45	1.33
3	D	3887	OMC	C4-N4	4.76	1.45	1.33
3	D	3718	A2M	O5'-C5'	-4.75	1.33	1.44
3	D	2861	OMC	C4-N4	4.75	1.45	1.33
2	B	34	56B	C2-N2	4.75	1.45	1.34
3	D	3841	OMC	C4-N4	4.74	1.45	1.33
3	D	2365	OMC	C4-N3	4.74	1.44	1.34
3	D	1340	OMC	C4-N4	4.72	1.45	1.33
3	D	4536	OMC	C4-N4	4.72	1.45	1.33
3	D	2363	A2M	O5'-C5'	-4.72	1.33	1.44
3	D	2824	OMC	C4-N4	4.71	1.45	1.33
48	w	484	A2M	O5'-C5'	-4.71	1.33	1.44
3	D	2804	OMC	C4-N4	4.71	1.45	1.33
48	w	166	A2M	O5'-C5'	-4.71	1.33	1.44
3	D	3724	A2M	O5'-C5'	-4.70	1.33	1.44
48	w	1031	A2M	O5'-C5'	-4.70	1.33	1.44
3	D	4456	OMC	C4-N4	4.70	1.45	1.33
3	D	3808	OMC	C4-N4	4.69	1.45	1.33
3	D	2365	OMC	C4-N4	4.69	1.45	1.33
3	D	2804	OMC	C4-N3	4.69	1.44	1.34
48	w	590	A2M	O5'-C5'	-4.68	1.33	1.44
3	D	4536	OMC	C4-N3	4.68	1.43	1.34
48	w	1383	A2M	O5'-C5'	-4.67	1.33	1.44
3	D	3808	OMC	C4-N3	4.67	1.43	1.34
3	D	3841	OMC	C4-N3	4.66	1.43	1.34
48	w	1678	A2M	O5'-C5'	-4.65	1.33	1.44
3	D	4456	OMC	C4-N3	4.64	1.43	1.34
3	D	2351	OMC	C4-N4	4.60	1.44	1.33
3	D	2351	OMC	C4-N3	4.58	1.43	1.34
48	w	462	OMC	C2-N1	4.55	1.49	1.40
48	w	576	A2M	O5'-C5'	-4.54	1.33	1.44
3	D	1534	A2M	O5'-C5'	-4.52	1.33	1.44
48	w	174	OMC	C2-N1	4.51	1.49	1.40
48	w	1391	OMC	C2-N1	4.49	1.49	1.40
48	w	517	OMC	C2-N1	4.48	1.49	1.40
48	w	1639	G7M	C5-N7	-4.46	1.34	1.39
48	w	1703	OMC	C2-N1	4.29	1.49	1.40
3	D	2824	OMC	C2-N1	4.28	1.49	1.40
2	B	46	G7M	C5-N7	-4.27	1.34	1.39
2	B	48	5MC	C2-N1	4.26	1.49	1.40
3	D	2351	OMC	C2-N1	4.24	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3808	OMC	C2-N1	4.22	1.49	1.40
2	B	48	5MC	C4-N4	4.21	1.45	1.34
3	D	2422	OMC	C2-N1	4.20	1.49	1.40
3	D	2804	OMC	C2-N1	4.19	1.49	1.40
3	D	4456	OMC	C2-N1	4.19	1.49	1.40
3	D	4536	OMC	C2-N1	4.13	1.48	1.40
3	D	3841	OMC	C2-N1	4.11	1.48	1.40
2	B	34	56B	C5-C6	4.09	1.53	1.44
3	D	2861	OMC	C2-N1	4.07	1.48	1.40
3	D	3887	OMC	C2-N1	4.05	1.48	1.40
3	D	2365	OMC	C2-N1	4.04	1.48	1.40
3	D	1340	OMC	C2-N1	4.01	1.48	1.40
3	D	3782	5MC	C2-N1	4.00	1.48	1.40
3	D	3701	OMC	C2-N1	4.00	1.48	1.40
3	D	3782	5MC	C4-N4	3.94	1.44	1.34
2	B	46	G7M	C5-C6	3.89	1.54	1.43
3	D	4447	5MC	C2-N1	3.89	1.48	1.40
3	D	4447	5MC	C4-N4	3.89	1.44	1.34
48	w	1639	G7M	C5-C6	3.83	1.54	1.43
2	B	20	3AU	C4-N3	3.68	1.46	1.40
2	B	39	UY1	C2-N1	3.65	1.41	1.36
2	B	20	3AU	C6-N1	3.63	1.46	1.38
2	B	55	PSU	C6-C5	3.60	1.39	1.35
48	w	822	PSU	C6-C5	3.60	1.39	1.35
48	w	627	OMU	C4-N3	3.57	1.45	1.38
48	w	801	PSU	C6-C5	3.57	1.39	1.35
48	w	1288	OMU	C4-N3	3.57	1.45	1.38
48	w	210	PSU	C6-C5	3.57	1.39	1.35
2	B	20	3AU	O2-C2	-3.56	1.16	1.22
48	w	572	PSU	C6-C5	3.56	1.39	1.35
3	D	3762	PSU	C6-C5	3.48	1.39	1.35
3	D	1773	OMU	C4-N3	3.47	1.44	1.38
48	w	1326	OMU	C4-N3	3.44	1.44	1.38
3	D	3818	UY1	C2-N1	3.44	1.41	1.36
48	w	172	OMU	C4-N3	3.44	1.44	1.38
48	w	799	OMU	C4-N3	3.43	1.44	1.38
48	w	34	PSU	C6-C5	3.43	1.39	1.35
48	w	116	OMU	C4-N3	3.43	1.44	1.38
48	w	866	PSU	C6-C5	3.43	1.39	1.35
48	w	1625	PSU	C6-C5	3.42	1.39	1.35
48	w	1643	PSU	C6-C5	3.42	1.39	1.35
48	w	428	OMU	C4-N3	3.40	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	121	OMU	C4-N3	3.40	1.44	1.38
48	w	1244	PSU	C6-C5	3.39	1.39	1.35
48	w	1442	OMU	C4-N3	3.39	1.44	1.38
48	w	119	PSU	C6-C5	3.37	1.39	1.35
3	D	4420	PSU	C6-C5	3.37	1.39	1.35
48	w	1232	PSU	C6-C5	3.36	1.39	1.35
48	w	609	PSU	C6-C5	3.35	1.39	1.35
48	w	863	PSU	C6-C5	3.34	1.39	1.35
48	w	1367	PSU	C6-C5	3.34	1.39	1.35
48	w	36	PSU	C6-C5	3.33	1.39	1.35
48	w	1056	PSU	C6-C5	3.33	1.39	1.35
48	w	1445	PSU	C6-C5	3.33	1.39	1.35
48	w	1804	OMU	C4-N3	3.32	1.44	1.38
48	w	109	PSU	C6-C5	3.31	1.39	1.35
48	w	218	PSU	C6-C5	3.31	1.39	1.35
48	w	649	PSU	C6-C5	3.31	1.39	1.35
48	w	686	PSU	C6-C5	3.31	1.39	1.35
48	w	1238	PSU	C6-C5	3.31	1.39	1.35
48	w	93	PSU	C6-C5	3.30	1.39	1.35
3	D	3768	PSU	C6-C5	3.29	1.39	1.35
2	B	35	PSU	C6-C5	3.29	1.39	1.35
3	D	3734	PSU	C6-C5	3.29	1.39	1.35
48	w	815	PSU	C6-C5	3.28	1.39	1.35
48	w	966	PSU	C6-C5	3.27	1.39	1.35
48	w	105	PSU	C6-C5	3.27	1.39	1.35
3	D	2415	OMU	C4-N3	3.24	1.44	1.38
48	w	1347	PSU	C6-C5	3.24	1.39	1.35
3	D	4423	PSU	C6-C5	3.23	1.39	1.35
48	w	174	OMC	C6-N1	3.23	1.45	1.38
3	D	3770	PSU	C6-C5	3.22	1.39	1.35
3	D	1316	OMG	C5-N7	-3.22	1.32	1.39
3	D	4196	OMG	C5-N7	-3.21	1.32	1.39
48	w	517	OMC	C6-N1	3.20	1.45	1.38
48	w	681	PSU	C6-C5	3.20	1.39	1.35
3	D	4392	OMG	C5-N7	-3.19	1.32	1.39
3	D	2632	PSU	C6-C5	3.19	1.39	1.35
48	w	462	OMC	C6-N1	3.18	1.45	1.38
48	w	651	PSU	C6-C5	3.18	1.39	1.35
48	w	1045	PSU	C6-C5	3.18	1.39	1.35
48	w	814	PSU	C6-C5	3.18	1.39	1.35
3	D	3792	OMG	C5-N7	-3.17	1.32	1.39
48	w	406	PSU	C6-C5	3.17	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	1MG	C5-C6	3.17	1.53	1.45
3	D	3715	PSU	C6-C5	3.16	1.39	1.35
3	D	1683	PSU	C6-C5	3.16	1.39	1.35
48	w	1391	OMC	C6-N1	3.15	1.45	1.38
3	D	1781	PSU	C6-C5	3.15	1.39	1.35
3	D	3730	PSU	C6-C5	3.15	1.39	1.35
3	D	3920	PSU	C6-C5	3.15	1.39	1.35
3	D	1625	OMG	C5-N7	-3.14	1.33	1.39
48	w	1046	PSU	C6-C5	3.14	1.39	1.35
48	w	1177	PSU	C6-C5	3.14	1.39	1.35
48	w	1174	PSU	C6-C5	3.13	1.39	1.35
3	D	2364	OMG	C5-N7	-3.12	1.33	1.39
3	D	4500	PSU	C6-C5	3.12	1.39	1.35
3	D	4361	PSU	C6-C5	3.11	1.38	1.35
3	D	1782	PSU	C6-C5	3.11	1.38	1.35
3	D	4623	OMG	C5-N7	-3.11	1.33	1.39
3	D	4392	OMG	O6-C6	-3.11	1.17	1.23
3	D	4296	PSU	C6-C5	3.11	1.38	1.35
3	D	3764	PSU	C6-C5	3.10	1.38	1.35
48	w	1004	PSU	C6-C5	3.10	1.38	1.35
3	D	4227	OMU	C4-N3	3.10	1.44	1.38
3	D	4637	OMG	C5-N7	-3.10	1.33	1.39
3	D	1862	PSU	C6-C5	3.10	1.38	1.35
3	D	4552	PSU	C6-C5	3.10	1.38	1.35
3	D	4972	PSU	C6-C5	3.10	1.38	1.35
3	D	5010	PSU	C6-C5	3.09	1.38	1.35
48	w	1703	OMC	C6-N1	3.09	1.45	1.38
3	D	1792	PSU	C6-C5	3.09	1.38	1.35
3	D	1522	OMG	C5-N7	-3.09	1.33	1.39
2	B	34	56B	C11-C12	3.09	1.58	1.53
3	D	2424	OMG	C5-N7	-3.08	1.33	1.39
3	D	4353	PSU	C6-C5	3.08	1.38	1.35
2	B	20	3AU	C11-C10	3.08	1.59	1.52
3	D	4689	PSU	C6-C5	3.08	1.38	1.35
3	D	3887	OMC	C6-N1	3.07	1.45	1.38
3	D	3627	OMG	C5-N7	-3.05	1.33	1.39
48	w	1692	PSU	C6-C5	3.05	1.38	1.35
3	D	4618	OMG	C5-N7	-3.05	1.33	1.39
3	D	2351	OMC	O2-C2	-3.05	1.18	1.23
3	D	2351	OMC	C6-N1	3.05	1.45	1.38
48	w	1850	MA6	C8-N9	-3.04	1.32	1.37
3	D	4403	PSU	C6-C5	3.04	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3808	OMC	O2-C2	-3.04	1.18	1.23
3	D	4494	OMG	C5-N7	-3.04	1.33	1.39
3	D	5001	PSU	C6-C5	3.04	1.38	1.35
3	D	4498	OMU	C4-N3	3.04	1.44	1.38
3	D	2861	OMC	C6-N1	3.04	1.45	1.38
2	B	37	1MG	C5-N7	-3.04	1.33	1.39
3	D	2422	OMC	C6-N1	3.04	1.45	1.38
3	D	4312	PSU	C6-C5	3.03	1.38	1.35
3	D	4521	PSU	C6-C5	3.03	1.38	1.35
3	D	4494	OMG	O6-C6	-3.03	1.17	1.23
3	D	3841	OMC	O2-C2	-3.03	1.18	1.23
5	F	75	OMG	C5-N7	-3.03	1.33	1.39
48	w	1081	PSU	C6-C5	3.03	1.38	1.35
3	D	3744	OMG	C5-N7	-3.03	1.33	1.39
48	w	1850	MA6	C6-N6	3.02	1.45	1.36
3	D	4471	PSU	C6-C5	3.02	1.38	1.35
3	D	2837	OMU	C4-N3	3.02	1.44	1.38
3	D	3925	OMU	O2-C2	-3.02	1.17	1.23
3	D	1744	PSU	C6-C5	3.02	1.38	1.35
3	D	3899	OMG	C5-N7	-3.02	1.33	1.39
48	w	683	OMG	C5-N7	-3.01	1.33	1.39
3	D	4456	OMC	O2-C2	-3.01	1.18	1.23
3	D	2824	OMC	C6-N1	3.00	1.45	1.38
48	w	1490	OMG	C5-N7	-3.00	1.33	1.39
3	D	4499	OMG	C5-N7	-3.00	1.33	1.39
3	D	1860	PSU	C6-C5	3.00	1.38	1.35
3	D	4536	OMC	C6-N1	3.00	1.45	1.38
3	D	4306	OMU	C4-N3	3.00	1.43	1.38
3	D	2861	OMC	O2-C2	-2.99	1.18	1.23
3	D	4620	OMU	C4-N3	2.99	1.43	1.38
3	D	4532	PSU	C6-C5	2.99	1.38	1.35
3	D	3701	OMC	C6-N1	2.99	1.45	1.38
3	D	4370	OMG	C5-N7	-2.99	1.33	1.39
3	D	2365	OMC	O2-C2	-2.99	1.18	1.23
3	D	2365	OMC	C6-N1	2.99	1.45	1.38
3	D	3695	PSU	C6-C5	2.98	1.38	1.35
3	D	2804	OMC	O2-C2	-2.98	1.18	1.23
3	D	4299	PSU	C6-C5	2.97	1.38	1.35
3	D	1316	OMG	O6-C6	-2.97	1.17	1.23
3	D	3627	OMG	O6-C6	-2.97	1.17	1.23
3	D	3841	OMC	C6-N1	2.97	1.45	1.38
3	D	2364	OMG	O6-C6	-2.97	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4431	PSU	C6-C5	2.97	1.38	1.35
3	D	2508	PSU	C6-C5	2.97	1.38	1.35
3	D	1522	OMG	O6-C6	-2.97	1.17	1.23
3	D	3899	OMG	O6-C6	-2.97	1.17	1.23
48	w	1639	G7M	C2-N1	2.96	1.45	1.37
3	D	4498	OMU	O2-C2	-2.96	1.17	1.23
3	D	3808	OMC	C6-N1	2.95	1.45	1.38
2	B	46	G7M	C2-N1	2.95	1.45	1.37
3	D	4576	PSU	C6-C5	2.95	1.38	1.35
3	D	4228	OMG	O6-C6	-2.95	1.18	1.23
3	D	1340	OMC	O2-C2	-2.95	1.18	1.23
48	w	1851	MA6	C5-C4	-2.95	1.33	1.39
3	D	4579	PSU	C6-C5	2.95	1.38	1.35
3	D	3925	OMU	O4-C4	-2.94	1.18	1.24
3	D	4536	OMC	O2-C2	-2.94	1.18	1.23
2	B	46	G7M	C6-N1	2.94	1.44	1.38
3	D	4456	OMC	C6-N1	2.94	1.45	1.38
3	D	4623	OMG	O6-C6	-2.93	1.18	1.23
3	D	4306	OMU	O2-C2	-2.93	1.17	1.23
3	D	4293	PSU	C6-C5	2.93	1.38	1.35
3	D	4370	OMG	O6-C6	-2.92	1.18	1.23
3	D	2804	OMC	C6-N1	2.92	1.45	1.38
3	D	3758	PSU	C6-C5	2.92	1.38	1.35
3	D	3637	PSU	C6-C5	2.92	1.38	1.35
3	D	4228	OMG	C5-N7	-2.92	1.33	1.39
3	D	3792	OMG	O6-C6	-2.92	1.18	1.23
3	D	3944	OMG	C5-N7	-2.92	1.33	1.39
48	w	601	OMG	C5-N7	-2.92	1.33	1.39
2	B	27	M2G	C2-N2	2.92	1.40	1.35
3	D	3887	OMC	O2-C2	-2.92	1.18	1.23
3	D	4637	OMG	O6-C6	-2.91	1.18	1.23
3	D	4196	OMG	O6-C6	-2.91	1.18	1.23
3	D	1760	OMG	C5-C6	2.91	1.55	1.44
48	w	436	OMG	C5-N7	-2.91	1.33	1.39
3	D	4457	PSU	C6-C5	2.91	1.38	1.35
3	D	4618	OMG	O6-C6	-2.91	1.18	1.23
3	D	2837	OMU	O4-C4	-2.91	1.18	1.24
3	D	3851	PSU	C6-C5	2.91	1.38	1.35
3	D	2422	OMC	O2-C2	-2.90	1.18	1.23
48	w	1328	OMG	C5-C6	2.90	1.55	1.44
3	D	3701	OMC	O2-C2	-2.90	1.18	1.23
3	D	4628	PSU	C6-C5	2.89	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	58	1MA	C2-N1	2.89	1.41	1.35
48	w	1639	G7M	C6-N1	2.89	1.44	1.38
3	D	4620	OMU	O2-C2	-2.88	1.17	1.23
3	D	2837	OMU	O2-C2	-2.88	1.17	1.23
48	w	509	OMG	C5-C6	2.88	1.55	1.44
3	D	3925	OMU	C4-N3	2.88	1.43	1.38
3	D	2824	OMC	O2-C2	-2.87	1.18	1.23
48	w	644	OMG	C5-N7	-2.87	1.33	1.39
3	D	3944	OMG	C5-C6	2.87	1.55	1.44
3	D	1625	OMG	O6-C6	-2.87	1.18	1.23
3	D	4620	OMU	O4-C4	-2.86	1.18	1.24
48	w	1851	MA6	C6-N6	2.86	1.45	1.36
48	w	1703	OMC	O2-C2	-2.86	1.18	1.23
3	D	4306	OMU	O4-C4	-2.86	1.18	1.24
48	w	644	OMG	C5-C6	2.86	1.55	1.44
3	D	4530	UR3	C6-N1	2.86	1.44	1.38
3	D	3639	PSU	C6-C5	2.86	1.38	1.35
3	D	4498	OMU	O4-C4	-2.86	1.19	1.24
48	w	509	OMG	C5-N7	-2.85	1.33	1.39
3	D	1536	PSU	C6-C5	2.85	1.38	1.35
3	D	1340	OMC	C6-N1	2.85	1.44	1.38
3	D	3744	OMG	O6-C6	-2.85	1.18	1.23
48	w	436	OMG	C5-C6	2.84	1.54	1.44
3	D	1760	OMG	C6-N1	2.84	1.44	1.38
48	w	1490	OMG	C5-C6	2.84	1.54	1.44
2	B	6	2MG	C5-N7	-2.84	1.33	1.39
48	w	1328	OMG	C5-N7	-2.84	1.33	1.39
3	D	4227	OMU	O4-C4	-2.84	1.19	1.24
3	D	4227	OMU	O2-C2	-2.83	1.17	1.23
48	w	601	OMG	C5-C6	2.83	1.54	1.44
3	D	4442	PSU	C6-C5	2.83	1.38	1.35
3	D	4499	OMG	O6-C6	-2.83	1.18	1.23
3	D	3853	PSU	C6-C5	2.81	1.38	1.35
48	w	683	OMG	C5-C6	2.81	1.54	1.44
2	B	10	2MG	C5-N7	-2.81	1.33	1.39
3	D	3744	OMG	C5-C6	2.80	1.54	1.44
3	D	2415	OMU	O4-C4	-2.80	1.19	1.24
5	F	75	OMG	O6-C6	-2.80	1.18	1.23
5	F	75	OMG	C5-C6	2.80	1.54	1.44
48	w	1850	MA6	C5-N7	-2.79	1.33	1.39
3	D	4228	OMG	C5-C6	2.78	1.54	1.44
48	w	436	OMG	O6-C6	-2.78	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3792	OMG	C5-C6	2.78	1.54	1.44
3	D	4499	OMG	C5-C6	2.77	1.54	1.44
3	D	1760	OMG	C5-N7	-2.77	1.33	1.39
3	D	2415	OMU	O2-C2	-2.77	1.18	1.23
3	D	4392	OMG	C5-C6	2.76	1.54	1.44
3	D	2424	OMG	O6-C6	-2.76	1.18	1.23
3	D	4618	OMG	C5-C6	2.76	1.54	1.44
3	D	4494	OMG	C5-C6	2.76	1.54	1.44
3	D	1522	OMG	C5-C6	2.76	1.54	1.44
3	D	4370	OMG	C5-C6	2.75	1.54	1.44
3	D	3899	OMG	C5-C6	2.75	1.54	1.44
3	D	4623	OMG	C5-C6	2.75	1.54	1.44
48	w	509	OMG	O6-C6	-2.75	1.18	1.23
48	w	1490	OMG	O6-C6	-2.74	1.18	1.23
48	w	683	OMG	O6-C6	-2.74	1.18	1.23
3	D	3627	OMG	C5-C6	2.74	1.54	1.44
2	B	34	56B	C2-N1	2.73	1.44	1.37
3	D	2364	OMG	C5-C6	2.73	1.54	1.44
3	D	4637	OMG	C5-C6	2.73	1.54	1.44
3	D	4196	OMG	C5-C6	2.73	1.54	1.44
48	w	601	OMG	O6-C6	-2.72	1.18	1.23
3	D	1316	OMG	C5-C6	2.72	1.54	1.44
3	D	1625	OMG	C5-C6	2.71	1.54	1.44
3	D	2424	OMG	C5-C6	2.71	1.54	1.44
48	w	428	OMU	O4-C4	-2.70	1.19	1.24
2	B	47	H2U	C2-N3	-2.70	1.33	1.38
3	D	3944	OMG	O6-C6	-2.70	1.18	1.23
48	w	116	OMU	O4-C4	-2.69	1.19	1.24
48	w	517	OMC	O2-C2	-2.69	1.18	1.23
48	w	1850	MA6	C5-C4	-2.68	1.34	1.39
48	w	509	OMG	C6-N1	2.68	1.43	1.38
3	D	1677	PSU	C6-C5	2.68	1.38	1.35
48	w	644	OMG	O6-C6	-2.68	1.18	1.23
48	w	172	OMU	O4-C4	-2.67	1.19	1.24
3	D	4447	5MC	O2-C2	-2.67	1.18	1.23
2	B	17	H2U	C2-N3	-2.67	1.33	1.38
48	w	644	OMG	C6-N1	2.67	1.43	1.38
48	w	1804	OMU	O4-C4	-2.66	1.19	1.24
48	w	1326	OMU	O4-C4	-2.66	1.19	1.24
48	w	1442	OMU	O4-C4	-2.65	1.19	1.24
48	w	121	OMU	O4-C4	-2.65	1.19	1.24
48	w	1328	OMG	C6-N1	2.65	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	M2G	C2-N2	2.65	1.40	1.35
48	w	462	OMC	O2-C2	-2.64	1.18	1.23
3	D	3944	OMG	C6-N1	2.64	1.43	1.38
48	w	436	OMG	C6-N1	2.64	1.43	1.38
48	w	683	OMG	C6-N1	2.64	1.43	1.38
2	B	10	2MG	C5-C6	2.64	1.54	1.44
2	B	6	2MG	C5-C6	2.64	1.54	1.44
48	w	116	OMU	O2-C2	-2.63	1.18	1.23
48	w	174	OMC	O2-C2	-2.63	1.18	1.23
48	w	1326	OMU	O2-C2	-2.62	1.18	1.23
48	w	1391	OMC	O2-C2	-2.62	1.18	1.23
48	w	172	OMU	O2-C2	-2.62	1.18	1.23
2	B	16	H2U	C2-N3	-2.62	1.33	1.38
48	w	1328	OMG	O6-C6	-2.61	1.18	1.23
48	w	1804	OMU	O2-C2	-2.61	1.18	1.23
48	w	799	OMU	O4-C4	-2.61	1.19	1.24
48	w	1442	OMU	O2-C2	-2.61	1.18	1.23
3	D	1760	OMG	O6-C6	-2.61	1.18	1.23
48	w	1328	OMG	C2-N1	2.60	1.44	1.37
2	B	16	H2U	C4-N3	-2.60	1.33	1.37
48	w	1288	OMU	O4-C4	-2.60	1.19	1.24
48	w	1288	OMU	O2-C2	-2.59	1.18	1.23
48	w	627	OMU	O4-C4	-2.59	1.19	1.24
48	w	121	OMU	O2-C2	-2.59	1.18	1.23
3	D	2424	OMG	C6-N1	2.59	1.43	1.38
3	D	1760	OMG	C2-N1	2.59	1.44	1.37
2	B	34	56B	O6-C6	-2.58	1.18	1.23
48	w	601	OMG	C6-N1	2.58	1.43	1.38
3	D	1773	OMU	O4-C4	-2.58	1.19	1.24
3	D	1773	OMU	O2-C2	-2.58	1.18	1.23
48	w	627	OMU	O2-C2	-2.58	1.18	1.23
48	w	1832	6MZ	C5-C4	-2.56	1.34	1.39
48	w	174	OMC	C5-C4	2.56	1.48	1.42
48	w	428	OMU	O2-C2	-2.56	1.18	1.23
48	w	1490	OMG	C6-N1	2.56	1.43	1.38
3	D	4220	6MZ	C5-C4	-2.55	1.34	1.39
48	w	509	OMG	C2-N1	2.54	1.44	1.37
2	B	17	H2U	C4-N3	-2.54	1.33	1.37
2	B	27	M2G	C6-N1	2.54	1.43	1.38
48	w	1851	MA6	C5-N7	-2.53	1.34	1.39
48	w	601	OMG	C2-N1	2.53	1.43	1.37
48	w	799	OMU	O2-C2	-2.53	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	644	OMG	C2-N1	2.52	1.43	1.37
48	w	462	OMC	C5-C4	2.51	1.48	1.42
48	w	436	OMG	C2-N1	2.50	1.43	1.37
5	F	75	OMG	C6-N1	2.50	1.43	1.38
3	D	3944	OMG	C2-N1	2.48	1.43	1.37
3	D	4618	OMG	C6-N1	2.48	1.43	1.38
3	D	4499	OMG	C6-N1	2.48	1.43	1.38
48	w	1639	G7M	O6-C6	-2.47	1.18	1.23
48	w	1490	OMG	C2-N1	2.46	1.43	1.37
48	w	683	OMG	C2-N1	2.46	1.43	1.37
2	B	10	2MG	C6-N1	2.46	1.43	1.38
2	B	47	H2U	C4-N3	-2.45	1.33	1.37
3	D	1625	OMG	C6-N1	2.45	1.43	1.38
3	D	3782	5MC	O2-C2	-2.45	1.19	1.23
2	B	26	M2G	C6-N1	2.44	1.43	1.38
3	D	4499	OMG	C2-N1	2.42	1.43	1.37
48	w	517	OMC	C5-C4	2.42	1.48	1.42
5	F	75	OMG	C2-N1	2.42	1.43	1.37
3	D	3744	OMG	C6-N1	2.42	1.43	1.38
3	D	1522	OMG	C6-N1	2.41	1.43	1.38
48	w	668	A2M	O4'-C4'	-2.41	1.39	1.45
2	B	6	2MG	C6-N1	2.41	1.43	1.38
3	D	4370	OMG	C6-N1	2.40	1.43	1.38
48	w	576	A2M	C5-C4	2.40	1.43	1.39
3	D	4228	OMG	C6-N1	2.40	1.43	1.38
48	w	1391	OMC	C5-C4	2.40	1.48	1.42
2	B	46	G7M	O6-C6	-2.40	1.19	1.23
48	w	1703	OMC	C5-C4	2.39	1.48	1.42
3	D	2424	OMG	C2-N1	2.39	1.43	1.37
2	B	20	3AU	O4-C4	-2.39	1.18	1.23
48	w	166	A2M	C5-C4	2.38	1.43	1.39
3	D	3627	OMG	C6-N1	2.38	1.43	1.38
3	D	3899	OMG	C6-N1	2.37	1.43	1.38
48	w	1851	MA6	C8-N9	-2.37	1.33	1.37
3	D	4618	OMG	C2-N1	2.37	1.43	1.37
2	B	34	56B	C6-N1	2.36	1.43	1.38
3	D	3792	OMG	C6-N1	2.36	1.43	1.38
3	D	4530	UR3	O2-C2	-2.36	1.18	1.22
3	D	3744	OMG	C2-N1	2.36	1.43	1.37
3	D	4228	OMG	C2-N1	2.35	1.43	1.37
3	D	4370	OMG	C2-N1	2.35	1.43	1.37
3	D	2364	OMG	C6-N1	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3701	OMC	C5-C4	2.34	1.48	1.42
3	D	1625	OMG	C2-N1	2.34	1.43	1.37
3	D	4494	OMG	C6-N1	2.33	1.43	1.38
3	D	4637	OMG	C6-N1	2.32	1.43	1.38
3	D	4530	UR3	O4-C4	-2.31	1.18	1.23
3	D	3627	OMG	C2-N1	2.30	1.43	1.37
3	D	4623	OMG	C6-N1	2.30	1.43	1.38
48	w	1248	B8N	O4'-C1'	-2.30	1.40	1.43
3	D	4494	OMG	C2-N1	2.30	1.43	1.37
3	D	4623	OMG	C2-N1	2.29	1.43	1.37
3	D	4220	6MZ	C8-N9	-2.29	1.33	1.37
2	B	20	3AU	O30-C13	2.29	1.29	1.22
48	w	1678	A2M	O4'-C4'	-2.28	1.39	1.45
3	D	1316	OMG	C6-N1	2.28	1.43	1.38
3	D	3760	A2M	C5-C4	2.28	1.43	1.39
2	B	48	5MC	CM5-C5	2.27	1.56	1.50
3	D	3792	OMG	C2-N1	2.27	1.43	1.37
3	D	4196	OMG	C2-N1	2.26	1.43	1.37
3	D	2422	OMC	C5-C4	2.26	1.48	1.42
3	D	1316	OMG	C4-N9	-2.25	1.32	1.38
3	D	3841	OMC	C5-C4	2.25	1.48	1.42
48	w	159	A2M	C2'-C1'	2.25	1.58	1.53
3	D	4536	OMC	C5-C4	2.25	1.48	1.42
3	D	4392	OMG	C6-N1	2.24	1.43	1.38
3	D	3899	OMG	C4-N9	-2.24	1.32	1.38
3	D	4220	6MZ	C5-N7	-2.24	1.34	1.39
3	D	3887	OMC	C5-C4	2.24	1.48	1.42
3	D	1522	OMG	C2-N1	2.23	1.43	1.37
3	D	1524	A2M	O4'-C4'	-2.23	1.40	1.45
3	D	2364	OMG	C2-N1	2.23	1.43	1.37
48	w	166	A2M	C8-N9	2.23	1.41	1.37
3	D	2861	OMC	C5-C4	2.23	1.48	1.42
3	D	4392	OMG	C2-N1	2.23	1.43	1.37
3	D	3899	OMG	C2-N1	2.23	1.43	1.37
3	D	3627	OMG	C4-N9	-2.22	1.32	1.38
3	D	2365	OMC	C5-C4	2.22	1.48	1.42
3	D	4196	OMG	C6-N1	2.22	1.43	1.38
3	D	4637	OMG	C2-N1	2.22	1.43	1.37
3	D	4228	OMG	C4-N9	-2.21	1.32	1.38
3	D	1522	OMG	C4-N9	-2.21	1.32	1.38
3	D	3808	OMC	C5-C4	2.21	1.48	1.42
48	w	1832	6MZ	C5-N7	-2.20	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	159	A2M	O3'-C3'	-2.20	1.37	1.43
3	D	4499	OMG	C4-N9	-2.19	1.32	1.38
3	D	1316	OMG	C2-N1	2.19	1.43	1.37
3	D	2363	A2M	O4'-C4'	-2.19	1.40	1.45
2	B	10	2MG	O6-C6	-2.19	1.19	1.23
3	D	4456	OMC	C5-C4	2.19	1.47	1.42
48	w	1832	6MZ	C8-N9	-2.18	1.33	1.37
3	D	4392	OMG	C4-N9	-2.18	1.32	1.38
3	D	2824	OMC	C5-C4	2.17	1.47	1.42
2	B	6	2MG	O6-C6	-2.17	1.19	1.23
48	w	799	OMU	C6-N1	2.16	1.43	1.38
3	D	4623	OMG	C4-N9	-2.16	1.32	1.38
2	B	48	5MC	O2-C2	-2.15	1.19	1.23
3	D	2364	OMG	C4-N9	-2.14	1.32	1.38
3	D	1773	OMU	C5-C4	2.14	1.48	1.43
2	B	46	G7M	C8-N7	2.14	1.36	1.33
48	w	627	OMU	C6-N1	2.14	1.43	1.38
2	B	37	1MG	O6-C6	-2.14	1.18	1.23
48	w	1288	OMU	C6-N1	2.13	1.43	1.38
3	D	2424	OMG	C4-N9	-2.13	1.32	1.38
48	w	159	A2M	C5-C4	2.13	1.43	1.39
3	D	1773	OMU	C6-N1	2.13	1.43	1.38
3	D	2804	OMC	C5-C4	2.11	1.47	1.42
48	w	799	OMU	C5-C4	2.10	1.48	1.43
3	D	2351	OMC	C5-C4	2.10	1.47	1.42
3	D	4494	OMG	C4-N9	-2.09	1.32	1.38
48	w	1288	OMU	C5-C4	2.09	1.48	1.43
2	B	39	UY1	C4-N3	2.08	1.42	1.38
48	w	1442	OMU	C6-N1	2.08	1.43	1.38
3	D	4442	PSU	O4'-C1'	-2.08	1.41	1.43
48	w	172	OMU	C5-C4	2.08	1.48	1.43
48	w	627	OMU	C5-C4	2.07	1.48	1.43
3	D	1316	OMG	C8-N9	-2.07	1.32	1.37
3	D	3760	A2M	C8-N9	2.07	1.41	1.37
3	D	1871	A2M	O3'-C3'	-2.07	1.38	1.43
48	w	1442	OMU	C5-C4	2.06	1.48	1.43
3	D	3744	OMG	C4-N9	-2.06	1.32	1.38
3	D	4530	UR3	C5-C4	2.06	1.49	1.43
3	D	4370	OMG	C4-N9	-2.06	1.32	1.38
48	w	428	OMU	C5-C4	2.05	1.48	1.43
48	w	468	A2M	C5-C4	2.05	1.42	1.39
48	w	1326	OMU	C6-N1	2.04	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1340	OMC	C5-C4	2.04	1.47	1.42
48	w	1804	OMU	C5-C4	2.04	1.48	1.43
3	D	4618	OMG	C4-N9	-2.04	1.32	1.38
3	D	3782	5MC	CM5-C5	2.03	1.55	1.50
48	w	1326	OMU	C5-C4	2.02	1.48	1.43
3	D	4637	OMG	C4-N9	-2.01	1.32	1.38
48	w	590	A2M	C5-C4	2.01	1.42	1.39
2	B	37	1MG	C4-N9	-2.01	1.32	1.38
48	w	1804	OMU	C6-N1	2.01	1.42	1.38
48	w	116	OMU	C6-N1	2.01	1.42	1.38
3	D	1322	1MA	C2-N1	2.01	1.39	1.35
48	w	1678	A2M	C5-C4	2.01	1.42	1.39
2	B	58	1MA	C4-N3	2.00	1.40	1.35

All (925) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	5MU	C5-C4-N3	12.08	125.63	115.31
2	B	54	5MU	C5-C6-N1	-9.63	113.43	123.34
2	B	34	56B	C1'-N9-C4	-7.46	104.36	126.50
2	B	34	56B	C5-C4-N3	-6.44	119.98	127.52
2	B	10	2MG	C2-N3-C4	6.38	119.95	112.04
2	B	6	2MG	C2-N3-C4	6.34	119.91	112.04
48	w	1851	MA6	N1-C2-N3	-5.71	119.67	128.60
3	D	2415	OMU	C4-N3-C2	-5.71	119.05	126.58
3	D	4220	6MZ	N1-C2-N3	-5.70	119.69	128.60
3	D	4227	OMU	C4-N3-C2	-5.64	119.15	126.58
48	w	1850	MA6	N1-C2-N3	-5.54	119.94	128.60
3	D	3944	OMG	C5-C4-N3	-5.53	119.48	128.46
3	D	2837	OMU	C4-N3-C2	-5.53	119.28	126.58
48	w	1832	6MZ	N1-C2-N3	-5.53	119.96	128.60
3	D	4498	OMU	C4-N3-C2	-5.42	119.43	126.58
48	w	1804	OMU	C4-N3-C2	-5.40	119.45	126.58
3	D	4196	OMG	C5-C4-N3	-5.40	119.70	128.46
3	D	3792	OMG	C5-C4-N3	-5.39	119.72	128.46
3	D	1760	OMG	C5-C4-N3	-5.34	119.79	128.46
3	D	1625	OMG	C5-C4-N3	-5.34	119.80	128.46
3	D	3925	OMU	C4-N3-C2	-5.32	119.56	126.58
3	D	4637	OMG	C5-C4-N3	-5.30	119.86	128.46
48	w	428	OMU	C4-N3-C2	-5.29	119.60	126.58
3	D	4306	OMU	C4-N3-C2	-5.28	119.61	126.58
48	w	172	OMU	C4-N3-C2	-5.27	119.62	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	683	OMG	C5-C4-N3	-5.27	119.92	128.46
48	w	1490	OMG	C5-C4-N3	-5.23	119.98	128.46
48	w	436	OMG	C5-C4-N3	-5.23	119.98	128.46
48	w	1832	6MZ	C5-C4-N3	-5.22	119.94	126.75
48	w	799	OMU	C4-N3-C2	-5.21	119.71	126.58
3	D	4620	OMU	C4-N3-C2	-5.20	119.72	126.58
48	w	1442	OMU	C4-N3-C2	-5.20	119.73	126.58
5	F	75	OMG	C5-C4-N3	-5.19	120.03	128.46
2	B	54	5MU	O4-C4-C5	-5.17	118.91	124.90
3	D	4618	OMG	C5-C4-N3	-5.17	120.07	128.46
48	w	1328	OMG	C5-C4-N3	-5.17	120.07	128.46
2	B	10	2MG	C5-C4-N3	-5.17	120.08	128.46
48	w	1326	OMU	C4-N3-C2	-5.13	119.81	126.58
3	D	4494	OMG	C5-C4-N3	-5.13	120.14	128.46
48	w	601	OMG	C5-C4-N3	-5.11	120.16	128.46
3	D	2364	OMG	C5-C4-N3	-5.11	120.17	128.46
48	w	627	OMU	C4-N3-C2	-5.11	119.84	126.58
3	D	4392	OMG	C5-C4-N3	-5.10	120.19	128.46
3	D	1316	OMG	C5-C4-N3	-5.10	120.19	128.46
3	D	4370	OMG	C5-C4-N3	-5.09	120.21	128.46
48	w	1288	OMU	C4-N3-C2	-5.08	119.88	126.58
48	w	509	OMG	C5-C4-N3	-5.08	120.22	128.46
48	w	116	OMU	C4-N3-C2	-5.07	119.89	126.58
3	D	4623	OMG	C5-C4-N3	-5.03	120.30	128.46
3	D	3744	OMG	C5-C4-N3	-5.02	120.32	128.46
3	D	2424	OMG	C5-C4-N3	-5.02	120.33	128.46
3	D	3627	OMG	C5-C4-N3	-5.01	120.34	128.46
3	D	3899	OMG	C5-C4-N3	-4.98	120.37	128.46
3	D	1773	OMU	C4-N3-C2	-4.96	120.04	126.58
2	B	37	1MG	C5-C4-N3	-4.95	120.44	128.46
48	w	644	OMG	C5-C4-N3	-4.94	120.45	128.46
2	B	6	2MG	C5-C4-N3	-4.93	120.47	128.46
3	D	4499	OMG	C5-C4-N3	-4.92	120.49	128.46
3	D	1522	OMG	C5-C4-N3	-4.91	120.50	128.46
3	D	1683	PSU	N1-C2-N3	4.89	120.67	115.13
48	w	121	OMU	C4-N3-C2	-4.87	120.15	126.58
48	w	1851	MA6	C5-C4-N3	-4.85	120.43	126.75
3	D	1677	PSU	C4-N3-C2	-4.84	119.36	126.34
3	D	1744	PSU	N1-C2-N3	4.82	120.59	115.13
3	D	4552	PSU	C4-N3-C2	-4.82	119.40	126.34
48	w	609	PSU	N1-C2-N3	4.81	120.58	115.13
48	w	815	PSU	C4-N3-C2	-4.81	119.41	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3637	PSU	N1-C2-N3	4.81	120.58	115.13
3	D	4500	PSU	N1-C2-N3	4.80	120.57	115.13
3	D	4228	OMG	C5-C4-N3	-4.79	120.69	128.46
3	D	1860	PSU	N1-C2-N3	4.78	120.54	115.13
3	D	4220	6MZ	C5-C4-N3	-4.78	120.52	126.75
3	D	4353	PSU	C4-N3-C2	-4.77	119.47	126.34
3	D	4521	PSU	N1-C2-N3	4.76	120.53	115.13
3	D	3758	PSU	C4-N3-C2	-4.76	119.48	126.34
3	D	1536	PSU	N1-C2-N3	4.75	120.51	115.13
3	D	3637	PSU	C4-N3-C2	-4.75	119.50	126.34
3	D	4521	PSU	C4-N3-C2	-4.74	119.51	126.34
3	D	3851	PSU	C4-N3-C2	-4.74	119.51	126.34
3	D	4353	PSU	N1-C2-N3	4.74	120.50	115.13
3	D	1536	PSU	C4-N3-C2	-4.74	119.51	126.34
3	D	1744	PSU	C4-N3-C2	-4.74	119.52	126.34
48	w	406	PSU	C4-N3-C2	-4.73	119.52	126.34
3	D	4500	PSU	C4-N3-C2	-4.73	119.52	126.34
3	D	3770	PSU	N1-C2-N3	4.73	120.49	115.13
3	D	1862	PSU	N1-C2-N3	4.71	120.47	115.13
48	w	686	PSU	C4-N3-C2	-4.71	119.55	126.34
2	B	54	5MU	C4-N3-C2	-4.71	121.25	127.35
48	w	572	PSU	C4-N3-C2	-4.71	119.55	126.34
3	D	4530	UR3	C4-N3-C2	-4.71	120.13	124.56
3	D	1683	PSU	C4-N3-C2	-4.70	119.57	126.34
3	D	3734	PSU	N1-C2-N3	4.70	120.45	115.13
3	D	4312	PSU	C4-N3-C2	-4.69	119.58	126.34
3	D	4431	PSU	N1-C2-N3	4.69	120.44	115.13
3	D	4552	PSU	N1-C2-N3	4.69	120.44	115.13
48	w	1692	PSU	C4-N3-C2	-4.69	119.58	126.34
48	w	1081	PSU	C4-N3-C2	-4.69	119.59	126.34
2	B	35	PSU	C4-N3-C2	-4.68	119.59	126.34
3	D	4312	PSU	N1-C2-N3	4.68	120.43	115.13
3	D	4431	PSU	C4-N3-C2	-4.68	119.60	126.34
3	D	4361	PSU	C4-N3-C2	-4.67	119.60	126.34
3	D	4442	PSU	N1-C2-N3	4.67	120.42	115.13
48	w	815	PSU	N1-C2-N3	4.67	120.42	115.13
3	D	4689	PSU	C4-N3-C2	-4.67	119.61	126.34
3	D	3920	PSU	C4-N3-C2	-4.67	119.62	126.34
3	D	4442	PSU	C4-N3-C2	-4.66	119.62	126.34
3	D	4403	PSU	C4-N3-C2	-4.66	119.62	126.34
3	D	4689	PSU	N1-C2-N3	4.66	120.41	115.13
3	D	3695	PSU	C4-N3-C2	-4.66	119.62	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1174	PSU	C4-N3-C2	-4.66	119.62	126.34
48	w	109	PSU	C4-N3-C2	-4.66	119.63	126.34
3	D	1782	PSU	C4-N3-C2	-4.66	119.63	126.34
48	w	1177	PSU	C4-N3-C2	-4.65	119.64	126.34
3	D	1860	PSU	C4-N3-C2	-4.65	119.64	126.34
3	D	4579	PSU	N1-C2-N3	4.65	120.40	115.13
3	D	3639	PSU	C4-N3-C2	-4.65	119.64	126.34
48	w	866	PSU	C4-N3-C2	-4.65	119.65	126.34
3	D	2508	PSU	C4-N3-C2	-4.64	119.65	126.34
3	D	3851	PSU	N1-C2-N3	4.64	120.39	115.13
3	D	3734	PSU	C4-N3-C2	-4.64	119.66	126.34
48	w	649	PSU	C4-N3-C2	-4.64	119.66	126.34
3	D	1862	PSU	C4-N3-C2	-4.64	119.66	126.34
3	D	4471	PSU	C4-N3-C2	-4.64	119.66	126.34
48	w	1850	MA6	C5-C4-N3	-4.64	120.70	126.75
48	w	105	PSU	N1-C2-N3	4.64	120.38	115.13
48	w	966	PSU	C4-N3-C2	-4.63	119.66	126.34
3	D	4576	PSU	C4-N3-C2	-4.63	119.67	126.34
3	D	5010	PSU	N1-C2-N3	4.63	120.38	115.13
3	D	3762	PSU	N1-C2-N3	4.63	120.38	115.13
48	w	1244	PSU	C4-N3-C2	-4.63	119.67	126.34
3	D	4457	PSU	C4-N3-C2	-4.63	119.67	126.34
48	w	109	PSU	N1-C2-N3	4.63	120.37	115.13
48	w	218	PSU	C4-N3-C2	-4.63	119.67	126.34
48	w	1367	PSU	C4-N3-C2	-4.63	119.67	126.34
3	D	4972	PSU	C4-N3-C2	-4.62	119.68	126.34
48	w	966	PSU	N1-C2-N3	4.62	120.37	115.13
48	w	609	PSU	C4-N3-C2	-4.62	119.68	126.34
48	w	863	PSU	C4-N3-C2	-4.62	119.69	126.34
3	D	5001	PSU	C4-N3-C2	-4.61	119.69	126.34
3	D	4361	PSU	N1-C2-N3	4.61	120.36	115.13
48	w	863	PSU	N1-C2-N3	4.61	120.36	115.13
48	w	1347	PSU	C4-N3-C2	-4.61	119.70	126.34
48	w	1081	PSU	N1-C2-N3	4.61	120.35	115.13
48	w	1174	PSU	N1-C2-N3	4.61	120.35	115.13
3	D	4972	PSU	N1-C2-N3	4.61	120.35	115.13
3	D	3695	PSU	N1-C2-N3	4.60	120.35	115.13
3	D	4471	PSU	N1-C2-N3	4.60	120.35	115.13
48	w	681	PSU	C4-N3-C2	-4.60	119.71	126.34
48	w	406	PSU	N1-C2-N3	4.60	120.34	115.13
48	w	686	PSU	N1-C2-N3	4.60	120.34	115.13
48	w	1045	PSU	C4-N3-C2	-4.60	119.71	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2508	PSU	N1-C2-N3	4.60	120.34	115.13
48	w	1367	PSU	N1-C2-N3	4.59	120.34	115.13
3	D	3768	PSU	C4-N3-C2	-4.59	119.73	126.34
2	B	55	PSU	C4-N3-C2	-4.58	119.74	126.34
48	w	1445	PSU	C4-N3-C2	-4.58	119.74	126.34
3	D	3768	PSU	N1-C2-N3	4.58	120.32	115.13
48	w	1056	PSU	C4-N3-C2	-4.58	119.74	126.34
48	w	1850	MA6	C2-N1-C6	4.58	122.57	111.75
48	w	651	PSU	C4-N3-C2	-4.58	119.74	126.34
3	D	4423	PSU	C4-N3-C2	-4.58	119.74	126.34
3	D	1792	PSU	C4-N3-C2	-4.58	119.75	126.34
3	D	4628	PSU	N1-C2-N3	4.58	120.31	115.13
48	w	649	PSU	N1-C2-N3	4.57	120.31	115.13
48	w	1850	MA6	C4-C5-C6	4.57	121.00	115.88
48	w	681	PSU	N1-C2-N3	4.57	120.31	115.13
3	D	4220	6MZ	N9-C8-N7	-4.57	107.67	113.91
3	D	3944	OMG	C2-N3-C4	4.57	120.44	112.30
3	D	3639	PSU	N1-C2-N3	4.57	120.30	115.13
3	D	3920	PSU	N1-C2-N3	4.56	120.30	115.13
3	D	1782	PSU	N1-C2-N3	4.56	120.30	115.13
48	w	801	PSU	N1-C2-N3	4.56	120.30	115.13
3	D	3730	PSU	C4-N3-C2	-4.56	119.77	126.34
3	D	4628	PSU	C4-N3-C2	-4.56	119.77	126.34
3	D	4296	PSU	N1-C2-N3	4.56	120.30	115.13
3	D	4423	PSU	N1-C2-N3	4.56	120.29	115.13
48	w	1177	PSU	N1-C2-N3	4.55	120.29	115.13
48	w	866	PSU	N1-C2-N3	4.55	120.28	115.13
48	w	1056	PSU	N1-C2-N3	4.55	120.28	115.13
3	D	3770	PSU	C4-N3-C2	-4.55	119.79	126.34
48	w	105	PSU	C4-N3-C2	-4.54	119.79	126.34
2	B	35	PSU	N1-C2-N3	4.54	120.28	115.13
3	D	1677	PSU	N1-C2-N3	4.54	120.28	115.13
3	D	5010	PSU	C4-N3-C2	-4.54	119.80	126.34
3	D	1781	PSU	C4-N3-C2	-4.54	119.80	126.34
3	D	5001	PSU	N1-C2-N3	4.53	120.26	115.13
48	w	36	PSU	N1-C2-N3	4.53	120.26	115.13
3	D	4532	PSU	C4-N3-C2	-4.53	119.81	126.34
48	w	210	PSU	C4-N3-C2	-4.53	119.81	126.34
48	w	1046	PSU	C4-N3-C2	-4.53	119.81	126.34
3	D	4579	PSU	C4-N3-C2	-4.53	119.82	126.34
48	w	651	PSU	N1-C2-N3	4.53	120.26	115.13
48	w	34	PSU	N1-C2-N3	4.52	120.25	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1004	PSU	N1-C2-N3	4.52	120.25	115.13
48	w	814	PSU	C4-N3-C2	-4.52	119.82	126.34
3	D	1781	PSU	N1-C2-N3	4.52	120.25	115.13
48	w	1045	PSU	N1-C2-N3	4.52	120.25	115.13
48	w	218	PSU	N1-C2-N3	4.51	120.24	115.13
3	D	3762	PSU	C4-N3-C2	-4.51	119.84	126.34
48	w	1004	PSU	C4-N3-C2	-4.51	119.84	126.34
48	w	1347	PSU	N1-C2-N3	4.50	120.23	115.13
3	D	4576	PSU	N1-C2-N3	4.50	120.23	115.13
48	w	822	PSU	C4-N3-C2	-4.50	119.86	126.34
3	D	4296	PSU	C4-N3-C2	-4.50	119.86	126.34
3	D	3715	PSU	N1-C2-N3	4.50	120.22	115.13
3	D	4299	PSU	N1-C2-N3	4.49	120.22	115.13
3	D	1792	PSU	N1-C2-N3	4.48	120.21	115.13
48	w	1244	PSU	N1-C2-N3	4.48	120.21	115.13
48	w	1692	PSU	N1-C2-N3	4.48	120.20	115.13
48	w	1232	PSU	C4-N3-C2	-4.48	119.89	126.34
3	D	4403	PSU	N1-C2-N3	4.48	120.20	115.13
3	D	2632	PSU	C4-N3-C2	-4.47	119.89	126.34
3	D	4299	PSU	C4-N3-C2	-4.47	119.89	126.34
3	D	3764	PSU	C4-N3-C2	-4.47	119.89	126.34
48	w	1643	PSU	N1-C2-N3	4.47	120.19	115.13
48	w	1232	PSU	N1-C2-N3	4.47	120.19	115.13
48	w	1238	PSU	C4-N3-C2	-4.47	119.90	126.34
48	w	1643	PSU	C4-N3-C2	-4.46	119.91	126.34
48	w	119	PSU	N1-C2-N3	4.46	120.18	115.13
3	D	3715	PSU	C4-N3-C2	-4.46	119.92	126.34
3	D	3758	PSU	N1-C2-N3	4.46	120.18	115.13
3	D	1760	OMG	C2-N3-C4	4.45	120.23	112.30
3	D	4618	OMG	C2-N3-C4	4.43	120.20	112.30
3	D	2632	PSU	N1-C2-N3	4.43	120.15	115.13
48	w	119	PSU	C4-N3-C2	-4.43	119.95	126.34
48	w	572	PSU	N1-C2-N3	4.42	120.14	115.13
48	w	36	PSU	C4-N3-C2	-4.42	119.97	126.34
3	D	3730	PSU	N1-C2-N3	4.42	120.13	115.13
3	D	3792	OMG	C2-N3-C4	4.41	120.17	112.30
3	D	4457	PSU	N1-C2-N3	4.41	120.13	115.13
3	D	2364	OMG	C2-N3-C4	4.41	120.16	112.30
48	w	1445	PSU	N1-C2-N3	4.41	120.12	115.13
48	w	1851	MA6	N9-C8-N7	-4.41	107.89	113.91
3	D	4392	OMG	C2-N3-C4	4.41	120.15	112.30
2	B	54	5MU	N3-C2-N1	4.40	120.73	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4532	PSU	N1-C2-N3	4.40	120.12	115.13
48	w	1625	PSU	C4-N3-C2	-4.39	120.01	126.34
48	w	210	PSU	N1-C2-N3	4.39	120.11	115.13
48	w	1238	PSU	N1-C2-N3	4.39	120.11	115.13
48	w	1046	PSU	N1-C2-N3	4.39	120.11	115.13
48	w	436	OMG	C2-N3-C4	4.39	120.12	112.30
48	w	93	PSU	C4-N3-C2	-4.38	120.02	126.34
3	D	3764	PSU	N1-C2-N3	4.38	120.10	115.13
3	D	3627	OMG	C2-N3-C4	4.38	120.11	112.30
3	D	3744	OMG	C2-N3-C4	4.38	120.10	112.30
3	D	3899	OMG	C2-N3-C4	4.38	120.10	112.30
3	D	1316	OMG	C2-N3-C4	4.38	120.10	112.30
48	w	683	OMG	C2-N3-C4	4.37	120.09	112.30
48	w	1851	MA6	C2-N1-C6	4.37	122.08	111.75
2	B	34	56B	C2-N3-C4	4.37	120.08	112.30
3	D	4196	OMG	C2-N3-C4	4.36	120.06	112.30
3	D	3853	PSU	C4-N3-C2	-4.35	120.07	126.34
48	w	1490	OMG	C2-N3-C4	4.35	120.04	112.30
48	w	1832	6MZ	N9-C8-N7	-4.34	107.97	113.91
3	D	1522	OMG	C2-N3-C4	4.34	120.03	112.30
3	D	4370	OMG	C2-N3-C4	4.34	120.03	112.30
2	B	46	G7M	C2-N3-C4	4.34	120.03	112.30
48	w	1328	OMG	C2-N3-C4	4.34	120.03	112.30
2	B	55	PSU	N1-C2-N3	4.34	120.05	115.13
3	D	1625	OMG	C2-N3-C4	4.33	120.02	112.30
48	w	1625	PSU	N1-C2-N3	4.33	120.04	115.13
3	D	4293	PSU	N1-C2-N3	4.33	120.03	115.13
3	D	4499	OMG	C2-N3-C4	4.33	120.01	112.30
3	D	4637	OMG	C2-N3-C4	4.33	120.01	112.30
48	w	601	OMG	C2-N3-C4	4.33	120.01	112.30
48	w	814	PSU	N1-C2-N3	4.32	120.03	115.13
3	D	4293	PSU	C4-N3-C2	-4.32	120.11	126.34
48	w	822	PSU	N1-C2-N3	4.32	120.02	115.13
48	w	509	OMG	C2-N3-C4	4.31	119.99	112.30
3	D	4623	OMG	C2-N3-C4	4.30	119.96	112.30
5	F	75	OMG	C2-N3-C4	4.28	119.93	112.30
3	D	4420	PSU	C4-N3-C2	-4.28	120.17	126.34
48	w	1639	G7M	C2-N3-C4	4.28	119.93	112.30
3	D	4494	OMG	C2-N3-C4	4.28	119.93	112.30
3	D	3853	PSU	N1-C2-N3	4.28	119.98	115.13
48	w	801	PSU	C4-N3-C2	-4.28	120.17	126.34
48	w	93	PSU	N1-C2-N3	4.25	119.95	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	644	OMG	C2-N3-C4	4.25	119.87	112.30
2	B	10	2MG	C2-N1-C6	-4.25	119.59	124.48
48	w	34	PSU	C4-N3-C2	-4.24	120.23	126.34
3	D	2424	OMG	C2-N3-C4	4.23	119.84	112.30
2	B	54	5MU	C5M-C5-C4	4.22	123.41	118.77
48	w	1851	MA6	C4-C5-C6	4.17	120.55	115.88
3	D	4228	OMG	C2-N3-C4	4.16	119.71	112.30
3	D	4420	PSU	N1-C2-N3	4.16	119.84	115.13
2	B	54	5MU	C5M-C5-C6	-4.11	117.36	122.85
2	B	6	2MG	C2-N1-C6	-4.07	119.80	124.48
3	D	4227	OMU	N3-C2-N1	4.06	120.28	114.89
3	D	2415	OMU	N3-C2-N1	4.04	120.26	114.89
3	D	3925	OMU	N3-C2-N1	4.03	120.25	114.89
2	B	34	56B	C7-C5-C4	-4.03	108.00	112.66
48	w	1639	G7M	C5-C4-N3	-4.01	120.45	128.15
3	D	4447	5MC	C5-C6-N1	-4.01	119.21	123.34
3	D	2837	OMU	N3-C2-N1	4.00	120.21	114.89
3	D	4620	OMU	N3-C2-N1	3.98	120.18	114.89
3	D	4306	OMU	N3-C2-N1	3.98	120.17	114.89
3	D	3944	OMG	N9-C4-N3	3.93	133.83	125.94
3	D	4498	OMU	N3-C2-N1	3.90	120.07	114.89
48	w	1832	6MZ	C4-C5-C6	3.88	119.81	116.81
48	w	1804	OMU	N3-C2-N1	3.87	120.03	114.89
48	w	172	OMU	N3-C2-N1	3.85	120.00	114.89
48	w	1639	G7M	C5-C6-N1	3.84	119.81	111.79
48	w	1850	MA6	N9-C8-N7	-3.83	108.67	113.91
48	w	1442	OMU	N3-C2-N1	3.83	119.97	114.89
2	B	46	G7M	C5-C4-N3	-3.82	120.83	128.15
3	D	1625	OMG	N9-C4-N3	3.82	133.60	125.94
2	B	16	H2U	C4-N3-C2	-3.81	122.63	125.79
48	w	428	OMU	N3-C2-N1	3.78	119.90	114.89
3	D	3792	OMG	N9-C4-N3	3.77	133.51	125.94
2	B	46	G7M	C5-C6-N1	3.77	119.66	111.79
48	w	799	OMU	N3-C2-N1	3.76	119.88	114.89
3	D	1773	OMU	N3-C2-N1	3.71	119.82	114.89
3	D	4196	OMG	N9-C4-N3	3.71	133.39	125.94
48	w	1326	OMU	N3-C2-N1	3.71	119.81	114.89
48	w	1288	OMU	N3-C2-N1	3.70	119.81	114.89
3	D	1760	OMG	N9-C4-N3	3.70	133.36	125.94
3	D	4220	6MZ	C5-N7-C8	3.66	108.71	103.51
2	B	20	3AU	C4-N3-C2	-3.65	120.05	124.63
48	w	1851	MA6	C5-N7-C8	3.64	108.68	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2415	OMU	C5-C4-N3	3.63	120.27	114.84
48	w	116	OMU	N3-C2-N1	3.62	119.70	114.89
3	D	4637	OMG	N9-C4-N3	3.62	133.21	125.94
48	w	627	OMU	N3-C2-N1	3.62	119.69	114.89
48	w	683	OMG	N9-C4-N3	3.61	133.19	125.94
48	w	1832	6MZ	C2-N3-C4	3.59	120.23	111.75
48	w	436	OMG	N9-C4-N3	3.58	133.12	125.94
2	B	37	1MG	C2-N3-C4	3.57	120.00	111.98
3	D	4220	6MZ	C2-N3-C4	3.57	120.17	111.75
3	D	4498	OMU	C5-C4-N3	3.56	120.17	114.84
48	w	1490	OMG	N9-C4-N3	3.55	133.07	125.94
3	D	4228	OMG	N9-C8-N7	-3.54	106.72	113.39
2	B	34	56B	C7-C8-N9	-3.54	107.59	111.06
48	w	1337	4AC	O7-C7-N4	3.54	127.54	121.82
3	D	4227	OMU	C5-C4-N3	3.54	120.13	114.84
48	w	1842	4AC	O7-C7-N4	3.53	127.53	121.82
5	F	75	OMG	N9-C4-N3	3.51	133.00	125.94
3	D	3899	OMG	N9-C8-N7	-3.51	106.78	113.39
3	D	1522	OMG	N9-C8-N7	-3.50	106.80	113.39
3	D	4370	OMG	N9-C8-N7	-3.48	106.84	113.39
48	w	1328	OMG	N9-C4-N3	3.46	132.89	125.94
48	w	121	OMU	N3-C2-N1	3.46	119.48	114.89
3	D	2837	OMU	C5-C4-N3	3.46	120.01	114.84
3	D	4623	OMG	N9-C8-N7	-3.45	106.89	113.39
48	w	1804	OMU	C5-C4-N3	3.44	119.98	114.84
48	w	436	OMG	N9-C8-N7	-3.44	106.92	113.39
2	B	10	2MG	N9-C4-N3	3.43	132.83	125.94
48	w	601	OMG	N9-C4-N3	3.43	132.83	125.94
48	w	644	OMG	N9-C8-N7	-3.42	106.94	113.39
3	D	4370	OMG	N9-C4-N3	3.41	132.79	125.94
3	D	4499	OMG	N9-C8-N7	-3.41	106.97	113.39
3	D	1316	OMG	N9-C4-N3	3.41	132.78	125.94
3	D	4618	OMG	N9-C4-N3	3.40	132.77	125.94
48	w	1832	6MZ	C5-N7-C8	3.40	108.34	103.51
3	D	1316	OMG	N9-C8-N7	-3.39	107.01	113.39
48	w	428	OMU	C5-C4-N3	3.39	119.91	114.84
48	w	1328	OMG	N9-C8-N7	-3.38	107.03	113.39
48	w	799	OMU	C5-C4-N3	3.38	119.89	114.84
2	B	34	56B	N9-C4-N3	3.38	132.72	125.94
48	w	509	OMG	N9-C8-N7	-3.38	107.03	113.39
3	D	3627	OMG	N9-C8-N7	-3.37	107.04	113.39
48	w	509	OMG	N9-C4-N3	3.37	132.71	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1851	MA6	C2-N3-C4	3.37	119.72	111.75
3	D	3925	OMU	C5-C4-N3	3.35	119.86	114.84
3	D	2424	OMG	N9-C4-N3	3.35	132.67	125.94
3	D	4494	OMG	N9-C4-N3	3.34	132.65	125.94
3	D	3744	OMG	N9-C8-N7	-3.34	107.10	113.39
3	D	2364	OMG	N9-C8-N7	-3.34	107.11	113.39
48	w	1326	OMU	C5-C4-N3	3.34	119.83	114.84
3	D	4392	OMG	N9-C4-N3	3.33	132.63	125.94
48	w	116	OMU	C5-C4-N3	3.32	119.81	114.84
3	D	2364	OMG	N9-C4-N3	3.32	132.61	125.94
48	w	609	PSU	O2-C2-N1	-3.32	119.14	122.79
3	D	4494	OMG	N9-C8-N7	-3.32	107.14	113.39
3	D	4392	OMG	N9-C8-N7	-3.32	107.14	113.39
3	D	3782	5MC	C5-C6-N1	-3.31	119.93	123.34
3	D	4618	OMG	N9-C8-N7	-3.31	107.16	113.39
3	D	4228	OMG	C1'-N9-C4	-3.31	116.68	126.50
48	w	172	OMU	C5-C4-N3	3.31	119.79	114.84
3	D	4637	OMG	N9-C8-N7	-3.30	107.17	113.39
48	w	1639	G7M	O6-C6-C5	-3.30	120.61	128.06
48	w	683	OMG	N9-C8-N7	-3.30	107.18	113.39
3	D	4620	OMU	C5-C4-N3	3.29	119.77	114.84
3	D	2424	OMG	N9-C8-N7	-3.29	107.19	113.39
48	w	627	OMU	C5-C4-N3	3.29	119.77	114.84
3	D	1760	OMG	N9-C8-N7	-3.29	107.19	113.39
2	B	46	G7M	O6-C6-C5	-3.29	120.64	128.06
3	D	4306	OMU	C5-C4-N3	3.29	119.75	114.84
48	w	601	OMG	N9-C8-N7	-3.28	107.20	113.39
48	w	1442	OMU	C5-C4-N3	3.28	119.75	114.84
48	w	121	OMU	C5-C4-N3	3.28	119.75	114.84
3	D	4499	OMG	N9-C4-N3	3.28	132.52	125.94
48	w	1288	OMU	C5-C4-N3	3.27	119.73	114.84
48	w	644	OMG	N9-C4-N3	3.27	132.50	125.94
2	B	6	2MG	N9-C8-N7	-3.26	107.24	113.39
3	D	3944	OMG	N9-C8-N7	-3.26	107.25	113.39
5	F	75	OMG	N9-C8-N7	-3.26	107.25	113.39
48	w	1850	MA6	C5-N7-C8	3.26	108.14	103.51
2	B	20	3AU	C5-C4-N3	3.25	119.79	115.50
3	D	4623	OMG	N9-C4-N3	3.25	132.46	125.94
3	D	3744	OMG	N9-C4-N3	3.23	132.43	125.94
3	D	3627	OMG	N9-C4-N3	3.23	132.42	125.94
3	D	1522	OMG	N9-C4-N3	3.22	132.41	125.94
3	D	3899	OMG	N9-C4-N3	3.22	132.41	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1522	OMG	C1'-N9-C4	-3.22	116.94	126.50
2	B	6	2MG	N9-C4-N3	3.22	132.40	125.94
3	D	2424	OMG	C2-N1-C6	-3.20	119.26	125.10
3	D	1625	OMG	N9-C8-N7	-3.19	107.38	113.39
3	D	4196	OMG	C2-N1-C6	-3.19	119.29	125.10
2	B	10	2MG	N9-C8-N7	-3.17	107.41	113.39
48	w	1490	OMG	N9-C8-N7	-3.17	107.42	113.39
2	B	37	1MG	N9-C8-N7	-3.16	107.44	113.39
3	D	4228	OMG	N9-C4-N3	3.16	132.28	125.94
48	w	683	OMG	C2-N1-C6	-3.15	119.36	125.10
3	D	4196	OMG	N9-C8-N7	-3.14	107.48	113.39
3	D	3792	OMG	N9-C8-N7	-3.13	107.50	113.39
3	D	4637	OMG	C2-N1-C6	-3.11	119.42	125.10
3	D	3627	OMG	C1'-N9-C4	-3.11	117.27	126.50
3	D	1773	OMU	C5-C4-N3	3.10	119.48	114.84
3	D	4392	OMG	C2-N1-C6	-3.10	119.45	125.10
3	D	1625	OMG	C2-N1-C6	-3.10	119.45	125.10
3	D	4220	6MZ	C4-C5-N7	-3.09	106.85	110.62
48	w	1328	OMG	C2-N1-C6	-3.09	119.47	125.10
48	w	1851	MA6	C4-C5-N7	-3.08	106.86	110.62
3	D	3899	OMG	C1'-N9-C4	-3.08	117.35	126.50
3	D	4220	6MZ	C4-C5-C6	3.08	119.20	116.81
48	w	509	OMG	C2-N1-C6	-3.08	119.48	125.10
48	w	644	OMG	C1'-N9-C4	-3.08	117.36	126.50
2	B	34	56B	C2-N1-C6	-3.07	119.50	125.10
48	w	1850	MA6	C2-N3-C4	3.06	118.98	111.75
48	w	436	OMG	C2-N1-C6	-3.06	119.53	125.10
3	D	3944	OMG	C2-N1-C6	-3.05	119.53	125.10
3	D	4618	OMG	C2-N1-C6	-3.05	119.53	125.10
3	D	3627	OMG	C2-N1-C6	-3.05	119.54	125.10
3	D	2364	OMG	C2-N1-C6	-3.04	119.55	125.10
5	F	75	OMG	C2-N1-C6	-3.04	119.56	125.10
48	w	1639	G7M	N9-C4-N3	3.02	132.01	125.94
48	w	34	PSU	O2-C2-N1	-3.02	119.47	122.79
3	D	1760	OMG	C2-N1-C6	-3.02	119.60	125.10
3	D	4623	OMG	C2-N1-C6	-3.01	119.60	125.10
3	D	4370	OMG	C2-N1-C6	-3.01	119.60	125.10
3	D	4494	OMG	C2-N1-C6	-3.01	119.62	125.10
48	w	644	OMG	C2-N1-C6	-3.00	119.63	125.10
3	D	1316	OMG	C2-N1-C6	-2.99	119.65	125.10
48	w	601	OMG	C2-N1-C6	-2.99	119.66	125.10
3	D	4499	OMG	C2-N1-C6	-2.98	119.67	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4499	OMG	C1'-N9-C4	-2.97	117.67	126.50
48	w	1639	G7M	C2-N1-C6	-2.97	119.68	125.10
3	D	3792	OMG	C2-N1-C6	-2.96	119.70	125.10
2	B	48	5MC	C5-C6-N1	-2.96	120.30	123.34
2	B	37	1MG	N9-C4-N3	2.95	131.87	125.94
3	D	1522	OMG	C2-N1-C6	-2.95	119.73	125.10
2	B	46	G7M	N9-C4-N3	2.94	131.85	125.94
48	w	116	OMU	O4-C4-C5	-2.93	120.00	125.16
3	D	4623	OMG	C1'-N9-C4	-2.93	117.80	126.50
3	D	2837	OMU	O4-C4-C5	-2.93	120.01	125.16
3	D	1536	PSU	O2-C2-N1	-2.93	119.57	122.79
3	D	3744	OMG	C2-N1-C6	-2.92	119.78	125.10
3	D	3899	OMG	C2-N1-C6	-2.92	119.78	125.10
3	D	1534	A2M	C3'-C2'-C1'	-2.91	97.41	102.89
48	w	1490	OMG	C2-N1-C6	-2.91	119.79	125.10
3	D	3744	OMG	C1'-N9-C4	-2.91	117.86	126.50
48	w	627	OMU	O4-C4-C5	-2.90	120.06	125.16
48	w	428	OMU	O4-C4-C5	-2.90	120.07	125.16
3	D	4370	OMG	C1'-N9-C4	-2.89	117.91	126.50
3	D	4228	OMG	C2-N1-C6	-2.89	119.83	125.10
2	B	37	1MG	C1'-N9-C8	-2.89	118.48	126.70
3	D	2415	OMU	O4-C4-C5	-2.87	120.11	125.16
48	w	509	OMG	C1'-N9-C4	-2.87	117.98	126.50
3	D	4500	PSU	O2-C2-N1	-2.87	119.63	122.79
3	D	3785	A2M	C2'-C1'-N9	-2.86	108.71	113.53
48	w	1850	MA6	C4-C5-N7	-2.86	107.14	110.62
48	w	1832	6MZ	N3-C4-N9	2.86	131.79	127.08
3	D	4392	OMG	C5-C6-N1	2.84	120.40	113.19
48	w	1804	OMU	O4-C4-C5	-2.84	120.17	125.16
48	w	1326	OMU	O4-C4-C5	-2.83	120.19	125.16
3	D	4498	OMU	O4-C4-C5	-2.83	120.19	125.16
3	D	3734	PSU	O2-C2-N1	-2.83	119.68	122.79
3	D	4579	PSU	O2-C2-N1	-2.83	119.68	122.79
3	D	4392	OMG	C1'-N9-C4	-2.82	118.11	126.50
48	w	1288	OMU	O4-C4-C5	-2.82	120.20	125.16
48	w	121	OMU	O4-C4-C5	-2.81	120.22	125.16
3	D	3627	OMG	C5-C6-N1	2.81	120.32	113.19
3	D	2424	OMG	C1'-N9-C4	-2.81	118.16	126.50
2	B	20	3AU	C6-N1-C2	-2.80	119.28	121.79
48	w	172	OMU	O4-C4-C5	-2.80	120.23	125.16
3	D	4196	OMG	C5-C6-N1	2.80	120.30	113.19
3	D	4227	OMU	O4-C4-C5	-2.80	120.24	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1534	A2M	O2'-C2'-C1'	2.80	114.54	109.08
3	D	2424	OMG	C5-C6-N1	2.79	120.28	113.19
3	D	4618	OMG	C1'-N9-C4	-2.78	118.24	126.50
3	D	3770	PSU	O2-C2-N1	-2.78	119.73	122.79
3	D	1522	OMG	C5-C6-N1	2.78	120.24	113.19
3	D	2364	OMG	C5-C6-N1	2.78	120.24	113.19
3	D	1683	PSU	O2-C2-N1	-2.76	119.75	122.79
48	w	576	A2M	C3'-C2'-C1'	-2.76	97.69	102.89
3	D	4499	OMG	C5-C6-N1	2.76	120.19	113.19
3	D	4618	OMG	C5-C6-N1	2.75	120.18	113.19
48	w	799	OMU	O4-C4-C5	-2.75	120.32	125.16
3	D	4637	OMG	C5-C6-N1	2.75	120.17	113.19
3	D	3744	OMG	C5-C6-N1	2.75	120.17	113.19
48	w	683	OMG	C5-C6-N1	2.75	120.17	113.19
48	w	109	PSU	O2-C2-N1	-2.74	119.77	122.79
3	D	4370	OMG	C5-C6-N1	2.74	120.15	113.19
48	w	509	OMG	C5-C6-N1	2.74	120.14	113.19
3	D	4494	OMG	C1'-N9-C4	-2.74	118.37	126.50
48	w	644	OMG	C5-C6-N1	2.74	120.14	113.19
48	w	1328	OMG	C5-C6-N1	2.74	120.14	113.19
48	w	36	PSU	O2-C2-N1	-2.73	119.78	122.79
3	D	1316	OMG	C5-C6-N1	2.73	120.13	113.19
48	w	436	OMG	C5-C6-N1	2.73	120.12	113.19
3	D	4623	OMG	C5-C6-N1	2.73	120.12	113.19
48	w	1442	OMU	O4-C4-C5	-2.73	120.36	125.16
48	w	601	OMG	C5-C6-N1	2.72	120.11	113.19
3	D	3944	OMG	C5-C6-N1	2.72	120.11	113.19
3	D	4494	OMG	C5-C6-N1	2.72	120.11	113.19
48	w	1232	PSU	O2-C2-N1	-2.72	119.79	122.79
3	D	3925	OMU	O4-C4-C5	-2.72	120.38	125.16
3	D	1625	OMG	C5-C6-N1	2.71	120.08	113.19
3	D	2364	OMG	C1'-N9-C4	-2.71	118.45	126.50
3	D	4306	OMU	O4-C4-C5	-2.71	120.40	125.16
3	D	4431	PSU	O2-C2-N1	-2.70	119.81	122.79
3	D	3899	OMG	C5-C6-N1	2.70	120.05	113.19
48	w	1328	OMG	C1'-N9-C4	-2.70	118.48	126.50
48	w	686	PSU	O2-C2-N1	-2.70	119.82	122.79
3	D	4312	PSU	O2-C2-N1	-2.70	119.82	122.79
3	D	1773	OMU	O4-C4-C5	-2.70	120.42	125.16
3	D	1760	OMG	C5-C6-N1	2.70	120.03	113.19
3	D	4296	PSU	O2-C2-N1	-2.69	119.83	122.79
3	D	1862	PSU	O2-C2-N1	-2.69	119.83	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	75	OMG	C5-C6-N1	2.69	120.03	113.19
2	B	10	2MG	C5-C6-N1	2.69	120.02	113.19
3	D	3639	PSU	O2-C2-N1	-2.69	119.83	122.79
2	B	6	2MG	C5-C6-N1	2.68	120.01	113.19
3	D	4442	PSU	O2-C2-N1	-2.68	119.84	122.79
48	w	406	PSU	O2-C2-N1	-2.68	119.84	122.79
48	w	210	PSU	O2-C2-N1	-2.68	119.84	122.79
3	D	5010	PSU	O2-C2-N1	-2.67	119.85	122.79
3	D	4521	PSU	O2-C2-N1	-2.67	119.85	122.79
48	w	1238	PSU	O2-C2-N1	-2.66	119.86	122.79
3	D	3730	PSU	O2-C2-N1	-2.66	119.86	122.79
48	w	1639	G7M	CN7-N7-C5	2.65	130.07	126.77
3	D	4228	OMG	C5-C6-N1	2.65	119.93	113.19
3	D	1744	PSU	O2-C2-N1	-2.65	119.87	122.79
2	B	37	1MG	C5-C6-N1	2.65	120.04	114.91
48	w	436	OMG	C1'-N9-C4	-2.65	118.63	126.50
48	w	1490	OMG	C5-C6-N1	2.65	119.92	113.19
3	D	4576	PSU	O2-C2-N1	-2.65	119.87	122.79
48	w	1625	PSU	O2-C2-N1	-2.65	119.87	122.79
48	w	1643	PSU	O2-C2-N1	-2.65	119.87	122.79
3	D	4552	PSU	O2-C2-N1	-2.65	119.88	122.79
3	D	4353	PSU	O2-C2-N1	-2.65	119.88	122.79
3	D	3792	OMG	C5-C6-N1	2.64	119.90	113.19
2	B	46	G7M	C2-N1-C6	-2.64	120.28	125.10
3	D	1316	OMG	C1'-N9-C4	-2.64	118.66	126.50
3	D	2424	OMG	O6-C6-C5	-2.63	119.62	126.60
3	D	3764	PSU	O2-C2-N1	-2.63	119.90	122.79
48	w	966	PSU	O2-C2-N1	-2.62	119.90	122.79
48	w	34	PSU	C6-N1-C2	-2.62	120.00	122.68
48	w	119	PSU	O2-C2-N1	-2.62	119.90	122.79
3	D	1860	PSU	O2-C2-N1	-2.62	119.91	122.79
3	D	4403	PSU	O2-C2-N1	-2.61	119.91	122.79
48	w	1081	PSU	O2-C2-N1	-2.61	119.92	122.79
48	w	1851	MA6	C5-C4-N9	2.61	108.82	105.78
3	D	1625	OMG	O6-C6-C5	-2.61	119.69	126.60
48	w	105	PSU	O2-C2-N1	-2.60	119.92	122.79
48	w	649	PSU	O2-C2-N1	-2.60	119.92	122.79
48	w	1367	PSU	O2-C2-N1	-2.60	119.93	122.79
3	D	4220	6MZ	C5-C4-N9	2.59	108.80	105.78
48	w	863	PSU	O2-C2-N1	-2.59	119.94	122.79
3	D	1781	PSU	O2-C2-N1	-2.59	119.94	122.79
3	D	3762	PSU	O2-C2-N1	-2.59	119.94	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1174	PSU	O2-C2-N1	-2.58	119.95	122.79
3	D	4628	PSU	O2-C2-N1	-2.58	119.95	122.79
3	D	3768	PSU	O2-C2-N1	-2.57	119.96	122.79
3	D	4620	OMU	O4-C4-C5	-2.57	120.63	125.16
3	D	4579	PSU	C6-N1-C2	-2.57	120.05	122.68
3	D	4457	PSU	O2-C2-N1	-2.57	119.96	122.79
48	w	1004	PSU	O2-C2-N1	-2.57	119.96	122.79
48	w	601	OMG	C1'-N9-C4	-2.57	118.86	126.50
48	w	1832	6MZ	C4-C5-N7	-2.57	107.49	110.62
3	D	4532	PSU	O2-C2-N1	-2.57	119.96	122.79
48	w	866	PSU	O2-C2-N1	-2.56	119.97	122.79
48	w	1177	PSU	O2-C2-N1	-2.56	119.97	122.79
48	w	1347	PSU	O2-C2-N1	-2.56	119.97	122.79
2	B	55	PSU	O2-C2-N1	-2.56	119.97	122.79
3	D	1677	PSU	O2-C2-N1	-2.56	119.97	122.79
3	D	4499	OMG	O6-C6-C5	-2.55	119.84	126.60
2	B	6	2MG	N1-C2-N3	-2.55	120.01	123.95
48	w	509	OMG	O6-C6-C5	-2.55	119.84	126.60
48	w	801	PSU	C6-N1-C2	-2.54	120.08	122.68
5	F	75	OMG	C1'-N9-C4	-2.54	118.95	126.50
3	D	2508	PSU	O2-C2-N1	-2.54	119.99	122.79
3	D	3695	PSU	O2-C2-N1	-2.54	120.00	122.79
48	w	681	PSU	O2-C2-N1	-2.54	120.00	122.79
48	w	218	PSU	O2-C2-N1	-2.53	120.01	122.79
48	w	1383	A2M	C3'-C2'-C1'	-2.53	98.14	102.89
3	D	1683	PSU	C6-N1-C2	-2.53	120.10	122.68
3	D	4420	PSU	O2-C2-N1	-2.53	120.01	122.79
3	D	1760	OMG	O6-C6-C5	-2.52	119.91	126.60
48	w	1244	PSU	O2-C2-N1	-2.52	120.01	122.79
5	F	75	OMG	O6-C6-C5	-2.52	119.91	126.60
48	w	1851	MA6	N1-C6-N6	-2.52	114.33	117.08
3	D	4471	PSU	O2-C2-N1	-2.51	120.03	122.79
2	B	35	PSU	O2-C2-N1	-2.51	120.03	122.79
3	D	3770	PSU	C6-N1-C2	-2.50	120.12	122.68
3	D	4530	UR3	C6-N1-C2	-2.50	119.55	121.79
3	D	4423	PSU	O2-C2-N1	-2.50	120.04	122.79
48	w	683	OMG	O6-C6-C5	-2.50	119.97	126.60
48	w	1046	PSU	O2-C2-N1	-2.49	120.04	122.79
48	w	436	OMG	O6-C6-C5	-2.49	119.99	126.60
48	w	1045	PSU	O2-C2-N1	-2.49	120.05	122.79
48	w	1337	4AC	CM7-C7-N4	-2.48	111.00	115.29
48	w	1328	OMG	O6-C6-C5	-2.48	120.01	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	801	PSU	O2-C2-N1	-2.48	120.06	122.79
48	w	609	PSU	C6-C5-C4	2.48	119.93	118.20
2	B	10	2MG	O6-C6-C5	-2.48	120.02	126.60
2	B	6	2MG	O6-C6-C5	-2.48	120.02	126.60
48	w	644	OMG	O6-C6-C5	-2.48	120.02	126.60
48	w	1842	4AC	C5-C4-N4	-2.48	118.61	122.92
3	D	4689	PSU	O2-C2-N1	-2.47	120.07	122.79
48	w	815	PSU	O2-C2-N1	-2.47	120.07	122.79
48	w	1445	PSU	O2-C2-N1	-2.47	120.08	122.79
3	D	3944	OMG	O6-C6-C5	-2.46	120.06	126.60
3	D	2364	OMG	O6-C6-C5	-2.46	120.07	126.60
3	D	5010	PSU	C6-N1-C2	-2.46	120.17	122.68
48	w	1692	PSU	O2-C2-N1	-2.46	120.09	122.79
3	D	4370	OMG	O6-C6-C5	-2.46	120.08	126.60
48	w	651	PSU	O2-C2-N1	-2.45	120.09	122.79
3	D	3792	OMG	O6-C6-C5	-2.45	120.10	126.60
48	w	93	PSU	O2-C2-N1	-2.45	120.10	122.79
48	w	1490	OMG	O6-C6-C5	-2.44	120.11	126.60
2	B	46	G7M	CN7-N7-C5	2.44	129.80	126.77
3	D	3627	OMG	O6-C6-C5	-2.44	120.13	126.60
3	D	4637	OMG	C1'-N9-C4	-2.44	119.26	126.50
3	D	4618	OMG	O6-C6-C5	-2.44	120.14	126.60
3	D	4299	PSU	O2-C2-N1	-2.43	120.11	122.79
48	w	601	OMG	O6-C6-C5	-2.43	120.15	126.60
3	D	1782	PSU	O2-C2-N1	-2.43	120.11	122.79
48	w	1490	OMG	C1'-N9-C4	-2.43	119.28	126.50
2	B	54	5MU	O4-C4-N3	-2.43	115.47	120.12
3	D	1536	PSU	C6-N1-C2	-2.42	120.21	122.68
3	D	4361	PSU	O2-C2-N1	-2.42	120.12	122.79
48	w	1842	4AC	CM7-C7-N4	-2.42	111.11	115.29
3	D	4196	OMG	O6-C6-C5	-2.42	120.19	126.60
3	D	1522	OMG	O6-C6-C5	-2.42	120.19	126.60
3	D	4392	OMG	O6-C6-C5	-2.42	120.19	126.60
3	D	2815	A2M	N3-C4-N9	2.42	131.06	127.08
3	D	4623	OMG	O6-C6-C5	-2.41	120.20	126.60
3	D	1316	OMG	O6-C6-C5	-2.41	120.20	126.60
3	D	4500	PSU	C6-N1-C2	-2.41	120.22	122.68
3	D	1744	PSU	C6-N1-C2	-2.41	120.22	122.68
2	B	10	2MG	N1-C2-N3	-2.40	120.23	123.95
3	D	4228	OMG	C1'-N9-C8	2.40	133.52	126.70
3	D	4228	OMG	O6-C6-C5	-2.39	120.25	126.60
48	w	36	PSU	C6-N1-C2	-2.39	120.24	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4637	OMG	O6-C6-C5	-2.39	120.26	126.60
3	D	4689	PSU	C6-N1-C2	-2.39	120.24	122.68
3	D	2837	OMU	O2-C2-N1	-2.39	119.61	122.79
48	w	1056	PSU	O2-C2-N1	-2.39	120.16	122.79
48	w	1678	A2M	N3-C4-N9	2.39	131.01	127.08
3	D	3715	PSU	O2-C2-N1	-2.38	120.17	122.79
3	D	3851	PSU	O2-C2-N1	-2.38	120.17	122.79
3	D	4296	PSU	C6-N1-C2	-2.38	120.25	122.68
48	w	159	A2M	N3-C4-N9	2.38	131.00	127.08
48	w	1850	MA6	N3-C4-N9	2.37	130.99	127.08
48	w	512	A2M	N3-C4-N9	2.37	130.99	127.08
3	D	3853	PSU	O2-C2-N1	-2.36	120.19	122.79
3	D	1860	PSU	C6-N1-C2	-2.36	120.27	122.68
48	w	105	PSU	C6-N1-C2	-2.36	120.27	122.68
3	D	3715	PSU	C6-N1-C2	-2.36	120.27	122.68
3	D	1522	OMG	C1'-N9-C8	2.36	133.40	126.70
3	D	4494	OMG	O6-C6-C5	-2.36	120.35	126.60
3	D	3768	PSU	C6-N1-C2	-2.35	120.28	122.68
48	w	109	PSU	C6-N1-C2	-2.35	120.28	122.68
48	w	683	OMG	C1'-N9-C4	-2.35	119.53	126.50
2	B	20	3AU	O2-C2-N3	-2.34	118.73	121.99
2	B	20	3AU	C1'-N1-C2	2.34	120.94	116.99
3	D	2632	PSU	O2-C2-N1	-2.34	120.21	122.79
48	w	1004	PSU	C6-N1-C2	-2.34	120.29	122.68
3	D	3744	OMG	O6-C6-C5	-2.34	120.40	126.60
3	D	4442	PSU	C6-N1-C2	-2.34	120.29	122.68
3	D	3627	OMG	C1'-N9-C8	2.33	133.33	126.70
48	w	814	PSU	O2-C2-N1	-2.33	120.23	122.79
3	D	4442	PSU	O4'-C1'-C2'	2.33	108.42	105.14
3	D	3762	PSU	C6-N1-C2	-2.32	120.31	122.68
3	D	4420	PSU	O4'-C1'-C2'	2.32	108.41	105.14
48	w	822	PSU	O4'-C1'-C2'	2.32	108.41	105.14
48	w	576	A2M	N3-C4-N9	2.32	130.90	127.08
3	D	3734	PSU	C6-N1-C2	-2.32	120.32	122.68
3	D	1871	A2M	C3'-C2'-C1'	-2.31	98.54	102.89
3	D	3899	OMG	O6-C6-C5	-2.31	120.47	126.60
3	D	4423	PSU	C6-N1-C2	-2.31	120.33	122.68
3	D	1862	PSU	C6-N1-C2	-2.30	120.33	122.68
48	w	863	PSU	C6-N1-C2	-2.30	120.33	122.68
48	w	436	OMG	C8-N7-C5	2.30	108.41	104.24
3	D	4431	PSU	C6-N1-C2	-2.30	120.33	122.68
3	D	3785	A2M	N3-C4-N9	2.30	130.88	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1174	PSU	C6-N1-C2	-2.30	120.33	122.68
2	B	54	5MU	O2-C2-N1	-2.30	119.73	122.79
3	D	1781	PSU	C6-N1-C2	-2.30	120.33	122.68
3	D	4293	PSU	C6-N1-C2	-2.30	120.33	122.68
48	w	1232	PSU	C6-N1-C2	-2.30	120.33	122.68
3	D	3758	PSU	O2-C2-N1	-2.30	120.26	122.79
3	D	3920	PSU	O2-C2-N1	-2.30	120.26	122.79
3	D	1326	A2M	N3-C4-N9	2.29	130.86	127.08
3	D	4628	PSU	C6-N1-C2	-2.29	120.34	122.68
3	D	4972	PSU	O2-C2-N1	-2.29	120.27	122.79
48	w	119	PSU	C6-N1-C2	-2.29	120.34	122.68
3	D	4306	OMU	O2-C2-N1	-2.29	119.75	122.79
48	w	966	PSU	C6-N1-C2	-2.29	120.34	122.68
48	w	1328	OMG	C8-N7-C5	2.29	108.38	104.24
3	D	1760	OMG	C1'-N9-C4	-2.28	119.72	126.50
3	D	5001	PSU	O2-C2-N1	-2.28	120.28	122.79
48	w	822	PSU	O2-C2-N1	-2.28	120.28	122.79
3	D	2351	OMC	O2-C2-N3	-2.28	118.62	122.33
3	D	4623	OMG	C8-N7-C5	2.28	108.36	104.24
3	D	3782	5MC	CM5-C5-C6	-2.28	119.81	122.85
3	D	4370	OMG	C8-N7-C5	2.28	108.36	104.24
48	w	651	PSU	C6-N1-C2	-2.27	120.36	122.68
48	w	1643	PSU	C6-N1-C2	-2.27	120.36	122.68
3	D	2351	OMC	C1'-N1-C2	2.27	123.49	118.42
3	D	4299	PSU	C6-N1-C2	-2.27	120.37	122.68
48	w	681	PSU	C6-N1-C2	-2.26	120.37	122.68
3	D	4353	PSU	C6-N1-C2	-2.26	120.37	122.68
3	D	398	A2M	N3-C4-N9	2.26	130.81	127.08
3	D	4972	PSU	C6-N1-C2	-2.26	120.38	122.68
3	D	5001	PSU	C6-N1-C2	-2.25	120.38	122.68
48	w	572	PSU	O2-C2-N1	-2.25	120.31	122.79
3	D	4228	OMG	C8-N7-C5	2.25	108.32	104.24
3	D	1524	A2M	N3-C4-N9	2.25	130.79	127.08
3	D	4403	PSU	O4'-C1'-C2'	2.25	108.31	105.14
3	D	3695	PSU	C6-N1-C2	-2.25	120.38	122.68
3	D	3944	OMG	C8-N7-C5	2.25	108.31	104.24
48	w	1337	4AC	C5-C4-N4	-2.25	119.02	122.92
3	D	2508	PSU	C6-N1-C2	-2.25	120.39	122.68
48	w	644	OMG	C1'-N9-C8	2.24	133.09	126.70
3	D	4312	PSU	C6-N1-C2	-2.24	120.39	122.68
48	w	468	A2M	N3-C4-N9	2.24	130.78	127.08
3	D	3899	OMG	C8-N7-C5	2.24	108.30	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3920	PSU	C6-N1-C2	-2.24	120.39	122.68
48	w	509	OMG	C8-N7-C5	2.24	108.29	104.24
48	w	1056	PSU	C6-N1-C2	-2.23	120.40	122.68
48	w	609	PSU	C6-N1-C2	-2.23	120.40	122.68
48	w	644	OMG	C8-N7-C5	2.23	108.28	104.24
48	w	686	PSU	C6-N1-C2	-2.23	120.40	122.68
3	D	3744	OMG	C8-N7-C5	2.23	108.28	104.24
48	w	1238	PSU	C6-N1-C2	-2.23	120.41	122.68
48	w	1851	MA6	N3-C4-N9	2.23	130.75	127.08
48	w	1081	PSU	O4'-C1'-C2'	2.23	108.28	105.14
48	w	166	A2M	N3-C4-N9	2.23	130.75	127.08
3	D	4523	A2M	N3-C4-N9	2.23	130.75	127.08
3	D	4500	PSU	C6-C5-C4	2.23	119.75	118.20
3	D	1522	OMG	C8-N7-C5	2.22	108.26	104.24
3	D	2632	PSU	C6-N1-C2	-2.22	120.42	122.68
3	D	3734	PSU	C6-C5-C4	2.22	119.75	118.20
3	D	2815	A2M	C5-C4-N3	-2.22	123.86	126.75
3	D	4521	PSU	C6-N1-C2	-2.21	120.42	122.68
48	w	649	PSU	C6-N1-C2	-2.21	120.42	122.68
3	D	3899	OMG	C1'-N9-C8	2.21	132.99	126.70
48	w	1367	PSU	C6-N1-C2	-2.21	120.43	122.68
3	D	1760	OMG	C8-N7-C5	2.20	108.23	104.24
3	D	3818	UY1	O4-C4-N3	-2.20	115.90	120.12
2	B	39	UY1	O4-C4-N3	-2.20	115.90	120.12
3	D	3785	A2M	C2-N1-C6	-2.20	114.99	118.77
2	B	16	H2U	O4-C4-N3	2.20	123.77	120.28
2	B	37	1MG	C8-N7-C5	2.20	108.22	104.24
2	B	6	2MG	C8-N7-C5	2.19	108.21	104.24
3	D	4392	OMG	C8-N7-C5	2.19	108.21	104.24
3	D	3760	A2M	N3-C4-N9	2.19	130.69	127.08
48	w	1383	A2M	C2'-C1'-N9	-2.19	109.84	113.53
3	D	4576	PSU	C6-N1-C2	-2.19	120.44	122.68
3	D	2815	A2M	C2-N1-C6	-2.19	115.01	118.77
3	D	4637	OMG	C8-N7-C5	2.19	108.20	104.24
48	w	683	OMG	C8-N7-C5	2.19	108.20	104.24
3	D	4494	OMG	C8-N7-C5	2.19	108.19	104.24
5	F	75	OMG	C8-N7-C5	2.19	108.19	104.24
3	D	4220	6MZ	N3-C4-N9	2.18	130.68	127.08
48	w	1177	PSU	C6-N1-C2	-2.18	120.45	122.68
48	w	1046	PSU	C6-N1-C2	-2.18	120.45	122.68
3	D	3724	A2M	N3-C4-N9	2.18	130.68	127.08
3	D	3760	A2M	C3'-C2'-C1'	-2.18	98.79	102.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1316	OMG	C8-N7-C5	2.18	108.19	104.24
3	D	3825	A2M	N3-C4-N9	2.18	130.67	127.08
48	w	484	A2M	N3-C4-N9	2.18	130.67	127.08
3	D	4361	PSU	C6-N1-C2	-2.18	120.46	122.68
3	D	2364	OMG	C8-N7-C5	2.18	108.18	104.24
2	B	10	2MG	C8-N7-C5	2.17	108.17	104.24
3	D	4293	PSU	O2-C2-N1	-2.17	120.40	122.79
48	w	1850	MA6	C5-C4-N9	2.17	108.31	105.78
3	D	3637	PSU	C6-N1-C2	-2.17	120.46	122.68
48	w	601	OMG	C8-N7-C5	2.17	108.17	104.24
3	D	3764	PSU	C6-N1-C2	-2.17	120.46	122.68
3	D	400	A2M	N3-C4-N9	2.17	130.66	127.08
3	D	1782	PSU	C6-N1-C2	-2.17	120.47	122.68
3	D	3851	PSU	C6-N1-C2	-2.17	120.47	122.68
48	w	1625	PSU	C6-N1-C2	-2.17	120.47	122.68
48	w	1248	B8N	O4'-C1'-C2'	2.17	108.20	105.14
2	B	55	PSU	C6-N1-C2	-2.16	120.47	122.68
3	D	3853	PSU	C6-N1-C2	-2.16	120.47	122.68
48	w	1347	PSU	C6-N1-C2	-2.16	120.47	122.68
3	D	4618	OMG	C8-N7-C5	2.16	108.15	104.24
3	D	4471	PSU	C6-N1-C2	-2.16	120.48	122.68
48	w	815	PSU	C6-C5-C4	2.16	119.71	118.20
3	D	4499	OMG	C8-N7-C5	2.16	108.14	104.24
3	D	3825	A2M	C2-N1-C6	-2.16	115.07	118.77
48	w	1678	A2M	C2-N1-C6	-2.16	115.07	118.77
3	D	3744	OMG	C1'-N9-C8	2.16	132.83	126.70
3	D	1534	A2M	N3-C4-N9	2.15	130.63	127.08
3	D	2787	A2M	N3-C4-N9	2.15	130.62	127.08
48	w	668	A2M	N3-C4-N9	2.15	130.62	127.08
3	D	3718	A2M	N3-C4-N9	2.15	130.62	127.08
48	w	1842	4AC	C4-N3-C2	-2.15	117.19	120.12
48	w	99	A2M	N3-C4-N9	2.15	130.62	127.08
3	D	4196	OMG	C1'-N9-C4	-2.14	120.13	126.50
48	w	866	PSU	C6-N1-C2	-2.14	120.49	122.68
3	D	1871	A2M	N3-C4-N9	2.14	130.61	127.08
3	D	1792	PSU	O2-C2-N1	-2.14	120.43	122.79
3	D	2401	A2M	N3-C4-N9	2.14	130.61	127.08
48	w	406	PSU	C6-N1-C2	-2.14	120.50	122.68
48	w	1832	6MZ	C5-C4-N9	2.14	108.27	105.78
3	D	3639	PSU	C6-N1-C2	-2.14	120.50	122.68
48	w	1445	PSU	C6-N1-C2	-2.14	120.50	122.68
3	D	3627	OMG	C8-N7-C5	2.14	108.11	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4623	OMG	C1'-N9-C8	2.14	132.78	126.70
48	w	27	A2M	N3-C4-N9	2.14	130.60	127.08
3	D	1326	A2M	C2-N1-C6	-2.14	115.10	118.77
3	D	1524	A2M	C2-N1-C6	-2.13	115.10	118.77
3	D	1792	PSU	C6-N1-C2	-2.13	120.50	122.68
3	D	3718	A2M	C2-N1-C6	-2.13	115.11	118.77
3	D	3730	PSU	C6-N1-C2	-2.13	120.50	122.68
3	D	4532	PSU	C6-N1-C2	-2.13	120.51	122.68
48	w	1678	A2M	C5-C4-N3	-2.13	123.97	126.75
48	w	210	PSU	C6-N1-C2	-2.13	120.51	122.68
48	w	159	A2M	C5-C4-N3	-2.13	123.97	126.75
48	w	815	PSU	C6-N1-C2	-2.13	120.51	122.68
3	D	1534	A2M	C2-N1-C6	-2.13	115.12	118.77
3	D	2363	A2M	N3-C4-N9	2.12	130.58	127.08
48	w	166	A2M	O4'-C4'-C3'	2.12	109.32	105.11
2	B	37	1MG	C1'-N9-C4	2.12	132.81	126.50
3	D	2787	A2M	C2-N1-C6	-2.12	115.12	118.77
48	w	93	PSU	C6-N1-C2	-2.12	120.52	122.68
3	D	4523	A2M	C2-N1-C6	-2.12	115.13	118.77
48	w	799	OMU	O2-C2-N1	-2.12	119.97	122.79
3	D	4552	PSU	C6-N1-C2	-2.11	120.52	122.68
3	D	4499	OMG	C1'-N9-C8	2.11	132.72	126.70
3	D	2804	OMC	O2-C2-N3	-2.11	118.89	122.33
48	w	1244	PSU	C6-C5-C4	2.11	119.67	118.20
48	w	484	A2M	C2-N1-C6	-2.11	115.14	118.77
3	D	3830	A2M	N3-C4-N9	2.11	130.56	127.08
48	w	99	A2M	C2-N1-C6	-2.11	115.14	118.77
48	w	166	A2M	C2-N1-C6	-2.11	115.14	118.77
3	D	4498	OMU	O2-C2-N1	-2.11	119.98	122.79
3	D	398	A2M	C2-N1-C6	-2.10	115.16	118.77
3	D	4403	PSU	C6-N1-C2	-2.10	120.53	122.68
48	w	1031	A2M	N3-C4-N9	2.10	130.54	127.08
48	w	1490	OMG	C8-N7-C5	2.10	108.04	104.24
3	D	3758	PSU	C6-N1-C2	-2.10	120.54	122.68
3	D	3724	A2M	C2-N1-C6	-2.10	115.17	118.77
48	w	218	PSU	C6-N1-C2	-2.10	120.54	122.68
48	w	172	OMU	O2-C2-N1	-2.09	120.00	122.79
2	B	48	5MC	CM5-C5-C6	-2.09	120.05	122.85
48	w	468	A2M	C2-N1-C6	-2.09	115.18	118.77
3	D	1534	A2M	C5-C4-N3	-2.08	124.03	126.75
48	w	1045	PSU	C6-N1-C2	-2.08	120.56	122.68
3	D	400	A2M	C2-N1-C6	-2.08	115.19	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	576	A2M	C5-C4-N3	-2.08	124.04	126.75
48	w	1081	PSU	C6-N1-C2	-2.08	120.56	122.68
3	D	4392	OMG	C1'-N9-C8	2.08	132.61	126.70
3	D	4620	OMU	O2-C2-N1	-2.08	120.03	122.79
3	D	4220	6MZ	C4-N9-C8	2.08	107.98	105.73
3	D	3760	A2M	C2-N1-C6	-2.07	115.21	118.77
3	D	2415	OMU	O2-C2-N1	-2.07	120.03	122.79
3	D	2401	A2M	C2-N1-C6	-2.07	115.21	118.77
48	w	109	PSU	C6-C5-C4	2.07	119.64	118.20
48	w	159	A2M	C2-N1-C6	-2.07	115.21	118.77
48	w	590	A2M	C2-N1-C6	-2.07	115.22	118.77
3	D	398	A2M	C5-C4-N3	-2.07	124.05	126.75
48	w	1244	PSU	C6-N1-C2	-2.07	120.57	122.68
2	B	35	PSU	C6-N1-C2	-2.06	120.57	122.68
3	D	1534	A2M	O4'-C1'-N9	-2.06	104.00	108.06
3	D	2424	OMG	C8-N7-C5	2.06	107.97	104.24
3	D	2363	A2M	C2-N1-C6	-2.06	115.23	118.77
3	D	1625	OMG	C8-N7-C5	2.06	107.96	104.24
3	D	4457	PSU	C6-N1-C2	-2.06	120.58	122.68
48	w	576	A2M	C2-N1-C6	-2.05	115.24	118.77
48	w	509	OMG	C1'-N9-C8	2.05	132.54	126.70
3	D	4196	OMG	C8-N7-C5	2.05	107.95	104.24
3	D	3792	OMG	C1'-N9-C4	-2.05	120.42	126.50
3	D	3792	OMG	C8-N7-C5	2.05	107.95	104.24
3	D	1322	1MA	C6-C5-N7	-2.05	128.47	132.20
2	B	26	M2G	O6-C6-N1	-2.04	116.20	120.12
48	w	649	PSU	C6-C5-C4	2.04	119.63	118.20
48	w	1692	PSU	C6-N1-C2	-2.04	120.59	122.68
48	w	121	OMU	O2-C2-N1	-2.04	120.07	122.79
3	D	4618	OMG	C1'-N9-C8	2.04	132.51	126.70
3	D	3944	OMG	C1'-N9-C4	-2.04	120.44	126.50
3	D	3830	A2M	C2-N1-C6	-2.04	115.27	118.77
3	D	3637	PSU	O2-C2-N1	-2.04	120.55	122.79
48	w	36	PSU	C6-C5-C4	2.04	119.62	118.20
48	w	1337	4AC	C4-N3-C2	-2.03	117.35	120.12
48	w	1639	G7M	CN7-N7-C8	-2.03	121.70	124.84
3	D	4370	OMG	C1'-N9-C8	2.03	132.48	126.70
48	w	1383	A2M	N3-C4-N9	2.03	130.43	127.08
48	w	1383	A2M	C2-N1-C6	-2.03	115.28	118.77
2	B	27	M2G	O6-C6-N1	-2.03	116.23	120.12
48	w	1832	6MZ	C4-N9-C8	2.03	107.92	105.73
3	D	3718	A2M	N3-C2-N1	2.03	131.78	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	572	PSU	O4'-C1'-C2'	2.03	108.00	105.14
48	w	814	PSU	C6-N1-C2	-2.03	120.61	122.68
48	w	166	A2M	C5-C4-N3	-2.03	124.11	126.75
3	D	2424	OMG	C1'-N9-C8	2.02	132.46	126.70
48	w	1337	4AC	C5-C4-N3	2.02	125.85	122.59
3	D	1860	PSU	C6-C5-C4	2.02	119.61	118.20
2	B	17	H2U	C4-N3-C2	-2.02	124.12	125.79
2	B	17	H2U	O4-C4-N3	2.01	123.47	120.28
3	D	1524	A2M	C5-C4-N3	-2.01	124.12	126.75
3	D	3724	A2M	C5-C4-N3	-2.01	124.12	126.75
3	D	1625	OMG	C1'-N9-C4	-2.01	120.52	126.50
48	w	1367	PSU	C6-C5-C4	2.01	119.61	118.20
2	B	10	2MG	O3'-C3'-C2'	2.01	118.33	111.82
3	D	4457	PSU	O4'-C1'-C2'	2.01	107.97	105.14
48	w	1804	OMU	O2-C2-N1	-2.01	120.12	122.79
3	D	4523	A2M	C2'-C1'-N9	-2.01	110.15	113.53
2	B	46	G7M	N9-C8-N7	-2.00	107.26	112.21
48	w	512	A2M	C5-C4-N3	-2.00	124.14	126.75

There are no chirality outliers.

All (158) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6	2MG	O4'-C4'-C5'-O5'
2	B	6	2MG	C3'-C4'-C5'-O5'
2	B	16	H2U	O4'-C1'-N1-C2
2	B	16	H2U	O4'-C1'-N1-C6
2	B	20	3AU	O4'-C1'-N1-C2
2	B	20	3AU	O4'-C1'-N1-C6
2	B	20	3AU	C10-C11-C12-C13
2	B	20	3AU	C10-C11-C12-N40
2	B	34	56B	C11-C10-N10-C9
2	B	34	56B	C5-C7-C9-N10
3	D	1534	A2M	C1'-C2'-O2'-CM'
3	D	1677	PSU	C2'-C1'-C5-C6
3	D	1760	OMG	C3'-C4'-C5'-O5'
3	D	2364	OMG	C1'-C2'-O2'-CM2
3	D	2415	OMU	C1'-C2'-O2'-CM2
3	D	2424	OMG	O4'-C4'-C5'-O5'
3	D	2424	OMG	C3'-C4'-C5'-O5'
3	D	2815	A2M	O4'-C4'-C5'-O5'
3	D	2815	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	D	2824	OMC	C1'-C2'-O2'-CM2
3	D	3701	OMC	C2'-C1'-N1-C6
3	D	3724	A2M	C1'-C2'-O2'-CM'
3	D	3818	UY1	C3'-C4'-C5'-O5'
3	D	3818	UY1	O4'-C4'-C5'-O5'
3	D	3925	OMU	C1'-C2'-O2'-CM2
3	D	3944	OMG	O4'-C4'-C5'-O5'
3	D	3944	OMG	C3'-C4'-C5'-O5'
3	D	4196	OMG	C1'-C2'-O2'-CM2
3	D	4500	PSU	C3'-C4'-C5'-O5'
3	D	4500	PSU	O4'-C4'-C5'-O5'
3	D	4637	OMG	C1'-C2'-O2'-CM2
48	w	34	PSU	C3'-C4'-C5'-O5'
48	w	34	PSU	O4'-C4'-C5'-O5'
48	w	116	OMU	C1'-C2'-O2'-CM2
48	w	159	A2M	O4'-C4'-C5'-O5'
48	w	159	A2M	C3'-C4'-C5'-O5'
48	w	159	A2M	C1'-C2'-O2'-CM'
48	w	166	A2M	O4'-C4'-C5'-O5'
48	w	166	A2M	C3'-C4'-C5'-O5'
48	w	428	OMU	C2'-C1'-N1-C6
48	w	428	OMU	C1'-C2'-O2'-CM2
48	w	468	A2M	C3'-C4'-C5'-O5'
48	w	576	A2M	C3'-C4'-C5'-O5'
48	w	590	A2M	C1'-C2'-O2'-CM'
48	w	590	A2M	C2'-C1'-N9-C8
48	w	601	OMG	C1'-C2'-O2'-CM2
48	w	644	OMG	C3'-C4'-C5'-O5'
48	w	644	OMG	C1'-C2'-O2'-CM2
48	w	668	A2M	O4'-C4'-C5'-O5'
48	w	799	OMU	C1'-C2'-O2'-CM2
48	w	1328	OMG	C1'-C2'-O2'-CM2
48	w	1442	OMU	C1'-C2'-O2'-CM2
48	w	1639	G7M	O4'-C4'-C5'-O5'
48	w	1678	A2M	C1'-C2'-O2'-CM'
48	w	1804	OMU	C1'-C2'-O2'-CM2
48	w	1832	6MZ	C5-C6-N6-C9
48	w	1832	6MZ	N1-C6-N6-C9
48	w	1851	MA6	O4'-C4'-C5'-O5'
3	D	3701	OMC	C2'-C1'-N1-C2
2	B	16	H2U	O4'-C4'-C5'-O5'
2	B	46	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	D	3785	A2M	O4'-C4'-C5'-O5'
3	D	3785	A2M	C3'-C4'-C5'-O5'
48	w	468	A2M	O4'-C4'-C5'-O5'
48	w	799	OMU	O4'-C4'-C5'-O5'
48	w	1238	PSU	C3'-C4'-C5'-O5'
48	w	1490	OMG	C3'-C4'-C5'-O5'
48	w	1851	MA6	C3'-C4'-C5'-O5'
2	B	20	3AU	C2'-C1'-N1-C6
48	w	428	OMU	C2'-C1'-N1-C2
2	B	16	H2U	C3'-C4'-C5'-O5'
3	D	1760	OMG	O4'-C4'-C5'-O5'
3	D	3760	A2M	O4'-C4'-C5'-O5'
48	w	644	OMG	O4'-C4'-C5'-O5'
48	w	668	A2M	C3'-C4'-C5'-O5'
48	w	1238	PSU	O4'-C4'-C5'-O5'
48	w	1490	OMG	O4'-C4'-C5'-O5'
48	w	1639	G7M	C3'-C4'-C5'-O5'
48	w	590	A2M	C2'-C1'-N9-C4
2	B	39	UY1	C1'-C2'-O2'-CM2
2	B	20	3AU	C2'-C1'-N1-C2
3	D	3760	A2M	C3'-C4'-C5'-O5'
3	D	4447	5MC	C2'-C1'-N1-C6
48	w	428	OMU	C3'-C4'-C5'-O5'
48	w	1248	B8N	C32-C31-N3-C4
2	B	46	G7M	C4'-C5'-O5'-P
2	B	46	G7M	O4'-C4'-C5'-O5'
3	D	1677	PSU	O4'-C4'-C5'-O5'
48	w	428	OMU	O4'-C4'-C5'-O5'
48	w	576	A2M	O4'-C4'-C5'-O5'
48	w	1703	OMC	O4'-C4'-C5'-O5'
3	D	1524	A2M	C3'-C4'-C5'-O5'
3	D	2787	A2M	C2'-C1'-N9-C8
2	B	20	3AU	N40-C12-C13-O30
3	D	1524	A2M	O4'-C4'-C5'-O5'
3	D	1534	A2M	O4'-C4'-C5'-O5'
3	D	1677	PSU	C3'-C4'-C5'-O5'
3	D	3744	OMG	C1'-C2'-O2'-CM2
3	D	4447	5MC	O4'-C1'-N1-C6
3	D	4447	5MC	C2'-C1'-N1-C2
48	w	34	PSU	C4'-C5'-O5'-P
3	D	3701	OMC	O4'-C1'-N1-C2
3	D	2401	A2M	C3'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
48	w	462	OMC	C3'-C2'-O2'-CM2
48	w	1326	OMU	O4'-C1'-N1-C6
48	w	799	OMU	C3'-C4'-C5'-O5'
3	D	3701	OMC	O4'-C1'-N1-C6
3	D	4500	PSU	C4'-C5'-O5'-P
48	w	428	OMU	O4'-C1'-N1-C2
48	w	1490	OMG	C4'-C5'-O5'-P
48	w	99	A2M	O4'-C4'-C5'-O5'
48	w	428	OMU	O4'-C1'-N1-C6
3	D	4447	5MC	O4'-C1'-N1-C2
2	B	16	H2U	C4'-C5'-O5'-P
3	D	4494	OMG	C3'-C2'-O2'-CM2
3	D	1534	A2M	C4'-C5'-O5'-P
3	D	2815	A2M	C4'-C5'-O5'-P
48	w	159	A2M	C4'-C5'-O5'-P
48	w	590	A2M	O4'-C4'-C5'-O5'
3	D	2787	A2M	C2'-C1'-N9-C4
48	w	1248	B8N	C32-C31-N3-C2
3	D	3944	OMG	C4'-C5'-O5'-P
48	w	1326	OMU	O4'-C1'-N1-C2
2	B	55	PSU	O4'-C1'-C5-C4
3	D	3818	UY1	O4'-C1'-C5-C4
3	D	4500	PSU	O4'-C1'-C5-C4
48	w	572	PSU	O4'-C1'-C5-C4
3	D	3785	A2M	C3'-C2'-O2'-CM'
3	D	4370	OMG	C3'-C2'-O2'-CM2
48	w	1326	OMU	C3'-C2'-O2'-CM2
3	D	2351	OMC	C2'-C1'-N1-C6
3	D	1322	1MA	C2'-C1'-N9-C8
3	D	1322	1MA	C2'-C1'-N9-C4
48	w	166	A2M	C4'-C5'-O5'-P
3	D	2364	OMG	O4'-C4'-C5'-O5'
3	D	1524	A2M	O4'-C1'-N9-C8
2	B	16	H2U	C2'-C1'-N1-C6
2	B	20	3AU	N40-C12-C13-O31
48	w	1703	OMC	C3'-C4'-C5'-O5'
3	D	4370	OMG	C1'-C2'-O2'-CM2
48	w	468	A2M	C1'-C2'-O2'-CM'
48	w	1851	MA6	C5-C6-N6-C9
48	w	1326	OMU	C2'-C1'-N1-C2
3	D	2787	A2M	O4'-C1'-N9-C8
3	D	2422	OMC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	47	H2U	O4'-C1'-N1-C6
3	D	1677	PSU	O4'-C1'-C5-C6
3	D	3818	UY1	O4'-C1'-C5-C6
48	w	572	PSU	O4'-C1'-C5-C6
3	D	1326	A2M	C4'-C5'-O5'-P
3	D	398	A2M	O4'-C4'-C5'-O5'
3	D	2351	OMC	O4'-C4'-C5'-O5'
3	D	2351	OMC	C2'-C1'-N1-C2
3	D	2351	OMC	C3'-C2'-O2'-CM2
2	B	17	H2U	O4'-C4'-C5'-O5'
48	w	1383	A2M	C3'-C4'-C5'-O5'
2	B	47	H2U	C2'-C1'-N1-C2
48	w	1288	OMU	C2'-C1'-N1-C2

There are no ring outliers.

78 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	w	121	OMU	1	0
3	D	4220	6MZ	1	0
48	w	468	A2M	1	0
3	D	3825	A2M	1	0
3	D	3724	A2M	2	0
48	w	1678	A2M	2	0
48	w	1031	A2M	1	0
48	w	686	PSU	1	0
5	F	75	OMG	1	0
48	w	159	A2M	2	0
3	D	2424	OMG	1	0
3	D	4620	OMU	2	0
48	w	1442	OMU	1	0
3	D	3734	PSU	1	0
48	w	1490	OMG	1	0
3	D	2815	A2M	1	0
3	D	2351	OMC	3	0
3	D	3944	OMG	2	0
3	D	4494	OMG	1	0
3	D	4447	5MC	1	0
3	D	1326	A2M	2	0
48	w	1639	G7M	2	0
48	w	116	OMU	3	0
48	w	1004	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	w	1842	4AC	1	0
3	D	4457	PSU	1	0
3	D	4536	OMC	1	0
3	D	5001	PSU	1	0
48	w	801	PSU	1	0
48	w	512	A2M	1	0
3	D	4196	OMG	1	0
2	B	10	2MG	1	0
2	B	16	H2U	1	0
48	w	815	PSU	1	0
48	w	1328	OMG	1	0
48	w	627	OMU	1	0
2	B	6	2MG	1	0
48	w	166	A2M	1	0
3	D	4623	OMG	1	0
48	w	509	OMG	2	0
48	w	34	PSU	1	0
48	w	1288	OMU	1	0
3	D	1760	OMG	1	0
3	D	3818	UY1	1	0
48	w	174	OMC	1	0
48	w	27	A2M	1	0
3	D	1677	PSU	1	0
3	D	1773	OMU	2	0
3	D	3718	A2M	3	0
48	w	1391	OMC	2	0
3	D	4689	PSU	1	0
48	w	428	OMU	1	0
48	w	462	OMC	1	0
48	w	644	OMG	2	0
3	D	4579	PSU	2	0
48	w	799	OMU	1	0
48	w	576	A2M	3	0
3	D	1871	A2M	1	0
3	D	2364	OMG	1	0
3	D	3744	OMG	1	0
48	w	1692	PSU	1	0
3	D	2422	OMC	1	0
3	D	3925	OMU	1	0
48	w	572	PSU	2	0
48	w	1643	PSU	1	0
3	D	1534	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	w	1703	OMC	1	0
3	D	2824	OMC	1	0
3	D	2415	OMU	5	0
48	w	590	A2M	4	0
48	w	1850	MA6	1	0
3	D	2363	A2M	1	0
48	w	1804	OMU	2	0
48	w	36	PSU	1	0
3	D	4637	OMG	2	0
3	D	1340	OMC	1	0
3	D	2804	OMC	1	0
3	D	2632	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 546 ligands modelled in this entry, 545 are monoatomic - leaving 1 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
81	GAL	B	101	2	11,11,12	2.07	4 (36%)	15,15,17	1.69	4 (26%)

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
81	GAL	B	101	2	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	B	101	GAL	O5-C1	-3.53	1.38	1.43
81	B	101	GAL	C2-C3	3.31	1.57	1.52
81	B	101	GAL	C4-C5	2.61	1.58	1.53
81	B	101	GAL	C1-C2	2.14	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	B	101	GAL	O2-C2-C3	-3.29	103.56	110.14
81	B	101	GAL	O4-C4-C5	-2.55	102.97	109.30
81	B	101	GAL	C2-C3-C4	-2.40	106.75	110.89
81	B	101	GAL	C6-C5-C4	-2.14	108.00	113.00

There are no chirality outliers.

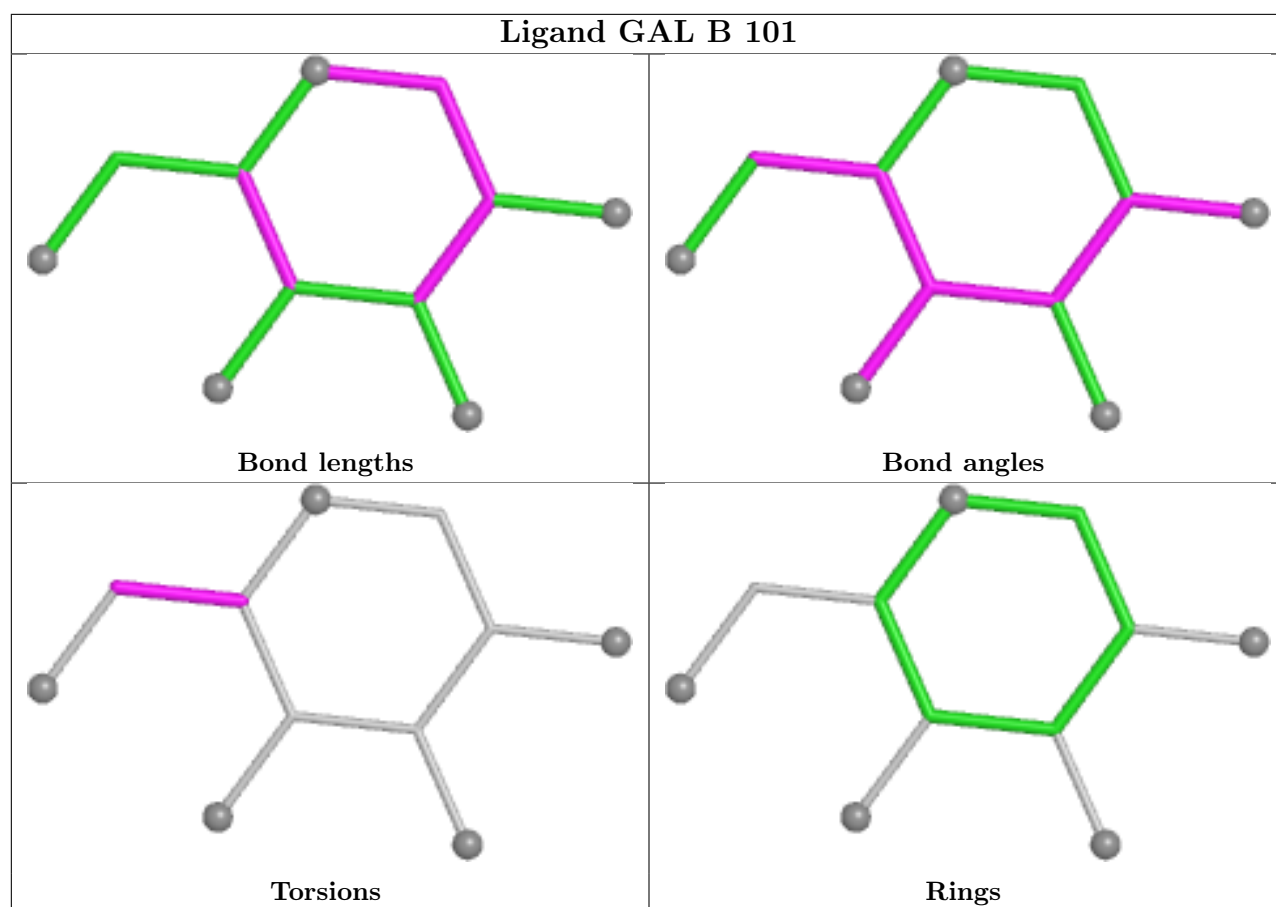
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	B	101	GAL	O5-C5-C6-O6
81	B	101	GAL	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

There are no chain breaks in this entry.

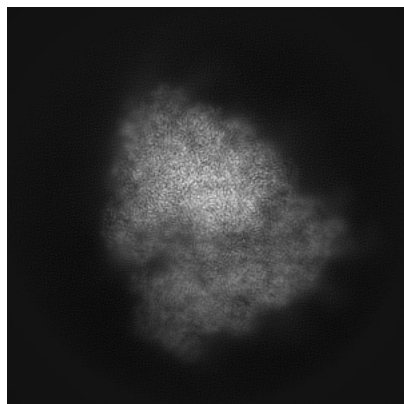
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36180. These allow visual inspection of the internal detail of the map and identification of artifacts.

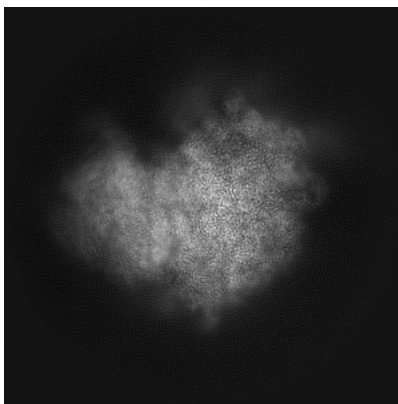
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

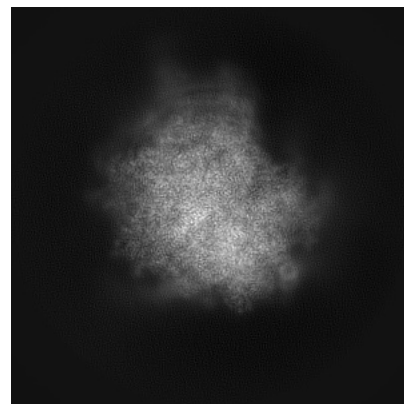
6.1.1 Primary map



X

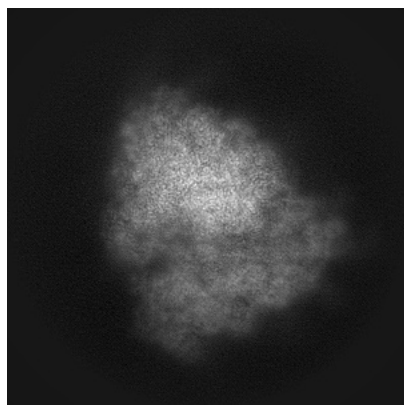


Y

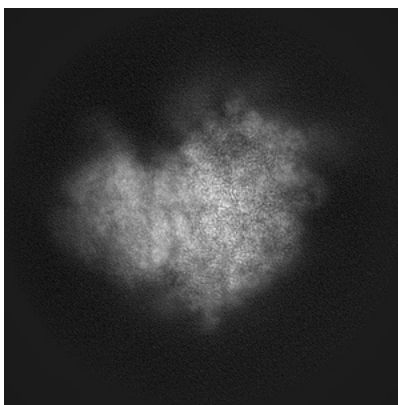


Z

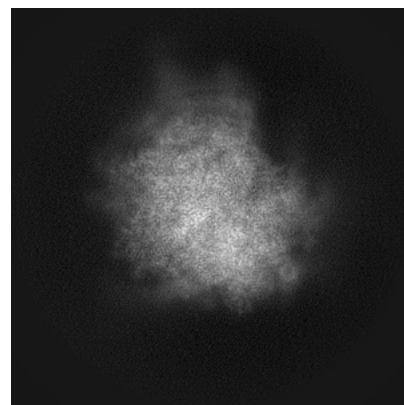
6.1.2 Raw map



X



Y

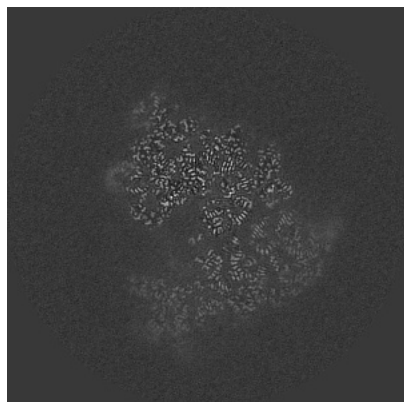


Z

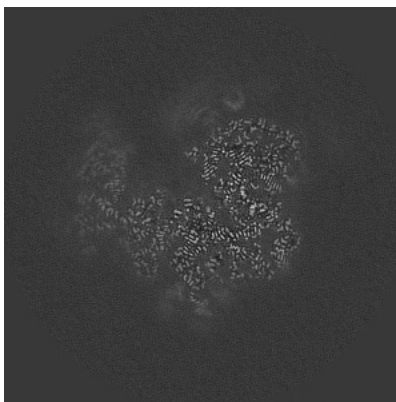
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

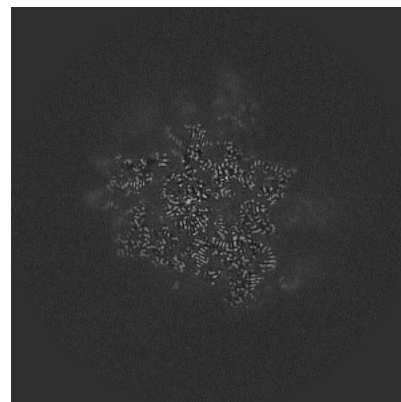
6.2.1 Primary map



X Index: 265

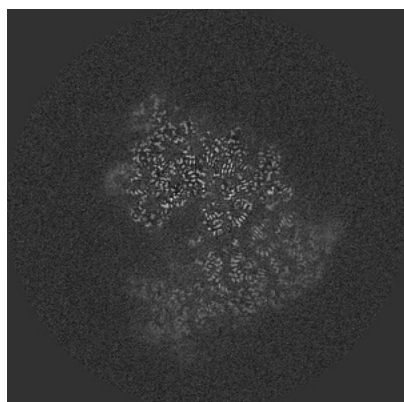


Y Index: 265

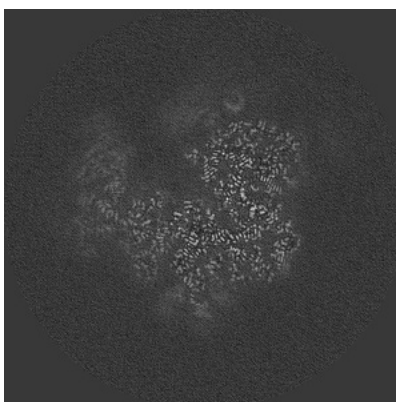


Z Index: 265

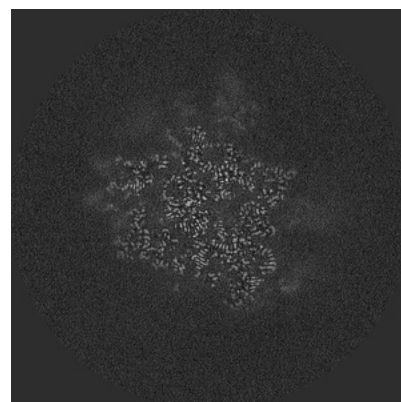
6.2.2 Raw map



X Index: 265



Y Index: 265

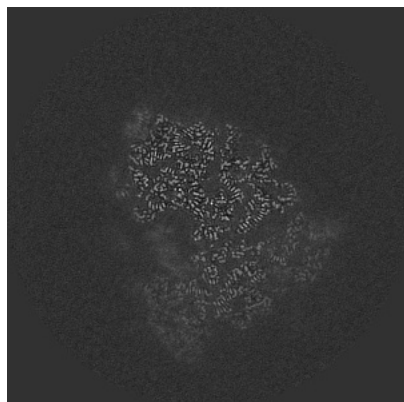


Z Index: 265

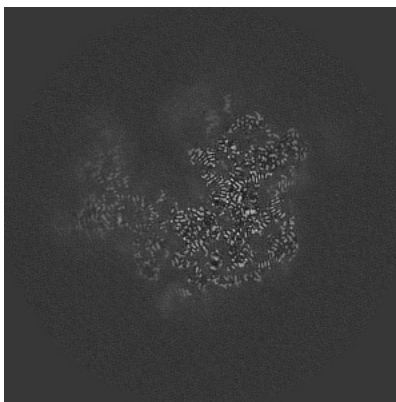
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

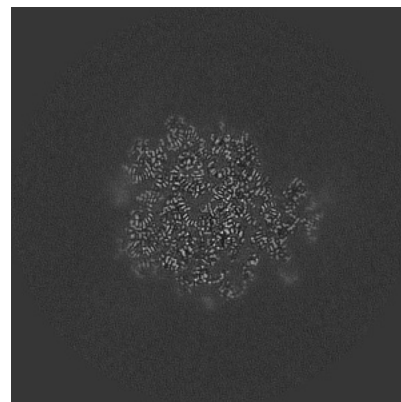
6.3.1 Primary map



X Index: 253

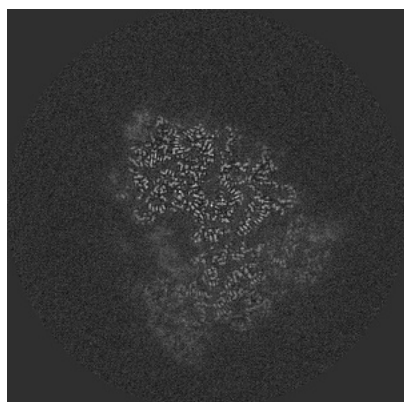


Y Index: 258

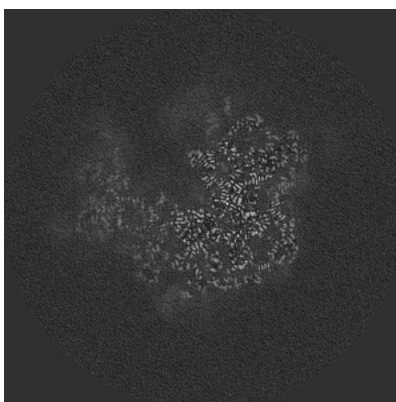


Z Index: 300

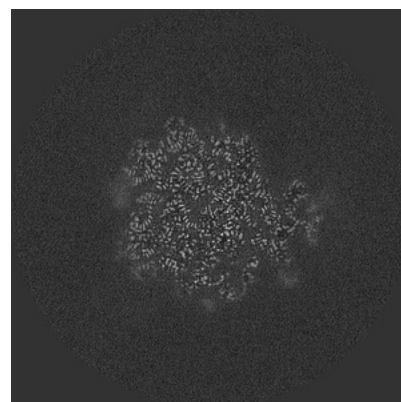
6.3.2 Raw map



X Index: 253



Y Index: 258

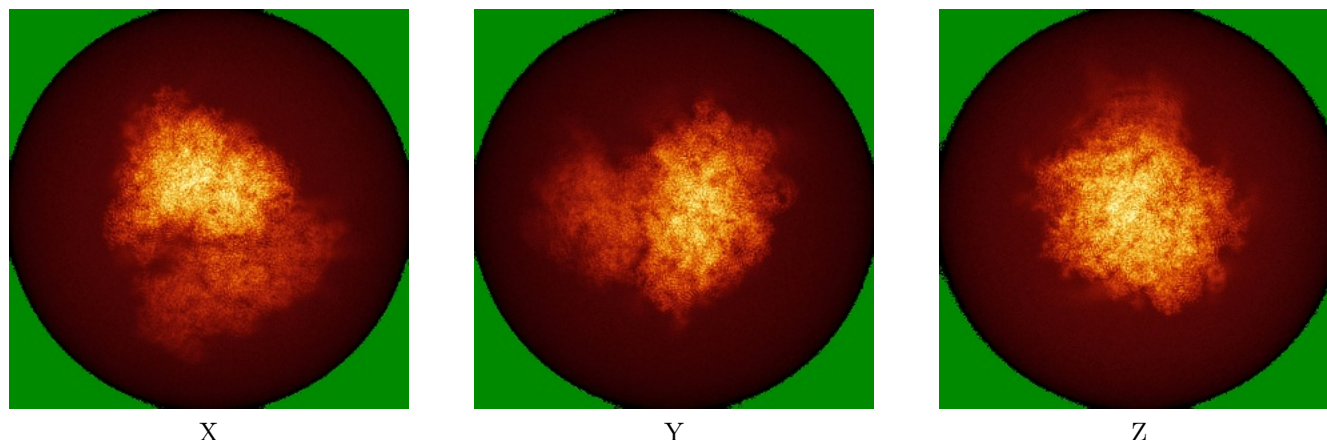


Z Index: 300

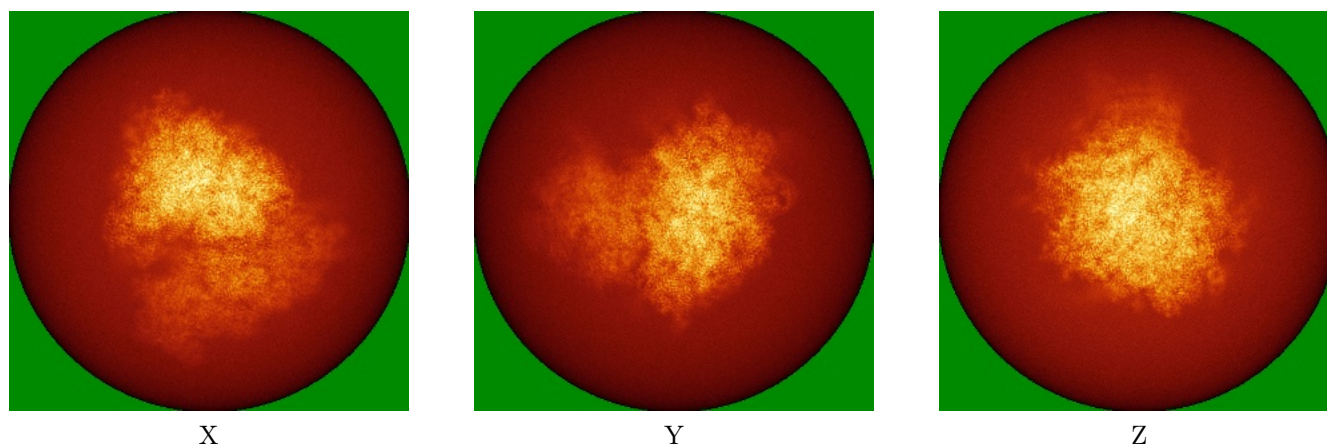
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



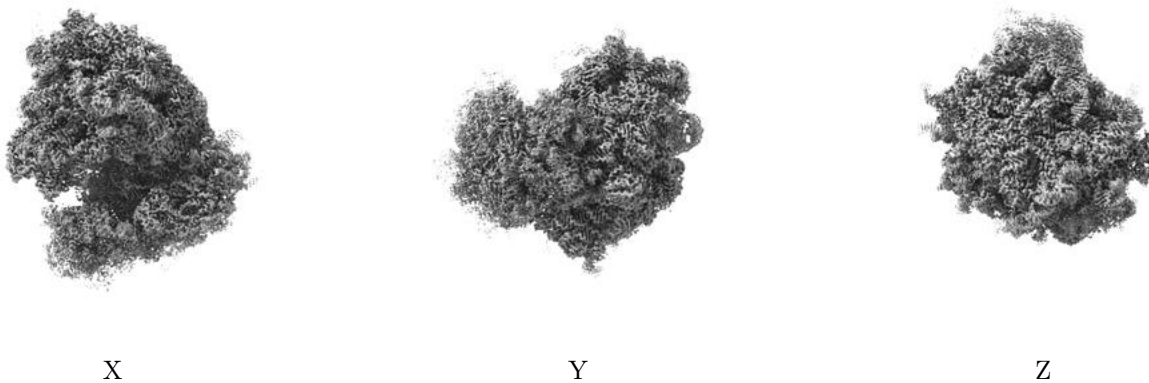
6.4.2 Raw map



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

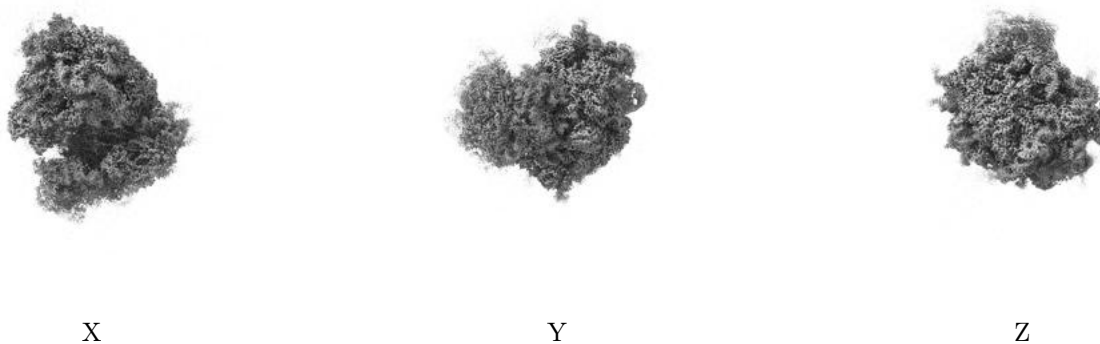
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0191. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

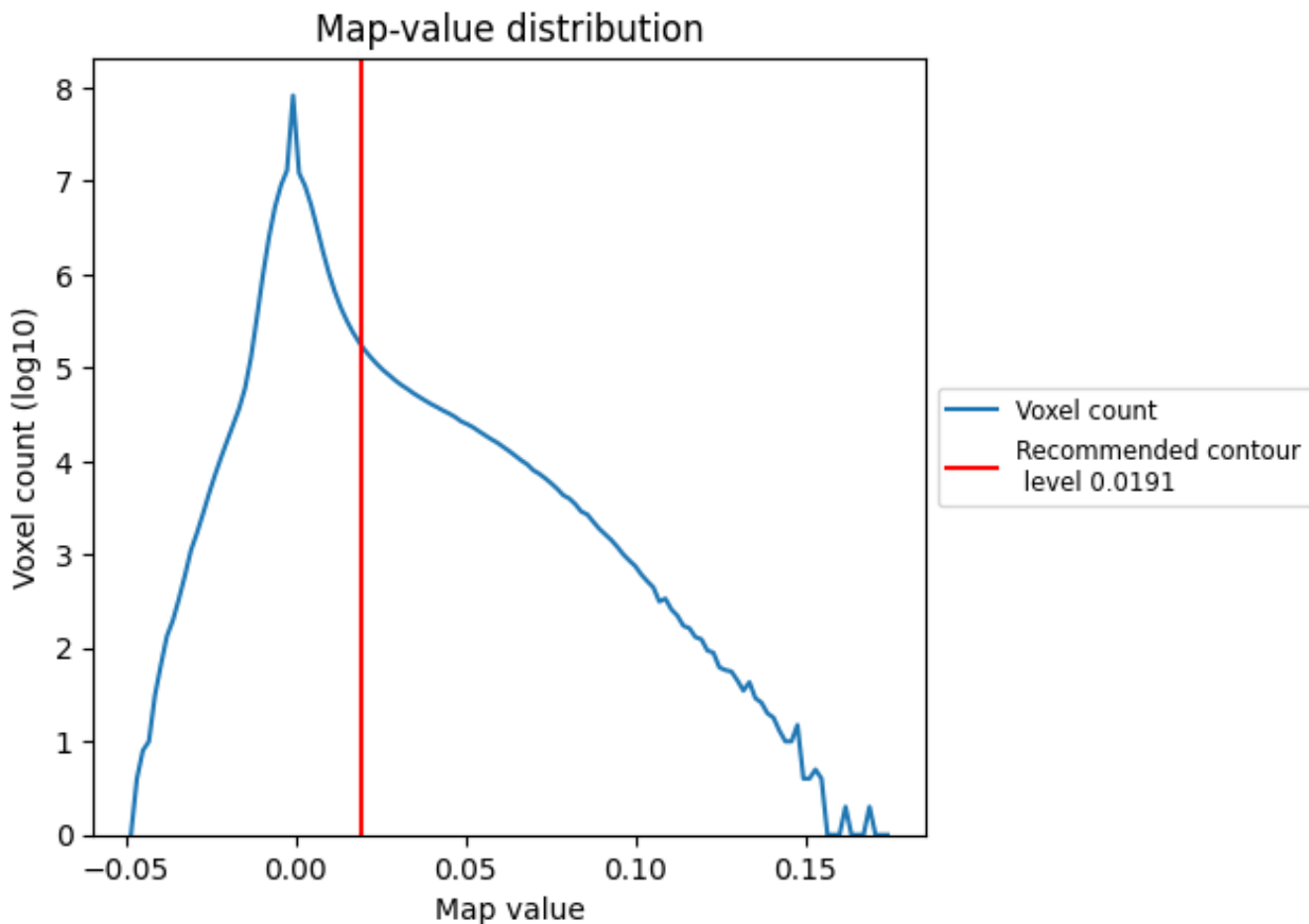
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

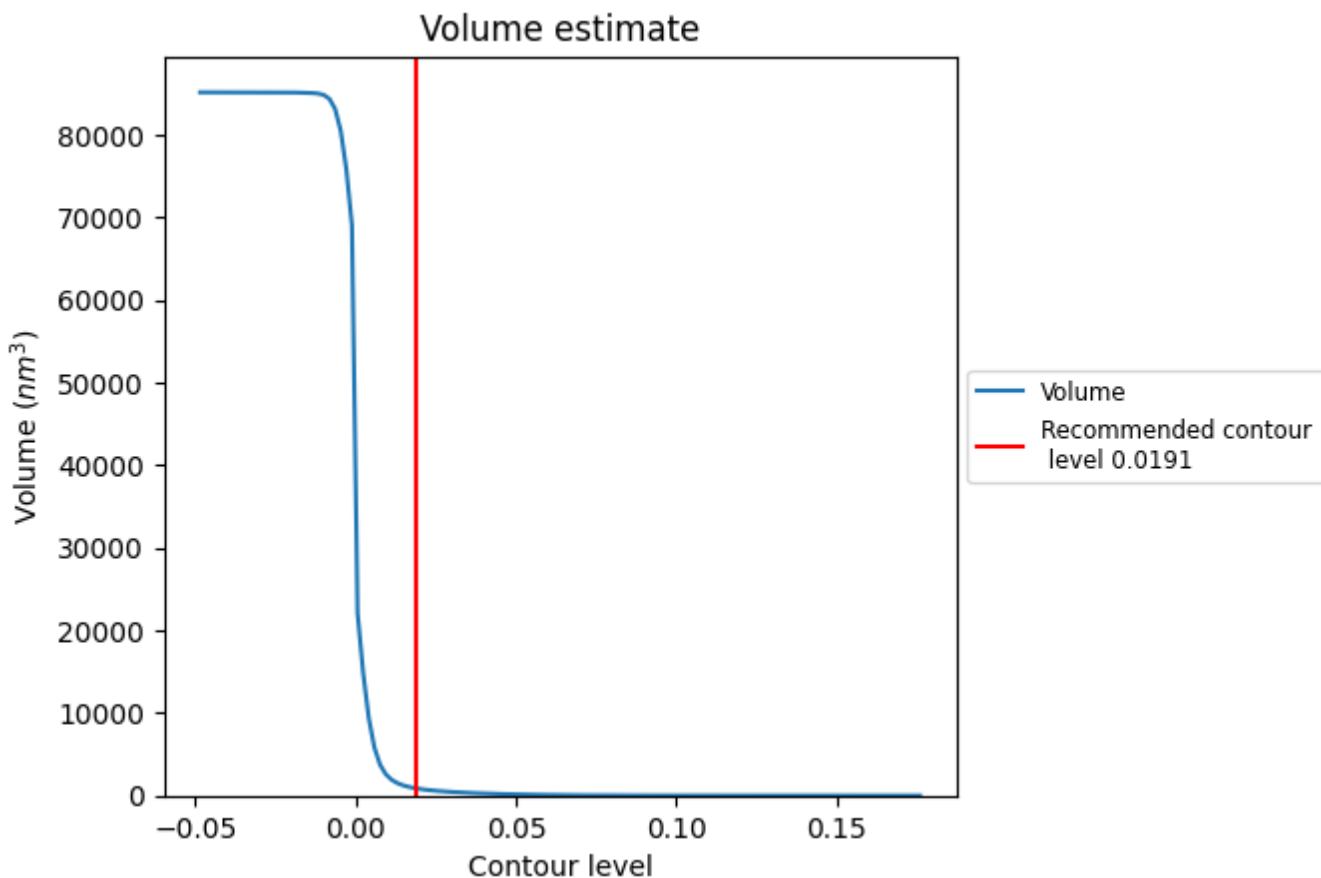
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

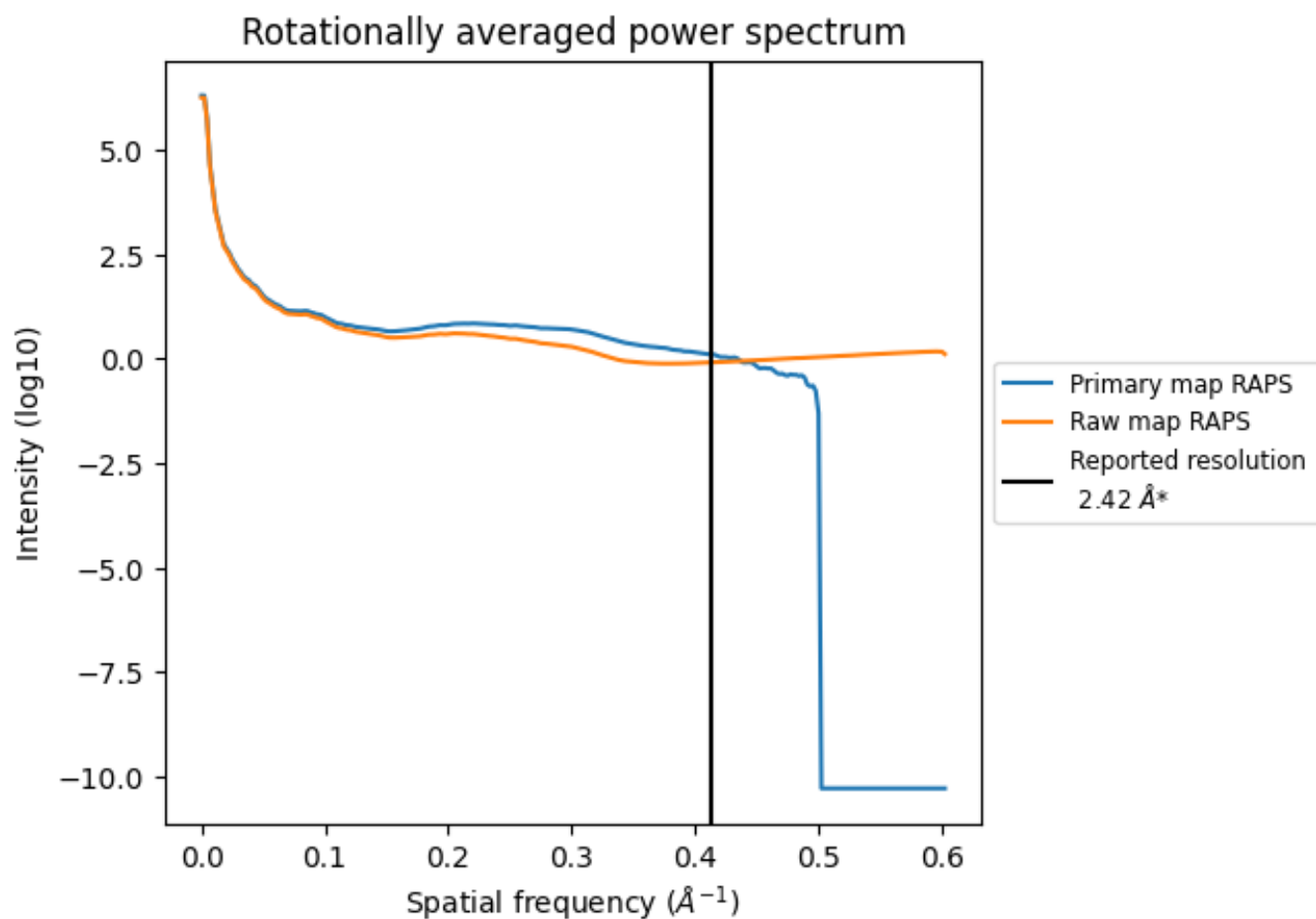
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 860 nm³; this corresponds to an approximate mass of 777 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 [i](#)

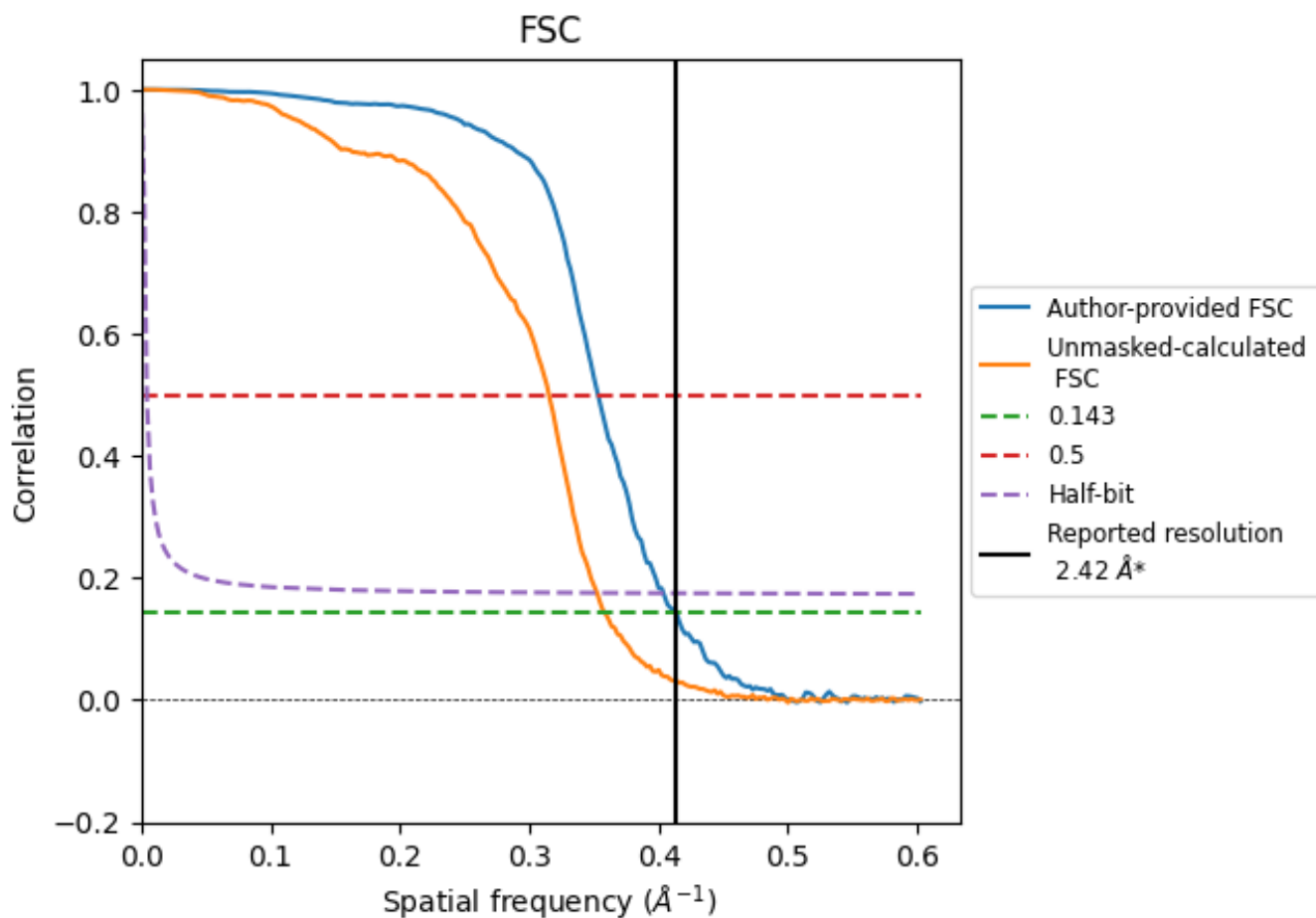


*Reported resolution corresponds to spatial frequency of 0.413 Å⁻¹

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 0.413 Å⁻¹

8.2 Resolution estimates [i](#)

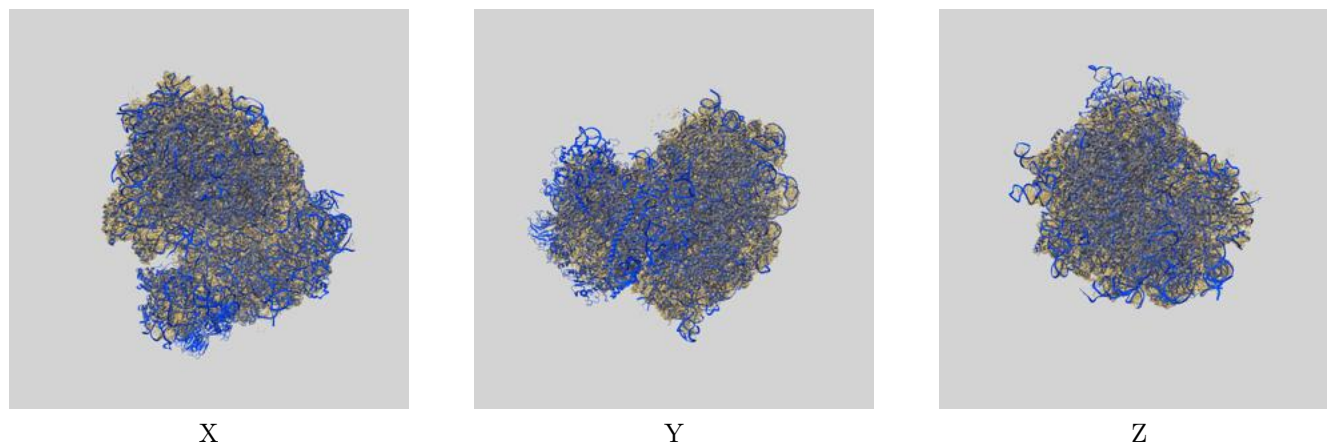
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.83	2.48
Unmasked-calculated*	2.79	3.17	2.84

*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 2.79 differs from the reported value 2.42 by more than 10 %

9 Map-model fit [i](#)

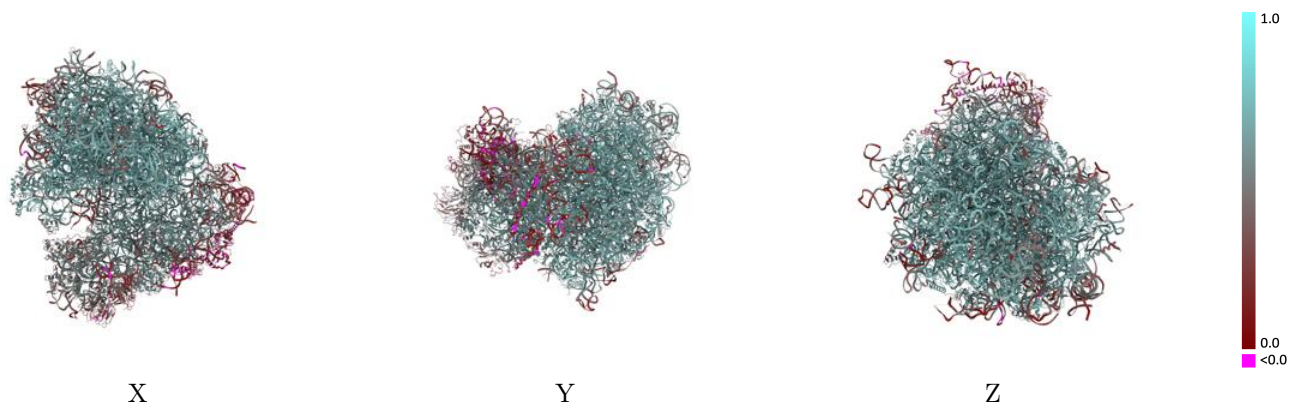
This section contains information regarding the fit between EMDB map EMD-36180 and PDB model 8JDL. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



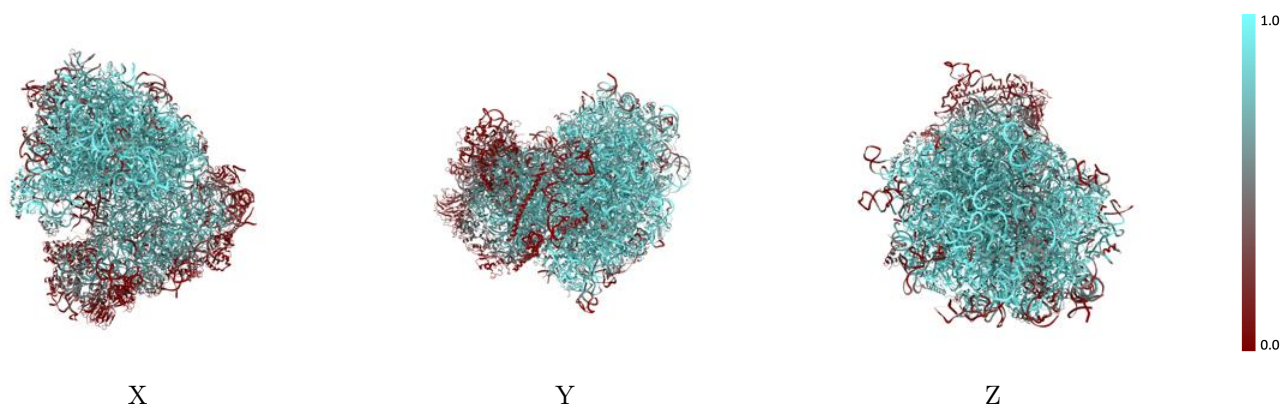
The images above show the 3D surface view of the map at the recommended contour level 0.0191 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



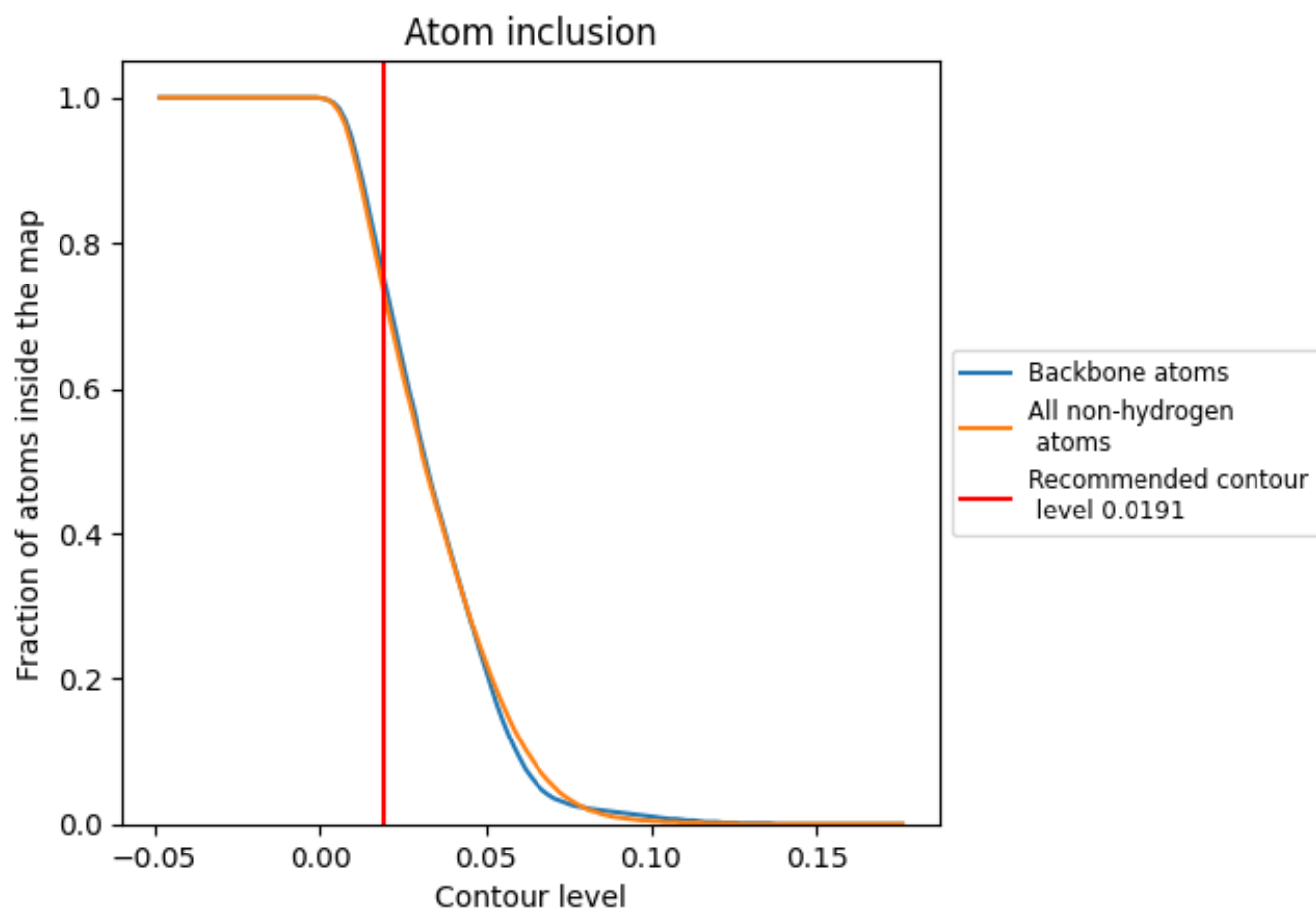
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0191).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.0191) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7350	 0.5730
0	 0.2460	 0.4230
1	 0.3220	 0.3450
2	 0.3830	 0.4840
3	 0.1560	 0.2800
4	 0.2200	 0.4010
5	 0.5270	 0.5120
6	 0.2500	 0.2290
7	 0.0520	 0.3010
8	 0.6910	 0.5920
9	 0.6360	 0.5790
A	 0.4890	 0.4710
AA	 0.6660	 0.5800
AB	 0.1410	 0.3950
AC	 0.3210	 0.4620
AD	 0.2250	 0.4190
AE	 0.2540	 0.4570
AF	 0.2730	 0.4540
AG	 0.2290	 0.3700
AH	 0.4820	 0.5530
AI	 0.7290	 0.6070
AJ	 0.6450	 0.5500
AK	 0.1130	 0.1930
AL	 0.1580	 0.3970
AM	 0.7120	 0.5870
AN	 0.4150	 0.4820
AO	 0.3510	 0.4680
AP	 0.5180	 0.5330
AQ	 0.1330	 0.2160
AR	 0.0240	 0.2980
B	 0.2670	 0.3860
D	 0.8520	 0.6160
E	 0.9700	 0.6660
F	 0.9050	 0.6340
G	 0.9540	 0.6890









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Chain	Atom inclusion	Q-score
H	 0.8850	 0.6660
I	 0.9040	 0.6550
J	 0.7840	 0.6120
K	 0.7610	 0.6050
L	 0.9050	 0.6690
M	 0.7080	 0.5780
N	 0.8240	 0.6330
O	 0.8550	 0.6460
P	 0.6500	 0.5430
Q	 0.8040	 0.6190
R	 0.8570	 0.6290
S	 0.9640	 0.6900
T	 0.9120	 0.6760
U	 0.8900	 0.6710
V	 0.9410	 0.6790
W	 0.7820	 0.6030
X	 0.9260	 0.6730
Y	 0.8550	 0.6440
Z	 0.5890	 0.5300
a	 0.9130	 0.6770
b	 0.8660	 0.6640
c	 0.8430	 0.6310
d	 0.8170	 0.6280
e	 0.8170	 0.6280
f	 0.9070	 0.6730
g	 0.7150	 0.5750
h	 0.8350	 0.6270
i	 0.8310	 0.6390
j	 0.9450	 0.6880
k	 0.9410	 0.6780
l	 0.8570	 0.6390
m	 0.8290	 0.6290
n	 0.7720	 0.6160
o	 0.9500	 0.6850
p	 0.6460	 0.5650
q	 0.9010	 0.6590
r	 0.8750	 0.6560
s	 0.8810	 0.6610
t	 0.8060	 0.6260
u	 0.8790	 0.6670
v	 0.9020	 0.6410
w	 0.6880	 0.5150

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Chain	Atom inclusion	Q-score
x	 0.4640	 0.5430
y	 0.5690	 0.5650
z	 0.6350	 0.5760