



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 05:42 PM JST

PDB ID : 8JDM / pdb_00008jdm
EMDB ID : EMD-36181
Title : Structure of the Human cytoplasmic Ribosome with human tRNA
Tyr(GalQ34) and mRNA(UAU) (rotated state)
Authors : Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.
Deposited on : 2023-05-14
Resolution : 2.67 Å(reported)
Based on initial models : 6Y57, 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:

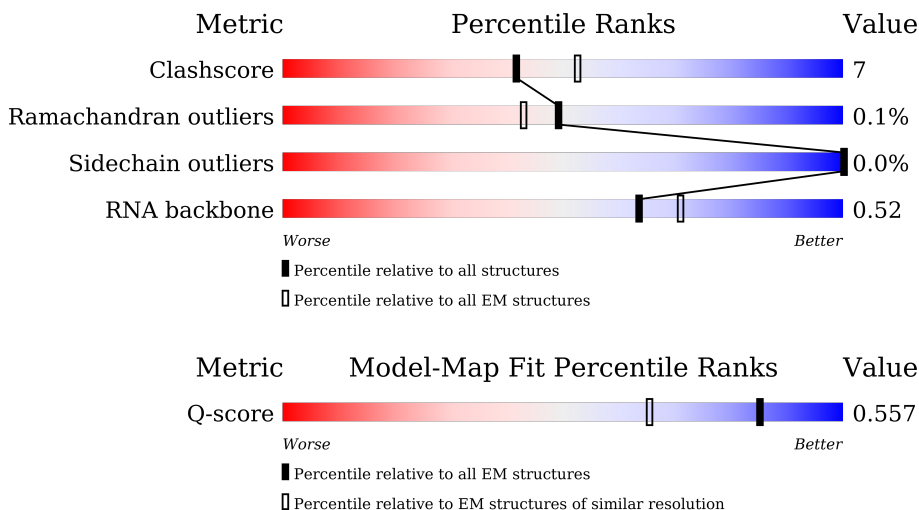
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

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

The reported resolution of this entry is 2.67 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.











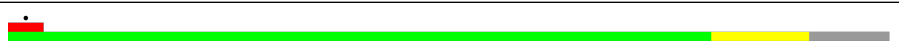

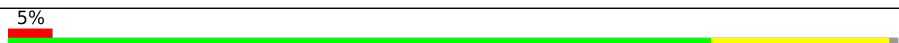


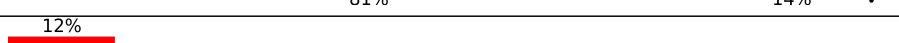
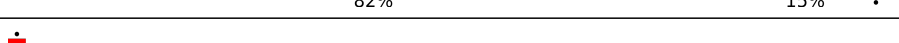
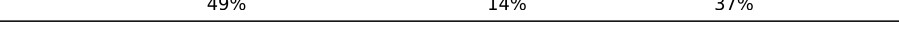
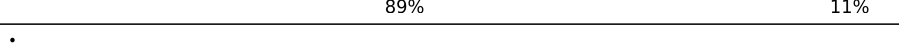
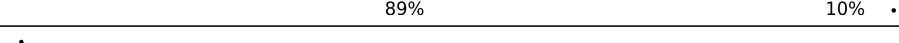
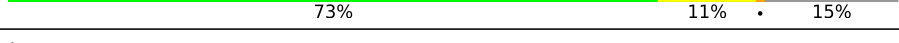



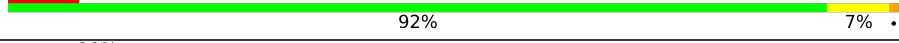


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9182 (2.17 - 3.17)

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	
2	B	76	
2	C	76	








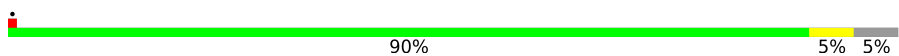


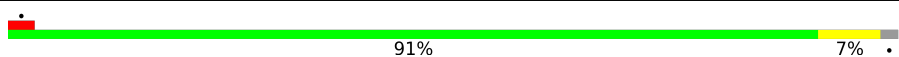

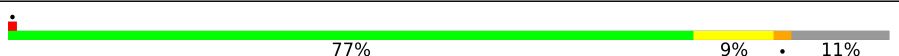
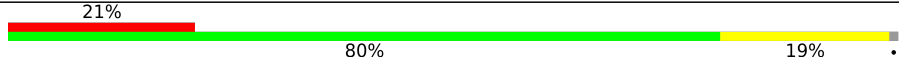
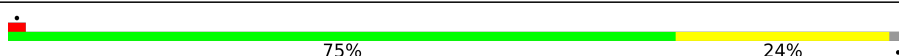
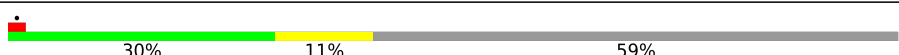

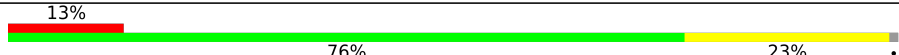
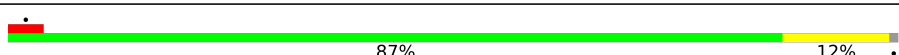
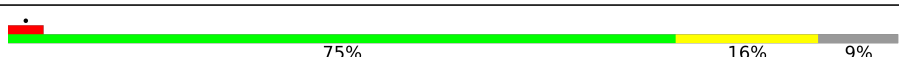





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Mol	Chain	Length	Quality of chain
3	D	5070	
4	E	120	
5	F	156	
6	G	257	
7	H	403	
8	I	427	
9	J	297	
10	K	288	
11	L	248	
12	M	266	
13	N	192	
14	O	214	
15	P	178	
16	Q	211	
17	R	215	
18	S	204	
19	T	203	
20	U	184	
21	V	188	
22	W	196	
23	X	176	
24	Y	160	
25	Z	128	
26	a	140	
27	b	157	

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Mol	Chain	Length	Quality of chain
28	c	156	
29	d	145	
30	e	136	
31	f	148	
32	g	159	
33	h	115	
34	i	125	
35	j	135	
36	k	110	
37	l	117	
38	m	123	
39	n	105	
40	o	97	
41	p	70	
42	q	51	
43	r	128	
44	s	25	
45	t	106	
46	u	92	
47	v	137	
48	w	1869	
49	x	295	
50	y	264	
51	z	293	
52	0	243	

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Mol	Chain	Length	Quality of chain
53	1	263	73% 72% 27%
54	2	204	61% 70% 22% 8%
55	3	249	86% 64% 31% 5%
56	4	194	80% 61% 35%
57	5	208	67% 68% 31%
58	6	194	66% 64% 30% 6%
59	7	165	55% 41% 17% 42%
60	8	158	30% 76% 14% 10%
61	9	151	34% 79% 20%
62	AA	151	22% 66% 23% 11%
63	AB	145	59% 68% 25% 8%
64	AC	146	63% 73% 25%
65	AD	135	73% 71% 24%
66	AE	152	64% 59% 36% 5%
67	AF	145	62% 79% 19%
68	AG	119	64% 51% 34% 14%
69	AH	83	39% 76% 24%
70	AI	130	8% 75% 24%
71	AJ	143	21% 85% 13%
72	AK	133	86% 56% 36% 8%
73	AL	125	54% 43% 14% 42%
74	AM	115	21% 69% 17% 14%
75	AN	84	56% 63% 36%
76	AO	69	57% 59% 29% 12%
77	AP	56	18% 61% 20% 20%

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Mol	Chain	Length	Quality of chain
78	AQ	59	
79	AR	317	

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 209349 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	14	288	130	40	104	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	73	1580	715	281	512	72	0	0
2	C	73	1580	715	281	512	72	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
6	G	247	Total	C	N	O	S	0	0
			1891	1185	388	312	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
21	V	187	1513	944	314	250	5	0	0

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

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

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

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

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

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

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

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

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

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

- 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
28	c	120	Total	C	N	O	S	0	0
			981	628	185	167	1		

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

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

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

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

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

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

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

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

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

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

- 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
41	p	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- 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
			Total	C	N	O	P		
48	w	1634	34933	15622	6267	11411	1633	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
62	AA	134	1002	612	197	187	6	0	0

- 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	72	574	368	104	101	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
			Total	C	N	O	S		
77	AP	45	370	228	77	60	5	0	0

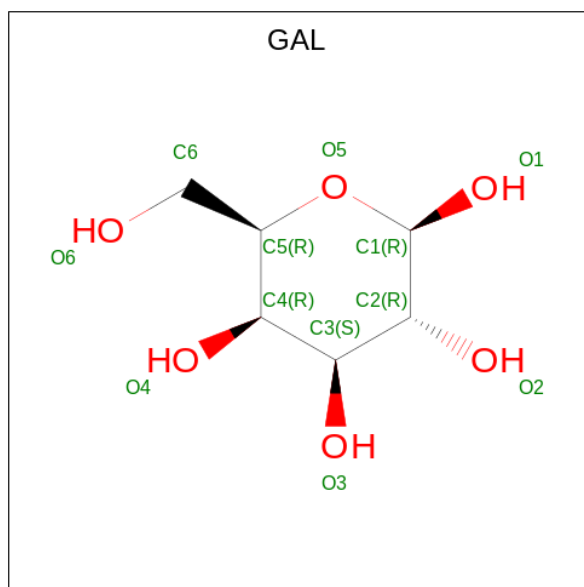
- Molecule 78 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	AQ	55	438	271	95	71	1	0	0

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

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

- Molecule 80 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	D	391	Total	Mg	0
			391	391	
81	E	10	Total	Mg	0
			10	10	
81	F	5	Total	Mg	0
			5	5	
81	G	2	Total	Mg	0
			2	2	
81	H	1	Total	Mg	0
			1	1	
81	I	1	Total	Mg	0
			1	1	
81	N	1	Total	Mg	0
			1	1	
81	O	1	Total	Mg	0
			1	1	
81	S	1	Total	Mg	0
			1	1	
81	U	1	Total	Mg	0
			1	1	
81	V	2	Total	Mg	0
			2	2	
81	W	1	Total	Mg	0
			1	1	
81	X	1	Total	Mg	0
			1	1	
81	a	1	Total	Mg	0
			1	1	
81	g	1	Total	Mg	0
			1	1	
81	j	1	Total	Mg	0
			1	1	
81	k	1	Total	Mg	0
			1	1	
81	l	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
81	w	93	Total 93	Mg 93	0
81	2	1	Total 1	Mg 1	0
81	AA	1	Total 1	Mg 1	0
81	AG	1	Total 1	Mg 1	0
81	AM	1	Total 1	Mg 1	0

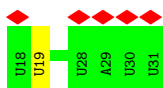
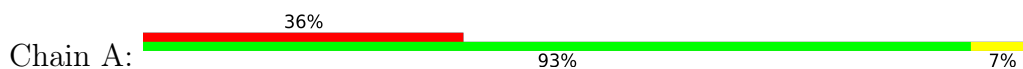
- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	o	1	Total 1	Zn 1	0
82	r	1	Total 1	Zn 1	0
82	t	1	Total 1	Zn 1	0
82	u	1	Total 1	Zn 1	0
82	w	1	Total 1	Zn 1	0
82	AA	1	Total 1	Zn 1	0

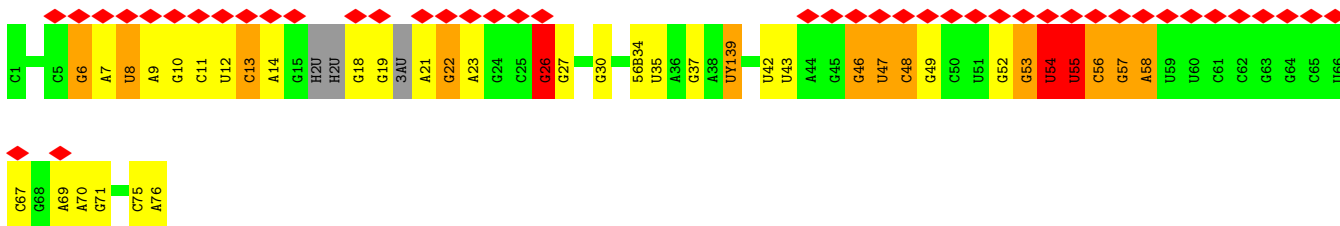
3 Residue-property plots [i](#)

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

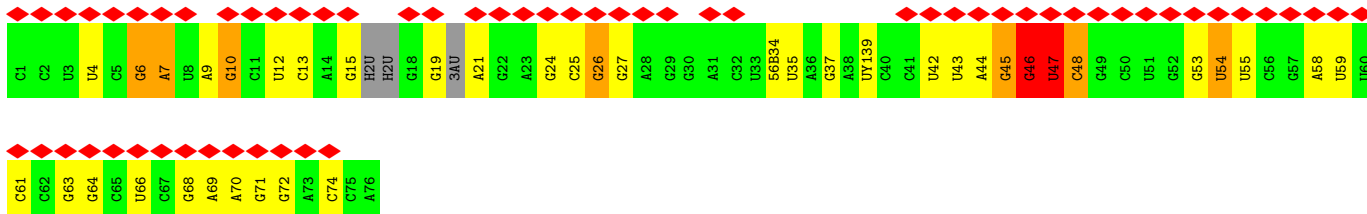
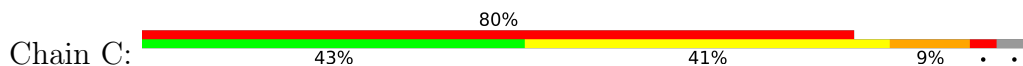
- Molecule 1: mRNA



- Molecule 2: tRNA (Tyr)

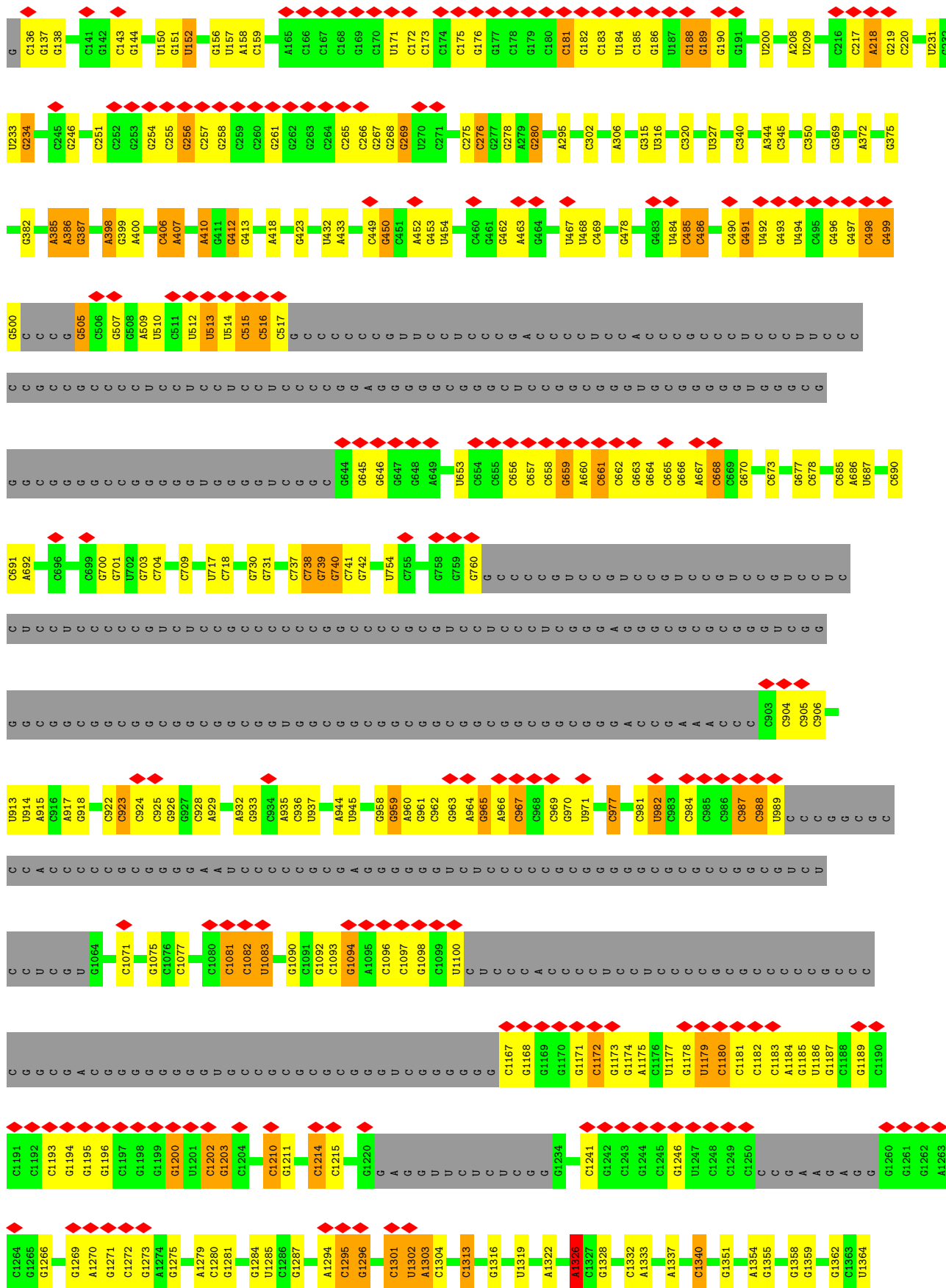


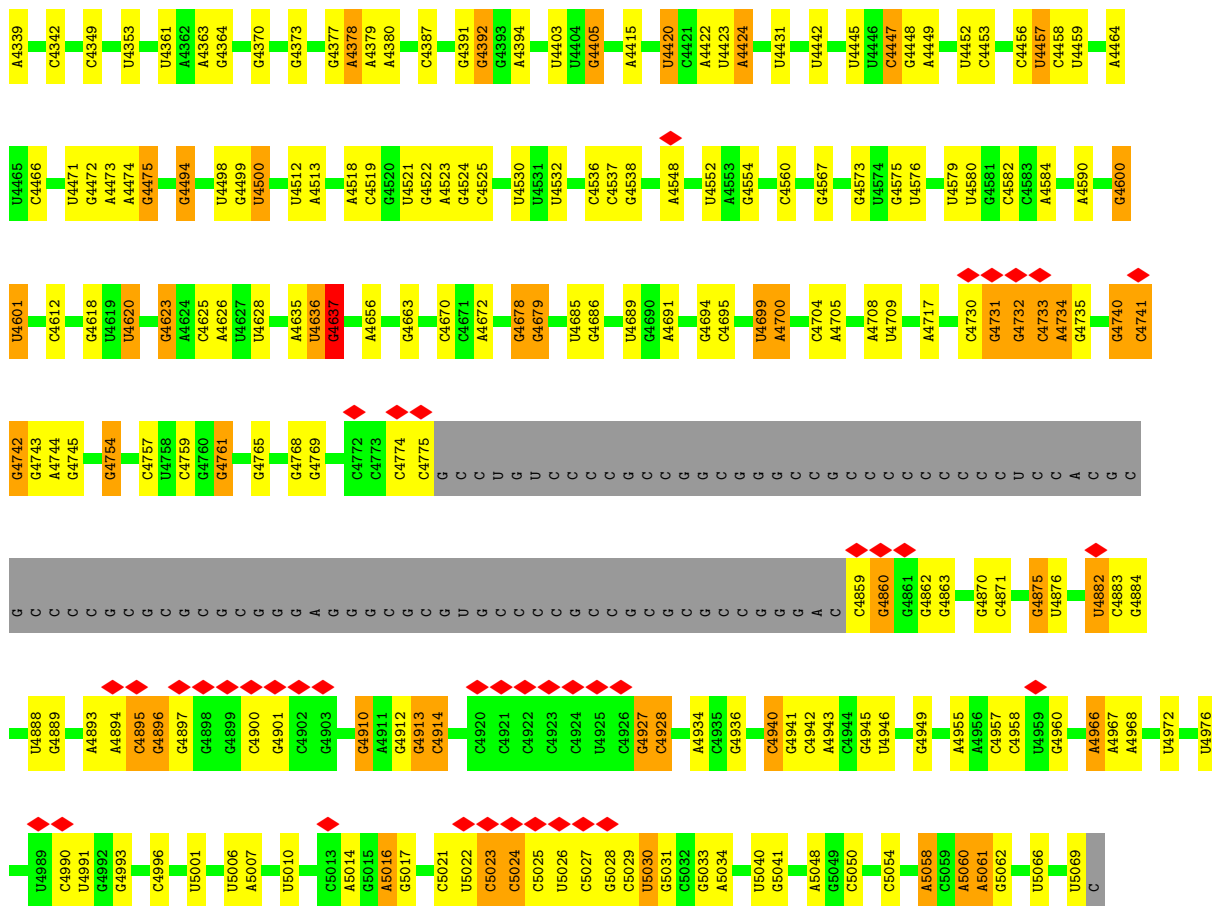
- Molecule 2: tRNA (Tyr)



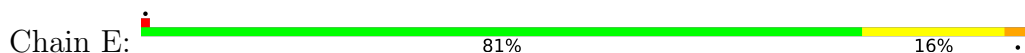
- Molecule 3: 28S ribosomal RNA



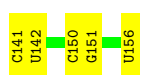
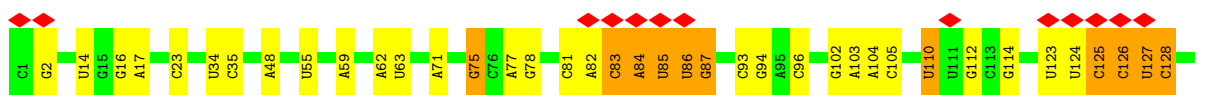




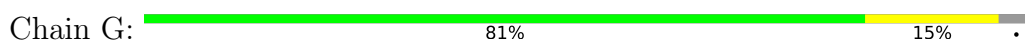
• Molecule 4: 5S ribosomal RNA

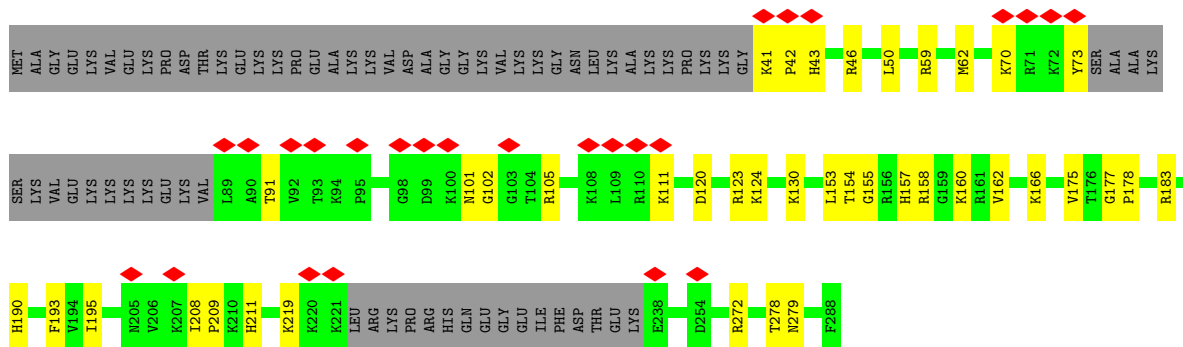


• Molecule 5: 5.8S ribosomal RNA

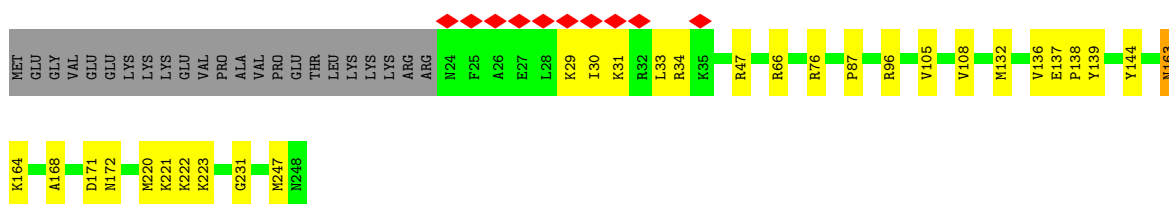
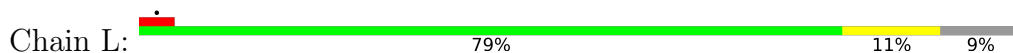


• Molecule 6: 60S ribosomal protein L8

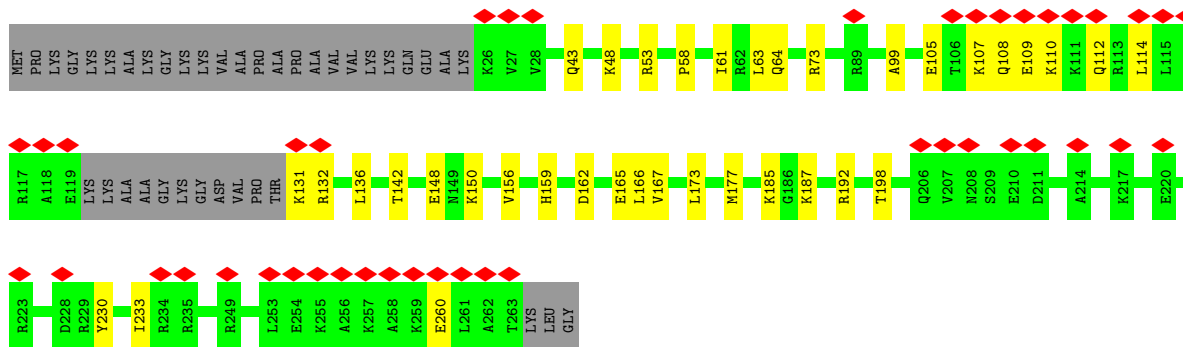




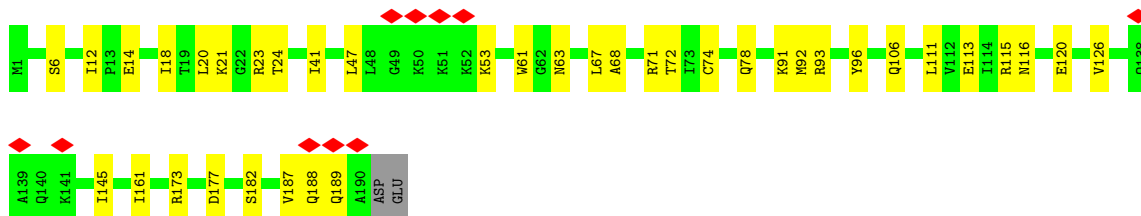
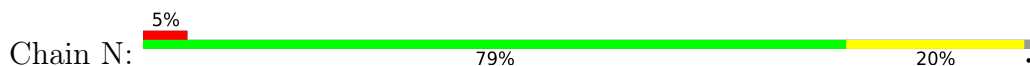
• Molecule 11: 60S ribosomal protein L7



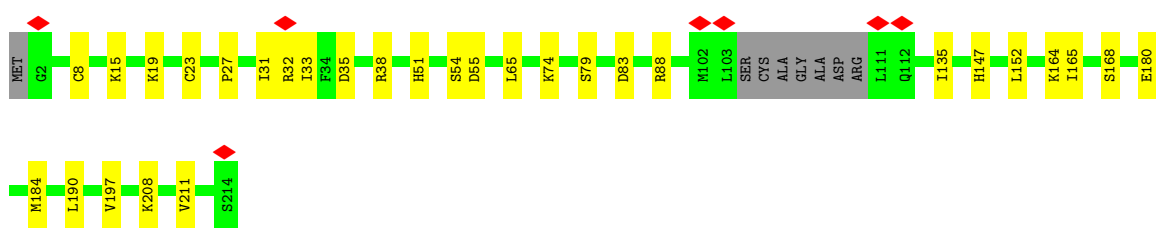
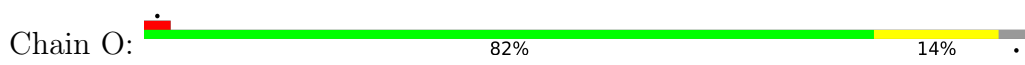
• Molecule 12: 60S ribosomal protein L7a



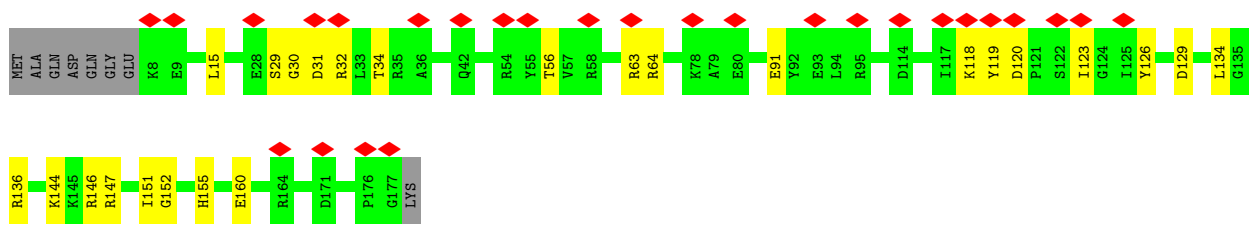
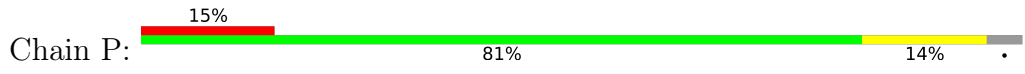
• Molecule 13: 60S ribosomal protein L9



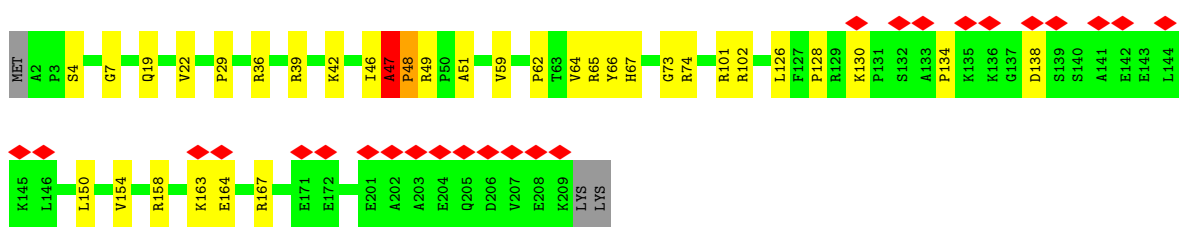
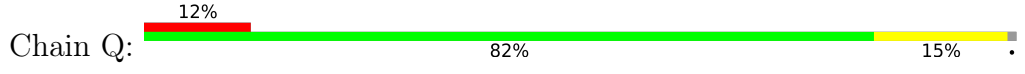
• Molecule 14: 60S ribosomal protein L10-like



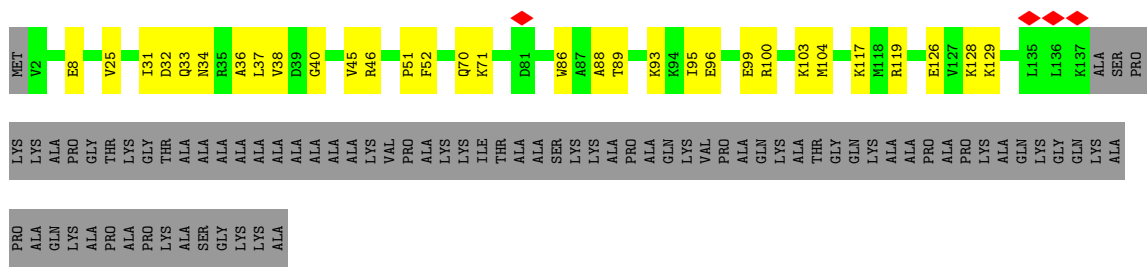
• Molecule 15: 60S ribosomal protein L11



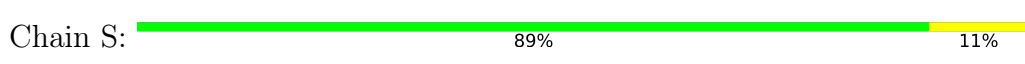
• Molecule 16: 60S ribosomal protein L13



• Molecule 17: 60S ribosomal protein L14



• Molecule 18: 60S ribosomal protein L15

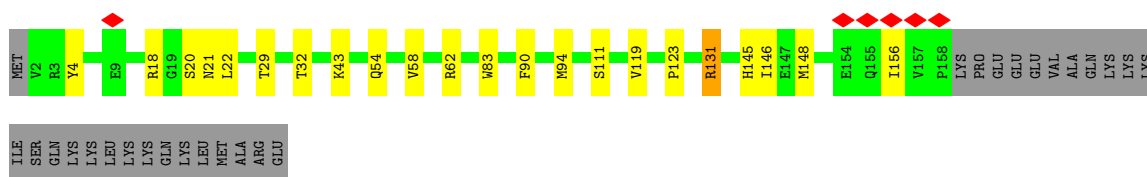




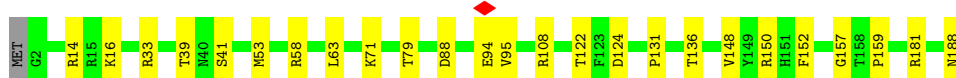
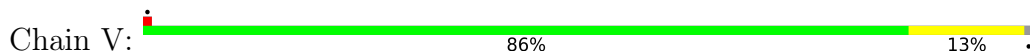
• Molecule 19: 60S ribosomal protein L13a



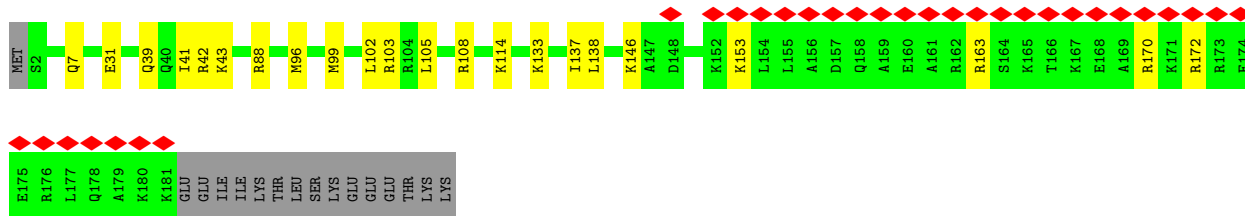
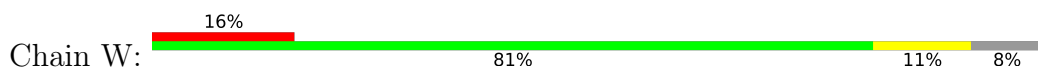
• Molecule 20: 60S ribosomal protein L17



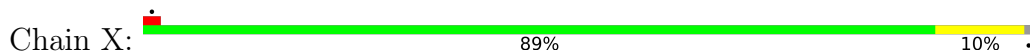
• Molecule 21: 60S ribosomal protein L18



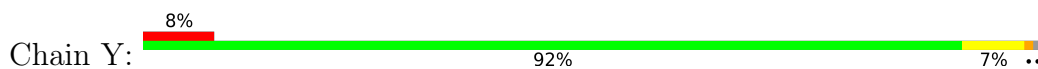
• Molecule 22: 60S ribosomal protein L19

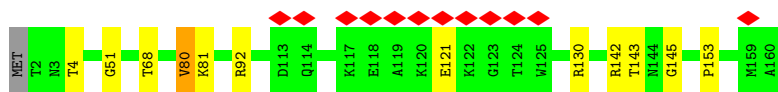


• Molecule 23: 60S ribosomal protein L18a

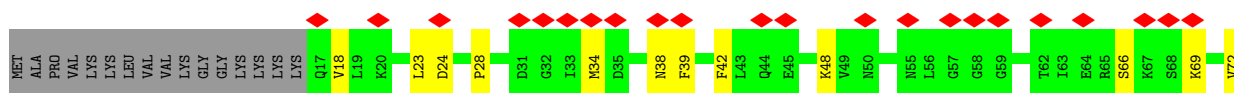


• Molecule 24: 60S ribosomal protein L21

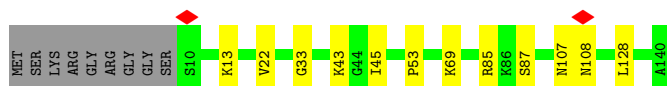
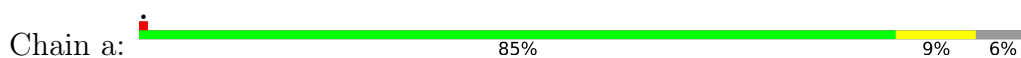




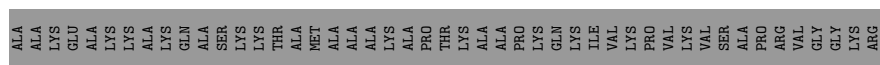
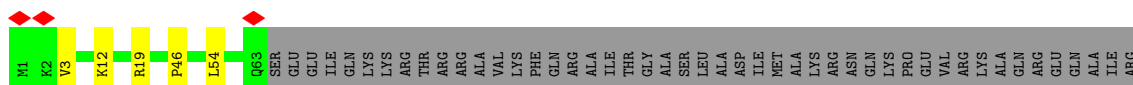
• Molecule 25: 60S ribosomal protein L22



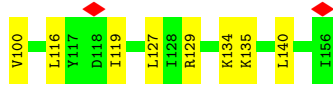
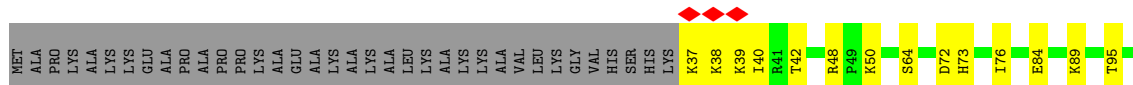
• Molecule 26: 60S ribosomal protein L23



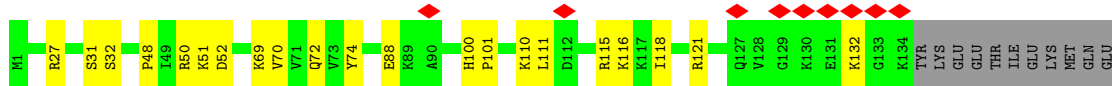
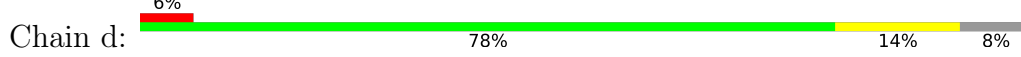
• Molecule 27: 60S ribosomal protein L24



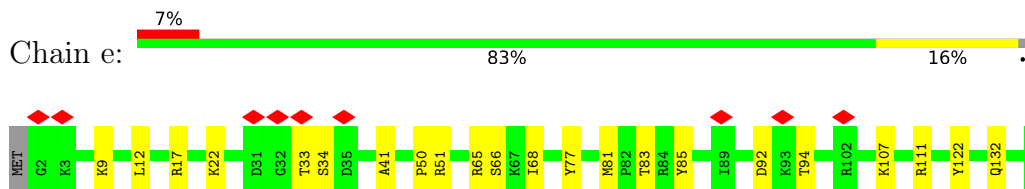
• Molecule 28: 60S ribosomal protein L23a



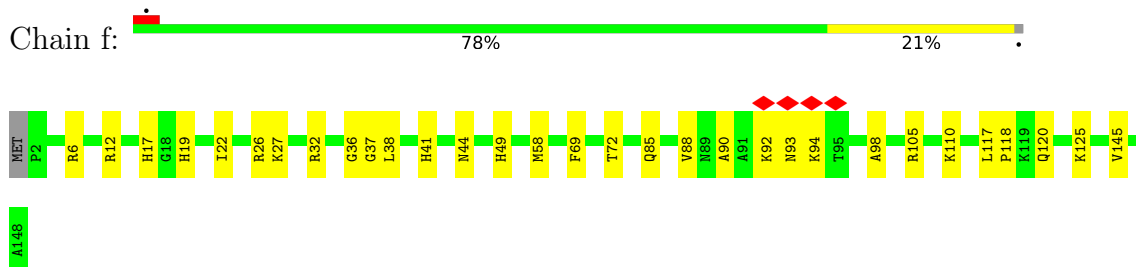
• Molecule 29: 60S ribosomal protein L26



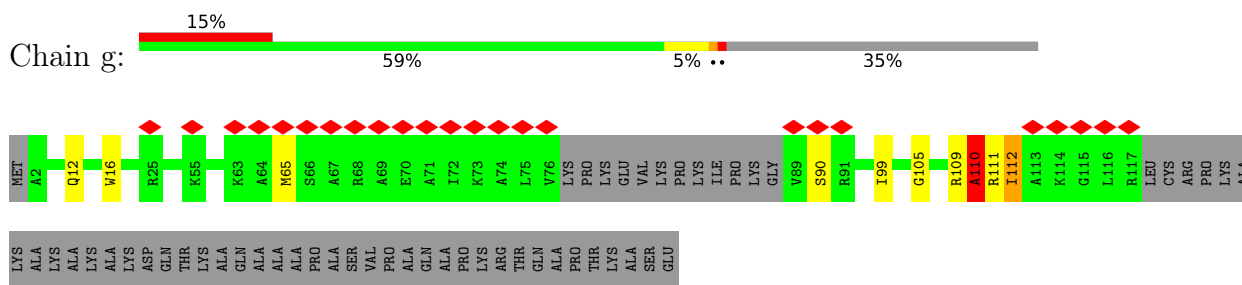
• Molecule 30: 60S ribosomal protein L27



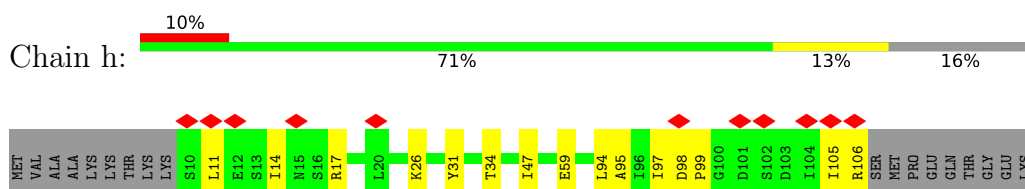
• Molecule 31: 60S ribosomal protein L27a



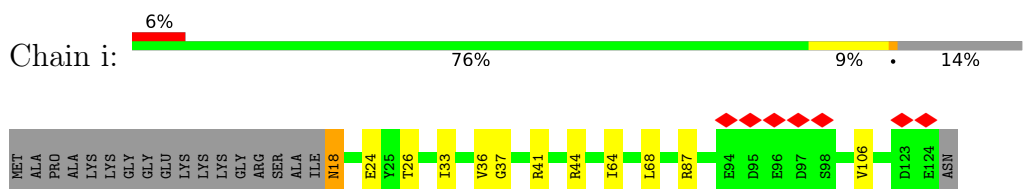
• Molecule 32: 60S ribosomal protein L29



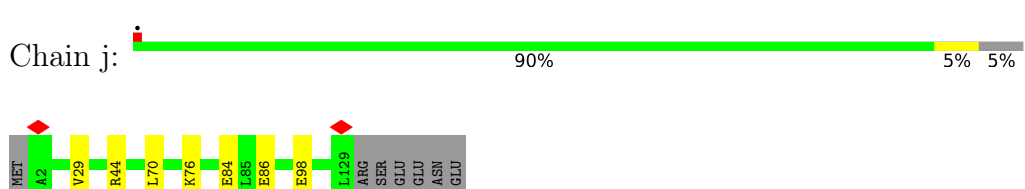
• Molecule 33: 60S ribosomal protein L30



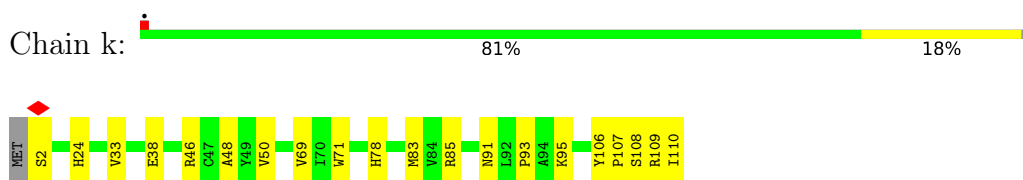
• Molecule 34: 60S ribosomal protein L31



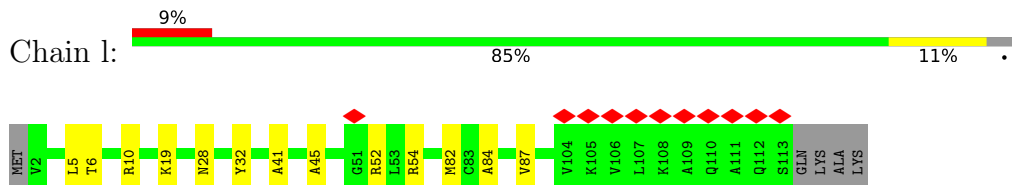
• Molecule 35: 60S ribosomal protein L32



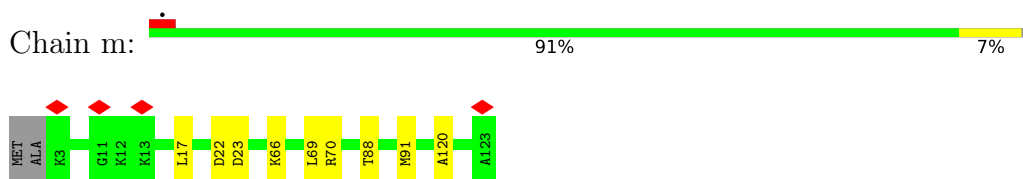
- Molecule 36: 60S ribosomal protein L35a



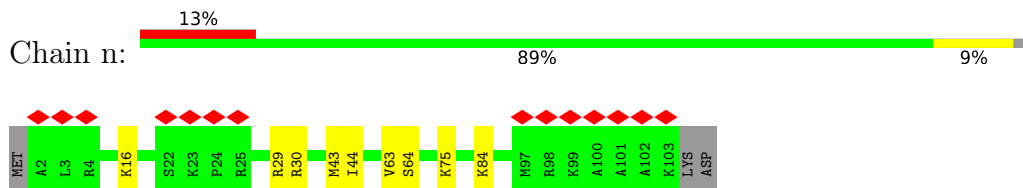
- Molecule 37: 60S ribosomal protein L34



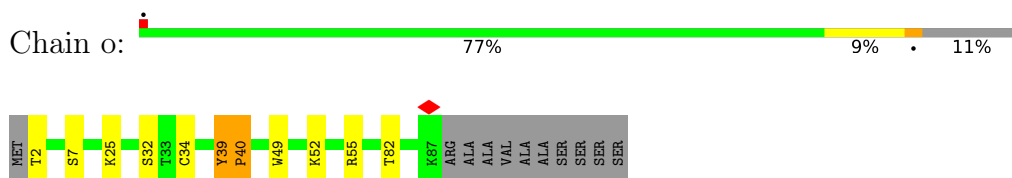
- Molecule 38: 60S ribosomal protein L35



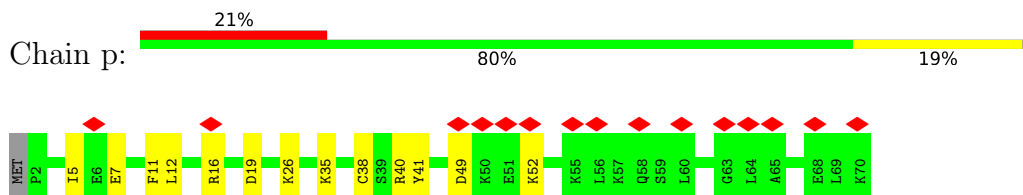
- Molecule 39: 60S ribosomal protein L36



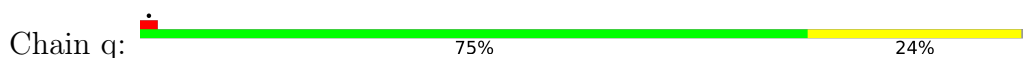
- Molecule 40: 60S ribosomal protein L37



- Molecule 41: 60S ribosomal protein L38

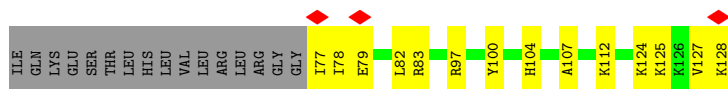
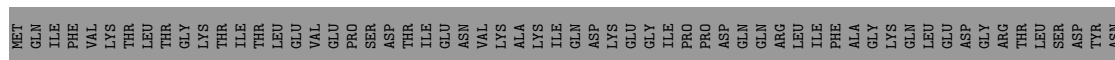


- Molecule 42: 60S ribosomal protein L39





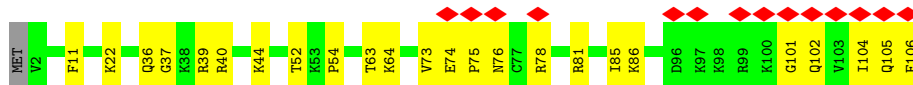
• Molecule 43: Ubiquitin-60S ribosomal protein L40



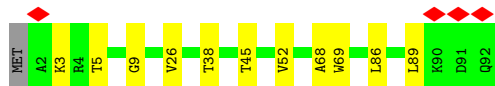
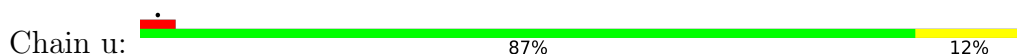
• Molecule 44: 60S ribosomal protein L41



• Molecule 45: 60S ribosomal protein L36a



• Molecule 46: 60S ribosomal protein L37a

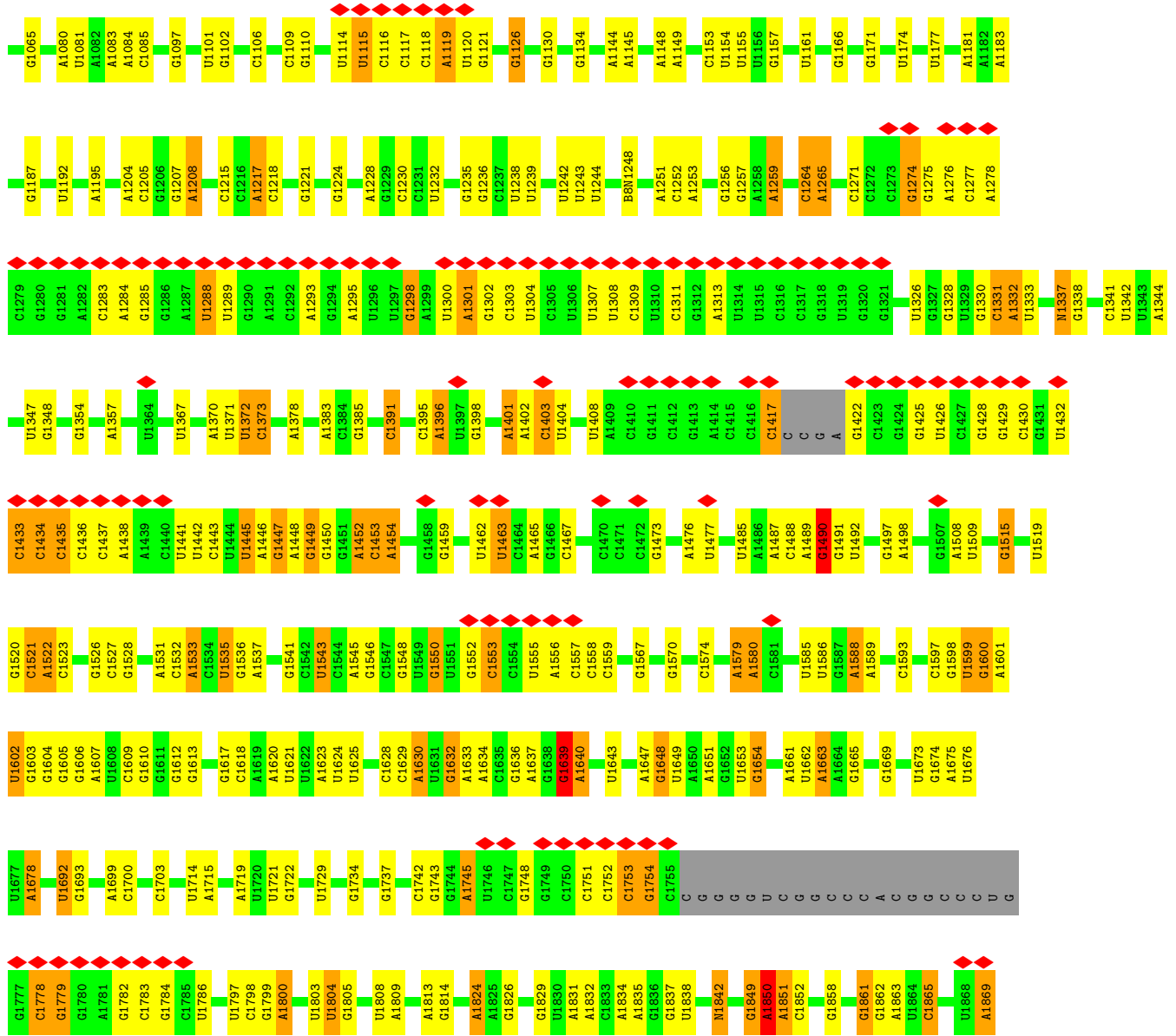


• Molecule 47: 60S ribosomal protein L28

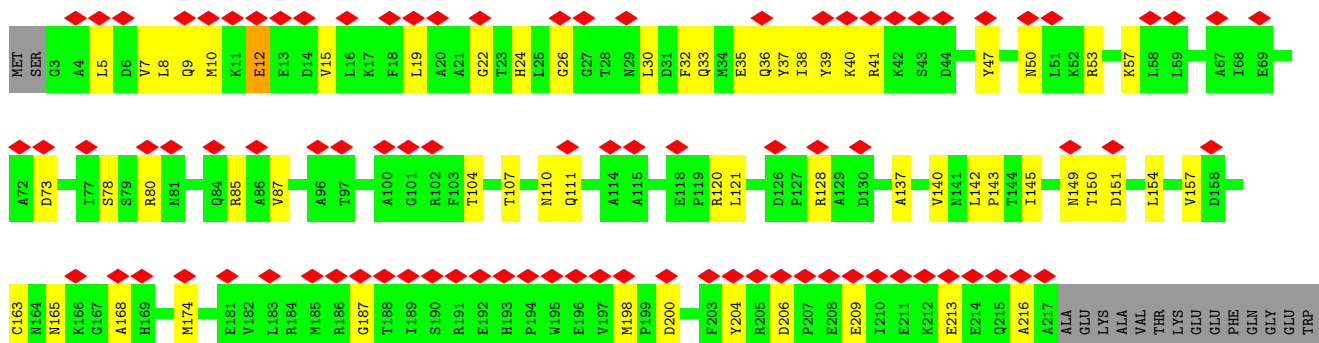


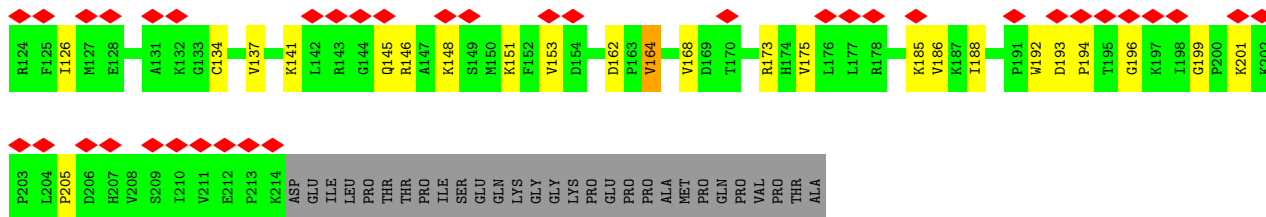
• Molecule 48: 18S ribosomal RNA



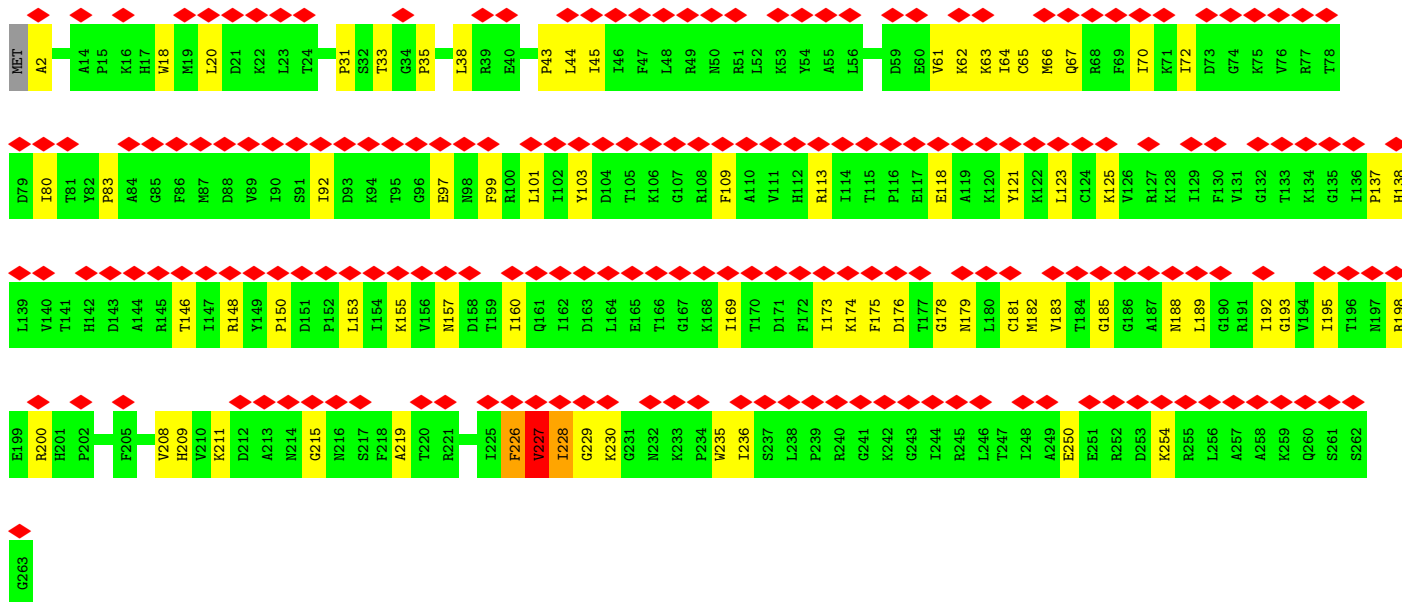


● Molecule 49: 40S ribosomal protein SA

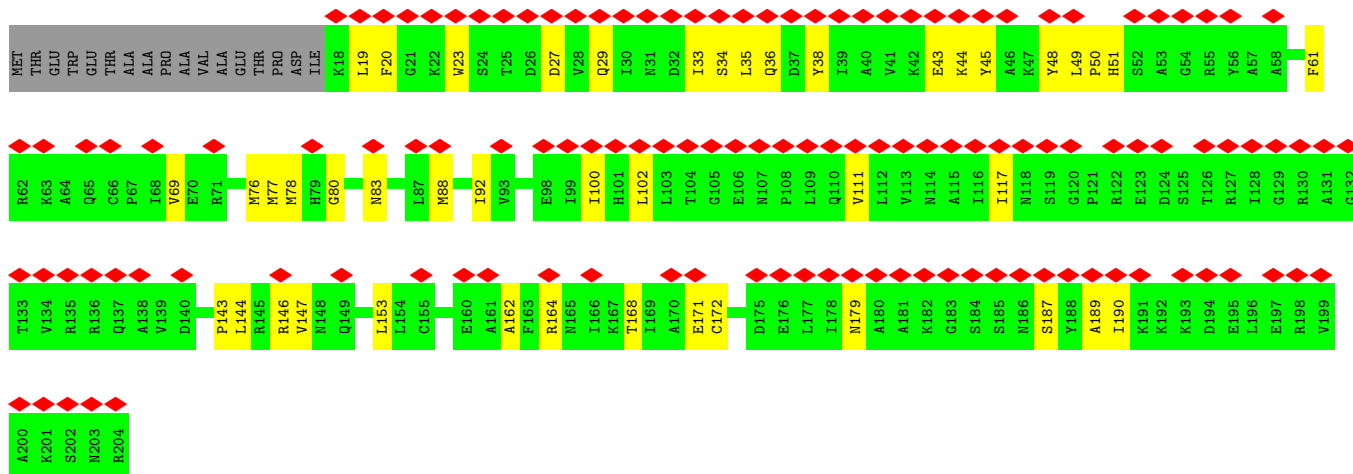




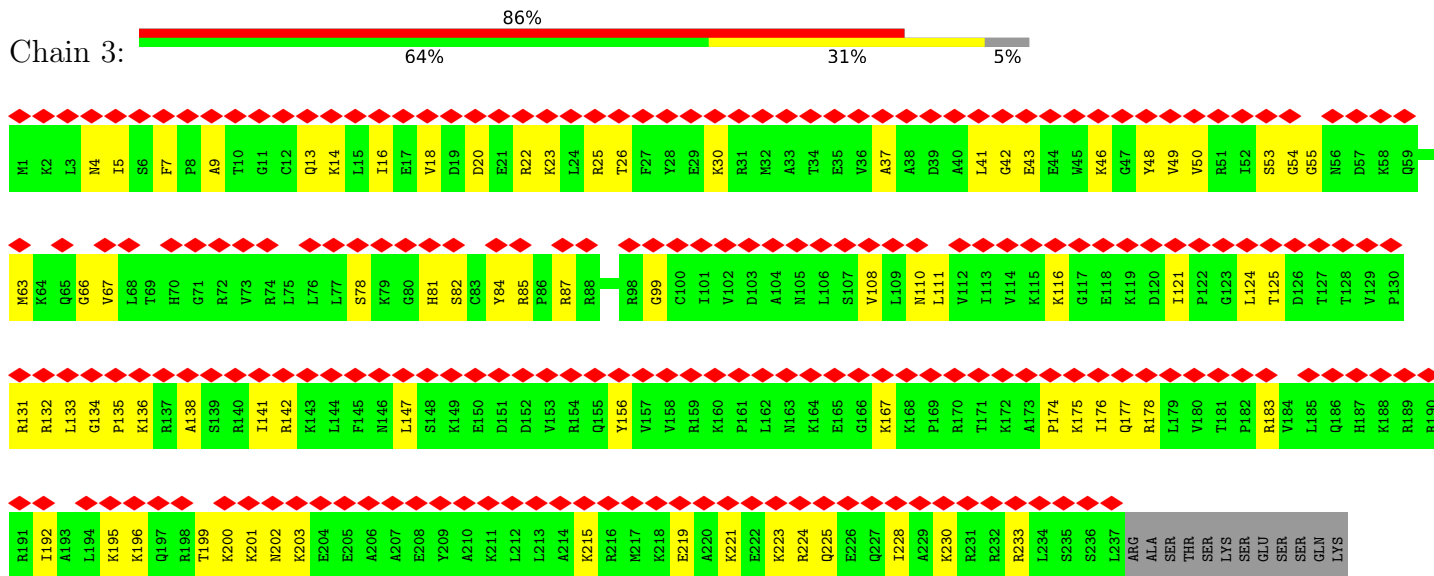
• Molecule 53: 40S ribosomal protein S4, X isoform



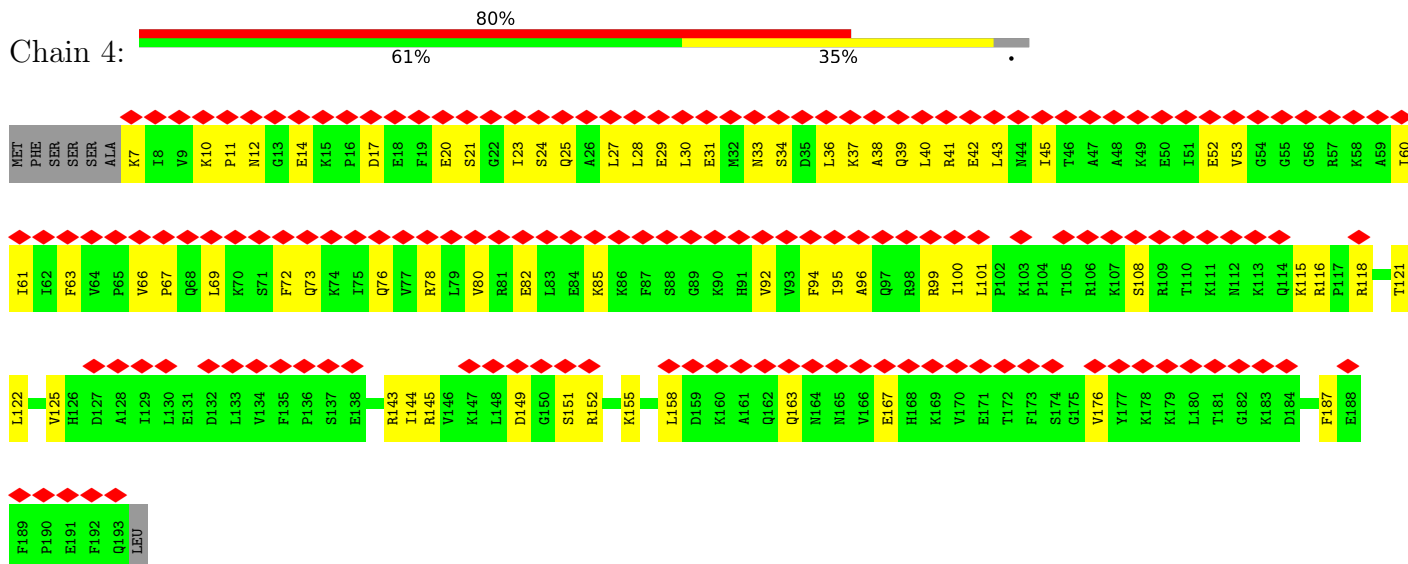
• Molecule 54: 40S ribosomal protein S5



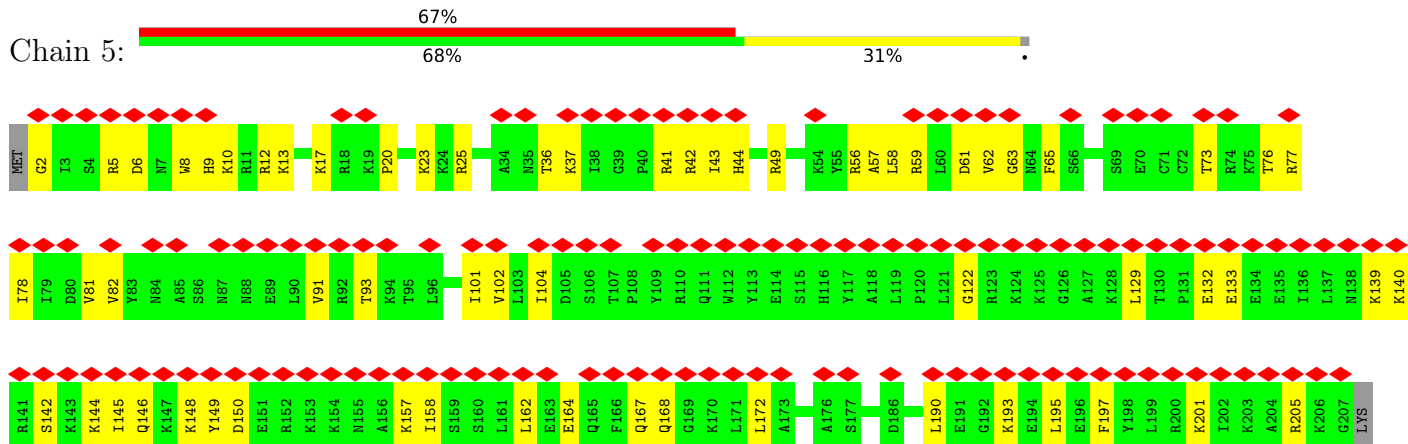
• Molecule 55: 40S ribosomal protein S6



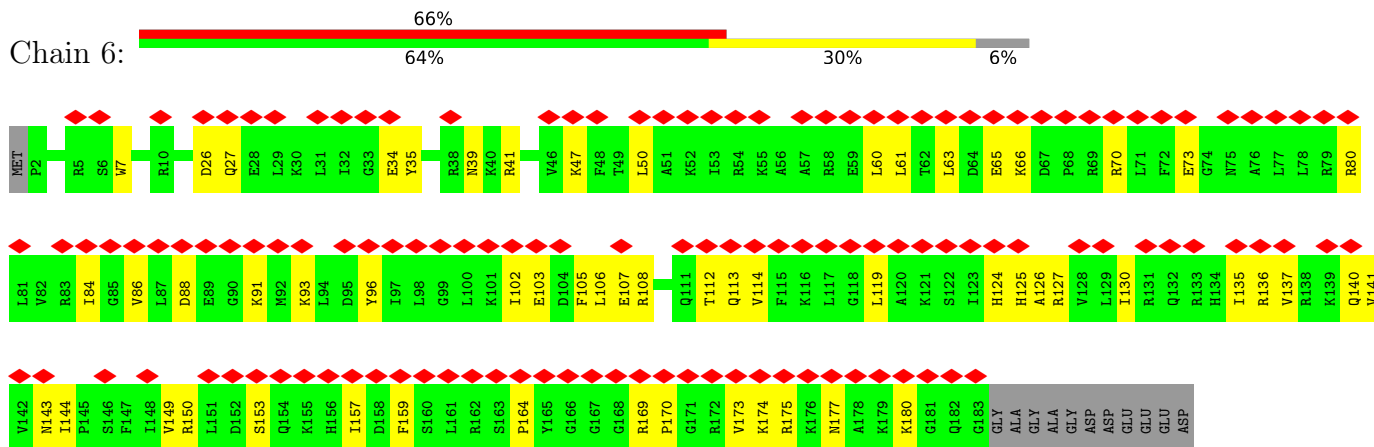
• Molecule 56: 40S ribosomal protein S7



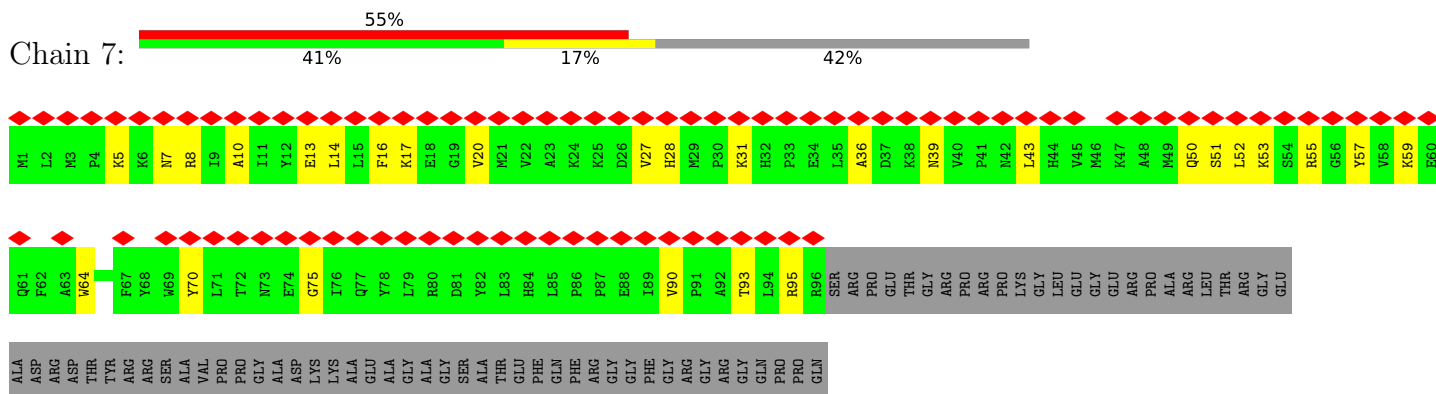
• Molecule 57: 40S ribosomal protein S8



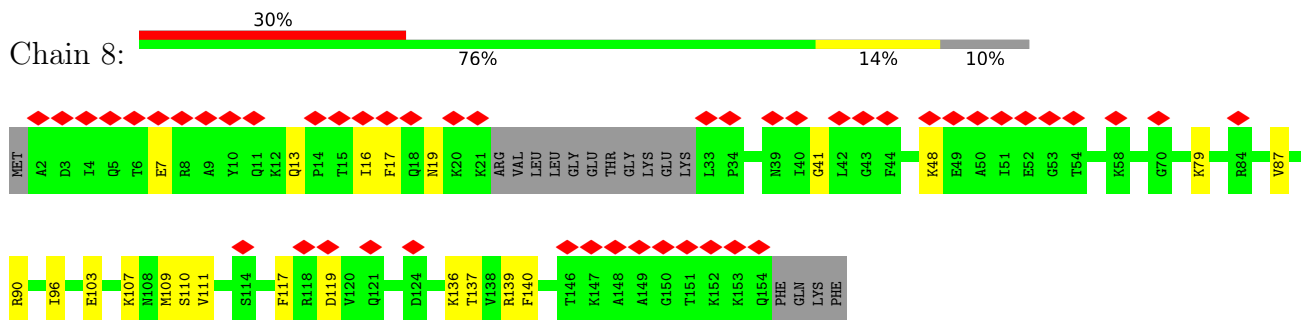
- Molecule 58: 40S ribosomal protein S9



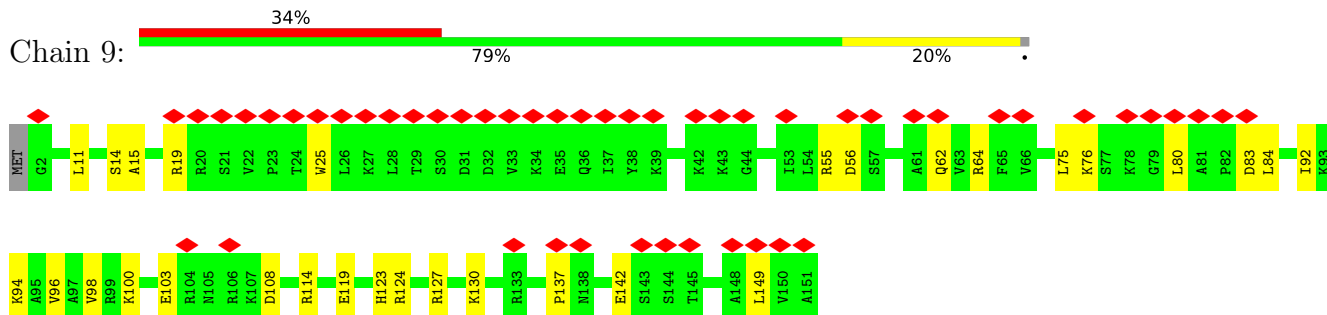
- Molecule 59: 40S ribosomal protein S10



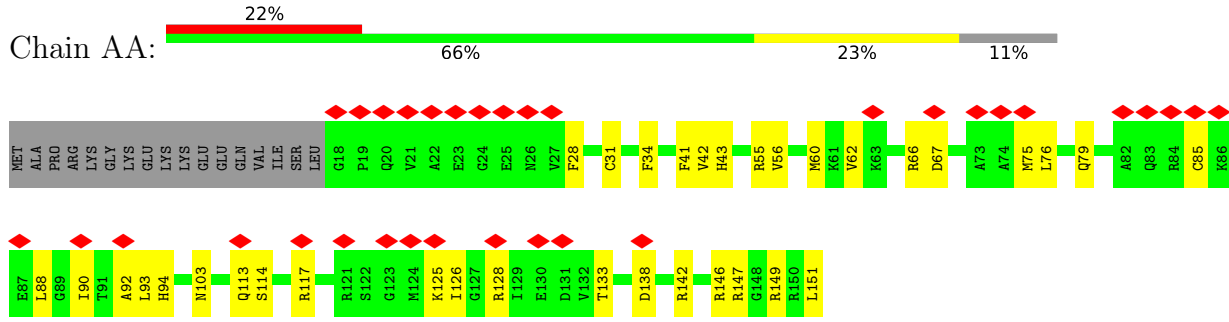
- Molecule 60: 40S ribosomal protein S11



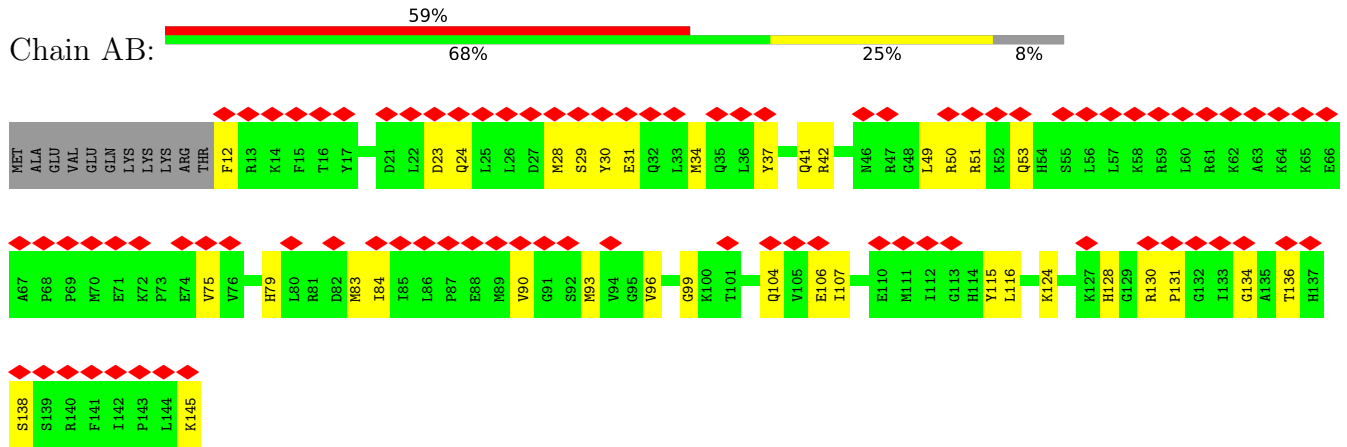
- Molecule 61: 40S ribosomal protein S13



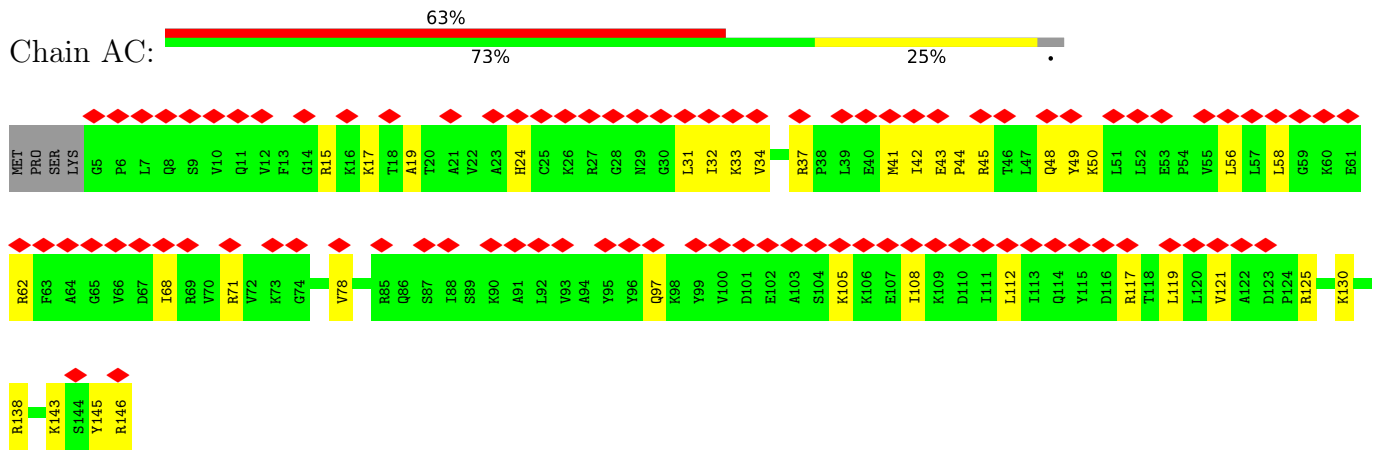
• Molecule 62: 40S ribosomal protein S14



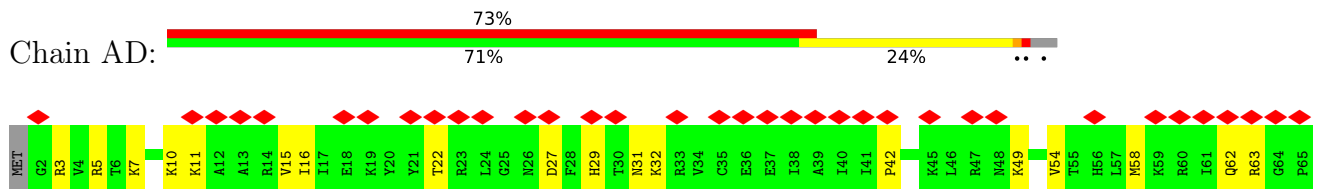
• Molecule 63: 40S ribosomal protein S15

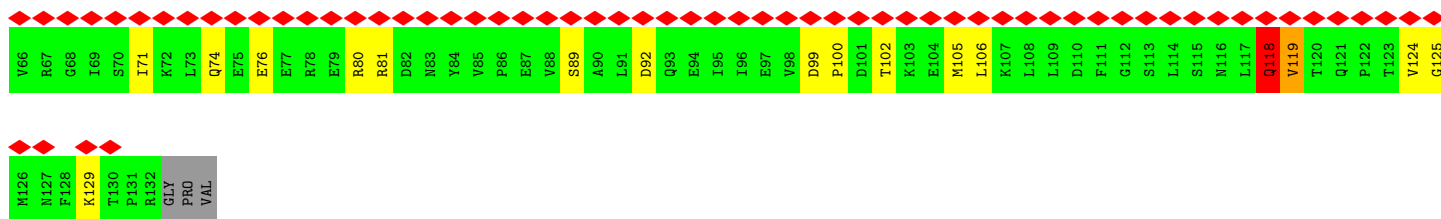


• Molecule 64: 40S ribosomal protein S16



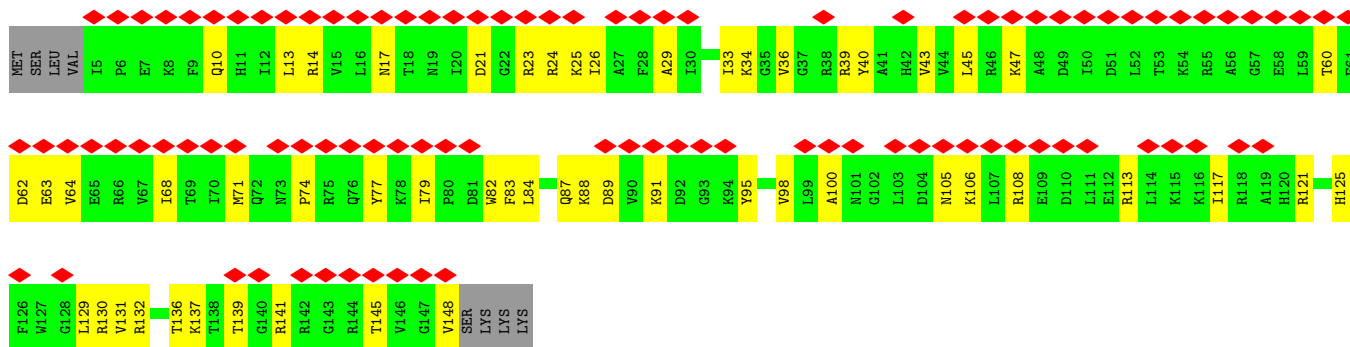
• Molecule 65: 40S ribosomal protein S17





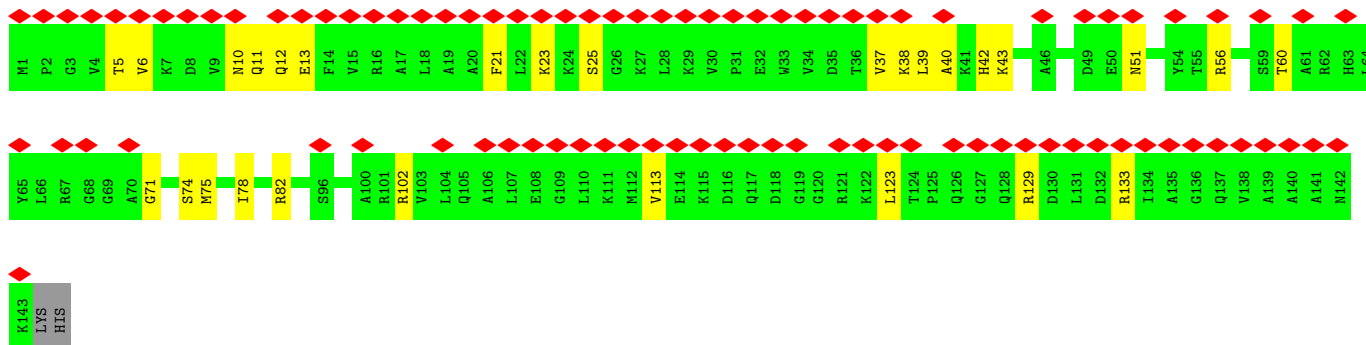
- Molecule 66: 40S ribosomal protein S18

Chain AE: 64% 59% 36% 5%



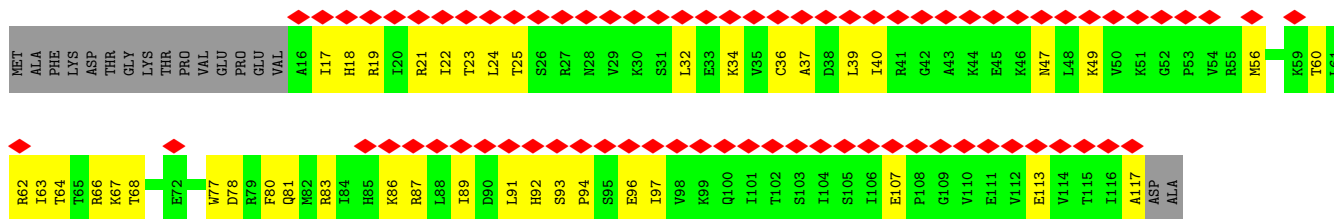
- Molecule 67: 40S ribosomal protein S19

Chain AF: 62% 79% 19%

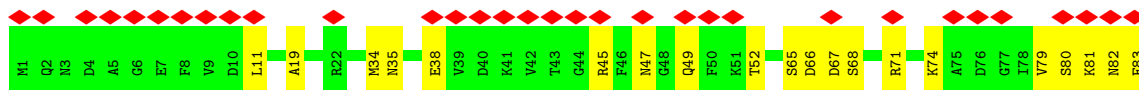
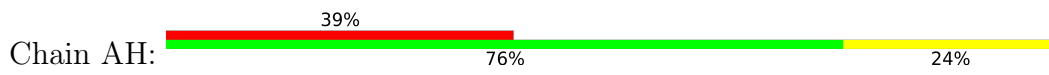


- Molecule 68: 40S ribosomal protein S20

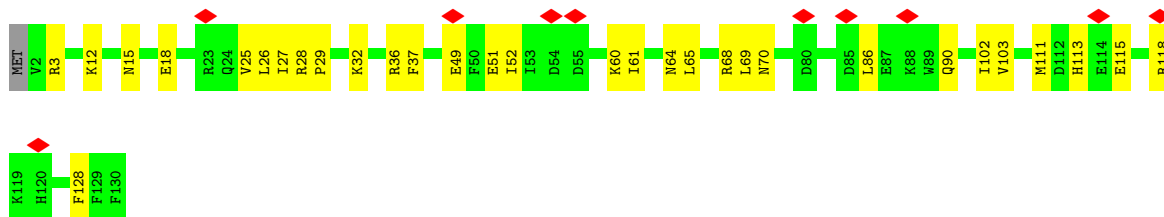
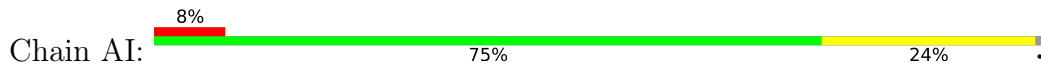
Chain AG: 64% 51% 34% 14%



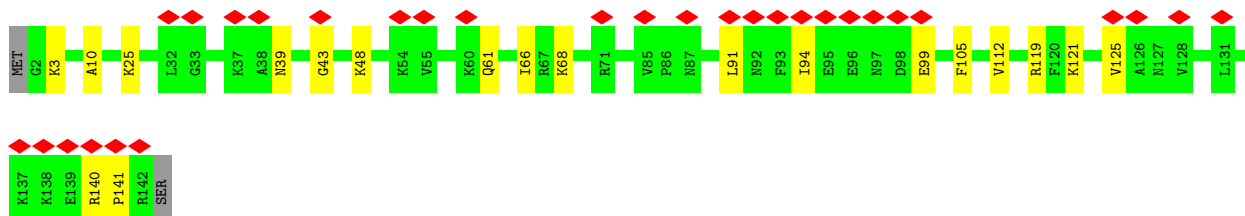
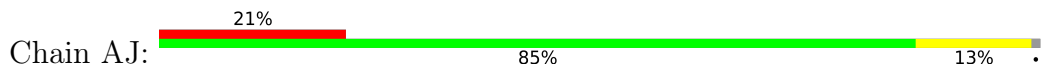
- Molecule 69: 40S ribosomal protein S21



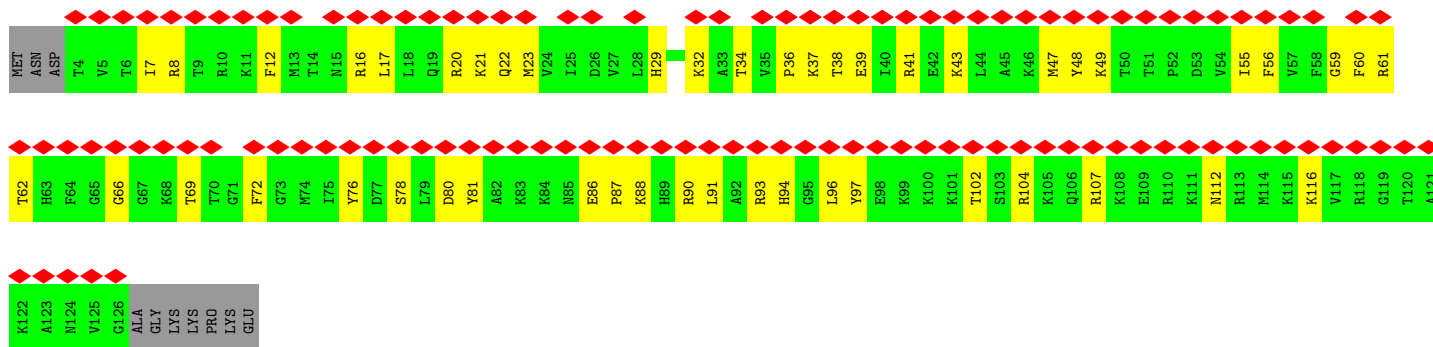
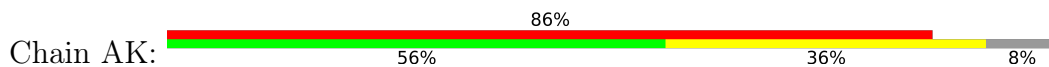
• Molecule 70: 40S ribosomal protein S15a



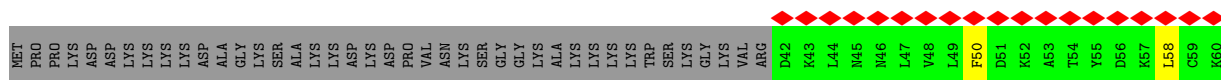
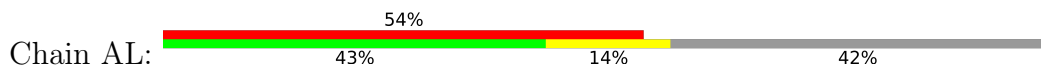
• Molecule 71: 40S ribosomal protein S23

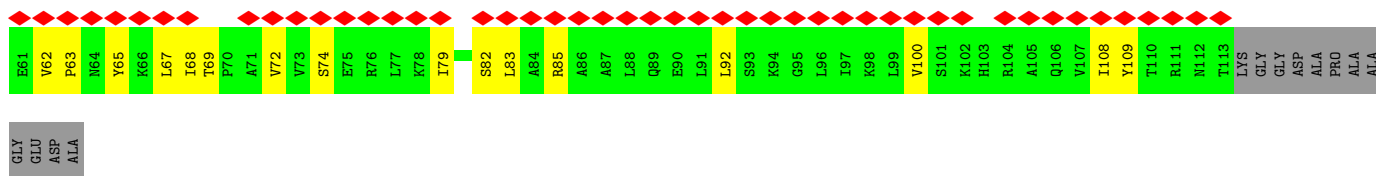


• Molecule 72: 40S ribosomal protein S24

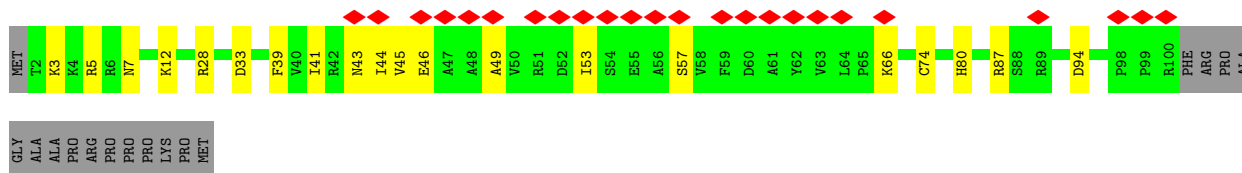


• Molecule 73: 40S ribosomal protein S25

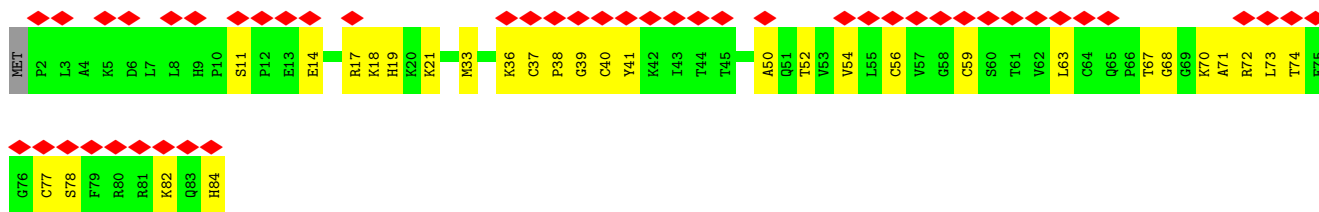




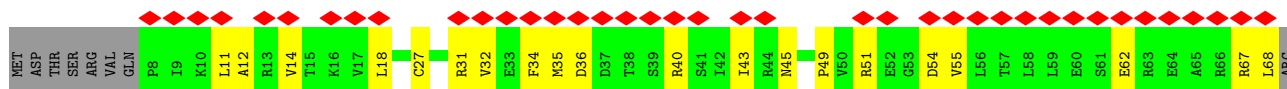
● Molecule 74: 40S ribosomal protein S26



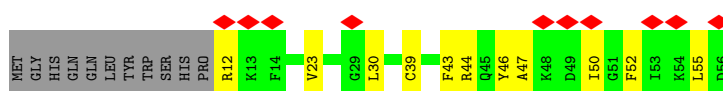
● Molecule 75: 40S ribosomal protein S27



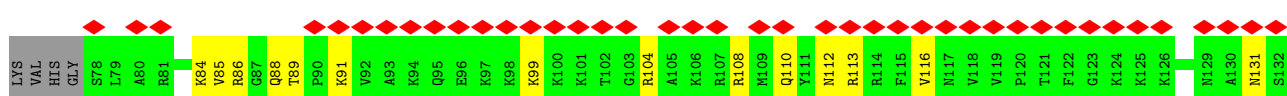
● Molecule 76: 40S ribosomal protein S28



● Molecule 77: 40S ribosomal protein S29



● Molecule 78: 40S ribosomal protein S30



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75250	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	0.142	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0183	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: UY1, 1MA, 56B, ZN, 2MG, M2G, B8N, 5MU, MA6, OMC, H2U, 4AC, A2M, PSU, 6MZ, G7M, OMG, 5MC, 1MG, GAL, MG, OMU, 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	0.14	0/319	0.15	0/492
2	B	0.19	0/1401	0.19	0/2175
2	C	0.16	0/1401	0.18	0/2175
3	D	0.31	1/81567 (0.0%)	0.26	6/127232 (0.0%)
4	E	0.30	0/2858	0.22	0/4455
5	F	0.30	0/3675	0.24	0/5725
6	G	0.31	0/1929	0.45	0/2586
7	H	0.29	0/3279	0.42	0/4388
8	I	0.30	0/2938	0.42	0/3946
9	J	0.25	0/2425	0.40	0/3248
10	K	0.24	0/1785	0.45	0/2394
11	L	0.31	0/1905	0.43	0/2539
12	M	0.24	0/1863	0.41	0/2510
13	N	0.26	0/1537	0.42	0/2066
14	O	0.26	0/1699	0.41	0/2270
15	P	0.20	0/1385	0.40	0/1852
16	Q	0.27	0/1713	0.46	1/2293 (0.0%)
17	R	0.26	0/1142	0.42	0/1527
18	S	0.32	0/1746	0.41	0/2338
19	T	0.31	0/1673	0.40	0/2238
20	U	0.29	0/1300	0.41	0/1746
21	V	0.31	0/1537	0.44	0/2052
22	W	0.25	0/1524	0.39	0/2013
23	X	0.30	0/1493	0.41	0/2003
24	Y	0.28	0/1326	0.38	0/1770
25	Z	0.20	0/835	0.39	0/1122
26	a	0.28	0/993	0.39	0/1332
27	b	0.26	0/541	0.41	0/720
28	c	0.24	0/998	0.36	0/1340
29	d	0.26	0/1132	0.40	0/1504
30	e	0.25	0/1130	0.37	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.30	0/1191	0.40	0/1591
32	g	0.24	0/844	0.52	1/1115 (0.1%)
33	h	0.25	0/765	0.33	0/1027
34	i	0.28	0/903	0.38	0/1216
35	j	0.30	0/1071	0.39	0/1429
36	k	0.32	0/895	0.50	0/1198
37	l	0.28	0/898	0.44	0/1197
38	m	0.24	0/1018	0.34	0/1344
39	n	0.21	0/843	0.37	0/1115
40	o	0.31	0/720	0.47	0/952
41	p	0.25	0/575	0.47	0/761
42	q	0.28	0/454	0.36	0/599
43	r	0.26	0/435	0.41	0/575
44	s	0.23	0/240	0.39	0/305
45	t	0.27	0/876	0.43	0/1156
46	u	0.28	0/718	0.37	0/953
47	v	0.30	0/1017	0.42	0/1364
48	w	0.21	0/37158	0.23	0/57908
49	x	0.18	0/1732	0.39	0/2355
50	y	0.17	0/1752	0.34	0/2345
51	z	0.18	0/1668	0.36	0/2254
52	0	0.15	0/1672	0.41	1/2250 (0.0%)
53	1	0.15	0/2112	0.37	0/2842
54	2	0.15	0/1485	0.38	0/1998
55	3	0.14	0/1940	0.36	0/2583
56	4	0.15	0/1533	0.39	0/2053
57	5	0.14	0/1703	0.40	0/2275
58	6	0.15	0/1531	0.40	0/2045
59	7	0.13	0/834	0.38	0/1125
60	8	0.18	0/1170	0.38	0/1568
61	9	0.17	0/1232	0.35	0/1656
62	AA	0.19	0/1015	0.44	0/1361
63	AB	0.16	0/1126	0.36	0/1505
64	AC	0.14	0/1146	0.38	0/1534
65	AD	0.18	0/1071	0.51	2/1438 (0.1%)
66	AE	0.17	0/1187	0.45	0/1593
67	AF	0.14	0/1130	0.36	0/1515
68	AG	0.15	0/809	0.40	0/1087
69	AH	0.18	0/643	0.40	0/860
70	AI	0.20	0/1051	0.38	0/1406
71	AJ	0.17	0/1116	0.35	0/1490
72	AK	0.14	0/1019	0.36	0/1355
73	AL	0.14	0/580	0.41	0/780

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	AM	0.20	0/805	0.42	0/1079
75	AN	0.19	0/657	0.42	0/883
76	AO	0.16	0/481	0.44	0/643
77	AP	0.18	0/375	0.40	0/492
78	AQ	0.13	0/443	0.41	0/582
79	AR	0.16	0/2493	0.45	0/3394
All	All	0.26	1/219181 (0.0%)	0.32	11/321709 (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	2
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
32	g	0	1
40	o	0	1
53	1	0	2
65	AD	0	1
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3785	A2M	O3'-P	5.11	1.61	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2101	C	OP1-P-OP2	-13.37	79.50	119.60
3	D	2100	A	OP2-P-O3'	-11.89	72.33	108.00
3	D	2101	C	O5'-P-OP1	-10.47	76.58	108.00
3	D	2100	A	OP1-P-O3'	9.64	136.93	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	0	164	VAL	N-CA-C	-7.71	106.39	113.71
3	D	2101	C	O5'-P-OP2	6.86	128.57	108.00
32	g	112	ILE	N-CA-C	-6.74	107.31	113.71
16	Q	134	PRO	CA-N-CD	-5.74	103.96	112.00
65	AD	118	GLN	CA-C-N	5.35	131.60	121.97
65	AD	118	GLN	C-N-CA	5.35	131.60	121.97
3	D	2100	A	O3'-P-O5'	-5.21	96.19	104.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	1	226	PHE	Peptide
53	1	227	VAL	Peptide
65	AD	118	GLN	Peptide
6	G	123	ARG	Peptide
6	G	239	ALA	Peptide
7	H	16	PHE	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
32	g	110	ALA	Peptide
40	o	39	TYR	Peptide

5.2 Too-close contacts [\(i\)](#)

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	288	0	145	0	0
2	B	1580	0	794	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1580	0	794	12	0
3	D	75336	0	38156	479	0
4	E	2558	0	1296	14	0
5	F	3315	0	1685	27	0
6	G	1891	0	1986	28	0
7	H	3211	0	3356	37	0
8	I	2884	0	3060	44	0
9	J	2379	0	2408	42	0
10	K	1751	0	1905	32	0
11	L	1870	0	1996	22	0
12	M	1832	0	1962	28	0
13	N	1518	0	1601	28	0
14	O	1660	0	1692	20	0
15	P	1362	0	1399	21	0
16	Q	1682	0	1792	31	0
17	R	1120	0	1187	24	0
18	S	1701	0	1749	21	0
19	T	1641	0	1788	15	0
20	U	1273	0	1304	18	0
21	V	1513	0	1628	16	0
22	W	1508	0	1664	19	0
23	X	1453	0	1490	13	0
24	Y	1298	0	1366	9	0
25	Z	821	0	839	15	0
26	a	979	0	1039	8	0
27	b	528	0	541	3	0
28	c	981	0	1062	18	0
29	d	1115	0	1205	17	0
30	e	1107	0	1182	15	0
31	f	1162	0	1213	24	0
32	g	832	0	883	7	0
33	h	755	0	791	8	0
34	i	888	0	930	10	0
35	j	1053	0	1147	7	0
36	k	876	0	912	13	0
37	l	888	0	981	12	0
38	m	1010	0	1143	8	0
39	n	832	0	917	8	0
40	o	705	0	737	8	0
41	p	569	0	637	9	0
42	q	444	0	483	9	0
43	r	429	0	466	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	s	239	0	289	0	0
45	t	862	0	930	17	0
46	u	708	0	756	9	0
47	v	1002	0	1068	16	0
48	w	34933	0	17693	406	0
49	x	1695	0	1690	45	0
50	y	1725	0	1800	40	0
51	z	1633	0	1716	21	0
52	0	1646	0	1734	33	0
53	1	2070	0	2166	54	0
54	2	1464	0	1505	39	0
55	3	1917	0	2078	63	0
56	4	1510	0	1606	49	0
57	5	1674	0	1739	52	0
58	6	1506	0	1618	47	0
59	7	810	0	836	22	0
60	8	1150	0	1199	16	0
61	9	1208	0	1294	22	0
62	AA	1002	0	1023	28	0
63	AB	1103	0	1156	29	0
64	AC	1128	0	1195	29	0
65	AD	1057	0	1110	30	0
66	AE	1169	0	1198	39	0
67	AF	1111	0	1144	22	0
68	AG	799	0	850	33	0
69	AH	636	0	637	14	0
70	AI	1034	0	1080	25	0
71	AJ	1098	0	1167	14	0
72	AK	1002	0	1067	37	0
73	AL	574	0	627	14	0
74	AM	792	0	845	16	0
75	AN	643	0	650	25	0
76	AO	479	0	507	16	0
77	AP	370	0	377	11	0
78	AQ	438	0	484	11	0
79	AR	2436	0	2393	116	0
80	B	11	0	10	0	0
80	C	11	0	10	0	0
81	2	1	0	0	0	0
81	AA	1	0	0	0	0
81	AG	1	0	0	0	0
81	AM	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	D	391	0	0	0	0
81	E	10	0	0	0	0
81	F	5	0	0	0	0
81	G	2	0	0	0	0
81	H	1	0	0	0	0
81	I	1	0	0	0	0
81	N	1	0	0	0	0
81	O	1	0	0	0	0
81	S	1	0	0	0	0
81	U	1	0	0	0	0
81	V	2	0	0	0	0
81	W	1	0	0	0	0
81	X	1	0	0	0	0
81	a	1	0	0	0	0
81	g	1	0	0	0	0
81	j	1	0	0	0	0
81	k	1	0	0	0	0
81	l	1	0	0	0	0
81	w	93	0	0	0	0
82	AA	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
82	w	1	0	0	0	0
All	All	209349	0	154558	2220	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 7.

All (2220) 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:1:C:H42	5:F:156:U:H3	1.15	0.95
34:i:18:ASN:HD22	34:i:18:ASN:N	1.66	0.93
3:D:1303:A:N6	3:D:2316:G:N7	2.16	0.92
3:D:4092:G:H21	3:D:4093:G:H1	1.20	0.89
17:R:96:GLU:HA	17:R:99:GLU:HG3	1.56	0.88
3:D:1656:U:OP2	31:f:26:ARG:NH2	2.10	0.85
3:D:4946:U:HO2'	36:k:2:SER:N	1.75	0.84
53:1:173:ILE:HD13	53:1:229:GLY:HA2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:82:A:N7	29:d:50:ARG:NH2	2.27	0.83
3:D:1701:A:H5'	3:D:2096:G:H22	1.43	0.82
48:w:1612:G:H1'	66:AE:87:GLN:HE21	1.45	0.81
3:D:4742:G:N2	3:D:4958:C:O2	2.13	0.81
48:w:566:U:H3	48:w:584:G:H1	1.29	0.81
3:D:2472:A:H1'	28:c:48:ARG:HB3	1.63	0.80
48:w:568:C:H42	48:w:582:C:H42	1.30	0.79
79:AR:26:GLN:NE2	79:AR:73:SER:O	2.15	0.79
22:W:39:GLN:OE1	22:W:42:ARG:NH2	2.15	0.79
48:w:560:A:H61	48:w:588:G:H1	1.30	0.79
6:G:117:GLU:HB2	6:G:162:ASN:HB2	1.64	0.78
56:4:12:ASN:ND2	56:4:14:GLU:O	2.16	0.78
3:D:505:G:H1	3:D:653:U:H3	1.32	0.78
72:AK:7:ILE:HD13	72:AK:43:LYS:HG2	1.66	0.78
6:G:31:ALA:HB2	6:G:123:ARG:HH21	1.48	0.77
6:G:30:ARG:O	6:G:163:ARG:NH2	2.18	0.77
70:AI:25:VAL:HG23	70:AI:65:LEU:HD21	1.66	0.77
8:I:110:ARG:O	8:I:113:ARG:NH1	2.16	0.76
20:U:94:MET:HE1	20:U:146:ILE:HB	1.65	0.76
31:f:17:HIS:O	31:f:19:HIS:N	2.18	0.76
62:AA:92:ALA:HB2	62:AA:125:LYS:HB2	1.68	0.75
79:AR:111:VAL:HG12	79:AR:122:SER:HA	1.68	0.75
52:0:101:GLN:HG3	52:0:126:ILE:HD11	1.67	0.75
3:D:3937:C:H1'	18:S:125:SER:HB2	1.69	0.75
79:AR:108:VAL:HA	79:AR:124:SER:HA	1.68	0.75
49:x:80:ARG:NH2	49:x:165:ASN:O	2.19	0.74
14:O:32:ARG:HG3	14:O:33:ILE:H	1.51	0.74
74:AM:43:ASN:HB2	74:AM:46:GLU:HG3	1.69	0.74
48:w:1488:C:O2'	48:w:1490:OMG:OP2	2.05	0.74
3:D:3751:G:H21	3:D:3775:A:H8	1.33	0.74
48:w:1396:A:O2'	48:w:1398:G:N7	2.21	0.74
76:AO:67:ARG:HG2	76:AO:68:LEU:HG	1.70	0.74
3:D:1518:A:OP1	31:f:27:LYS:NZ	2.20	0.74
64:AC:43:GLU:HG2	64:AC:44:PRO:HD3	1.69	0.74
3:D:4894:A:H3'	3:D:4895:C:H5'	1.70	0.73
3:D:4882:U:OP1	17:R:117:LYS:NZ	2.21	0.73
52:0:193:ASP:HB3	52:0:199:GLY:HA3	1.70	0.73
72:AK:91:LEU:HD22	72:AK:96:LEU:HD11	1.70	0.73
3:D:1391:A:OP1	21:V:181:ARG:NH1	2.21	0.73
3:D:4494:OMG:HM21	26:a:22:VAL:HG11	1.69	0.73
49:x:38:ILE:HD11	49:x:47:TYR:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:176:ASP:O	53:1:179:ASN:ND2	2.22	0.73
7:H:107:ALA:HB2	7:H:201:LEU:HD22	1.71	0.73
57:5:76:THR:HG22	57:5:77:ARG:H	1.54	0.72
69:AH:66:ASP:OD1	69:AH:67:ASP:N	2.21	0.72
48:w:1354:G:N2	48:w:1357:A:OP2	2.22	0.72
53:1:92:ILE:HD11	72:AK:17:LEU:HD11	1.70	0.72
76:AO:18:LEU:HD22	76:AO:67:ARG:HH12	1.54	0.72
3:D:2479:G:N2	3:D:2499:C:O2	2.16	0.72
48:w:152:U:H3	48:w:166:A2M:H62	1.37	0.72
2:B:18:G:H1	2:B:55:PSU:HN3	1.35	0.72
68:AG:78:ASP:OD2	77:AP:44:ARG:NH1	2.23	0.72
48:w:643:A:OP1	58:6:41:ARG:NH2	2.23	0.72
79:AR:244:ASN:HB3	79:AR:245:ARG:HE	1.54	0.71
45:t:36:GLN:OE1	45:t:40:ARG:NH1	2.23	0.71
48:w:1264:C:H4'	48:w:1265:A:H5'	1.73	0.71
56:4:145:ARG:NH1	70:AI:51:GLU:OE2	2.23	0.71
79:AR:44:LYS:HG3	79:AR:56:GLN:HG3	1.72	0.71
61:9:55:ARG:NE	61:9:56:ASP:OD1	2.16	0.71
79:AR:120:ILE:HB	79:AR:132:TRP:HB2	1.73	0.71
4:E:12:U:O3'	4:E:109:U:O2'	2.08	0.70
53:1:125:LYS:HB2	53:1:226:PHE:HD1	1.54	0.70
3:D:963:G:O6	3:D:2095:A:N6	2.24	0.70
63:AB:93:MET:SD	63:AB:104:GLN:NE2	2.65	0.70
3:D:3689:G:O2'	3:D:3818:UY1:OP2	2.08	0.70
79:AR:7:LEU:HD11	79:AR:308:ARG:HD3	1.73	0.70
14:O:79:SER:OG	14:O:147:HIS:ND1	2.23	0.70
48:w:1647:A:OP1	64:AC:138:ARG:NH1	2.23	0.70
56:4:36:LEU:HD21	56:4:40:LEU:HD13	1.74	0.70
8:I:298:ILE:HG22	21:V:131:PRO:HB3	1.72	0.70
48:w:1745:A:H1'	55:3:66:GLY:HA2	1.72	0.70
63:AB:130:ARG:NH1	66:AE:148:VAL:O	2.24	0.70
3:D:2591:A:N6	3:D:2754:G:O2'	2.25	0.69
75:AN:11:SER:OG	75:AN:14:GLU:OE1	2.09	0.69
48:w:345:U:O2	53:1:33:THR:OG1	2.10	0.69
58:6:88:ASP:OD1	58:6:91:LYS:NZ	2.19	0.69
48:w:525:A:OP2	78:AQ:99:LYS:NZ	2.25	0.69
48:w:571:U:O2'	72:AK:60:PHE:O	2.11	0.69
48:w:552:G:OP2	78:AQ:112:ASN:ND2	2.26	0.69
48:w:170:A:O2'	55:3:136:LYS:NZ	2.25	0.69
48:w:1729:U:H3	48:w:1805:G:H1	1.41	0.69
79:AR:93:THR:HG23	79:AR:94:THR:HG23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:836:G:N2	48:w:839:C:O5'	2.26	0.69
53:1:181:CYS:HA	53:1:227:VAL:HA	1.74	0.69
32:g:110:ALA:O	32:g:112:ILE:N	2.15	0.69
3:D:184:U:O2	3:D:254:G:N2	2.25	0.68
3:D:4940:C:OP2	10:K:219:LYS:NZ	2.26	0.68
68:AG:23:THR:HB	68:AG:113:GLU:HB2	1.75	0.68
2:C:44:A:H2'	2:C:45:G:H4'	1.75	0.68
3:D:1364:U:OP2	16:Q:36:ARG:NH2	2.26	0.68
3:D:4092:G:N3	3:D:4093:G:N2	2.37	0.68
46:u:5:THR:HG21	46:u:9:GLY:H	1.57	0.68
50:y:71:LEU:HA	50:y:74:LEU:HB2	1.75	0.68
3:D:5022:U:O2'	3:D:5024:C:OP2	2.12	0.68
48:w:1288:OMU:HN3	48:w:1311:C:H42	1.42	0.68
48:w:1192:U:OP1	71:AJ:119:ARG:NH1	2.25	0.68
3:D:4635:A:H2	3:D:4663:G:H21	1.41	0.68
7:H:222:VAL:O	7:H:343:ARG:NH1	2.26	0.68
48:w:581:U:H4'	72:AK:66:GLY:HA3	1.75	0.68
68:AG:47:ASN:HB3	68:AG:91:LEU:HD22	1.74	0.68
48:w:561:A:H5''	58:6:164:PRO:HG2	1.76	0.68
9:J:209:ARG:NH2	9:J:234:ASP:OD1	2.27	0.68
50:y:57:ILE:HG13	50:y:58:ALA:H	1.57	0.68
3:D:121:A:OP2	12:M:107:LYS:NZ	2.27	0.67
19:T:47:PHE:HZ	19:T:144:GLU:HG3	1.60	0.67
48:w:1230:C:OP1	66:AE:130:ARG:NH2	2.27	0.67
48:w:1332:A:O2'	52:0:145:GLN:OE1	2.11	0.67
79:AR:217:MET:SD	79:AR:219:TRP:NE1	2.67	0.67
3:D:2739:C:H4'	46:u:52:VAL:HG21	1.77	0.67
75:AN:36:LYS:HE2	75:AN:41:TYR:HA	1.76	0.67
9:J:155:THR:OG1	9:J:179:ARG:NH2	2.27	0.67
22:W:114:LYS:O	22:W:146:LYS:NZ	2.21	0.67
56:4:27:LEU:HA	56:4:30:LEU:HD23	1.75	0.67
3:D:4875:G:H2'	23:X:169:THR:HG22	1.77	0.67
3:D:1179:U:H3'	3:D:1180:C:H5''	1.77	0.67
3:D:4942:C:H5''	10:K:155:GLY:HA2	1.76	0.67
3:D:3641:U:OP2	3:D:3646:A:N6	2.27	0.67
8:I:46:LYS:HD2	8:I:113:ARG:HD3	1.76	0.67
48:w:830:A:OP2	48:w:846:G:N2	2.25	0.67
3:D:2469:C:H5	3:D:2471:G:H1	1.43	0.67
3:D:478:G:OP1	47:v:66:ARG:NH2	2.28	0.67
3:D:739:G:O2'	3:D:740:G:O5'	2.10	0.67
8:I:140:LYS:O	8:I:204:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:x:149:ASN:OD1	49:x:150:THR:N	2.24	0.67
58:6:84:ILE:HA	58:6:150:ARG:HA	1.77	0.66
48:w:925:G:H1	48:w:1017:U:H3	1.41	0.66
74:AM:5:ARG:HG3	74:AM:7:ASN:O	1.96	0.66
48:w:1161:U:O4	71:AJ:3:LYS:NZ	2.28	0.66
9:J:202:GLN:NE2	9:J:237:GLU:OE1	2.28	0.66
10:K:101:ASN:OD1	10:K:105:ARG:NH2	2.28	0.66
67:AF:113:VAL:HA	67:AF:123:LEU:HA	1.76	0.66
79:AR:302:TYR:HE2	79:AR:308:ARG:HD2	1.61	0.66
12:M:260:GLU:HG3	50:y:57:ILE:HD12	1.76	0.66
48:w:1543:U:OP1	64:AC:37:ARG:NH1	2.28	0.66
59:7:27:VAL:HB	59:7:43:LEU:HD12	1.75	0.66
48:w:1401:A:N6	48:w:1441:U:O2'	2.29	0.66
41:p:40:ARG:NH1	41:p:41:TYR:OH	2.28	0.66
42:q:30:LYS:HB2	42:q:33:ASN:HB2	1.76	0.66
16:Q:47:ALA:O	16:Q:49:ARG:N	2.28	0.66
48:w:570:C:H4'	72:AK:36:PRO:HG3	1.76	0.66
3:D:3681:G:OP2	6:G:128:ARG:NH1	2.29	0.66
54:2:35:LEU:HD12	54:2:117:ILE:HD13	1.76	0.66
48:w:1276:A:H4'	59:7:50:GLN:HE22	1.61	0.66
53:1:125:LYS:NZ	53:1:157:ASN:OD1	2.29	0.66
56:4:42:GLU:HG2	56:4:43:LEU:HD12	1.77	0.66
79:AR:82:SER:OG	79:AR:84:ASP:OD1	2.13	0.66
22:W:170:ARG:NH2	48:w:914:U:O4	2.28	0.65
65:AD:16:ILE:HD11	65:AD:54:VAL:HG21	1.77	0.65
3:D:1676:C:O2'	3:D:3914:U:N3	2.29	0.65
11:L:171:ASP:OD1	11:L:172:ASN:N	2.29	0.65
49:x:128:ARG:NH2	49:x:151:ASP:O	2.28	0.65
48:w:289:G:OP1	53:1:155:LYS:NZ	2.30	0.65
58:6:107:GLU:O	58:6:113:GLN:NE2	2.30	0.65
48:w:165:G:H1'	55:3:110:ASN:HD22	1.62	0.65
48:w:943:U:OP2	50:y:216:LYS:NZ	2.28	0.65
50:y:107:ARG:NH2	62:AA:133:THR:O	2.27	0.65
48:w:571:U:H5''	72:AK:37:LYS:HG3	1.77	0.65
52:0:47:GLU:HG2	52:0:85:GLU:HB2	1.78	0.65
3:D:2262:G:OP2	47:v:98:ARG:NH2	2.27	0.65
16:Q:64:VAL:HA	16:Q:67:HIS:CD2	2.31	0.65
48:w:65:C:N4	55:3:134:GLY:O	2.30	0.65
51:z:146:GLU:HB3	51:z:149:THR:HG22	1.78	0.65
79:AR:29:ASP:OD1	79:AR:47:ARG:NH1	2.29	0.65
3:D:1351:G:OP1	8:I:33:ARG:NH1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:u:89:LEU:O	50:y:219:LYS:NZ	2.29	0.65
3:D:2848:G:O2'	3:D:3838:U:O4	2.15	0.65
56:4:25:GLN:HA	56:4:28:LEU:HD22	1.79	0.65
3:D:492:U:O2	3:D:663:G:N2	2.30	0.64
6:G:27:ALA:O	6:G:128:ARG:NH2	2.30	0.64
6:G:101:VAL:HG22	6:G:165:VAL:HG22	1.78	0.64
61:9:75:LEU:HD22	61:9:80:LEU:HD11	1.78	0.64
3:D:977:C:OP2	10:K:59:ARG:NH1	2.30	0.64
3:D:2562:G:N2	3:D:2565:A:OP2	2.30	0.64
59:7:31:LYS:NZ	59:7:36:ALA:O	2.30	0.64
3:D:1570:G:N7	46:u:3:LYS:NZ	2.44	0.64
3:D:4775:C:N3	3:D:4859:C:N4	2.45	0.64
11:L:30:ILE:HD13	11:L:33:LEU:HD21	1.79	0.64
13:N:106:GLN:NE2	13:N:113:GLU:OE2	2.30	0.64
17:R:95:ILE:O	17:R:96:GLU:HG3	1.97	0.64
56:4:69:LEU:HD13	56:4:96:ALA:HB2	1.79	0.64
48:w:1373:C:OP1	65:AD:7:LYS:N	2.28	0.64
3:D:3651:A:OP2	6:G:200:ARG:NH1	2.30	0.64
3:D:491:G:H1	3:D:663:G:H1	1.46	0.64
3:D:3756:A:H61	3:D:3768:PSU:HN3	1.44	0.64
6:G:137:ILE:HD11	6:G:149:LYS:HB2	1.79	0.64
48:w:974:C:O2	62:AA:55:ARG:NH1	2.30	0.64
79:AR:143:GLN:HE21	79:AR:145:GLU:HG2	1.62	0.64
30:e:83:THR:HG22	30:e:85:TYR:H	1.62	0.64
62:AA:56:VAL:HA	62:AA:60:MET:HE2	1.78	0.64
3:D:4141:G:H5''	3:D:4142:C:H5'	1.79	0.63
54:2:100:ILE:HG21	54:2:111:VAL:HG11	1.80	0.63
3:D:4945:G:H1'	10:K:158:ARG:HH22	1.63	0.63
9:J:208:MET:HE1	9:J:236:MET:HE1	1.81	0.63
48:w:921:G:OP2	75:AN:21:LYS:NZ	2.30	0.63
62:AA:76:LEU:HA	62:AA:79:GLN:HG2	1.80	0.63
62:AA:117:ARG:HH12	76:AO:62:GLU:HB3	1.63	0.63
72:AK:12:PHE:HD1	72:AK:23:MET:HB3	1.63	0.63
11:L:222:LYS:HB3	11:L:231:GLY:HA2	1.80	0.63
47:v:26:SER:OG	47:v:28:GLU:OE1	2.12	0.63
48:w:179:C:H3'	48:w:180:G:H8	1.63	0.63
10:K:46:ARG:HG3	10:K:62:MET:HE1	1.79	0.63
43:r:127:VAL:HG13	43:r:128:LYS:HG2	1.80	0.63
48:w:380:G:OP1	57:5:56:ARG:NH2	2.31	0.63
3:D:3614:G:O2'	3:D:3615:G:OP1	2.17	0.63
18:S:120:TRP:HE1	18:S:123:GLU:HG3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:76:A:N7	16:Q:74:ARG:NH2	2.47	0.63
3:D:2658:G:N2	3:D:2676:A:OP2	2.23	0.63
48:w:818:A:OP1	58:6:80:ARG:NH2	2.32	0.63
6:G:28:ARG:HB2	6:G:123:ARG:HB3	1.81	0.63
48:w:372:U:OP1	60:8:136:LYS:NZ	2.29	0.63
3:D:496:G:H2'	3:D:497:G:C8	2.33	0.63
5:F:96:C:H5''	38:m:66:LYS:HD2	1.81	0.63
52:0:106:ARG:HG3	52:0:175:VAL:HG12	1.81	0.63
3:D:4893:A:OP1	19:T:188:LYS:NZ	2.28	0.62
49:x:5:LEU:O	49:x:9:GLN:NE2	2.24	0.62
55:3:136:LYS:HG2	55:3:176:ILE:HA	1.79	0.62
65:AD:118:GLN:O	65:AD:119:VAL:HG23	1.98	0.62
3:D:5016:A:H2	3:D:5033:G:H21	1.47	0.62
48:w:384:U:O4	57:5:5:ARG:NH2	2.27	0.62
49:x:37:TYR:OH	49:x:57:LYS:NZ	2.31	0.62
3:D:4424:A:OP2	43:r:97:ARG:NH2	2.31	0.62
48:w:1404:U:OP2	68:AG:21:ARG:NH1	2.32	0.62
61:9:123:HIS:HB3	61:9:127:ARG:HH21	1.64	0.62
3:D:490:C:O2	3:D:664:G:N2	2.30	0.62
12:M:150:LYS:HE3	12:M:177:MET:HE3	1.82	0.62
41:p:12:LEU:HB3	41:p:16:ARG:HH12	1.63	0.62
48:w:317:C:OP2	55:3:183:ARG:NH2	2.31	0.62
57:5:81:VAL:HG22	57:5:102:VAL:HG12	1.80	0.62
79:AR:256:ILE:HB	79:AR:270:LEU:HD12	1.82	0.62
19:T:37:ARG:HD2	19:T:108:ILE:HD11	1.82	0.62
2:B:14:A:H61	2:B:21:A:H2	1.47	0.62
53:1:123:LEU:HB3	53:1:226:PHE:HZ	1.64	0.62
56:4:144:ILE:HG23	70:AI:52:ILE:HB	1.81	0.62
68:AG:80:PHE:HB3	77:AP:52:PHE:HB3	1.82	0.62
70:AI:49:GLU:O	70:AI:64:ASN:ND2	2.33	0.62
48:w:196:C:N4	48:w:201:C:OP1	2.33	0.62
12:M:58:PRO:HD2	12:M:61:ILE:HD11	1.81	0.61
53:1:44:LEU:HD11	53:1:72:ILE:HD11	1.82	0.61
3:D:1100:U:H3	3:D:1194:G:H1	1.48	0.61
13:N:187:VAL:HG12	13:N:188:GLN:H	1.65	0.61
50:y:112:SER:O	50:y:115:LYS:NZ	2.33	0.61
8:I:204:ARG:NH2	8:I:205:ARG:O	2.33	0.61
48:w:1834:A:H2	48:w:1837:G:H1	1.47	0.61
55:3:121:ILE:N	55:3:125:THR:OG1	2.33	0.61
15:P:56:THR:HG23	15:P:63:ARG:HA	1.81	0.61
41:p:5:ILE:HD11	41:p:11:PHE:HD1	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:5:164:GLU:O	57:5:168:GLN:NE2	2.34	0.61
34:i:18:ASN:N	34:i:18:ASN:ND2	2.40	0.61
79:AR:289:LEU:HD22	79:AR:298:LEU:HD21	1.81	0.61
3:D:937:U:OP1	17:R:46:ARG:NH1	2.33	0.61
3:D:1591:U:OP2	3:D:2856:C:O2'	2.18	0.61
4:E:23:A:N3	4:E:118:C:O2'	2.32	0.61
48:w:799:OMU:OP2	56:4:108:SER:OG	2.19	0.61
51:z:113:GLN:HB3	51:z:122:THR:HG22	1.81	0.61
72:AK:86:GLU:OE2	72:AK:90:ARG:NH1	2.28	0.61
79:AR:217:MET:HE1	79:AR:219:TRP:CZ2	2.35	0.61
3:D:982:U:O2	10:K:70:LYS:NZ	2.33	0.61
48:w:594:A:H61	48:w:643:A:H5''	1.65	0.61
3:D:188:G:N2	3:D:190:G:O6	2.33	0.61
3:D:2899:C:OP1	22:W:108:ARG:NH2	2.33	0.61
68:AG:56:MET:HB2	68:AG:86:LYS:HB3	1.83	0.61
79:AR:168:CYS:HA	79:AR:174:VAL:HG12	1.82	0.61
3:D:2578:G:N7	30:e:17:ARG:NH1	2.49	0.61
8:I:156:ASP:OD1	8:I:255:SER:OG	2.19	0.61
30:e:107:LYS:HZ2	30:e:111:ARG:HH21	1.47	0.61
79:AR:217:MET:HG2	79:AR:226:HIS:HE1	1.66	0.61
32:g:110:ALA:C	32:g:112:ILE:H	2.08	0.60
56:4:145:ARG:HE	70:AI:49:GLU:CD	2.08	0.60
37:l:5:LEU:HD11	37:l:32:TYR:CE1	2.36	0.60
48:w:560:A:H2'	48:w:561:A:H8	1.66	0.60
52:0:39:VAL:HG22	52:0:48:ILE:HG22	1.83	0.60
5:F:55:U:H3	5:F:62:A:H2	1.47	0.60
15:P:15:LEU:HD12	15:P:134:LEU:HD13	1.83	0.60
19:T:61:ARG:HD2	19:T:66:PRO:HB3	1.83	0.60
22:W:172:ARG:NH2	48:w:909:G:OP2	2.33	0.60
48:w:346:C:OP1	53:1:38:LEU:N	2.35	0.60
48:w:1239:U:H5''	63:AB:124:LYS:HD2	1.84	0.60
49:x:85:ARG:NH1	65:AD:81:ARG:O	2.34	0.60
3:D:2601:A:N6	3:D:2744:A:OP2	2.32	0.60
67:AF:10:ASN:HB3	67:AF:13:GLU:HG2	1.84	0.60
3:D:181:C:N4	3:D:254:G:O6	2.34	0.60
3:D:5040:U:OP2	7:H:396:ARG:NH1	2.34	0.60
8:I:195:LYS:HB2	8:I:200:ARG:HD2	1.83	0.60
28:c:64:SER:HB2	38:m:69:LEU:HD13	1.83	0.60
47:v:97:ILE:HG21	47:v:107:ARG:HB3	1.84	0.60
79:AR:166:VAL:HG12	79:AR:176:VAL:HG12	1.83	0.60
51:z:166:ARG:HB2	51:z:248:TYR:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:0:196:GLY:O	52:0:201:LYS:NZ	2.32	0.60
79:AR:101:PHE:HE1	79:AR:136:GLY:HA2	1.66	0.60
3:D:150:U:H3	12:M:162:ASP:HB2	1.65	0.60
3:D:4092:G:H1'	3:D:4093:G:H21	1.67	0.60
53:1:125:LYS:HB2	53:1:226:PHE:CD1	2.36	0.60
70:AI:111:MET:HB2	70:AI:115:GLU:OE2	2.02	0.60
3:D:1214:C:N4	32:g:90:SER:OG	2.31	0.60
15:P:118:LYS:HD2	15:P:119:TYR:N	2.17	0.60
63:AB:75:VAL:HG12	63:AB:93:MET:HB3	1.82	0.60
79:AR:231:ASP:OD1	79:AR:232:GLY:N	2.35	0.60
3:D:4474:A:H5''	43:r:125:LYS:HD2	1.84	0.60
48:w:1835:A:N1	74:AM:80:HIS:ND1	2.47	0.60
57:5:41:ARG:HD3	57:5:43:ILE:HD12	1.83	0.60
72:AK:22:GLN:HG3	72:AK:72:PHE:HZ	1.66	0.60
79:AR:128:THR:HB	79:AR:130:LYS:HZ1	1.65	0.60
5:F:96:C:OP1	38:m:70:ARG:NH1	2.35	0.59
48:w:39:A:H62	48:w:515:G:H21	1.48	0.59
48:w:190:G:OP2	57:5:148:LYS:NZ	2.28	0.59
55:3:42:GLY:O	55:3:46:LYS:NZ	2.34	0.59
3:D:1447:C:H2'	3:D:1448:G:H8	1.66	0.59
3:D:3896:C:O2'	7:H:268:ARG:NH2	2.30	0.59
3:D:4734:A:H1'	3:D:4735:G:C8	2.37	0.59
13:N:91:LYS:HG2	13:N:145:ILE:HG12	1.84	0.59
21:V:157:GLY:O	21:V:188:ASN:ND2	2.35	0.59
50:y:175:GLU:OE2	50:y:187:LYS:NZ	2.29	0.59
3:D:2095:A:H4'	3:D:2096:G:N7	2.17	0.59
9:J:118:ILE:HD11	9:J:135:ILE:HD12	1.83	0.59
51:z:256:TRP:CD2	70:AI:68:ARG:HD3	2.37	0.59
56:4:158:LEU:HD21	56:4:187:PHE:HD2	1.66	0.59
3:D:184:U:O2'	3:D:189:G:O4'	2.17	0.59
3:D:1090:G:OP1	24:Y:142:ARG:NH1	2.34	0.59
48:w:884:C:O2	48:w:902:G:N2	2.19	0.59
48:w:499:G:H2'	48:w:501:C:O2	2.03	0.59
35:j:84:GLU:OE2	47:v:20:ARG:NH2	2.35	0.59
76:AO:40:ARG:HH12	76:AO:62:GLU:CD	2.10	0.59
48:w:163:U:OP2	55:3:87:ARG:NH2	2.34	0.59
54:2:168:THR:OG1	54:2:171:GLU:OE1	2.21	0.59
65:AD:99:ASP:OD1	65:AD:102:THR:N	2.22	0.59
79:AR:201:SER:OG	79:AR:203:ASP:OD1	2.18	0.59
3:D:2485:U:H2'	3:D:2486:G:H8	1.67	0.59
5:F:75:OMG:OP2	29:d:74:TYR:OH	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:6:169:ARG:NH2	58:6:175:ARG:HH12	2.01	0.59
3:D:1096:C:O2	3:D:1200:G:N2	2.36	0.59
3:D:2083:C:OP2	21:V:14:ARG:NH1	2.36	0.59
48:w:1550:G:H3'	48:w:1579:A:H61	1.68	0.59
79:AR:127:LYS:HD2	79:AR:149:GLU:HA	1.85	0.59
3:D:4966:A:H5'	7:H:128:LYS:HD3	1.84	0.59
8:I:293:LEU:HA	8:I:298:ILE:HD11	1.85	0.59
48:w:943:U:OP1	50:y:214:LYS:NZ	2.36	0.59
48:w:1858:G:OP2	62:AA:146:ARG:NH2	2.34	0.59
48:w:1236:G:O2'	63:AB:131:PRO:O	2.17	0.58
53:1:181:CYS:N	53:1:193:GLY:O	2.36	0.58
57:5:129:LEU:HG	57:5:132:GLU:HB2	1.85	0.58
34:i:24:GLU:OE1	34:i:87:ARG:NH2	2.36	0.58
48:w:1849:G:O2'	48:w:1850:MA6:H8	2.03	0.58
59:7:59:LYS:HG2	59:7:70:TYR:HB2	1.84	0.58
61:9:130:LYS:NZ	61:9:137:PRO:O	2.36	0.58
62:AA:117:ARG:HD2	74:AM:49:ALA:HB2	1.85	0.58
65:AD:124:VAL:HG13	65:AD:125:GLY:H	1.68	0.58
3:D:375:G:OP2	40:o:52:LYS:NZ	2.33	0.58
48:w:1673:U:H5''	64:AC:78:VAL:HG12	1.84	0.58
3:D:3607:U:OP1	22:W:88:ARG:NH1	2.36	0.58
48:w:96:C:O2	48:w:473:A:O2'	2.20	0.58
68:AG:60:THR:HG22	68:AG:83:ARG:HG2	1.84	0.58
13:N:21:LYS:HB2	13:N:24:THR:OG1	2.02	0.58
48:w:919:A:OP2	61:9:64:ARG:NH1	2.35	0.58
48:w:996:A:OP1	61:9:114:ARG:NH1	2.36	0.58
55:3:48:TYR:OH	55:3:116:LYS:NZ	2.32	0.58
79:AR:279:SER:HB2	79:AR:282:GLU:HB2	1.86	0.58
3:D:4717:A:OP2	7:H:30:LYS:NZ	2.32	0.58
5:F:14:U:H5''	20:U:123:PRO:HD3	1.85	0.58
16:Q:164:GLU:OE1	16:Q:164:GLU:N	2.37	0.58
57:5:6:ASP:OD1	57:5:9:HIS:ND1	2.25	0.58
58:6:130:ILE:HG23	58:6:135:ILE:HD11	1.85	0.58
48:w:198:U:O2'	48:w:202:G:O6	2.21	0.58
52:0:164:VAL:O	52:0:168:VAL:HG22	2.04	0.58
68:AG:62:ARG:HH11	68:AG:81:GLN:HE21	1.52	0.58
70:AI:102:ILE:HG13	70:AI:113:HIS:HB3	1.85	0.58
3:D:327:U:O2'	39:n:30:ARG:NH1	2.35	0.58
3:D:2334:C:OP2	8:I:195:LYS:NZ	2.35	0.58
48:w:928:G:H1	48:w:1013:U:H3	1.51	0.58
48:w:1252:C:N4	64:AC:146:ARG:OXT	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1734:G:O2'	48:w:1800:A:N6	2.36	0.58
3:D:1760:OMG:N2	3:D:1773:OMU:H1'	2.19	0.58
3:D:3720:G:OP1	39:n:75:LYS:NZ	2.37	0.58
14:O:35:ASP:OD1	14:O:88:ARG:HG2	2.04	0.58
26:a:45:ILE:HG21	26:a:53:PRO:HB3	1.84	0.58
48:w:65:C:H42	55:3:134:GLY:HA3	1.69	0.58
48:w:291:G:H1'	48:w:292:A:H2'	1.85	0.58
50:y:47:THR:OG1	50:y:65:ARG:NH1	2.37	0.58
79:AR:42:MET:HG3	79:AR:56:GLN:HB2	1.85	0.58
3:D:1175:A:H2	3:D:1185:G:H22	1.52	0.58
21:V:63:LEU:HB2	21:V:88:ASP:HA	1.85	0.58
28:c:37:LYS:HG3	28:c:38:LYS:HG2	1.86	0.58
51:z:104:ASP:HB3	51:z:130:ILE:HG13	1.86	0.58
55:3:26:THR:O	55:3:30:LYS:NZ	2.37	0.58
55:3:67:VAL:HG21	55:3:99:GLY:HA2	1.85	0.58
48:w:1826:G:OP1	63:AB:145:LYS:NZ	2.31	0.57
52:0:162:ASP:O	52:0:164:VAL:N	2.31	0.57
57:5:37:LYS:HE2	57:5:93:THR:HG22	1.86	0.57
3:D:739:G:O2'	3:D:740:G:H8	1.86	0.57
3:D:2623:A:OP1	25:Z:101:ARG:NH1	2.34	0.57
12:M:131:LYS:NZ	12:M:132:ARG:O	2.37	0.57
29:d:72:GLN:HE21	29:d:74:TYR:HD1	1.52	0.57
48:w:894:G:H3'	48:w:895:G:H5''	1.84	0.57
68:AG:24:LEU:HB2	68:AG:87:ARG:HB2	1.86	0.57
48:w:380:G:P	57:5:56:ARG:HH22	2.27	0.57
79:AR:284:PRO:O	79:AR:285:GLN:NE2	2.37	0.57
48:w:606:G:H8	78:AQ:131:ASN:HD21	1.52	0.57
48:w:1752:C:H2'	48:w:1753:C:C5	2.39	0.57
50:y:69:VAL:HG23	50:y:74:LEU:HD11	1.87	0.57
79:AR:8:ARG:HH12	79:AR:48:ASP:C	2.13	0.57
7:H:293:ILE:HG23	7:H:294:LYS:H	1.69	0.57
12:M:159:HIS:ND1	12:M:185:LYS:HA	2.19	0.57
48:w:371:A:OP2	57:5:10:LYS:HB2	2.04	0.57
48:w:851:C:H5''	48:w:852:G:H5'	1.85	0.57
54:2:38:TYR:OH	76:AO:54:ASP:OD1	2.22	0.57
58:6:61:LEU:HD23	58:6:70:ARG:HH12	1.70	0.57
9:J:236:MET:HA	9:J:239:MET:HB3	1.87	0.57
17:R:25:VAL:HG12	17:R:45:VAL:HG21	1.86	0.57
48:w:165:G:N2	48:w:165:G:OP2	2.36	0.57
54:2:80:GLY:HA2	54:2:83:ASN:HB2	1.85	0.57
79:AR:249:CYS:HA	79:AR:258:ILE:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:121:A:H62	3:D:152:U:H3	1.53	0.57
4:E:7:G:OP1	9:J:33:ARG:NE	2.34	0.57
11:L:105:VAL:HG13	11:L:136:VAL:HG12	1.85	0.57
49:x:206:ASP:N	49:x:209:GLU:OE2	2.36	0.57
55:3:230:LYS:HA	55:3:233:ARG:HG2	1.87	0.57
3:D:5066:U:OP1	20:U:43:LYS:NZ	2.30	0.57
48:w:604:A:N3	48:w:639:C:O2'	2.33	0.57
48:w:1473:G:N2	48:w:1476:A:OP2	2.32	0.57
48:w:1523:C:H4'	66:AE:145:THR:H	1.68	0.57
48:w:1536:G:H2'	48:w:1537:A:C8	2.39	0.57
3:D:2431:A:OP1	42:q:41:ARG:NH1	2.31	0.57
3:D:3906:A:H2'	8:I:69:THR:HG23	1.87	0.57
17:R:31:ILE:HD11	17:R:37:LEU:HB2	1.85	0.57
48:w:1344:A:N1	48:w:1385:G:O2'	2.33	0.57
48:w:1598:G:HO2'	48:w:1599:U:H6	1.52	0.57
79:AR:72:SER:OG	79:AR:74:ASP:O	2.23	0.57
79:AR:91:ASP:OD2	79:AR:94:THR:OG1	2.18	0.57
10:K:101:ASN:OD1	10:K:102:GLY:N	2.38	0.56
48:w:1628:C:OP1	67:AF:38:LYS:NZ	2.38	0.56
48:w:1752:C:H2'	48:w:1753:C:H5	1.70	0.56
3:D:173:C:OP1	16:Q:130:LYS:NZ	2.37	0.56
3:D:1077:C:H4'	3:D:1215:C:N4	2.19	0.56
3:D:3811:G:O2'	3:D:3814:U:OP2	2.23	0.56
3:D:4582:C:OP2	7:H:28:LYS:NZ	2.36	0.56
48:w:114:G:O2'	48:w:382:C:O2'	2.23	0.56
48:w:498:C:N4	48:w:504:G:O6	2.38	0.56
48:w:1110:G:O2'	65:AD:124:VAL:O	2.20	0.56
48:w:1541:G:OP1	67:AF:56:ARG:NH1	2.37	0.56
48:w:1609:C:H3'	66:AE:132:ARG:HH21	1.70	0.56
50:y:103:MET:HB3	50:y:215:VAL:HG22	1.87	0.56
3:D:418:A:N6	5:F:16:G:H1'	2.20	0.56
3:D:3669:G:H21	3:D:3672:G:N2	2.03	0.56
3:D:4084:G:O6	6:G:72:ARG:NH2	2.34	0.56
17:R:126:GLU:HG2	17:R:129:LYS:HE3	1.86	0.56
20:U:21:ASN:HB3	20:U:145:HIS:HE1	1.70	0.56
26:a:107:ASN:OD1	26:a:108:ASN:N	2.37	0.56
29:d:50:ARG:HD2	29:d:115:ARG:HH11	1.70	0.56
33:h:105:ILE:HG13	33:h:106:ARG:HD3	1.87	0.56
48:w:527:C:H5'	58:6:125:HIS:HB2	1.86	0.56
48:w:1120:U:H5'	75:AN:72:ARG:NH2	2.21	0.56
59:7:5:LYS:HZ3	59:7:8:ARG:HG2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AN:54:VAL:HG23	75:AN:63:LEU:HB2	1.87	0.56
79:AR:48:ASP:OD2	79:AR:51:ASN:ND2	2.39	0.56
3:D:967:C:O2'	3:D:969:C:OP2	2.24	0.56
3:D:1362:G:OP1	16:Q:39:ARG:NH2	2.39	0.56
8:I:218:ILE:HA	8:I:229:LEU:HD22	1.86	0.56
30:e:92:ASP:OD1	30:e:94:THR:OG1	2.22	0.56
58:6:113:GLN:HG3	58:6:149:VAL:HG21	1.87	0.56
3:D:175:C:H2'	3:D:176:G:H8	1.70	0.56
3:D:4884:G:N7	10:K:272:ARG:NH2	2.54	0.56
12:M:61:ILE:HA	12:M:64:GLN:HG2	1.87	0.56
20:U:32:THR:HA	20:U:58:VAL:HG21	1.87	0.56
23:X:127:MET:HB3	24:Y:153:PRO:HG2	1.88	0.56
79:AR:45:LEU:HD11	79:AR:52:TYR:CE2	2.40	0.56
3:D:2487:G:H22	3:D:2492:C:H1'	1.71	0.56
3:D:4910:G:H22	19:T:107:GLY:HA3	1.69	0.56
7:H:231:VAL:HG11	7:H:251:VAL:HG23	1.88	0.56
15:P:120:ASP:HB3	15:P:123:ILE:HG12	1.88	0.56
48:w:811:A:O2'	48:w:812:A:OP1	2.22	0.56
49:x:85:ARG:NH2	49:x:200:ASP:O	2.39	0.56
2:C:46:G7M:O2'	2:C:47:H2U:O5'	2.19	0.56
3:D:2475:G:O6	28:c:48:ARG:NH1	2.38	0.56
3:D:2696:A:OP1	41:p:26:LYS:NZ	2.31	0.56
8:I:76:ILE:HD12	8:I:77:PRO:HD2	1.86	0.56
13:N:106:GLN:HE21	13:N:111:LEU:HD23	1.70	0.56
29:d:52:ASP:OD2	29:d:110:LYS:HG2	2.06	0.56
65:AD:29:HIS:HA	65:AD:32:LYS:HE2	1.88	0.56
3:D:4093:G:H3'	3:D:4094:G:H8	1.71	0.56
22:W:105:LEU:HD23	22:W:138:LEU:HD23	1.88	0.56
31:f:117:LEU:HD12	31:f:118:PRO:HD2	1.88	0.56
48:w:169:U:H4'	55:3:135:PRO:HA	1.87	0.56
48:w:1003:U:H5''	50:y:165:ARG:NH2	2.21	0.56
48:w:1016:U:H5''	61:9:14:SER:HB3	1.87	0.56
62:AA:42:VAL:HG23	62:AA:43:HIS:H	1.70	0.56
66:AE:33:ILE:HD13	66:AE:71:MET:HE1	1.88	0.56
3:D:3641:U:H5	3:D:3646:A:N7	2.04	0.56
49:x:163:CYS:HB3	49:x:174:MET:HE3	1.88	0.56
52:0:61:GLU:H	52:0:64:ARG:HG2	1.71	0.56
60:8:111:VAL:HG12	60:8:140:PHE:HB2	1.88	0.56
65:AD:22:THR:O	79:AR:212:LYS:NZ	2.37	0.56
73:AL:50:PHE:CE2	73:AL:83:LEU:HD21	2.41	0.56
14:O:19:LYS:HA	14:O:23:CYS:SG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:0:58:VAL:HG13	52:0:59:LEU:HD12	1.88	0.56
56:4:100:ILE:HG12	56:4:125:VAL:HG21	1.88	0.56
3:D:2579:G:N2	3:D:2582:A:OP2	2.34	0.55
18:S:68:ARG:NH1	18:S:124:ASP:O	2.34	0.55
48:w:875:A:H61	48:w:911:C:H42	1.52	0.55
52:0:99:ILE:HG23	52:0:173:ARG:HH21	1.71	0.55
54:2:33:ILE:HD11	76:AO:11:LEU:HD13	1.87	0.55
65:AD:71:ILE:O	65:AD:74:GLN:HG3	2.06	0.55
79:AR:62:HIS:HE1	79:AR:86:THR:OG1	1.89	0.55
3:D:114:G:N2	3:D:158:A:H61	2.04	0.55
3:D:690:C:OP2	10:K:111:LYS:NZ	2.39	0.55
3:D:2474:G:N2	3:D:2502:G:O2'	2.39	0.55
9:J:107:ARG:NH2	9:J:116:ASP:OD1	2.39	0.55
48:w:974:C:O2'	62:AA:43:HIS:ND1	2.33	0.55
3:D:369:G:N2	3:D:372:A:OP2	2.37	0.55
31:f:37:GLY:H	31:f:41:HIS:HB2	1.71	0.55
48:w:1417:C:N4	48:w:1422:G:OP2	2.38	0.55
59:7:14:LEU:HD12	59:7:17:LYS:HE2	1.89	0.55
70:AI:28:ARG:HB3	70:AI:29:PRO:HD3	1.88	0.55
72:AK:20:ARG:NH1	72:AK:76:TYR:OH	2.36	0.55
3:D:1174:G:H1	3:D:1186:U:H3	1.54	0.55
3:D:4623:OMG:OP1	7:H:19:ARG:NH2	2.40	0.55
3:D:5024:C:N4	3:D:5029:C:O4'	2.37	0.55
48:w:436:OMG:OP2	48:w:471:G:O2'	2.24	0.55
51:z:121:ARG:HH22	51:z:123:ARG:HD3	1.70	0.55
60:8:136:LYS:O	60:8:139:ARG:NH1	2.38	0.55
14:O:38:ARG:HD3	14:O:83:ASP:HB2	1.88	0.55
21:V:16:LYS:O	21:V:33:ARG:NH2	2.39	0.55
48:w:953:C:O2	62:AA:55:ARG:NH2	2.39	0.55
25:Z:38:ASN:OD1	25:Z:39:PHE:N	2.39	0.55
48:w:113:G:N2	48:w:293:C:O4'	2.39	0.55
50:y:172:MET:HE2	50:y:212:VAL:HG22	1.89	0.55
56:4:144:ILE:HD11	56:4:152:ARG:HD3	1.89	0.55
3:D:1699:A:H3'	3:D:1700:G:H5''	1.88	0.55
25:Z:28:PRO:HB2	25:Z:34:MET:HG2	1.89	0.55
3:D:1574:G:O2'	3:D:1575:A:O5'	2.25	0.55
8:I:7:LEU:HG	8:I:21:ASN:HB3	1.89	0.55
49:x:36:GLN:O	49:x:53:ARG:NH1	2.40	0.55
3:D:664:G:H2'	3:D:666:G:C8	2.42	0.55
3:D:2485:U:H2'	3:D:2486:G:C8	2.41	0.55
3:D:4700:A:N1	13:N:72:THR:HG21	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:64:VAL:HA	16:Q:67:HIS:HD2	1.70	0.55
58:6:107:GLU:O	58:6:112:THR:OG1	2.24	0.55
3:D:2562:G:O2'	3:D:2565:A:N6	2.39	0.55
3:D:3765:G:O2'	3:D:3767:C:N4	2.40	0.55
4:E:117:G:OP1	9:J:253:TYR:OH	2.25	0.55
33:h:34:THR:HG23	33:h:95:ALA:HB2	1.89	0.55
55:3:85:ARG:O	55:3:87:ARG:NH1	2.40	0.55
3:D:151:G:OP2	18:S:4:TYR:OH	2.25	0.54
3:D:4936:G:N7	10:K:183:ARG:NH2	2.55	0.54
48:w:838:G:N1	48:w:840:C:O2'	2.39	0.54
48:w:1372:U:O2'	48:w:1373:C:O5'	2.22	0.54
63:AB:49:LEU:HA	63:AB:53:GLN:HE21	1.72	0.54
3:D:730:G:OP2	11:L:76:ARG:NE	2.40	0.54
36:k:78:HIS:HB3	36:k:83:MET:O	2.08	0.54
48:w:363:A:N6	48:w:400:C:O2'	2.41	0.54
48:w:568:C:H2'	48:w:569:A:C8	2.42	0.54
54:2:187:SER:HB3	54:2:190:ILE:HG12	1.89	0.54
70:AI:27:ILE:HB	70:AI:61:ILE:HG23	1.88	0.54
79:AR:21:ILE:HD11	79:AR:307:VAL:HG11	1.88	0.54
10:K:162:VAL:HG22	10:K:175:VAL:HG22	1.89	0.54
45:t:74:GLU:O	45:t:78:ARG:NH1	2.41	0.54
55:3:7:PHE:HB2	55:3:124:LEU:HD13	1.89	0.54
60:8:90:ARG:HD2	60:8:109:MET:HE2	1.88	0.54
68:AG:39:LEU:HD22	68:AG:89:ILE:HD12	1.89	0.54
3:D:75:G:O2'	16:Q:101:ARG:NH1	2.40	0.54
48:w:167:G:H22	55:3:132:ARG:HH11	1.54	0.54
76:AO:40:ARG:NH2	76:AO:62:GLU:OE2	2.35	0.54
3:D:4146:G:H2'	3:D:4147:G:H8	1.72	0.54
22:W:163:ARG:HD3	48:w:871:U:C2	2.43	0.54
55:3:221:LYS:O	55:3:224:ARG:HG3	2.07	0.54
66:AE:24:ARG:HB2	66:AE:29:ALA:HB2	1.90	0.54
68:AG:94:PRO:HD2	68:AG:97:ILE:HD11	1.88	0.54
78:AQ:110:GLN:HA	78:AQ:113:ARG:HG2	1.89	0.54
3:D:246:G:OP2	29:d:132:LYS:NZ	2.39	0.54
3:D:4537:C:H2'	3:D:4538:G:C8	2.43	0.54
12:M:99:ALA:HB1	12:M:136:LEU:HD11	1.89	0.54
25:Z:95:ASN:C	25:Z:95:ASN:HD22	2.14	0.54
48:w:168:C:H4'	55:3:131:ARG:HH11	1.72	0.54
64:AC:31:LEU:HD21	64:AC:33:LYS:HE2	1.90	0.54
3:D:1179:U:O2'	3:D:1180:C:OP1	2.23	0.54
8:I:262:GLU:HB3	8:I:273:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:126:G:O6	55:3:196:LYS:HG2	2.08	0.54
76:AO:14:VAL:HG22	76:AO:32:VAL:HG12	1.90	0.54
3:D:43:U:OP1	18:S:85:VAL:HG23	2.08	0.54
6:G:30:ARG:NH1	6:G:36:GLU:OE2	2.39	0.54
16:Q:126:LEU:N	16:Q:138:ASP:OD2	2.38	0.54
48:w:962:A:H5''	62:AA:66:ARG:HB2	1.89	0.54
53:1:179:ASN:OD1	53:1:230:LYS:NZ	2.35	0.54
79:AR:199:THR:HG21	79:AR:240:CYS:HA	1.89	0.54
3:D:2621:A:OP1	25:Z:80:LYS:NZ	2.39	0.54
3:D:4742:G:H2'	3:D:4743:G:H8	1.72	0.54
7:H:254:ILE:HG13	7:H:254:ILE:O	2.07	0.54
18:S:138:PHE:HA	18:S:143:ARG:HD2	1.88	0.54
20:U:22:LEU:HD13	20:U:90:PHE:CD2	2.42	0.54
43:r:83:ARG:HG3	43:r:83:ARG:HH11	1.73	0.54
48:w:1283:C:O2'	48:w:1313:A:N1	2.36	0.54
57:5:8:TRP:HZ3	57:5:20:PRO:HB3	1.73	0.54
63:AB:30:TYR:O	63:AB:34:MET:HG3	2.07	0.54
72:AK:104:ARG:HA	72:AK:107:ARG:HG2	1.90	0.54
3:D:1202:C:N3	3:D:1203:G:O2'	2.38	0.54
3:D:2089:G:O2'	8:I:307:LYS:NZ	2.32	0.54
16:Q:4:SER:O	31:f:44:ASN:ND2	2.39	0.54
25:Z:23:LEU:HD11	25:Z:83:LEU:HD12	1.90	0.54
29:d:111:LEU:HD13	29:d:116:LYS:HE3	1.90	0.54
48:w:1298:G:H1'	63:AB:79:HIS:H	1.73	0.54
48:w:1485:U:OP1	52:0:151:LYS:NZ	2.41	0.54
48:w:1630:A:OP1	66:AE:40:TYR:HB2	2.08	0.54
55:3:192:ILE:HD12	55:3:195:LYS:HD2	1.90	0.54
79:AR:153:CYS:HB2	79:AR:155:ARG:HH12	1.73	0.54
3:D:1414:C:H2'	3:D:1415:G:H8	1.72	0.53
72:AK:80:ASP:OD1	72:AK:81:TYR:N	2.39	0.53
79:AR:26:GLN:HE21	79:AR:75:GLY:N	2.05	0.53
3:D:1172:C:O2'	3:D:1189:G:N2	2.36	0.53
3:D:2743:A:O2'	6:G:21:LYS:NZ	2.42	0.53
3:D:3612:C:H1'	3:D:5016:A:C8	2.43	0.53
9:J:3:PHE:CD2	9:J:4:VAL:HG22	2.42	0.53
10:K:41:LYS:N	10:K:42:PRO:HD2	2.23	0.53
42:q:12:PHE:CE2	42:q:51:LEU:HD22	2.42	0.53
48:w:103:A:H5'	57:5:12:ARG:NH1	2.24	0.53
48:w:1155:U:OP1	51:z:185:THR:OG1	2.23	0.53
51:z:213:LEU:HD23	51:z:240:THR:HG23	1.90	0.53
54:2:179:ASN:HB3	54:2:187:SER:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4:34:SER:OG	56:4:78:ARG:NH1	2.41	0.53
56:4:143:ARG:HB2	56:4:155:LYS:HB2	1.90	0.53
79:AR:11:LEU:HD13	79:AR:307:VAL:HG23	1.90	0.53
3:D:387:G:O2'	3:D:412:G:O6	2.17	0.53
3:D:1574:G:HO2'	3:D:1575:A:P	2.32	0.53
53:1:138:HIS:CD2	53:1:148:ARG:HB3	2.44	0.53
3:D:515:C:O2'	3:D:646:G:N2	2.40	0.53
8:I:38:ASN:O	8:I:42:THR:HG23	2.08	0.53
31:f:92:LYS:HD2	31:f:92:LYS:O	2.08	0.53
32:g:12:GLN:HB3	32:g:16:TRP:CZ3	2.44	0.53
48:w:1662:U:O4	48:w:1663:A:N6	2.41	0.53
25:Z:95:ASN:O	25:Z:95:ASN:ND2	2.35	0.53
48:w:115:U:O2'	48:w:381:C:O2	2.26	0.53
48:w:148:U:H2'	48:w:149:A:H5''	1.90	0.53
58:6:124:HIS:NE2	78:AQ:108:ARG:HG3	2.24	0.53
3:D:1442:C:O2'	3:D:1443:A:H5'	2.09	0.53
3:D:2588:C:OP1	3:D:2768:C:O2'	2.23	0.53
3:D:2755:A:OP1	30:e:65:ARG:NH1	2.42	0.53
3:D:4378:A:O2'	3:D:4379:A:H2'	2.09	0.53
3:D:4731:G:N3	3:D:4732:G:H1'	2.23	0.53
42:q:12:PHE:HE2	42:q:51:LEU:HD22	1.73	0.53
79:AR:20:GLN:HG2	79:AR:69:VAL:H	1.73	0.53
20:U:22:LEU:HD13	20:U:90:PHE:HD2	1.74	0.53
30:e:66:SER:HB2	30:e:122:TYR:HE2	1.72	0.53
42:q:2:SER:O	42:q:5:LYS:NZ	2.37	0.53
48:w:152:U:O2	48:w:167:G:N2	2.41	0.53
50:y:139:CYS:HB3	50:y:172:MET:HE1	1.90	0.53
3:D:4754:G:N7	10:K:279:ASN:HB2	2.24	0.53
4:E:7:G:H4'	9:J:33:ARG:HH11	1.73	0.53
16:Q:46:ILE:HD11	16:Q:51:ALA:HA	1.90	0.53
27:b:3:VAL:HG11	27:b:12:LYS:NZ	2.23	0.53
48:w:1606:G:N2	48:w:1632:G:H2'	2.24	0.53
48:w:1617:G:N1	48:w:1620:A:OP2	2.42	0.53
49:x:30:LEU:HB3	49:x:47:TYR:CE2	2.44	0.53
49:x:198:MET:HE1	49:x:200:ASP:HB2	1.90	0.53
3:D:4472:G:O2'	43:r:100:TYR:O	2.25	0.53
23:X:85:ASP:OD1	23:X:123:SER:HB2	2.09	0.53
53:1:123:LEU:HD23	53:1:236:ILE:HD11	1.91	0.53
54:2:61:PHE:HB3	76:AO:51:ARG:NH2	2.23	0.53
48:w:1435:C:H4'	48:w:1437:C:H41	1.74	0.53
6:G:120:PRO:HA	6:G:162:ASN:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:42:LYS:O	16:Q:46:ILE:HG12	2.09	0.52
16:Q:65:ARG:HD2	16:Q:66:TYR:CZ	2.45	0.52
73:AL:92:LEU:HD22	73:AL:109:TYR:HE2	1.73	0.52
75:AN:36:LYS:N	75:AN:78:SER:OG	2.41	0.52
3:D:2667:C:O4'	22:W:96:MET:HG3	2.08	0.52
3:D:4146:G:H2'	3:D:4147:G:C8	2.45	0.52
68:AG:93:SER:HB3	68:AG:97:ILE:HD11	1.91	0.52
3:D:1301:C:H2'	3:D:1302:U:H4'	1.91	0.52
3:D:2400:G:H21	37:l:6:THR:HG22	1.73	0.52
3:D:4140:C:O2'	3:D:4143:G:O6	2.19	0.52
10:K:166:LYS:HD3	10:K:208:ILE:HD12	1.91	0.52
48:w:168:C:O2'	55:3:133:LEU:HA	2.09	0.52
59:7:5:LYS:HA	59:7:8:ARG:HB3	1.90	0.52
59:7:64:TRP:CD2	77:AP:23:VAL:HG12	2.44	0.52
62:AA:85:CYS:HB3	62:AA:90:ILE:HB	1.91	0.52
75:AN:74:THR:HG23	75:AN:77:CYS:HB2	1.92	0.52
79:AR:62:HIS:CE1	79:AR:82:SER:OG	2.63	0.52
3:D:1553:A:N6	3:D:1574:G:H1'	2.24	0.52
3:D:1819:G:O4'	9:J:142:PHE:HB3	2.09	0.52
3:D:4364:G:H1'	31:f:58:MET:HE2	1.91	0.52
3:D:4635:A:H8	3:D:5048:A:H61	1.58	0.52
48:w:11:A:H8	48:w:1357:A:O2'	1.93	0.52
48:w:1607:A:H61	48:w:1632:G:H1'	1.74	0.52
3:D:1772:C:H2'	3:D:1773:OMU:H6	1.91	0.52
3:D:2611:A:H5'	3:D:2688:G:H4'	1.91	0.52
4:E:119:U:H2'	9:J:261:VAL:HG11	1.90	0.52
7:H:47:LEU:HD11	7:H:181:MET:SD	2.49	0.52
8:I:64:ALA:HB3	8:I:92:PHE:CE2	2.45	0.52
20:U:21:ASN:HB3	20:U:145:HIS:CE1	2.45	0.52
48:w:560:A:H5'	58:6:174:LYS:HB3	1.92	0.52
48:w:871:U:OP2	61:9:76:LYS:NZ	2.43	0.52
79:AR:87:LEU:HB2	79:AR:101:PHE:HB2	1.91	0.52
3:D:268:G:H2'	3:D:269:G:H8	1.73	0.52
3:D:280:G:H5''	18:S:14:LYS:HE2	1.91	0.52
3:D:462:G:H2'	3:D:463:A:C8	2.45	0.52
8:I:330:PRO:HG3	11:L:47:ARG:NH2	2.25	0.52
48:w:53:C:H5'	72:AK:112:ASN:OD1	2.08	0.52
48:w:1463:U:H3'	65:AD:63:ARG:HH22	1.74	0.52
56:4:76:GLN:HG2	56:4:94:PHE:HD2	1.74	0.52
64:AC:97:GLN:HB2	64:AC:105:LYS:HD2	1.92	0.52
66:AE:136:THR:HA	66:AE:139:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AR:73:SER:HB3	79:AR:117:ASN:HD21	1.73	0.52
3:D:1701:A:H5''	8:I:304:ALA:HB3	1.90	0.52
3:D:4473:A:OP1	43:r:124:LYS:NZ	2.43	0.52
51:z:198:ALA:HB1	51:z:202:THR:HG21	1.91	0.52
63:AB:93:MET:HE1	63:AB:106:GLU:HG3	1.90	0.52
69:AH:80:SER:O	69:AH:83:PHE:N	2.42	0.52
3:D:1498:G:OP1	21:V:150:ARG:NH1	2.43	0.52
3:D:2724:G:O2'	3:D:2726:G:OP2	2.27	0.52
5:F:16:G:HO2'	5:F:17:A:H8	1.57	0.52
16:Q:65:ARG:HD2	16:Q:66:TYR:CE2	2.44	0.52
48:w:33:G:HO2'	48:w:564:A:HO2'	1.57	0.52
74:AM:12:LYS:HB2	74:AM:33:ASP:OD2	2.09	0.52
3:D:1821:G:N3	3:D:1821:G:H2'	2.25	0.52
3:D:4691:A:H5'	13:N:71:ARG:HH11	1.74	0.52
3:D:4761:G:OP2	19:T:37:ARG:NH1	2.39	0.52
3:D:4913:G:H4'	3:D:4914:C:O5'	2.09	0.52
26:a:13:LYS:HD2	26:a:128:LEU:HD11	1.90	0.52
34:i:36:VAL:HG11	34:i:44:ARG:HD3	1.91	0.52
37:l:54:ARG:H	37:l:54:ARG:HD3	1.75	0.52
48:w:375:U:H1'	60:8:7:GLU:OE2	2.10	0.52
48:w:1454:A:H2	48:w:1476:A:H2'	1.75	0.52
48:w:1824:A:H5''	71:AJ:61:GLN:HA	1.92	0.52
3:D:175:C:H2'	3:D:176:G:C8	2.45	0.52
3:D:4635:A:O2'	3:D:4637:OMG:OP1	2.25	0.52
50:y:168:MET:HG2	50:y:197:ILE:HG21	1.92	0.52
56:4:7:LYS:HZ3	56:4:21:SER:HB2	1.75	0.52
56:4:61:ILE:HD11	56:4:176:VAL:HG22	1.92	0.52
3:D:295:A:OP2	45:t:39:ARG:NH1	2.43	0.51
48:w:388:U:H2'	48:w:389:A:C8	2.45	0.51
48:w:678:U:OP2	48:w:1026:C:N4	2.39	0.51
48:w:1144:A:H2'	48:w:1145:A:C8	2.45	0.51
48:w:1443:C:O2	64:AC:71:ARG:NH2	2.38	0.51
55:3:135:PRO:HG2	55:3:141:ILE:HD12	1.92	0.51
3:D:1279:A:O2'	3:D:1281:G:N7	2.36	0.51
3:D:1697:G:H22	3:D:2084:C:P	2.33	0.51
15:P:15:LEU:HD23	15:P:15:LEU:H	1.75	0.51
28:c:119:ILE:HD12	28:c:140:LEU:HD22	1.91	0.51
48:w:511:U:H2'	48:w:512:A2M:H8	1.92	0.51
59:7:31:LYS:NZ	59:7:39:ASN:OD1	2.28	0.51
61:9:83:ASP:N	61:9:83:ASP:OD1	2.42	0.51
64:AC:41:MET:HE1	67:AF:11:GLN:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3607:U:H2'	3:D:3608:A:C8	2.46	0.51
3:D:4092:G:H1'	3:D:4093:G:N2	2.25	0.51
4:E:24:C:H2'	4:E:25:G:O4'	2.10	0.51
15:P:118:LYS:HD2	15:P:119:TYR:H	1.75	0.51
15:P:160:GLU:OE1	15:P:160:GLU:N	2.37	0.51
34:i:64:ILE:HG23	34:i:68:LEU:HD23	1.93	0.51
40:o:2:THR:O	40:o:7:SER:OG	2.27	0.51
48:w:164:A:OP1	55:3:82:SER:OG	2.22	0.51
48:w:291:G:N2	48:w:293:C:OP2	2.36	0.51
53:1:160:ILE:HG21	53:1:169:ILE:HG22	1.92	0.51
79:AR:178:ASN:HB3	79:AR:183:LYS:H	1.75	0.51
3:D:4741:C:H4'	3:D:4742:G:H5'	1.91	0.51
4:E:47:G:C2	4:E:48:G:H1'	2.45	0.51
48:w:1553:C:H41	48:w:1557:C:H4'	1.75	0.51
48:w:1613:G:OP1	66:AE:88:LYS:NZ	2.36	0.51
49:x:12:GLU:O	49:x:15:VAL:HG22	2.10	0.51
53:1:178:GLY:H	53:1:195:ILE:HB	1.74	0.51
66:AE:98:VAL:HG21	66:AE:106:LYS:HD2	1.91	0.51
69:AH:79:VAL:O	69:AH:79:VAL:HG12	2.10	0.51
79:AR:126:ASP:OD1	79:AR:128:THR:OG1	2.28	0.51
3:D:969:C:O2'	10:K:123:ARG:NH1	2.35	0.51
3:D:1097:C:H2'	3:D:1098:G:C8	2.44	0.51
3:D:3607:U:H2'	3:D:3608:A:H8	1.75	0.51
48:w:355:G:OP2	60:8:107:LYS:NZ	2.40	0.51
48:w:613:G:N2	48:w:626:G:OP1	2.43	0.51
48:w:1448:A:H1'	48:w:1449:G:H5'	1.93	0.51
78:AQ:85:VAL:O	78:AQ:89:THR:HG23	2.10	0.51
79:AR:152:SER:HB2	79:AR:168:CYS:SG	2.50	0.51
2:C:7:A:H61	2:C:66:U:H3	1.58	0.51
3:D:2480:G:H2'	3:D:2481:G:H8	1.74	0.51
36:k:78:HIS:HB2	36:k:85:ARG:HG3	1.93	0.51
36:k:106:TYR:O	36:k:108:SER:N	2.42	0.51
48:w:145:G:H2'	48:w:146:G:C8	2.45	0.51
48:w:1669:G:OP2	64:AC:130:LYS:NZ	2.33	0.51
49:x:41:ARG:HB2	49:x:47:TYR:HE1	1.76	0.51
3:D:208:A:H2	3:D:233:U:H5''	1.75	0.51
3:D:2351:OMC:HM22	3:D:2352:U:H5'	1.92	0.51
14:O:190:LEU:HB3	14:O:197:VAL:HG22	1.92	0.51
48:w:1033:G:N1	48:w:1080:A:O2'	2.32	0.51
50:y:139:CYS:HB3	50:y:172:MET:CE	2.41	0.51
54:2:80:GLY:CA	54:2:83:ASN:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AN:37:CYS:HB3	75:AN:63:LEU:HD21	1.93	0.51
3:D:1406:G:H2'	3:D:1407:C:C5	2.45	0.51
3:D:4942:C:H4'	10:K:154:THR:HG23	1.92	0.51
7:H:322:HIS:O	7:H:342:LYS:NZ	2.40	0.51
19:T:61:ARG:HA	19:T:70:PRO:HD2	1.93	0.51
48:w:643:A:OP1	58:6:39:ASN:ND2	2.43	0.51
52:0:74:GLN:NE2	52:0:80:PRO:O	2.43	0.51
66:AE:62:ASP:N	66:AE:62:ASP:OD1	2.42	0.51
79:AR:27:PHE:HB3	79:AR:30:MET:HB3	1.93	0.51
15:P:31:ASP:HA	15:P:34:THR:HG22	1.93	0.51
19:T:54:TYR:OH	19:T:73:PHE:O	2.29	0.51
19:T:196:LEU:HG	19:T:201:LEU:HD11	1.93	0.51
33:h:31:TYR:OH	33:h:59:GLU:OE1	2.27	0.51
48:w:39:A:H62	48:w:515:G:N2	2.09	0.51
48:w:1259:A:N6	48:w:1519:U:O5'	2.44	0.51
63:AB:41:GLN:OE1	63:AB:84:ILE:HG12	2.09	0.51
71:AJ:105:PHE:CE2	71:AJ:112:VAL:HB	2.46	0.51
79:AR:64:HIS:ND1	79:AR:83:TRP:HB2	2.25	0.51
79:AR:170:TRP:HA	79:AR:194:TYR:HB2	1.93	0.51
2:B:56:C:N4	2:B:57:G:O6	2.44	0.51
3:D:3598:C:H2'	3:D:3599:A:C8	2.46	0.51
3:D:4742:G:H2'	3:D:4743:G:C8	2.46	0.51
16:Q:48:PRO:HB2	38:m:120:ALA:HB2	1.92	0.51
30:e:12:LEU:HB2	30:e:81:MET:HB3	1.92	0.51
36:k:24:HIS:HA	36:k:91:ASN:OD1	2.11	0.51
48:w:554:A:N7	48:w:555:A:N6	2.59	0.51
48:w:1520:G:O2'	48:w:1521:C:OP1	2.27	0.51
58:6:103:GLU:HA	58:6:106:LEU:HD12	1.93	0.51
76:AO:35:MET:HE1	76:AO:55:VAL:HG13	1.91	0.51
2:C:64:G:H4'	14:O:27:PRO:HA	1.92	0.50
3:D:485:C:H3'	3:D:486:C:H5''	1.92	0.50
3:D:1081:C:O2'	3:D:1082:C:H2'	2.10	0.50
3:D:1097:C:H2'	3:D:1098:G:H8	1.75	0.50
5:F:85:U:H4'	5:F:86:U:H5'	1.93	0.50
48:w:1536:G:H2'	48:w:1537:A:H8	1.75	0.50
51:z:85:SER:OG	51:z:85:SER:O	2.29	0.50
57:5:122:GLY:O	57:5:167:GLN:NE2	2.44	0.50
3:D:1705:G:H2'	3:D:1706:A:O4'	2.12	0.50
5:F:127:U:O2'	5:F:128:C:H6	1.94	0.50
14:O:31:ILE:HD12	14:O:65:LEU:HB3	1.91	0.50
23:X:99:ASP:OD1	23:X:100:LEU:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:912:C:H3'	48:w:913:A:H5''	1.92	0.50
56:4:10:LYS:HE3	56:4:20:GLU:HG3	1.91	0.50
9:J:33:ARG:O	9:J:37:VAL:HG12	2.11	0.50
48:w:1434:C:H4'	48:w:1435:C:O5'	2.10	0.50
48:w:1639:G7M:H2'	48:w:1640:A:C8	2.46	0.50
52:0:126:ILE:HG21	52:0:134:CYS:HB3	1.93	0.50
67:AF:40:ALA:HB3	67:AF:43:LYS:HG2	1.94	0.50
70:AI:3:ARG:HH22	70:AI:28:ARG:HH21	1.59	0.50
79:AR:17:TRP:HB2	79:AR:303:THR:HA	1.92	0.50
2:B:18:G:H22	2:B:55:PSU:HN3	1.58	0.50
3:D:492:U:H2'	3:D:493:G:C8	2.46	0.50
3:D:512:U:O2'	3:D:513:U:H5'	2.12	0.50
48:w:1618:C:H4'	63:AB:50:ARG:HH21	1.75	0.50
79:AR:68:ASP:OD1	79:AR:69:VAL:N	2.45	0.50
79:AR:199:THR:OG1	79:AR:239:LEU:O	2.26	0.50
3:D:1411:C:O2'	3:D:1412:G:O5'	2.29	0.50
12:M:187:LYS:HG3	12:M:198:THR:HB	1.93	0.50
18:S:120:TRP:NE1	18:S:123:GLU:HG3	2.27	0.50
30:e:51:ARG:HB2	30:e:65:ARG:HG2	1.93	0.50
48:w:560:A:N6	48:w:588:G:H1	2.05	0.50
48:w:1114:U:O2'	48:w:1115:U:H2'	2.11	0.50
49:x:33:GLN:HB3	49:x:154:LEU:HD12	1.92	0.50
62:AA:28:PHE:HA	62:AA:92:ALA:O	2.12	0.50
3:D:1442:C:N4	3:D:2104:G:O6	2.44	0.50
3:D:5006:U:H4'	3:D:5007:A:H5'	1.94	0.50
41:p:49:ASP:HB3	41:p:52:LYS:HG2	1.92	0.50
57:5:81:VAL:HG12	57:5:91:VAL:HG12	1.92	0.50
63:AB:29:SER:OG	63:AB:31:GLU:OE1	2.26	0.50
2:C:25:C:H2'	2:C:26:M2G:H8	1.77	0.50
3:D:406:C:O2'	3:D:407:A:OP1	2.30	0.50
3:D:4219:A:C6	3:D:4220:6MZ:H9	2.47	0.50
3:D:4743:G:H2'	3:D:4744:A:C8	2.47	0.50
10:K:190:HIS:HB3	10:K:193:PHE:HD2	1.77	0.50
16:Q:150:LEU:HD23	16:Q:154:VAL:HG12	1.92	0.50
37:l:45:ALA:HB3	37:l:82:MET:HG2	1.93	0.50
45:t:11:PHE:O	45:t:81:ARG:NH1	2.43	0.50
78:AQ:112:ASN:HA	78:AQ:116:VAL:HG22	1.93	0.50
2:B:69:A:H2'	2:B:70:A:H8	1.76	0.50
2:B:70:A:H2'	2:B:71:G:C8	2.47	0.50
3:D:1313:C:H5''	35:j:44:ARG:HH12	1.76	0.50
3:D:5023:C:OP1	3:D:5024:C:O2'	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:61:ASP:O	7:H:63:PRO:HD3	2.12	0.50
40:o:25:LYS:O	40:o:25:LYS:HD3	2.12	0.50
50:y:70:SER:HA	50:y:83:LYS:HA	1.94	0.50
50:y:122:GLU:OE1	50:y:140:VAL:HG12	2.12	0.50
56:4:29:GLU:OE1	56:4:33:ASN:ND2	2.44	0.50
57:5:101:ILE:HD12	57:5:190:LEU:HD11	1.94	0.50
68:AG:66:ARG:HG3	68:AG:68:THR:HG22	1.94	0.50
79:AR:11:LEU:HD23	79:AR:43:TRP:CE3	2.47	0.50
3:D:1759:G:H1	3:D:1773:OMU:C2	2.25	0.50
5:F:110:U:H5''	42:q:8:ARG:HH12	1.75	0.50
9:J:83:LEU:N	9:J:84:PRO:HD2	2.26	0.50
13:N:14:GLU:CD	13:N:14:GLU:H	2.20	0.50
48:w:124:U:OP1	53:1:148:ARG:NH2	2.45	0.50
56:4:145:ARG:HB2	70:AI:51:GLU:OE1	2.11	0.50
64:AC:34:VAL:N	64:AC:37:ARG:O	2.43	0.50
72:AK:102:THR:O	72:AK:107:ARG:NH1	2.44	0.50
76:AO:12:ALA:HB1	76:AO:32:VAL:HB	1.94	0.50
77:AP:46:TYR:O	77:AP:50:ILE:HG12	2.12	0.50
3:D:382:G:N1	3:D:385:A:OP2	2.44	0.49
3:D:515:C:H4'	3:D:516:C:OP1	2.12	0.49
3:D:737:C:C5	3:D:739:G:H5''	2.47	0.49
3:D:4580:U:O2'	7:H:182:GLU:OE2	2.19	0.49
7:H:29:VAL:HG12	7:H:31:SER:H	1.75	0.49
48:w:420:G:O2'	48:w:660:C:N3	2.39	0.49
53:1:230:LYS:H	53:1:235:TRP:NE1	2.10	0.49
59:7:53:LYS:HZ2	59:7:59:LYS:HA	1.77	0.49
64:AC:15:ARG:HA	64:AC:19:ALA:O	2.12	0.49
68:AG:96:GLU:HG2	68:AG:97:ILE:HG23	1.94	0.49
3:D:1319:U:OP2	31:f:22:ILE:HG22	2.12	0.49
3:D:1326:A2M:OP2	3:D:4445:U:O2'	2.25	0.49
45:t:74:GLU:CD	45:t:76:ASN:H	2.20	0.49
48:w:568:C:H2'	48:w:569:A:H8	1.76	0.49
55:3:37:ALA:HA	55:3:49:VAL:HA	1.94	0.49
66:AE:43:VAL:HG21	66:AE:83:PHE:CE2	2.47	0.49
79:AR:61:GLY:O	79:AR:88:ARG:NH1	2.45	0.49
79:AR:217:MET:HE1	79:AR:219:TRP:HZ2	1.77	0.49
79:AR:236:ILE:HA	79:AR:251:ALA:O	2.12	0.49
3:D:407:A:O2'	3:D:410:A:OP1	2.28	0.49
9:J:124:GLU:O	9:J:126:THR:HG23	2.12	0.49
14:O:152:LEU:HB3	14:O:165:ILE:HD12	1.94	0.49
49:x:110:ASN:O	49:x:111:GLN:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:3:67:VAL:CG2	55:3:99:GLY:HA2	2.42	0.49
62:AA:103:ASN:HD21	62:AA:142:ARG:HA	1.77	0.49
65:AD:5:ARG:HG3	65:AD:10:LYS:HE2	1.93	0.49
68:AG:63:ILE:HD11	77:AP:43:PHE:CZ	2.47	0.49
79:AR:174:VAL:CG2	79:AR:219:TRP:HZ3	2.25	0.49
3:D:738:C:O3'	17:R:71:LYS:NZ	2.46	0.49
3:D:1092:G:H2'	3:D:1093:C:C6	2.47	0.49
3:D:2097:U:O3'	3:D:2098:G:H4'	2.12	0.49
3:D:3654:G:O2'	3:D:3693:U:OP1	2.25	0.49
3:D:4092:G:O2'	3:D:4094:G:O6	2.30	0.49
31:f:90:ALA:HB3	31:f:120:GLN:HE21	1.76	0.49
45:t:101:GLY:HA2	45:t:102:GLN:HB2	1.93	0.49
48:w:190:G:O2'	48:w:208:G:N2	2.43	0.49
48:w:955:A:N1	48:w:968:U:O2'	2.44	0.49
56:4:69:LEU:O	56:4:73:GLN:HG2	2.12	0.49
59:7:55:ARG:HB3	59:7:57:TYR:CE2	2.47	0.49
3:D:3860:A:N3	20:U:131:ARG:NH1	2.59	0.49
25:Z:72:VAL:HG21	25:Z:83:LEU:HD11	1.95	0.49
48:w:579:C:O2	72:AK:61:ARG:NH1	2.30	0.49
48:w:594:A:N6	48:w:643:A:H5''	2.28	0.49
48:w:1533:A:OP2	54:2:164:ARG:NH2	2.45	0.49
53:1:185:GLY:H	53:1:189:LEU:HD13	1.75	0.49
54:2:35:LEU:HD22	54:2:147:VAL:HG23	1.95	0.49
65:AD:76:GLU:OE1	65:AD:80:ARG:NH1	2.43	0.49
70:AI:32:LYS:O	70:AI:36:ARG:HG2	2.13	0.49
74:AM:87:ARG:NH2	74:AM:94:ASP:OD1	2.43	0.49
15:P:29:SER:OG	15:P:30:GLY:N	2.44	0.49
32:g:99:ILE:HG23	32:g:109:ARG:HB3	1.95	0.49
48:w:1597:C:H4'	48:w:1603:G:C6	2.46	0.49
52:0:74:GLN:HG3	52:0:79:PHE:CE2	2.48	0.49
54:2:162:ALA:HB2	54:2:172:CYS:SG	2.53	0.49
60:8:103:GLU:HB2	71:AJ:10:ALA:HB3	1.94	0.49
64:AC:45:ARG:O	64:AC:48:GLN:HG2	2.12	0.49
66:AE:64:VAL:O	66:AE:68:ILE:HG12	2.13	0.49
79:AR:107:ASP:O	79:AR:125:ARG:N	2.41	0.49
3:D:490:C:H2'	3:D:491:G:C8	2.48	0.49
3:D:964:A:OP2	11:L:29:LYS:NZ	2.42	0.49
3:D:2779:C:O2'	5:F:112:G:OP1	2.17	0.49
48:w:1597:C:OP2	73:AL:85:ARG:NH2	2.41	0.49
55:3:200:LYS:C	55:3:202:ASN:H	2.19	0.49
57:5:157:LYS:NZ	57:5:158:ILE:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AF:60:THR:HG23	67:AF:75:MET:HE2	1.94	0.49
68:AG:34:LYS:NZ	68:AG:107:GLU:OE2	2.45	0.49
68:AG:36:CYS:SG	68:AG:37:ALA:N	2.86	0.49
79:AR:129:ILE:HD13	79:AR:154:VAL:HG11	1.95	0.49
2:B:69:A:H2'	2:B:70:A:C8	2.48	0.49
3:D:987:C:O2'	3:D:988:C:OP1	2.27	0.49
3:D:2474:G:H2'	3:D:2502:G:N2	2.28	0.49
3:D:2529:A:O2'	3:D:2531:C:OP2	2.31	0.49
3:D:4993:G:H1	3:D:5058:A:H61	1.60	0.49
7:H:17:LEU:O	7:H:19:ARG:N	2.45	0.49
12:M:165:GLU:C	12:M:167:VAL:H	2.20	0.49
28:c:129:ARG:HD3	28:c:135:LYS:HD2	1.93	0.49
48:w:591:U:H5'	48:w:593:C:H5'	1.95	0.49
48:w:1535:U:O2'	54:2:88:MET:SD	2.59	0.49
56:4:7:LYS:NZ	56:4:17:ASP:HB2	2.27	0.49
56:4:80:VAL:HG22	56:4:92:VAL:HG23	1.94	0.49
3:D:1830:G:H4'	32:g:65:MET:HE1	1.93	0.49
29:d:51:LYS:O	29:d:70:VAL:HG13	2.13	0.49
48:w:687:C:N3	56:4:118:ARG:NH2	2.61	0.49
48:w:1714:U:H2'	48:w:1715:A:C8	2.48	0.49
59:7:90:VAL:HG23	59:7:95:ARG:HB2	1.95	0.49
65:AD:124:VAL:HG13	65:AD:125:GLY:N	2.28	0.49
71:AJ:68:LYS:HB3	71:AJ:91:LEU:HD13	1.95	0.49
79:AR:87:LEU:HD21	79:AR:111:VAL:HG11	1.94	0.49
79:AR:104:HIS:CE1	79:AR:124:SER:HB3	2.48	0.49
3:D:1082:C:O2'	3:D:1083:U:O5'	2.29	0.49
3:D:2480:G:H2'	3:D:2481:G:C8	2.47	0.49
3:D:4093:G:H3'	3:D:4094:G:C8	2.48	0.49
13:N:189:GLN:H	13:N:189:GLN:CD	2.21	0.49
15:P:151:ILE:HG13	15:P:152:GLY:H	1.77	0.49
36:k:106:TYR:HB2	36:k:107:PRO:HD3	1.94	0.49
49:x:206:ASP:HB3	49:x:209:GLU:OE1	2.13	0.49
56:4:82:GLU:HA	56:4:85:LYS:HZ3	1.78	0.49
56:4:101:LEU:HD22	56:4:116:ARG:HD3	1.95	0.49
72:AK:12:PHE:HZ	72:AK:21:LYS:HD2	1.78	0.49
3:D:958:G:O2'	10:K:123:ARG:O	2.24	0.48
3:D:1402:C:H3'	3:D:1403:G:H5''	1.95	0.48
3:D:1927:U:OP1	3:D:1949:U:O2'	2.26	0.48
3:D:2475:G:OP1	3:D:2504:C:N4	2.46	0.48
5:F:71:A:OP1	29:d:27:ARG:NH2	2.46	0.48
13:N:126:VAL:HG11	13:N:161:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:32:ARG:NH1	15:P:126:TYR:HE2	2.11	0.48
16:Q:167:ARG:O	31:f:98:ALA:N	2.42	0.48
30:e:50:PRO:HD3	30:e:68:ILE:HG12	1.95	0.48
48:w:30:C:O2'	48:w:596:U:OP1	2.28	0.48
52:0:192:TRP:CZ3	52:0:194:PRO:HG3	2.48	0.48
77:AP:30:LEU:HA	77:AP:39:CYS:HA	1.94	0.48
79:AR:101:PHE:CE1	79:AR:136:GLY:HA2	2.46	0.48
79:AR:151:VAL:HG23	79:AR:168:CYS:O	2.13	0.48
79:AR:282:GLU:O	79:AR:284:PRO:HD3	2.13	0.48
2:C:25:C:H2'	2:C:26:M2G:C8	2.49	0.48
3:D:1332:C:H5''	35:j:29:VAL:HG23	1.95	0.48
3:D:1646:A:O2'	40:o:49:TRP:O	2.29	0.48
11:L:87:PRO:HG2	11:L:144:TYR:CD2	2.48	0.48
14:O:180:GLU:O	14:O:184:MET:HG3	2.11	0.48
52:0:37:VAL:HG12	52:0:50:ILE:HA	1.95	0.48
2:C:69:A:H2'	2:C:70:A:C8	2.48	0.48
3:D:1629:G:N1	6:G:208:GLU:OE1	2.39	0.48
9:J:62:CYS:HB3	9:J:105:LEU:HD22	1.95	0.48
11:L:220:MET:HE1	11:L:223:LYS:HD3	1.95	0.48
37:l:41:ALA:HB3	37:l:52:ARG:HG3	1.94	0.48
48:w:161:U:OP1	72:AK:116:LYS:NZ	2.37	0.48
52:0:186:VAL:O	52:0:186:VAL:HG12	2.14	0.48
53:1:227:VAL:HG13	53:1:228:ILE:N	2.28	0.48
54:2:48:TYR:CZ	64:AC:56:LEU:HD23	2.48	0.48
60:8:96:ILE:HG13	71:AJ:10:ALA:HB1	1.95	0.48
17:R:119:ARG:HG3	19:T:189:ILE:HG23	1.96	0.48
48:w:1543:U:H4'	64:AC:43:GLU:CD	2.38	0.48
48:w:1719:A:N6	48:w:1814:G:O2'	2.46	0.48
49:x:137:ALA:HB1	49:x:142:LEU:HB3	1.95	0.48
52:0:74:GLN:NE2	52:0:81:GLU:HA	2.29	0.48
3:D:2755:A:OP2	30:e:51:ARG:NH1	2.46	0.48
13:N:12:ILE:HG12	13:N:53:LYS:O	2.13	0.48
16:Q:163:LYS:HB2	31:f:105:ARG:HH12	1.79	0.48
48:w:190:G:H1'	48:w:209:A:N6	2.29	0.48
49:x:104:THR:O	49:x:107:THR:OG1	2.30	0.48
57:5:8:TRP:CZ3	57:5:20:PRO:HB3	2.47	0.48
3:D:5026:U:O2'	57:5:168:GLN:OE1	2.21	0.48
9:J:59:ASP:HB2	9:J:80:ALA:HB3	1.96	0.48
22:W:31:GLU:N	22:W:31:GLU:OE1	2.46	0.48
48:w:1060:A:H4'	48:w:1061:U:H5''	1.95	0.48
75:AN:50:ALA:H	75:AN:71:ALA:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:AO:31:ARG:HE	76:AO:43:ILE:HG13	1.78	0.48
3:D:4876:U:O4	23:X:161:ARG:NH2	2.47	0.48
8:I:150:LEU:HB3	8:I:151:PRO:HD3	1.96	0.48
9:J:217:ASP:OD2	9:J:218:ALA:N	2.47	0.48
43:r:77:ILE:HG13	43:r:78:ILE:HG22	1.95	0.48
48:w:96:C:H1'	48:w:474:G:H5'	1.96	0.48
48:w:1228:A:O2'	48:w:1634:A:N3	2.42	0.48
48:w:1274:G:H22	59:7:28:HIS:HE1	1.60	0.48
48:w:1648:G:O2'	48:w:1674:G:O6	2.28	0.48
50:y:52:THR:HA	50:y:57:ILE:HA	1.95	0.48
53:1:182:MET:N	53:1:227:VAL:O	2.46	0.48
56:4:122:LEU:HA	56:4:125:VAL:HG22	1.94	0.48
58:6:137:VAL:HG22	58:6:157:ILE:HG12	1.95	0.48
73:AL:58:LEU:HG	73:AL:62:VAL:HG21	1.95	0.48
73:AL:62:VAL:O	73:AL:65:TYR:HB2	2.14	0.48
79:AR:191:HIS:CD2	79:AR:195:LEU:HD11	2.48	0.48
8:I:232:VAL:O	8:I:233:SER:OG	2.27	0.48
16:Q:19:GLN:HA	16:Q:22:VAL:HG13	1.95	0.48
45:t:75:PRO:O	45:t:78:ARG:NH2	2.46	0.48
47:v:68:SER:OG	47:v:69:GLY:N	2.46	0.48
48:w:683:OMG:N1	48:w:1022:U:OP2	2.34	0.48
50:y:137:LEU:HG	50:y:215:VAL:HG12	1.96	0.48
50:y:175:GLU:HG2	50:y:193:ILE:HG21	1.95	0.48
51:z:79:GLU:HG2	69:AH:11:LEU:HG	1.96	0.48
72:AK:29:HIS:HB2	72:AK:32:LYS:HD2	1.95	0.48
74:AM:49:ALA:O	74:AM:53:ILE:HG12	2.13	0.48
3:D:469:C:N3	10:K:105:ARG:NH1	2.61	0.48
3:D:1355:G:OP1	21:V:108:ARG:NH2	2.30	0.48
3:D:4076:G:OP1	12:M:73:ARG:NE	2.30	0.48
8:I:66:SER:O	8:I:66:SER:OG	2.27	0.48
12:M:165:GLU:O	12:M:166:LEU:HB2	2.13	0.48
48:w:890:U:P	48:w:897:U:H3	2.37	0.48
48:w:1398:G:O2'	79:AR:88:ARG:NH2	2.46	0.48
48:w:1653:U:H2'	48:w:1654:G:C8	2.49	0.48
48:w:1834:A:H2	48:w:1837:G:H22	1.62	0.48
69:AH:38:GLU:OE2	69:AH:47:ASN:ND2	2.35	0.48
79:AR:222:ASN:OD1	79:AR:223:GLU:N	2.46	0.48
3:D:1660:U:H2'	31:f:12:ARG:O	2.13	0.48
13:N:6:SER:HB2	13:N:67:LEU:HD11	1.94	0.48
19:T:81:TRP:HB2	19:T:104:VAL:HG11	1.96	0.48
48:w:1620:A:OP1	63:AB:115:TYR:OH	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:x:19:LEU:HD21	65:AD:106:LEU:HD11	1.95	0.48
49:x:22:GLY:C	49:x:24:HIS:H	2.22	0.48
52:0:75:LYS:NZ	59:7:20:VAL:O	2.47	0.48
58:6:60:LEU:HA	58:6:63:LEU:HD12	1.96	0.48
63:AB:136:THR:HG22	63:AB:138:SER:H	1.79	0.48
3:D:276:C:H2'	39:n:29:ARG:NH2	2.29	0.47
3:D:691:C:H2'	3:D:692:A:C8	2.49	0.47
3:D:709:C:OP1	36:k:46:ARG:NH2	2.47	0.47
31:f:125:LYS:HA	31:f:145:VAL:O	2.14	0.47
37:l:84:ALA:O	37:l:87:VAL:HG12	2.14	0.47
48:w:26:U:H2'	48:w:27:A2M:H8	1.96	0.47
48:w:515:G:O2'	48:w:517:OMC:OP2	2.29	0.47
50:y:140:VAL:HG13	50:y:213:ARG:HB2	1.96	0.47
51:z:229:CYS:O	51:z:232:THR:HG22	2.14	0.47
53:1:174:LYS:HG3	53:1:175:PHE:N	2.29	0.47
56:4:31:GLU:HB3	56:4:41:ARG:HH11	1.78	0.47
61:9:11:LEU:HD12	61:9:11:LEU:O	2.14	0.47
68:AG:62:ARG:NH1	68:AG:81:GLN:HE21	2.11	0.47
71:AJ:66:ILE:O	71:AJ:68:LYS:NZ	2.47	0.47
3:D:959:G:N7	10:K:123:ARG:HG3	2.29	0.47
3:D:1094:G:N2	3:D:1203:G:H1'	2.29	0.47
3:D:2464:C:O2'	3:D:2465:C:H6	1.96	0.47
3:D:2669:C:H2'	3:D:2670:C:O4'	2.14	0.47
3:D:3717:A:H2'	3:D:3718:A2M:C8	2.44	0.47
8:I:109:ARG:HB3	8:I:111:TRP:CZ3	2.49	0.47
11:L:163:ASN:O	11:L:164:LYS:HG2	2.14	0.47
33:h:26:LYS:HG3	33:h:97:ILE:HB	1.96	0.47
36:k:33:VAL:HG23	36:k:38:GLU:HB2	1.97	0.47
48:w:337:C:H2'	48:w:338:G:H8	1.79	0.47
48:w:1114:U:HO2'	48:w:1115:U:H2'	1.78	0.47
48:w:1395:C:O2'	48:w:1396:A:OP1	2.30	0.47
56:4:118:ARG:O	56:4:121:THR:OG1	2.23	0.47
57:5:78:ILE:HA	57:5:104:ILE:HG22	1.96	0.47
68:AG:64:THR:HG22	68:AG:77:TRP:HE3	1.79	0.47
3:D:156:G:N2	3:D:157:U:O4	2.48	0.47
8:I:74:ALA:O	8:I:76:ILE:N	2.48	0.47
9:J:90:VAL:HG22	9:J:91:GLY:H	1.79	0.47
12:M:166:LEU:HD23	18:S:7:ILE:CD1	2.44	0.47
48:w:116:OMU:HN3	48:w:347:G:H1	1.61	0.47
48:w:1277:C:H2'	48:w:1278:A:H8	1.79	0.47
53:1:137:PRO:HB2	53:1:150:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2:38:TYR:CE1	54:2:143:PRO:HB2	2.48	0.47
56:4:66:VAL:N	56:4:67:PRO:HD2	2.29	0.47
72:AK:62:THR:HB	72:AK:69:THR:HG22	1.96	0.47
3:D:256:G:H2'	3:D:257:C:C6	2.50	0.47
3:D:2258:C:O2	10:K:91:THR:OG1	2.32	0.47
48:w:1598:G:O2'	48:w:1599:U:H6	1.97	0.47
58:6:136:ARG:NH1	58:6:159:PHE:O	2.47	0.47
72:AK:86:GLU:OE2	72:AK:87:PRO:HD2	2.15	0.47
79:AR:49:GLU:C	79:AR:51:ASN:H	2.22	0.47
79:AR:162:ASN:O	79:AR:164:ILE:N	2.45	0.47
2:B:75:C:O2'	45:t:54:PRO:O	2.26	0.47
9:J:121:GLY:HA3	9:J:168:ASP:O	2.14	0.47
48:w:1370:A:N3	48:w:1372:U:H5'	2.29	0.47
57:5:13:LYS:HG3	60:8:137:THR:HG21	1.96	0.47
63:AB:24:GLN:O	63:AB:28:MET:HG3	2.14	0.47
3:D:37:U:H4'	31:f:32:ARG:HD2	1.97	0.47
3:D:399:G:OP1	20:U:20:SER:HB2	2.14	0.47
3:D:662:C:H2'	3:D:663:G:C4	2.49	0.47
3:D:1415:G:H2'	3:D:1416:G:C8	2.50	0.47
7:H:293:ILE:HG23	7:H:294:LYS:N	2.29	0.47
7:H:294:LYS:O	7:H:294:LYS:HD3	2.15	0.47
14:O:55:ASP:OD1	14:O:55:ASP:N	2.46	0.47
36:k:50:VAL:HG22	36:k:69:VAL:HG12	1.96	0.47
48:w:587:A:O2'	48:w:588:G:N2	2.36	0.47
55:3:215:LYS:O	55:3:219:GLU:HG2	2.14	0.47
55:3:221:LYS:HE2	55:3:224:ARG:HH21	1.80	0.47
56:4:72:PHE:O	56:4:76:GLN:HG3	2.15	0.47
58:6:136:ARG:HA	58:6:141:VAL:HA	1.97	0.47
68:AG:19:ARG:HB2	68:AG:117:ALA:HB3	1.95	0.47
70:AI:102:ILE:HG22	70:AI:128:PHE:HB3	1.97	0.47
79:AR:202:PRO:HG2	79:AR:243:PRO:HA	1.96	0.47
4:E:23:A:HO2'	4:E:24:C:H6	1.61	0.47
21:V:79:THR:HB	21:V:136:THR:HG22	1.97	0.47
45:t:104:ILE:HA	45:t:105:GLN:HA	1.66	0.47
47:v:97:ILE:CG2	47:v:107:ARG:HB3	2.45	0.47
48:w:223:C:H2'	48:w:224:A:H8	1.79	0.47
48:w:869:A:C4	48:w:915:G:H1'	2.50	0.47
48:w:1171:G:O2'	48:w:1187:G:O6	2.32	0.47
48:w:1649:U:H3	48:w:1675:A:H2	1.62	0.47
48:w:1808:U:H2'	48:w:1809:A:C8	2.48	0.47
51:z:252:THR:HG22	51:z:254:ASP:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2:50:PRO:HB3	54:2:69:VAL:HG13	1.97	0.47
57:5:140:LYS:HZ1	57:5:145:ILE:HG13	1.79	0.47
60:8:13:GLN:O	60:8:16:ILE:HG22	2.14	0.47
63:AB:96:VAL:HG11	63:AB:116:LEU:HG	1.97	0.47
69:AH:38:GLU:OE2	69:AH:49:GLN:HB2	2.15	0.47
69:AH:67:ASP:OD2	69:AH:71:ARG:NH1	2.47	0.47
74:AM:28:ARG:HG2	74:AM:74:CYS:SG	2.55	0.47
76:AO:27:CYS:SG	76:AO:45:ASN:HB2	2.55	0.47
79:AR:68:ASP:HB2	79:AR:110:SER:HA	1.97	0.47
2:B:53:G:C4	2:B:54:5MU:H72	2.49	0.47
3:D:257:C:H2'	3:D:258:G:C8	2.49	0.47
3:D:661:C:H2'	3:D:662:C:C6	2.49	0.47
3:D:1852:U:H5''	31:f:22:ILE:HD11	1.96	0.47
3:D:3669:G:H21	3:D:3672:G:H21	1.62	0.47
35:j:76:LYS:NZ	35:j:98:GLU:OE1	2.42	0.47
48:w:441:C:OP2	57:5:2:GLY:N	2.47	0.47
53:1:227:VAL:HG13	53:1:228:ILE:H	1.79	0.47
69:AH:19:ALA:HB2	69:AH:68:SER:OG	2.15	0.47
73:AL:100:VAL:HB	73:AL:108:ILE:HG22	1.97	0.47
79:AR:3:GLU:HB3	79:AR:267:VAL:HG13	1.96	0.47
2:C:43:U:H2'	2:C:44:A:C8	2.50	0.47
3:D:385:A:N3	3:D:387:G:H5''	2.30	0.47
3:D:2083:C:P	21:V:14:ARG:HH12	2.38	0.47
3:D:4342:C:O3'	45:t:37:GLY:HA3	2.14	0.47
3:D:4620:OMU:O5'	3:D:4620:OMU:H6	2.14	0.47
3:D:5021:C:H3'	3:D:5022:U:H5''	1.97	0.47
24:Y:51:GLY:HA3	24:Y:92:ARG:HG3	1.97	0.47
25:Z:24:ASP:OD1	25:Z:111:GLU:HA	2.15	0.47
38:m:88:THR:OG1	38:m:91:MET:HG3	2.15	0.47
48:w:1331:C:O2'	48:w:1332:A:OP2	2.29	0.47
48:w:1432:U:H5''	48:w:1434:C:OP1	2.15	0.47
53:1:18:TRP:O	53:1:20:LEU:N	2.47	0.47
54:2:27:ASP:O	54:2:29:GLN:NE2	2.48	0.47
55:3:147:LEU:HD21	55:3:156:TYR:CE2	2.50	0.47
56:4:163:GLN:HA	56:4:167:GLU:OE2	2.14	0.47
63:AB:23:ASP:OD1	63:AB:24:GLN:N	2.48	0.47
72:AK:86:GLU:OE2	72:AK:90:ARG:HD2	2.15	0.47
79:AR:199:THR:HG21	79:AR:241:PHE:H	1.79	0.47
3:D:5:A:H4'	12:M:192:ARG:HH21	1.80	0.47
3:D:1633:G:H5'	3:D:1634:A:OP1	2.15	0.47
3:D:4088:C:O2	12:M:53:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4095:G:H1	3:D:4113:U:H3	1.62	0.47
8:I:67:TRP:HB2	8:I:71:ARG:NH1	2.30	0.47
35:j:86:GLU:OE1	35:j:86:GLU:N	2.48	0.47
48:w:591:U:H4'	48:w:592:C:O5'	2.14	0.47
48:w:985:G:H4'	62:AA:138:ASP:OD2	2.15	0.47
50:y:71:LEU:HD22	50:y:82:ARG:HB3	1.97	0.47
54:2:20:PHE:HD2	54:2:23:TRP:HD1	1.62	0.47
57:5:172:LEU:HD21	57:5:195:LEU:HD11	1.97	0.47
62:AA:34:PHE:HB3	62:AA:41:PHE:HB2	1.97	0.47
72:AK:16:ARG:H	72:AK:16:ARG:HD3	1.80	0.47
72:AK:78:SER:OG	72:AK:80:ASP:OD1	2.29	0.47
2:B:26:M2G:H5''	2:B:26:M2G:C8	2.50	0.46
3:D:75:G:N7	16:Q:102:ARG:HG2	2.30	0.46
3:D:3844:U:OP2	7:H:239:LYS:HG2	2.15	0.46
5:F:94:G:H21	40:o:82:THR:HB	1.80	0.46
18:S:159:ARG:HB2	18:S:164:LEU:HB2	1.96	0.46
37:l:41:ALA:O	37:l:52:ARG:HD2	2.15	0.46
48:w:1742:C:H2'	48:w:1743:G:O4'	2.15	0.46
55:3:219:GLU:O	55:3:223:LYS:HG2	2.15	0.46
72:AK:29:HIS:NE2	72:AK:69:THR:HG23	2.30	0.46
3:D:1370:G:OP2	8:I:48:ASN:ND2	2.41	0.46
3:D:1443:A:H2'	3:D:1444:G:O4'	2.15	0.46
3:D:4250:G:O2'	15:P:129:ASP:HB2	2.15	0.46
31:f:85:GLN:HA	31:f:88:VAL:HG22	1.96	0.46
48:w:472:C:H4'	48:w:474:G:OP1	2.15	0.46
48:w:1490:OMG:HM23	48:w:1490:OMG:H1'	1.73	0.46
49:x:41:ARG:HB2	49:x:47:TYR:CE1	2.51	0.46
56:4:82:GLU:HA	56:4:85:LYS:NZ	2.29	0.46
57:5:150:ASP:OD1	57:5:150:ASP:N	2.47	0.46
3:D:2096:G:N3	3:D:2096:G:H2'	2.30	0.46
3:D:4117:U:O4'	12:M:43:GLN:NE2	2.48	0.46
3:D:4140:C:H42	3:D:4146:G:H1'	1.80	0.46
3:D:4208:U:OP2	24:Y:4:THR:OG1	2.32	0.46
3:D:4325:A:N3	9:J:36:LEU:HB3	2.31	0.46
48:w:165:G:H4'	55:3:53:SER:OG	2.15	0.46
48:w:837:A:H62	72:AK:8:ARG:HG3	1.78	0.46
50:y:59:SER:HB3	50:y:63:LYS:NZ	2.30	0.46
55:3:85:ARG:HG3	55:3:87:ARG:NH1	2.30	0.46
66:AE:14:ARG:HH11	66:AE:17:ASN:HA	1.79	0.46
3:D:1100:U:H1'	3:D:1167:C:H42	1.79	0.46
8:I:235:LEU:HD23	8:I:240:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:151:ILE:HG13	15:P:152:GLY:N	2.30	0.46
17:R:99:GLU:O	17:R:103:LYS:HG2	2.15	0.46
23:X:15:ARG:HG3	23:X:16:CYS:O	2.16	0.46
48:w:570:C:O2'	72:AK:34:THR:O	2.31	0.46
48:w:1589:A:H4'	67:AF:82:ARG:HB3	1.96	0.46
48:w:1598:G:N7	73:AL:82:SER:N	2.64	0.46
49:x:10:MET:HE2	49:x:15:VAL:HG12	1.98	0.46
73:AL:74:SER:OG	73:AL:79:ILE:O	2.28	0.46
79:AR:195:LEU:HA	79:AR:211:GLY:HA3	1.97	0.46
79:AR:217:MET:CG	79:AR:226:HIS:HE1	2.28	0.46
3:D:496:G:H2'	3:D:497:G:H8	1.78	0.46
3:D:928:C:H2'	3:D:929:A:C8	2.51	0.46
3:D:2102:G:H2'	3:D:2102:G:N3	2.31	0.46
3:D:3746:A:H5''	6:G:244:GLY:HA3	1.97	0.46
3:D:4733:C:H1'	3:D:4734:A:H2'	1.96	0.46
28:c:38:LYS:O	28:c:40:ILE:HG12	2.15	0.46
48:w:212:C:H2'	48:w:213:G:C8	2.51	0.46
48:w:889:U:OP2	48:w:896:U:N3	2.42	0.46
48:w:1101:U:H2'	48:w:1102:G:C8	2.51	0.46
48:w:1629:C:H2'	48:w:1630:A:N3	2.30	0.46
52:0:151:LYS:O	52:0:153:VAL:HG13	2.15	0.46
58:6:170:PRO:HG2	58:6:175:ARG:HD3	1.97	0.46
75:AN:38:PRO:O	75:AN:40:CYS:N	2.48	0.46
79:AR:16:GLY:H	79:AR:305:ASN:CB	2.28	0.46
3:D:4678:G:O2'	3:D:4679:G:OP1	2.33	0.46
33:h:47:ILE:HD12	33:h:94:LEU:HD11	1.96	0.46
48:w:811:A:HO2'	48:w:812:A:P	2.39	0.46
48:w:836:G:H2'	48:w:836:G:N3	2.30	0.46
53:1:211:LYS:NZ	53:1:215:GLY:HA2	2.31	0.46
56:4:42:GLU:N	56:4:42:GLU:OE1	2.48	0.46
59:7:13:GLU:HA	59:7:16:PHE:HB3	1.98	0.46
69:AH:80:SER:O	69:AH:82:ASN:N	2.49	0.46
79:AR:76:GLN:HE22	79:AR:91:ASP:HB2	1.80	0.46
3:D:254:G:O2'	3:D:255:C:O4'	2.33	0.46
3:D:2486:G:N1	3:D:2493:G:N7	2.64	0.46
9:J:223:PHE:HB3	9:J:226:TYR:HB2	1.98	0.46
13:N:74:CYS:O	13:N:78:GLN:HG3	2.15	0.46
13:N:93:ARG:HG2	13:N:182:SER:HB3	1.98	0.46
16:Q:7:GLY:O	31:f:49:HIS:NE2	2.46	0.46
20:U:111:SER:HB3	20:U:156:ILE:HD13	1.96	0.46
29:d:31:SER:HA	29:d:48:PRO:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:22:LYS:NZ	30:e:132:GLN:O	2.37	0.46
48:w:493:A:H1'	48:w:574:A:H5'	1.98	0.46
53:1:31:PRO:HG3	53:1:43:PRO:HG3	1.98	0.46
53:1:64:ILE:HG12	53:1:70:ILE:HD11	1.98	0.46
57:5:172:LEU:HD23	57:5:172:LEU:H	1.80	0.46
60:8:17:PHE:CE1	60:8:19:ASN:HB2	2.50	0.46
3:D:3772:U:H5'	3:D:3773:U:OP2	2.16	0.46
3:D:4229:U:OP1	45:t:63:THR:OG1	2.33	0.46
3:D:4685:U:H2'	3:D:4686:G:C8	2.50	0.46
3:D:4769:G:H5''	19:T:176:ARG:HD3	1.96	0.46
10:K:41:LYS:HA	10:K:43:HIS:CE1	2.51	0.46
13:N:96:TYR:HA	13:N:177:ASP:OD1	2.16	0.46
38:m:22:ASP:OD1	38:m:23:ASP:N	2.49	0.46
48:w:97:U:H1'	48:w:473:A:H1'	1.97	0.46
48:w:165:G:H2'	48:w:166:A2M:O4'	2.15	0.46
48:w:502:C:C5	53:1:66:MET:HG2	2.51	0.46
48:w:616:A:H1'	78:AQ:85:VAL:HG23	1.98	0.46
48:w:1274:G:H1	59:7:28:HIS:CE1	2.33	0.46
51:z:76:LYS:HA	51:z:97:PHE:HE1	1.80	0.46
57:5:42:ARG:HE	57:5:59:ARG:CZ	2.29	0.46
79:AR:203:ASP:OD1	79:AR:204:GLY:N	2.49	0.46
3:D:1210:C:H41	11:L:66:ARG:CZ	2.29	0.46
3:D:1328:G:O2'	3:D:2349:A:OP1	2.31	0.46
3:D:1415:G:H2'	3:D:1416:G:H8	1.81	0.46
12:M:110:LYS:O	12:M:114:LEU:HD23	2.16	0.46
13:N:20:LEU:HD13	13:N:47:LEU:HD21	1.98	0.46
42:q:24:PRO:HG2	42:q:27:ILE:HG12	1.97	0.46
48:w:167:G:N2	55:3:132:ARG:HH11	2.14	0.46
55:3:50:VAL:HG21	55:3:111:LEU:HB3	1.96	0.46
79:AR:125:ARG:HA	79:AR:150:TRP:HB2	1.96	0.46
79:AR:153:CYS:SG	79:AR:197:THR:HA	2.55	0.46
3:D:1448:G:H2'	3:D:1449:C:C6	2.51	0.46
5:F:82:A:H4'	5:F:83:C:O4'	2.17	0.46
6:G:114:CYS:HB3	6:G:167:GLY:O	2.16	0.46
8:I:111:TRP:HD1	8:I:112:HIS:ND1	2.13	0.46
18:S:43:THR:OG1	18:S:131:GLU:OE1	2.30	0.46
58:6:47:LYS:HD3	58:6:102:ILE:HD12	1.98	0.46
68:AG:36:CYS:O	68:AG:40:ILE:HG12	2.16	0.46
3:D:659:G:H2'	3:D:660:A:C8	2.51	0.45
3:D:1443:A:C6	3:D:2103:G:C6	3.04	0.45
3:D:2542:G:H2'	3:D:2543:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2545:U:H2'	3:D:2546:G:C6	2.51	0.45
3:D:4731:G:H4'	3:D:4732:G:H4'	1.96	0.45
5:F:102:G:OP2	5:F:104:A:O2'	2.29	0.45
13:N:12:ILE:HG21	13:N:18:ILE:HD12	1.98	0.45
14:O:55:ASP:OD2	14:O:164:LYS:HE3	2.16	0.45
32:g:105:GLY:O	32:g:109:ARG:HG2	2.16	0.45
48:w:93:PSU:OP1	53:1:2:ALA:N	2.49	0.45
48:w:1003:U:H5''	50:y:165:ARG:HH22	1.80	0.45
50:y:224:GLU:HB2	50:y:227:LYS:HB2	1.98	0.45
53:1:118:GLU:HA	53:1:121:TYR:HE2	1.80	0.45
64:AC:112:LEU:HB3	64:AC:119:LEU:HD11	1.98	0.45
3:D:935:A:N1	17:R:70:GLN:NE2	2.61	0.45
3:D:1480:C:O2'	3:D:1482:G:OP2	2.35	0.45
3:D:2560:C:H2'	3:D:2561:C:C6	2.50	0.45
3:D:5016:A:N3	3:D:5016:A:H2'	2.30	0.45
5:F:83:C:O2'	5:F:84:A:H5''	2.16	0.45
6:G:82:ILE:HD11	6:G:99:GLY:HA3	1.98	0.45
7:H:224:LYS:HG2	7:H:340:THR:HG22	1.98	0.45
26:a:43:LYS:HB3	26:a:43:LYS:HE3	1.71	0.45
29:d:118:ILE:HG22	29:d:121:ARG:HH21	1.82	0.45
37:l:5:LEU:HD11	37:l:32:TYR:CZ	2.51	0.45
39:n:16:LYS:HA	39:n:16:LYS:HD3	1.80	0.45
48:w:196:C:O2	48:w:203:G:N1	2.40	0.45
48:w:935:G:O2'	61:9:108:ASP:OD1	2.32	0.45
48:w:1648:G:N7	64:AC:17:LYS:HD3	2.31	0.45
48:w:1676:U:H1'	54:2:78:MET:HE1	1.97	0.45
48:w:1754:G:N1	48:w:1779:G:O6	2.50	0.45
51:z:146:GLU:HG3	51:z:148:ALA:H	1.81	0.45
53:1:45:ILE:HG13	53:1:61:VAL:HG11	1.98	0.45
67:AF:42:HIS:NE2	67:AF:43:LYS:HE3	2.31	0.45
68:AG:64:THR:HG22	68:AG:77:TRP:CE3	2.51	0.45
3:D:398:A2M:HM'3	3:D:398:A2M:H1'	1.77	0.45
3:D:1194:G:H2'	3:D:1195:G:H8	1.81	0.45
47:v:47:LYS:HB2	47:v:102:TYR:CZ	2.50	0.45
48:w:1024:A:OP2	61:9:124:ARG:NH2	2.46	0.45
48:w:1106:C:H5''	75:AN:70:LYS:HD2	1.96	0.45
55:3:136:LYS:HG3	55:3:174:PRO:HB2	1.98	0.45
60:8:87:VAL:HA	60:8:110:SER:HA	1.98	0.45
61:9:92:ILE:O	61:9:96:VAL:HG23	2.16	0.45
65:AD:100:PRO:HD3	65:AD:119:VAL:HB	1.97	0.45
66:AE:113:ARG:HD3	66:AE:117:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:137:G:H2'	3:D:138:G:H8	1.82	0.45
3:D:433:A:C2	3:D:3867:A:H4'	2.51	0.45
3:D:4637:OMG:HM23	3:D:4637:OMG:H1'	1.71	0.45
3:D:4699:U:H1'	3:D:4700:A:H5''	1.98	0.45
3:D:4996:C:H4'	34:i:26:THR:HG23	1.97	0.45
16:Q:42:LYS:HE3	16:Q:46:ILE:HD13	1.97	0.45
48:w:195:C:O2	48:w:205:G:N2	2.49	0.45
51:z:77:SER:O	51:z:79:GLU:N	2.50	0.45
55:3:199:THR:O	55:3:203:LYS:NZ	2.49	0.45
3:D:4600:G:O2'	3:D:4601:U:P	2.75	0.45
28:c:73:HIS:HB3	28:c:116:LEU:HD23	1.98	0.45
40:o:34:CYS:HB3	40:o:39:TYR:H	1.81	0.45
48:w:1425:G:H2'	48:w:1426:U:C6	2.51	0.45
54:2:20:PHE:HE1	54:2:50:PRO:HD3	1.81	0.45
55:3:136:LYS:O	55:3:136:LYS:HD2	2.16	0.45
58:6:50:LEU:HD13	58:6:102:ILE:HA	1.99	0.45
75:AN:67:THR:HG22	75:AN:68:GLY:N	2.30	0.45
2:C:9:A:OP2	2:C:13:C:N4	2.50	0.45
3:D:668:C:H4'	8:I:6:PRO:HB3	1.98	0.45
3:D:958:G:N2	10:K:124:LYS:HB3	2.32	0.45
3:D:1370:G:P	8:I:48:ASN:HD22	2.40	0.45
3:D:4212:A:OP2	14:O:15:LYS:NZ	2.49	0.45
9:J:112:ARG:HE	9:J:112:ARG:HB3	1.61	0.45
12:M:105:GLU:HB2	12:M:109:GLU:HB2	1.99	0.45
12:M:166:LEU:HD23	18:S:7:ILE:HD11	1.99	0.45
13:N:61:TRP:CZ3	17:R:33:GLN:HG3	2.51	0.45
13:N:63:ASN:O	13:N:67:LEU:HB2	2.16	0.45
28:c:38:LYS:O	28:c:39:LYS:HG2	2.16	0.45
30:e:41:ALA:HB2	30:e:77:TYR:HE1	1.82	0.45
42:q:38:ASN:HB3	42:q:41:ARG:HG3	1.99	0.45
48:w:77:A:O2'	48:w:78:C:OP1	2.34	0.45
48:w:396:U:OP2	60:8:79:LYS:NZ	2.39	0.45
49:x:30:LEU:HD22	49:x:47:TYR:CE2	2.52	0.45
50:y:217:MET:HE2	50:y:217:MET:HB2	1.88	0.45
53:1:227:VAL:HG13	53:1:229:GLY:H	1.81	0.45
63:AB:49:LEU:HD12	63:AB:53:GLN:HG3	1.98	0.45
64:AC:32:ILE:HD12	64:AC:68:ILE:HD12	1.99	0.45
68:AG:63:ILE:HD11	77:AP:43:PHE:CE2	2.51	0.45
69:AH:35:ASN:OD1	69:AH:52:THR:HG22	2.16	0.45
70:AI:3:ARG:NH2	70:AI:28:ARG:HH21	2.15	0.45
73:AL:69:THR:HG22	73:AL:72:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:217:C:H5''	3:D:218:A:H4'	1.97	0.45
3:D:965:G:H2'	3:D:2092:G:N2	2.32	0.45
23:X:15:ARG:HB3	23:X:27:LEU:HD23	1.98	0.45
36:k:109:ARG:HG3	36:k:110:ILE:HD12	1.99	0.45
48:w:154:U:O2	55:3:4:ASN:ND2	2.44	0.45
48:w:656:G:H5'	48:w:662:G:N2	2.31	0.45
53:1:153:LEU:O	53:1:174:LYS:NZ	2.50	0.45
53:1:198:ARG:HB2	53:1:208:VAL:HG22	1.99	0.45
55:3:22:ARG:HA	55:3:25:ARG:HG3	1.99	0.45
55:3:200:LYS:O	55:3:201:LYS:HB3	2.17	0.45
66:AE:137:LYS:O	66:AE:141:ARG:NH2	2.37	0.45
6:G:205:ASN:HB2	6:G:206:PRO:HD2	1.98	0.45
11:L:96:ARG:HD2	11:L:139:TYR:CE2	2.52	0.45
12:M:173:LEU:HA	39:n:43:MET:HE2	1.97	0.45
13:N:12:ILE:HD11	13:N:53:LYS:HB2	1.98	0.45
14:O:54:SER:HB2	14:O:135:ILE:HD11	1.98	0.45
45:t:44:LYS:HE3	45:t:52:THR:HB	1.99	0.45
48:w:168:C:H2'	48:w:169:U:C6	2.52	0.45
48:w:179:C:H3'	48:w:180:G:C8	2.48	0.45
48:w:192:C:OP2	57:5:140:LYS:HD3	2.16	0.45
48:w:290:U:O2'	48:w:292:A:N7	2.48	0.45
48:w:434:G:H21	48:w:473:A:H8	1.65	0.45
48:w:1274:G:H22	59:7:28:HIS:CE1	2.35	0.45
48:w:1522:A:H5''	63:AB:128:HIS:CE1	2.52	0.45
48:w:1597:C:H4'	48:w:1603:G:O6	2.17	0.45
52:0:7:LYS:HA	52:0:7:LYS:HD3	1.75	0.45
55:3:41:LEU:HD23	55:3:41:LEU:H	1.81	0.45
57:5:82:VAL:O	57:5:205:ARG:NH1	2.49	0.45
63:AB:29:SER:OG	63:AB:30:TYR:N	2.50	0.45
72:AK:41:ARG:HA	72:AK:55:ILE:HD11	1.98	0.45
9:J:125:VAL:HG23	9:J:126:THR:H	1.81	0.45
29:d:50:ARG:HD2	29:d:115:ARG:NH1	2.31	0.45
37:l:19:LYS:HD3	37:l:19:LYS:HA	1.72	0.45
54:2:102:LEU:HD11	73:AL:67:LEU:HD13	1.99	0.45
58:6:119:LEU:H	58:6:119:LEU:HD23	1.82	0.45
61:9:94:LYS:O	61:9:98:VAL:HG23	2.17	0.45
65:AD:92:ASP:N	65:AD:92:ASP:OD1	2.50	0.45
66:AE:60:THR:N	66:AE:63:GLU:OE2	2.50	0.45
68:AG:22:ILE:HB	68:AG:89:ILE:HG13	1.98	0.45
75:AN:19:HIS:HB3	75:AN:21:LYS:O	2.17	0.45
3:D:3756:A:N6	3:D:3757:G:O6	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:220:MET:O	11:L:221:LYS:HG2	2.17	0.45
12:M:108:GLN:O	12:M:112:GLN:HG2	2.17	0.45
48:w:190:G:OP1	57:5:149:TYR:OH	2.34	0.45
48:w:1018:U:OP2	61:9:62:GLN:NE2	2.40	0.45
48:w:1535:U:H1'	54:2:92:ILE:HD11	1.97	0.45
49:x:35:GLU:O	49:x:38:ILE:HG22	2.17	0.45
50:y:89:GLU:HG3	50:y:223:PHE:HE1	1.82	0.45
51:z:88:ILE:HG21	51:z:94:ILE:HD11	1.98	0.45
54:2:144:LEU:HD23	76:AO:49:PRO:HG2	1.98	0.45
55:3:55:GLY:HA3	55:3:108:VAL:O	2.17	0.45
55:3:177:GLN:HG3	55:3:178:ARG:N	2.31	0.45
56:4:20:GLU:HA	56:4:23:ILE:HD13	1.98	0.45
58:6:26:ASP:OD1	58:6:27:GLN:N	2.50	0.45
58:6:73:GLU:OE2	58:6:73:GLU:N	2.49	0.45
71:AJ:39:ASN:HD22	71:AJ:43:GLY:H	1.64	0.45
79:AR:17:TRP:O	79:AR:36:ARG:HB2	2.17	0.45
79:AR:74:ASP:OD1	79:AR:74:ASP:N	2.46	0.45
79:AR:244:ASN:HB3	79:AR:245:ARG:NE	2.29	0.45
3:D:660:A:H3'	3:D:661:C:H5''	1.99	0.44
3:D:2693:G:OP1	41:p:35:LYS:NZ	2.40	0.44
3:D:4363:A:H5''	45:t:36:GLN:HG2	1.99	0.44
7:H:10:ARG:HG2	7:H:11:HIS:N	2.31	0.44
9:J:89:LYS:HE3	9:J:89:LYS:HB3	1.77	0.44
22:W:133:LYS:HB3	22:W:137:ILE:HD12	1.99	0.44
48:w:448:A:H5''	57:5:25:ARG:HA	1.99	0.44
48:w:526:A:O2'	58:6:125:HIS:ND1	2.42	0.44
48:w:1119:A:O2'	75:AN:72:ARG:NH2	2.48	0.44
64:AC:117:ARG:HH11	64:AC:121:VAL:HG21	1.82	0.44
74:AM:45:VAL:HG23	74:AM:46:GLU:H	1.82	0.44
79:AR:126:ASP:OD1	79:AR:126:ASP:N	2.49	0.44
79:AR:236:ILE:HG22	79:AR:252:THR:HG22	1.98	0.44
3:D:450:G:H8	3:D:450:G:OP2	2.01	0.44
3:D:1401:C:H2'	3:D:1402:C:C6	2.52	0.44
9:J:271:MET:HE2	9:J:276:LYS:HG3	1.99	0.44
10:K:120:ASP:OD1	10:K:120:ASP:N	2.49	0.44
45:t:64:LYS:HE2	45:t:64:LYS:HB3	1.82	0.44
48:w:1515:G:N2	63:AB:99:GLY:O	2.50	0.44
52:0:186:VAL:O	52:0:188:ILE:HG13	2.18	0.44
57:5:139:LYS:CE	57:5:146:GLN:HB2	2.47	0.44
75:AN:14:GLU:O	75:AN:18:LYS:HG3	2.16	0.44
79:AR:114:SER:OG	79:AR:116:ASP:OD1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1186:U:H2'	3:D:1187:G:N3	2.33	0.44
3:D:2382:A:N1	3:D:2829:U:O2'	2.45	0.44
17:R:40:GLY:H	17:R:45:VAL:HG23	1.81	0.44
24:Y:80:VAL:HG22	24:Y:81:LYS:H	1.82	0.44
25:Z:23:LEU:HD23	25:Z:110:TYR:HB2	1.99	0.44
48:w:1276:A:O2'	59:7:51:SER:HA	2.17	0.44
48:w:1842:4AC:O7	48:w:1842:4AC:H5	2.17	0.44
3:D:963:G:N7	3:D:964:A:N6	2.66	0.44
3:D:1408:G:H1'	3:D:1411:C:H42	1.82	0.44
3:D:1503:A:H4'	3:D:1504:G:H5'	1.99	0.44
3:D:2560:C:H2'	3:D:2561:C:H6	1.82	0.44
3:D:4859:C:H5''	3:D:4860:G:C8	2.53	0.44
11:L:247:MET:HE2	11:L:247:MET:HB3	1.91	0.44
13:N:173:ARG:HB3	43:r:127:VAL:HB	1.99	0.44
22:W:153:LYS:HD2	22:W:153:LYS:C	2.43	0.44
36:k:93:PRO:O	36:k:95:LYS:N	2.51	0.44
48:w:342:C:H2'	48:w:343:A:C8	2.53	0.44
48:w:1217:A:H2'	48:w:1218:C:C6	2.53	0.44
48:w:1391:OMC:H4'	77:AP:55:LEU:HD21	1.98	0.44
48:w:1417:C:OP1	67:AF:133:ARG:NH1	2.50	0.44
48:w:1446:A:O2'	48:w:1447:G:H5''	2.16	0.44
54:2:77:MET:HE2	54:2:83:ASN:O	2.17	0.44
56:4:76:GLN:HG2	56:4:94:PHE:CD2	2.52	0.44
67:AF:23:LYS:HE2	67:AF:51:ASN:HD22	1.83	0.44
72:AK:37:LYS:NZ	72:AK:93:ARG:HH11	2.14	0.44
79:AR:212:LYS:HD2	79:AR:235:ILE:HD12	1.99	0.44
3:D:181:C:H2'	3:D:182:G:C8	2.52	0.44
3:D:2263:A:OP1	47:v:107:ARG:NH2	2.51	0.44
3:D:2705:G:H1	3:D:2710:C:H42	1.64	0.44
3:D:4138:C:H2'	3:D:4139:G:C8	2.52	0.44
4:E:7:G:H4'	9:J:33:ARG:NH1	2.31	0.44
7:H:144:LYS:HE2	7:H:144:LYS:HB3	1.77	0.44
10:K:153:LEU:HD11	10:K:195:ILE:HG13	2.00	0.44
17:R:128:LYS:HE3	17:R:128:LYS:HB2	1.61	0.44
25:Z:38:ASN:O	25:Z:42:PHE:N	2.47	0.44
30:e:107:LYS:HZ2	30:e:111:ARG:NH2	2.13	0.44
48:w:28:U:H2'	48:w:29:G:H8	1.83	0.44
48:w:434:G:OP1	57:5:23:LYS:HG2	2.17	0.44
49:x:50:ASN:HA	65:AD:105:MET:HE3	1.99	0.44
49:x:198:MET:SD	65:AD:89:SER:HB3	2.57	0.44
53:1:183:VAL:HG11	53:1:188:ASN:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:5:158:ILE:HD12	57:5:162:LEU:HD23	1.99	0.44
58:6:177:ASN:HA	58:6:180:LYS:HG2	1.99	0.44
64:AC:58:LEU:HD22	64:AC:108:ILE:HG12	2.00	0.44
78:AQ:86:ARG:O	78:AQ:91:LYS:NZ	2.50	0.44
79:AR:78:ALA:HB2	79:AR:92:LEU:HD11	1.99	0.44
3:D:2637:U:OP1	37:l:28:ASN:ND2	2.50	0.44
3:D:4694:G:O2'	13:N:71:ARG:NH2	2.51	0.44
25:Z:18:VAL:HG22	25:Z:75:GLU:HG3	2.00	0.44
48:w:447:A:P	57:5:49:ARG:HH12	2.41	0.44
48:w:1126:G:OP2	65:AD:129:LYS:NZ	2.38	0.44
49:x:73:ASP:HB3	49:x:120:ARG:HB2	2.00	0.44
3:D:71:C:H1'	16:Q:62:PRO:O	2.17	0.44
3:D:3688:U:OP2	6:G:198:ARG:NH1	2.51	0.44
11:L:108:VAL:HG23	11:L:132:MET:HE2	1.99	0.44
37:l:82:MET:HE2	37:l:82:MET:HB3	1.79	0.44
48:w:28:U:H2'	48:w:29:G:C8	2.52	0.44
48:w:103:A:H5'	57:5:12:ARG:HH12	1.80	0.44
48:w:835:C:H5''	48:w:836:G:H5'	2.00	0.44
48:w:1204:A:O2'	48:w:1700:C:OP2	2.25	0.44
51:z:130:ILE:HD13	51:z:159:LYS:HG3	2.00	0.44
51:z:166:ARG:HB3	51:z:247:THR:HG22	1.99	0.44
54:2:20:PHE:HD2	54:2:23:TRP:CD1	2.35	0.44
55:3:124:LEU:HD12	55:3:125:THR:HG23	2.00	0.44
56:4:11:PRO:HD2	56:4:45:ILE:O	2.18	0.44
58:6:86:VAL:HG11	58:6:105:PHE:CE1	2.52	0.44
59:7:7:ASN:HA	59:7:10:ALA:HB3	1.99	0.44
70:AI:69:LEU:HG	70:AI:70:ASN:O	2.17	0.44
2:B:22:G:H2'	2:B:23:A:H8	1.83	0.44
3:D:320:C:OP1	39:n:84:LYS:NZ	2.44	0.44
11:L:87:PRO:HG2	11:L:144:TYR:CE2	2.53	0.44
16:Q:29:PRO:HD3	18:S:202:ARG:NH1	2.33	0.44
17:R:89:THR:O	17:R:93:LYS:HG2	2.18	0.44
21:V:148:VAL:HG12	21:V:152:PHE:CZ	2.53	0.44
24:Y:121:GLU:OE1	24:Y:121:GLU:N	2.51	0.44
39:n:63:VAL:O	39:n:64:SER:OG	2.28	0.44
48:w:1448:A:O2'	48:w:1449:G:H8	2.01	0.44
48:w:1865:C:C2	74:AM:5:ARG:HB2	2.52	0.44
54:2:51:HIS:O	64:AC:50:LYS:NZ	2.47	0.44
56:4:60:ILE:HD11	56:4:92:VAL:HG12	2.00	0.44
57:5:148:LYS:HZ2	57:5:149:TYR:HE1	1.65	0.44
68:AG:56:MET:HG3	68:AG:86:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AN:50:ALA:O	75:AN:52:THR:N	2.51	0.44
3:D:44:A:OP2	18:S:85:VAL:HG21	2.18	0.44
3:D:700:G:H2'	3:D:701:G:C8	2.53	0.44
3:D:981:C:H2'	10:K:73:TYR:HE1	1.82	0.44
3:D:3777:G:O2'	3:D:3815:G:O6	2.29	0.44
43:r:112:LYS:HA	43:r:112:LYS:HD3	1.90	0.44
45:t:105:GLN:NE2	45:t:106:PHE:H	2.16	0.44
48:w:223:C:H2'	48:w:224:A:C8	2.52	0.44
53:1:181:CYS:HA	53:1:227:VAL:CA	2.44	0.44
54:2:49:LEU:HG	64:AC:49:TYR:HB2	1.98	0.44
3:D:2094:G:C8	3:D:2095:A:C6	3.06	0.43
3:D:2363:A2M:H2'	3:D:2364:OMG:O4'	2.17	0.43
3:D:4322:G:N2	3:D:4325:A:OP2	2.49	0.43
17:R:96:GLU:HA	17:R:99:GLU:CG	2.37	0.43
27:b:46:PRO:HB2	27:b:54:LEU:HD12	2.00	0.43
48:w:606:G:O2'	48:w:608:C:OP1	2.36	0.43
48:w:960:U:H5''	62:AA:149:ARG:HH22	1.83	0.43
50:y:110:MET:HA	50:y:113:MET:HE2	1.99	0.43
54:2:76:MET:HG3	54:2:76:MET:O	2.18	0.43
55:3:43:GLU:HA	55:3:46:LYS:HZ3	1.83	0.43
58:6:93:LYS:HE3	58:6:93:LYS:HB3	1.84	0.43
67:AF:37:VAL:HG23	67:AF:38:LYS:N	2.32	0.43
70:AI:37:PHE:CE2	70:AI:103:VAL:HG11	2.53	0.43
78:AQ:84:LYS:O	78:AQ:88:GLN:HG2	2.18	0.43
2:C:42:U:H2'	2:C:43:U:O4'	2.18	0.43
3:D:497:G:C6	3:D:498:C:C2	3.07	0.43
8:I:73:VAL:HB	8:I:78:ARG:NH1	2.32	0.43
9:J:142:PHE:CZ	9:J:171:LEU:HD22	2.53	0.43
16:Q:158:ARG:HE	16:Q:158:ARG:HB3	1.53	0.43
17:R:104:MET:SD	19:T:199:HIS:HB3	2.59	0.43
48:w:1065:G:OP1	62:AA:149:ARG:NH1	2.51	0.43
48:w:1567:G:H1'	66:AE:82:TRP:CZ2	2.53	0.43
49:x:121:LEU:HD21	49:x:145:ILE:HD13	1.99	0.43
50:y:57:ILE:HG13	50:y:58:ALA:N	2.29	0.43
52:0:137:VAL:HG12	52:0:185:LYS:HB2	1.99	0.43
53:1:101:LEU:HD12	53:1:109:PHE:CD2	2.53	0.43
54:2:153:LEU:HG	54:2:189:ALA:HA	1.99	0.43
62:AA:151:LEU:HD23	62:AA:151:LEU:H	1.83	0.43
3:D:965:G:N2	3:D:2092:G:H1'	2.33	0.43
3:D:1412:G:H2'	3:D:1413:C:C6	2.53	0.43
3:D:2351:OMC:HM23	8:I:95:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3724:A2M:HM'3	3:D:3724:A2M:H1'	1.73	0.43
6:G:171:GLY:O	46:u:68:ALA:HB2	2.18	0.43
9:J:215:ASP:C	9:J:215:ASP:OD2	2.61	0.43
10:K:157:HIS:HB3	10:K:160:LYS:HD2	2.00	0.43
15:P:56:THR:OG1	15:P:64:ARG:HG3	2.18	0.43
38:m:91:MET:HE2	38:m:91:MET:HB3	1.87	0.43
48:w:877:C:H2'	48:w:878:G:O4'	2.17	0.43
48:w:1403:C:H2'	48:w:1433:C:N4	2.33	0.43
49:x:26:GLY:O	49:x:47:TYR:HB2	2.18	0.43
54:2:43:GLU:C	54:2:45:TYR:H	2.25	0.43
58:6:153:SER:O	58:6:153:SER:OG	2.35	0.43
63:AB:83:MET:HB3	63:AB:116:LEU:HB2	2.00	0.43
73:AL:68:ILE:CG2	73:AL:109:TYR:HB2	2.49	0.43
73:AL:69:THR:HG23	73:AL:72:VAL:H	1.82	0.43
3:D:188:G:H22	3:D:251:C:H42	1.66	0.43
3:D:1447:C:H2'	3:D:1448:G:C8	2.49	0.43
3:D:4138:C:H2'	3:D:4139:G:H8	1.82	0.43
3:D:4927:G:H5''	3:D:4928:C:H5	1.84	0.43
5:F:110:U:C5	5:F:112:G:H1'	2.53	0.43
48:w:116:OMU:HM23	48:w:116:OMU:H1'	1.87	0.43
48:w:130:G:H2'	48:w:130:G:N3	2.33	0.43
48:w:1332:A:H2'	52:0:141:LYS:HE2	2.01	0.43
50:y:39:PHE:CD2	50:y:74:LEU:HB3	2.53	0.43
50:y:39:PHE:HD2	50:y:74:LEU:HB3	1.82	0.43
77:AP:43:PHE:O	77:AP:47:ALA:N	2.50	0.43
3:D:6:C:H2'	3:D:7:C:C6	2.53	0.43
3:D:2493:G:H1'	5:F:127:U:OP1	2.17	0.43
4:E:48:G:C6	4:E:49:A:C6	3.07	0.43
5:F:93:C:O2'	5:F:94:G:H8	2.01	0.43
9:J:34:LYS:O	9:J:38:ILE:HG12	2.19	0.43
22:W:99:MET:HE2	22:W:99:MET:HA	2.01	0.43
26:a:87:SER:HB3	27:b:19:ARG:HH11	1.84	0.43
48:w:197:U:C5	48:w:198:U:H1'	2.53	0.43
50:y:167:LYS:O	50:y:171:ILE:HG12	2.19	0.43
51:z:202:THR:HG22	51:z:221:ASP:HB3	2.00	0.43
52:0:7:LYS:HE3	68:AG:25:THR:HG21	2.01	0.43
52:0:146:ARG:O	52:0:148:LYS:HD3	2.18	0.43
62:AA:31:CYS:HB2	62:AA:93:LEU:HD13	2.00	0.43
67:AF:21:PHE:O	67:AF:25:SER:OG	2.28	0.43
3:D:964:A:H3'	3:D:965:G:H4'	2.00	0.43
3:D:4392:OMG:N3	3:D:4447:5MC:HM52	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4768:G:OP1	19:T:168:TYR:OH	2.35	0.43
5:F:77:A:H2'	5:F:78:G:O4'	2.19	0.43
6:G:206:PRO:HD3	6:G:213:GLY:CA	2.48	0.43
17:R:96:GLU:O	17:R:100:ARG:HG3	2.18	0.43
29:d:32:SER:OG	29:d:101:PRO:O	2.32	0.43
48:w:301:A:N3	57:5:73:THR:HG21	2.33	0.43
48:w:419:G:N2	48:w:661:U:O2	2.52	0.43
48:w:686:PSU:OP1	70:AI:32:LYS:HG2	2.19	0.43
53:1:103:TYR:CE1	53:1:189:LEU:HD11	2.53	0.43
55:3:116:LYS:NZ	55:3:125:THR:HG21	2.33	0.43
64:AC:58:LEU:HB3	64:AC:62:ARG:HD2	2.00	0.43
79:AR:40:ILE:HB	79:AR:59:LEU:HB2	2.00	0.43
3:D:423:G:OP1	20:U:62:ARG:NH2	2.52	0.43
3:D:3776:G:OP2	3:D:3776:G:N2	2.50	0.43
4:E:55:A:H4'	15:P:155:HIS:HB2	2.01	0.43
11:L:31:LYS:HD3	11:L:31:LYS:HA	1.80	0.43
11:L:31:LYS:NZ	11:L:34:ARG:HH22	2.17	0.43
13:N:115:ARG:O	13:N:116:ASN:C	2.62	0.43
20:U:29:THR:HA	20:U:32:THR:HG22	2.00	0.43
35:j:84:GLU:CD	47:v:20:ARG:HH22	2.26	0.43
45:t:85:ILE:HG22	45:t:86:LYS:N	2.34	0.43
48:w:206:G:O6	57:5:144:LYS:NZ	2.51	0.43
48:w:338:G:H2'	48:w:339:A:H8	1.84	0.43
48:w:598:G:O2'	48:w:605:A:N1	2.48	0.43
48:w:1097:G:H4'	49:x:32:PHE:CD1	2.53	0.43
60:8:48:LYS:HE2	60:8:48:LYS:HB2	1.88	0.43
66:AE:105:ASN:OD1	66:AE:108:ARG:NH2	2.49	0.43
73:AL:62:VAL:HA	73:AL:65:TYR:CD2	2.54	0.43
79:AR:14:HIS:CE1	79:AR:18:VAL:HG22	2.54	0.43
3:D:492:U:H5'	8:I:268:ARG:HH11	1.83	0.43
3:D:4420:PSU:O2	3:D:4475:G:N2	2.52	0.43
7:H:370:THR:O	7:H:370:THR:HG22	2.19	0.43
12:M:48:LYS:HB3	28:c:42:THR:HG23	2.00	0.43
16:Q:65:ARG:HG3	31:f:69:PHE:CG	2.54	0.43
48:w:1300:U:O2	63:AB:51:ARG:NH2	2.51	0.43
48:w:1433:C:H4'	48:w:1435:C:H1'	2.00	0.43
48:w:1588:A:H2'	48:w:1589:A:C8	2.54	0.43
48:w:1639:G7M:HO2'	48:w:1640:A:P	2.41	0.43
50:y:71:LEU:CD2	50:y:82:ARG:HB3	2.49	0.43
53:1:65:CYS:SG	53:1:80:ILE:HG22	2.59	0.43
53:1:228:ILE:HD12	53:1:228:ILE:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AA:62:VAL:HG11	62:AA:67:ASP:OD2	2.19	0.43
66:AE:10:GLN:HB3	66:AE:13:LEU:HG	2.01	0.43
74:AM:41:ILE:HG22	74:AM:66:LYS:HD3	2.01	0.43
79:AR:89:LEU:HB2	79:AR:99:ARG:HB3	2.00	0.43
3:D:217:C:H5	3:D:219:G:H4'	1.82	0.43
3:D:1295:C:H4'	3:D:1296:G:C8	2.54	0.43
3:D:2478:C:N4	3:D:2479:G:O6	2.52	0.43
3:D:2561:C:H2'	3:D:2562:G:O4'	2.18	0.43
7:H:80:GLU:OE1	7:H:323:TYR:OH	2.23	0.43
43:r:83:ARG:HG3	43:r:83:ARG:NH1	2.34	0.43
48:w:560:A:H2'	48:w:561:A:C8	2.49	0.43
48:w:1648:G:H5''	64:AC:125:ARG:HB2	2.01	0.43
54:2:33:ILE:HA	54:2:36:GLN:HB2	2.01	0.43
56:4:52:GLU:HG3	56:4:53:VAL:O	2.19	0.43
61:9:84:LEU:HD21	61:9:149:LEU:HD21	2.01	0.43
64:AC:42:ILE:O	64:AC:45:ARG:HG3	2.19	0.43
66:AE:74:PRO:O	66:AE:79:ILE:HB	2.19	0.43
67:AF:39:LEU:HA	67:AF:39:LEU:HD23	1.79	0.43
68:AG:22:ILE:HB	68:AG:89:ILE:CG1	2.49	0.43
2:B:8:U:O2'	2:B:13:C:N4	2.52	0.43
3:D:1820:C:O2'	3:D:1821:G:N7	2.48	0.43
3:D:2415:OMU:HM23	3:D:2415:OMU:H1'	1.64	0.43
3:D:2570:U:H2'	3:D:2571:C:C6	2.54	0.43
3:D:4635:A:H3'	3:D:4636:U:H4'	2.00	0.43
3:D:4704:C:H2'	3:D:4705:A:C8	2.54	0.43
3:D:4896:G:H2'	3:D:4897:G:H8	1.84	0.43
15:P:32:ARG:HH12	15:P:126:TYR:HE2	1.67	0.43
28:c:89:LYS:HB3	28:c:95:THR:HG23	2.01	0.43
31:f:36:GLY:O	31:f:38:LEU:N	2.50	0.43
35:j:70:LEU:HD11	35:j:76:LYS:HB3	2.01	0.43
46:u:38:THR:HA	46:u:45:THR:HA	2.01	0.43
54:2:34:SER:HA	76:AO:55:VAL:HB	2.01	0.43
55:3:5:ILE:HD13	55:3:16:ILE:HD13	2.01	0.43
56:4:38:ALA:H	56:4:41:ARG:NH2	2.16	0.43
57:5:63:GLY:HA3	57:5:65:PHE:CE2	2.53	0.43
66:AE:84:LEU:HD12	66:AE:95:TYR:HB3	2.01	0.43
3:D:124:C:OP1	18:S:144:ARG:HD2	2.19	0.42
3:D:2059:C:O2	23:X:118:ARG:NH1	2.51	0.42
3:D:3925:OMU:HM23	3:D:3925:OMU:H1'	1.70	0.42
3:D:5029:C:O2'	3:D:5030:U:H6	2.01	0.42
5:F:126:C:H4'	5:F:127:U:OP1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:33:GLY:HA3	26:a:69:LYS:HE2	2.00	0.42
47:v:117:ILE:O	47:v:121:GLN:HG2	2.19	0.42
48:w:929:G:H2'	48:w:930:C:O4'	2.19	0.42
49:x:143:PRO:HB2	69:AH:34:MET:HE3	2.01	0.42
50:y:32:ASP:OD1	50:y:33:VAL:N	2.52	0.42
55:3:14:LYS:HB3	55:3:14:LYS:HE2	1.85	0.42
64:AC:143:LYS:HD3	64:AC:145:TYR:CZ	2.53	0.42
68:AG:18:HIS:NE2	68:AG:94:PRO:HA	2.34	0.42
70:AI:3:ARG:HH12	70:AI:28:ARG:HH21	1.67	0.42
75:AN:11:SER:N	75:AN:14:GLU:OE2	2.52	0.42
79:AR:128:THR:HB	79:AR:130:LYS:NZ	2.33	0.42
3:D:136:C:H2'	3:D:137:G:C8	2.54	0.42
3:D:717:U:H2'	3:D:718:C:C6	2.55	0.42
3:D:1818:G:O2'	3:D:1819:G:H5''	2.19	0.42
3:D:3759:A:HO2'	48:w:1826:G:HO2'	1.52	0.42
3:D:4145:C:H2'	3:D:4146:G:C8	2.54	0.42
3:D:4260:U:H2'	3:D:4261:C:C6	2.53	0.42
20:U:94:MET:SD	20:U:148:MET:HE3	2.59	0.42
21:V:39:THR:HG22	21:V:41:SER:H	1.84	0.42
21:V:94:GLU:O	21:V:95:VAL:C	2.62	0.42
28:c:72:ASP:O	28:c:76:ILE:HG12	2.19	0.42
31:f:72:THR:HG22	31:f:110:LYS:HB3	2.01	0.42
48:w:191:A:H5''	57:5:140:LYS:HE2	2.01	0.42
48:w:560:A:H61	48:w:588:G:H22	1.67	0.42
48:w:799:OMU:H1'	48:w:799:OMU:HM23	1.65	0.42
48:w:1208:A:H4'	48:w:1835:A:N7	2.34	0.42
48:w:1467:C:OP1	65:AD:3:ARG:N	2.45	0.42
62:AA:94:HIS:ND1	62:AA:128:ARG:HB2	2.34	0.42
66:AE:89:ASP:O	66:AE:91:LYS:N	2.52	0.42
68:AG:67:LYS:HG3	77:AP:44:ARG:NH1	2.33	0.42
75:AN:67:THR:HG22	75:AN:68:GLY:H	1.83	0.42
79:AR:132:TRP:CE3	79:AR:138:CYS:HB3	2.54	0.42
2:C:46:G7M:H4'	2:C:47:H2U:OP1	2.18	0.42
3:D:1534:A2M:HM'3	3:D:1534:A2M:H1'	1.90	0.42
3:D:4691:A:O2'	13:N:68:ALA:O	2.33	0.42
3:D:4895:C:H3'	3:D:4895:C:OP2	2.18	0.42
7:H:288:GLY:HA3	7:H:330:PHE:CE2	2.54	0.42
7:H:359:ALA:C	7:H:360:LEU:HD23	2.43	0.42
17:R:32:ASP:HA	23:X:145:PHE:CZ	2.54	0.42
34:i:106:VAL:O	34:i:106:VAL:HG12	2.20	0.42
40:o:52:LYS:HG2	40:o:55:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:t:22:LYS:HD3	45:t:73:VAL:HG12	2.01	0.42
50:y:219:LYS:HE2	50:y:219:LYS:HB2	1.94	0.42
52:0:205:PRO:HA	65:AD:42:PRO:HG2	2.00	0.42
58:6:84:ILE:O	58:6:108:ARG:NE	2.50	0.42
65:AD:11:LYS:O	65:AD:15:VAL:HG23	2.19	0.42
67:AF:74:SER:O	67:AF:78:ILE:HD12	2.19	0.42
70:AI:26:LEU:HD11	70:AI:60:LYS:HB3	2.00	0.42
79:AR:62:HIS:ND1	79:AR:62:HIS:O	2.50	0.42
3:D:498:C:H42	3:D:656:C:N4	2.16	0.42
3:D:1177:U:O2'	9:J:286:SER:OG	2.29	0.42
3:D:1743:A:O4'	9:J:15:ARG:HD2	2.20	0.42
3:D:4518:A:H8	3:D:4518:A:OP2	2.02	0.42
5:F:141:C:H2'	5:F:142:U:C6	2.54	0.42
6:G:54:ARG:HG3	6:G:56:ALA:H	1.84	0.42
6:G:108:PRO:HB2	46:u:86:LEU:HD22	2.01	0.42
7:H:154:LYS:HG3	7:H:191:ALA:HA	2.01	0.42
10:K:177:GLY:O	10:K:178:PRO:C	2.61	0.42
17:R:8:GLU:HB3	23:X:151:LYS:HG3	2.01	0.42
48:w:77:A:H8	55:3:175:LYS:HA	1.84	0.42
48:w:604:A:O2'	48:w:605:A:OP1	2.33	0.42
48:w:642:U:H5''	58:6:41:ARG:NH1	2.34	0.42
48:w:1204:A:H2'	48:w:1205:C:O4'	2.19	0.42
48:w:1452:A:H4'	48:w:1453:C:O5'	2.19	0.42
48:w:1558:C:H2'	48:w:1559:C:H6	1.85	0.42
48:w:1678:A2M:H1'	48:w:1678:A2M:HM'3	1.68	0.42
49:x:187:GLY:HA2	69:AH:45:ARG:NH1	2.35	0.42
58:6:114:VAL:HG13	58:6:126:ALA:HB1	2.01	0.42
66:AE:14:ARG:HE	66:AE:17:ASN:HA	1.84	0.42
67:AF:129:ARG:O	67:AF:133:ARG:HG3	2.20	0.42
70:AI:86:LEU:O	70:AI:90:GLN:HG2	2.19	0.42
72:AK:38:THR:OG1	72:AK:39:GLU:N	2.52	0.42
72:AK:86:GLU:CD	72:AK:87:PRO:HD2	2.45	0.42
79:AR:8:ARG:NH1	79:AR:48:ASP:O	2.51	0.42
79:AR:133:ASN:HD21	79:AR:139:LYS:HG2	1.84	0.42
79:AR:174:VAL:HG22	79:AR:219:TRP:HZ3	1.84	0.42
3:D:418:A:H62	5:F:16:G:H1'	1.81	0.42
3:D:739:G:HO2'	3:D:740:G:P	2.41	0.42
10:K:209:PRO:HB2	10:K:211:HIS:ND1	2.34	0.42
12:M:148:GLU:OE2	18:S:6:TYR:OH	2.24	0.42
17:R:25:VAL:HB	17:R:38:VAL:HG22	1.99	0.42
19:T:58:LEU:HD23	19:T:58:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:14:ILE:HD13	33:h:17:ARG:HH21	1.83	0.42
48:w:1166:G:N7	71:AJ:25:LYS:NZ	2.67	0.42
48:w:1778:C:H2'	48:w:1779:G:C8	2.53	0.42
55:3:18:VAL:HG12	55:3:20:ASP:H	1.85	0.42
55:3:225:GLN:HA	55:3:228:ILE:HG22	2.01	0.42
58:6:34:GLU:HG3	58:6:35:TYR:CD1	2.54	0.42
61:9:25:TRP:CG	75:AN:82:LYS:HD2	2.54	0.42
67:AF:37:VAL:C	67:AF:39:LEU:H	2.27	0.42
71:AJ:140:ARG:HD2	71:AJ:141:PRO:HD2	2.02	0.42
3:D:2705:G:H1	3:D:2710:C:N4	2.18	0.42
3:D:2739:C:H5''	46:u:69:TRP:CH2	2.55	0.42
3:D:3759:A:H5'	3:D:3765:G:H22	1.84	0.42
3:D:3896:C:HO2'	7:H:268:ARG:HH22	1.61	0.42
15:P:129:ASP:N	15:P:129:ASP:OD1	2.49	0.42
20:U:119:VAL:HG12	20:U:146:ILE:HG12	2.00	0.42
47:v:7:TRP:N	47:v:44:ILE:HD11	2.35	0.42
48:w:220:U:H2'	48:w:221:A:C8	2.55	0.42
48:w:474:G:O2'	48:w:508:A:OP2	2.25	0.42
48:w:1797:U:H2'	48:w:1798:C:C6	2.55	0.42
49:x:7:VAL:HG13	49:x:8:LEU:HG	2.02	0.42
58:6:127:ARG:HD3	78:AQ:104:ARG:HD3	2.02	0.42
58:6:143:ASN:C	58:6:144:ILE:HG13	2.45	0.42
60:8:117:PHE:C	60:8:119:ASP:H	2.28	0.42
69:AH:74:LYS:O	69:AH:81:LYS:HD2	2.20	0.42
75:AN:56:CYS:SG	75:AN:59:CYS:HB2	2.60	0.42
79:AR:225:LYS:NZ	79:AR:227:LEU:HD13	2.34	0.42
3:D:1837:A:OP2	24:Y:130:ARG:NH2	2.45	0.42
3:D:2899:C:P	22:W:108:ARG:HH22	2.43	0.42
9:J:41:LYS:HB2	24:Y:68:THR:O	2.19	0.42
12:M:63:LEU:HD12	18:S:32:GLN:HB2	2.02	0.42
15:P:91:GLU:OE2	63:AB:12:PHE:HA	2.20	0.42
34:i:37:GLY:O	34:i:41:ARG:HG3	2.19	0.42
48:w:1520:G:N3	48:w:1520:G:H2'	2.34	0.42
48:w:1693:G:H21	48:w:1834:A:H8	1.66	0.42
53:1:198:ARG:NE	53:1:200:ARG:HE	2.18	0.42
55:3:167:LYS:HE3	55:3:167:LYS:HB3	1.80	0.42
58:6:93:LYS:HG2	58:6:96:TYR:HD2	1.83	0.42
75:AN:50:ALA:C	75:AN:52:THR:H	2.28	0.42
79:AR:62:HIS:CD2	79:AR:82:SER:HB3	2.55	0.42
2:B:54:5MU:H2'	2:B:55:PSU:H4'	2.02	0.42
3:D:1340:OMC:OP1	31:f:6:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:79:TYR:O	9:J:82:GLU:HG2	2.20	0.42
48:w:440:G:O2'	48:w:1737:G:H1'	2.19	0.42
48:w:627:OMU:H6	48:w:627:OMU:H2'	1.90	0.42
48:w:823:U:H1'	58:6:140:GLN:HE22	1.84	0.42
48:w:991:G:C6	48:w:1134:G:H4'	2.54	0.42
48:w:1016:U:H5'	61:9:15:ALA:O	2.20	0.42
48:w:1465:A:O3'	65:AD:10:LYS:NZ	2.51	0.42
48:w:1490:OMG:OP2	48:w:1490:OMG:H8	2.03	0.42
49:x:39:TYR:CD2	49:x:40:LYS:HG2	2.55	0.42
49:x:213:GLU:HA	49:x:216:ALA:HB3	2.01	0.42
54:2:19:LEU:O	54:2:48:TYR:HA	2.20	0.42
55:3:7:PHE:CE2	55:3:9:ALA:HB3	2.55	0.42
55:3:54:GLY:O	55:3:110:ASN:HB2	2.20	0.42
56:4:149:ASP:C	56:4:151:SER:H	2.28	0.42
65:AD:27:ASP:O	65:AD:31:ASN:ND2	2.52	0.42
66:AE:34:LYS:HB2	66:AE:100:ALA:HA	2.02	0.42
2:B:13:C:H2'	2:B:14:A:H8	1.85	0.42
3:D:109:G:OP2	16:Q:74:ARG:NH1	2.38	0.42
3:D:677:G:H2'	3:D:678:C:C6	2.55	0.42
3:D:2403:A:OP1	37:I:10:ARG:HD2	2.20	0.42
3:D:3856:A:H5''	20:U:83:TRP:O	2.20	0.42
3:D:4733:C:O2	3:D:4734:A:H8	2.03	0.42
4:E:48:G:OP1	9:J:226:TYR:OH	2.37	0.42
6:G:125:LYS:HA	6:G:128:ARG:HD2	2.02	0.42
7:H:14:LEU:O	7:H:17:LEU:HB2	2.20	0.42
7:H:229:LYS:HG3	7:H:272:LYS:HD3	2.02	0.42
8:I:25:PRO:HG2	8:I:28:PHE:CE2	2.54	0.42
8:I:178:ASN:HA	8:I:181:LYS:HG2	2.02	0.42
11:L:30:ILE:HA	11:L:33:LEU:HG	2.01	0.42
11:L:137:GLU:N	11:L:138:PRO:HD2	2.33	0.42
14:O:51:HIS:CD2	14:O:168:SER:HB2	2.55	0.42
34:i:33:ILE:O	34:i:36:VAL:HG22	2.20	0.42
48:w:457:C:H2'	48:w:458:A:H8	1.85	0.42
48:w:517:OMC:H1'	48:w:517:OMC:HM23	1.75	0.42
48:w:1300:U:H5''	48:w:1301:A:H5'	2.01	0.42
48:w:1491:G:H2'	48:w:1492:U:C6	2.54	0.42
52:0:40:ARG:HH21	52:0:41:VAL:HG12	1.85	0.42
52:0:67:ARG:NE	59:7:93:THR:O	2.40	0.42
58:6:91:LYS:HB3	58:6:96:TYR:CD2	2.55	0.42
65:AD:58:MET:O	65:AD:62:GLN:HG2	2.20	0.42
66:AE:21:ASP:OD2	66:AE:23:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AE:36:VAL:HG21	66:AE:71:MET:HE3	2.01	0.42
66:AE:39:ARG:NH1	67:AF:38:LYS:HB2	2.35	0.42
72:AK:47:MET:SD	72:AK:48:TYR:HD1	2.43	0.42
79:AR:191:HIS:NE2	79:AR:209:SER:OG	2.44	0.42
3:D:1761:G:H1	3:D:1771:U:H3	1.68	0.42
3:D:2814:C:H5'	3:D:2815:A2M:OP2	2.19	0.42
3:D:4143:G:O2'	3:D:4144:C:H4'	2.20	0.42
16:Q:65:ARG:HG3	31:f:69:PHE:CD2	2.54	0.42
20:U:54:GLN:HA	20:U:83:TRP:CD1	2.55	0.42
48:w:153:G:N3	55:3:13:GLN:NE2	2.65	0.42
48:w:1102:G:H22	48:w:1130:G:N2	2.18	0.42
48:w:1834:A:H2	48:w:1837:G:N1	2.14	0.42
53:1:99:PHE:HE1	53:1:113:ARG:HG2	1.85	0.42
57:5:36:THR:OG1	57:5:57:ALA:O	2.28	0.42
66:AE:26:ILE:HG13	66:AE:45:LEU:HD11	2.02	0.42
79:AR:169:GLY:O	79:AR:195:LEU:HB2	2.20	0.42
3:D:231:U:H4'	29:d:100:HIS:CD2	2.54	0.41
3:D:385:A:H1'	3:D:386:A:H5''	2.02	0.41
3:D:2484:A:H3'	3:D:2485:U:O4'	2.20	0.41
6:G:116:LEU:HD23	6:G:164:ALA:HB2	2.02	0.41
6:G:117:GLU:HA	6:G:124:GLY:HA2	2.02	0.41
7:H:219:VAL:HG11	7:H:337:VAL:CG2	2.50	0.41
8:I:138:MET:HE1	8:I:145:GLU:OE2	2.20	0.41
28:c:127:LEU:HD11	28:c:135:LYS:HD3	2.01	0.41
29:d:50:ARG:HG2	29:d:51:LYS:H	1.85	0.41
41:p:7:GLU:OE1	41:p:7:GLU:N	2.53	0.41
41:p:12:LEU:HB3	41:p:16:ARG:NH1	2.33	0.41
42:q:38:ASN:C	42:q:40:LYS:H	2.28	0.41
48:w:428:OMU:H2'	48:w:428:OMU:H6	1.82	0.41
48:w:902:G:C6	48:w:903:A:H8	2.38	0.41
48:w:1610:G:P	66:AE:121:ARG:HH21	2.43	0.41
48:w:1651:A:H1'	54:2:83:ASN:ND2	2.35	0.41
49:x:30:LEU:HD22	49:x:47:TYR:HE2	1.84	0.41
51:z:108:LYS:HE3	51:z:110:MET:HB3	2.02	0.41
55:3:78:SER:OG	55:3:81:HIS:CE1	2.73	0.41
56:4:63:PHE:CE2	56:4:95:ILE:HD11	2.55	0.41
57:5:61:ASP:OD1	57:5:62:VAL:N	2.53	0.41
61:9:19:ARG:NH1	75:AN:84:HIS:OXT	2.43	0.41
72:AK:49:LYS:HE2	72:AK:49:LYS:HB2	1.91	0.41
3:D:1787:A:N3	3:D:4210:U:O2'	2.53	0.41
3:D:1961:G:H21	3:D:2025:A:H62	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3661:G:N7	6:G:152:SER:OG	2.46	0.41
10:K:278:THR:OG1	10:K:279:ASN:N	2.52	0.41
12:M:230:TYR:HA	12:M:233:ILE:HG12	2.03	0.41
15:P:146:ARG:HG2	15:P:147:ARG:HG2	2.02	0.41
17:R:34:ASN:O	17:R:51:PRO:HA	2.20	0.41
17:R:36:ALA:HB2	17:R:52:PHE:CZ	2.55	0.41
48:w:163:U:OP1	55:3:84:TYR:HA	2.20	0.41
48:w:292:A:H5'	60:8:41:GLY:H	1.85	0.41
48:w:522:A:N6	48:w:644:OMG:OP1	2.53	0.41
48:w:929:G:N2	48:w:1013:U:O2	2.53	0.41
48:w:1235:G:O2'	63:AB:134:GLY:O	2.29	0.41
48:w:1531:A:H2'	48:w:1532:C:C6	2.56	0.41
48:w:1692:PSU:H2'	48:w:1693:G:C8	2.54	0.41
48:w:1700:C:C2	48:w:1834:A:N6	2.88	0.41
58:6:119:LEU:HB2	58:6:159:PHE:CE2	2.55	0.41
64:AC:117:ARG:NH1	64:AC:121:VAL:HG21	2.34	0.41
67:AF:102:ARG:HD3	67:AF:102:ARG:HA	1.77	0.41
68:AG:49:LYS:HE3	68:AG:92:HIS:ND1	2.36	0.41
70:AI:15:ASN:C	70:AI:15:ASN:HD22	2.27	0.41
72:AK:76:TYR:OH	72:AK:86:GLU:OE1	2.28	0.41
79:AR:119:GLN:O	79:AR:120:ILE:HD13	2.20	0.41
3:D:302:C:OP1	18:S:68:ARG:HB2	2.20	0.41
3:D:499:G:H1'	3:D:656:C:O2	2.20	0.41
3:D:2498:C:H2'	3:D:2499:C:H6	1.85	0.41
5:F:125:C:O3'	5:F:126:C:H2'	2.19	0.41
12:M:156:VAL:O	12:M:156:VAL:HG12	2.19	0.41
21:V:122:THR:OG1	21:V:124:ASP:OD1	2.34	0.41
30:e:9:LYS:NZ	30:e:83:THR:O	2.38	0.41
30:e:33:THR:OG1	30:e:34:SER:N	2.53	0.41
48:w:601:OMG:HM23	48:w:601:OMG:H1'	1.85	0.41
48:w:913:A:OP1	56:4:99:ARG:NH2	2.52	0.41
48:w:1521:C:H5'	66:AE:129:LEU:HD22	2.02	0.41
50:y:87:ILE:HG22	50:y:101:HIS:HB2	2.02	0.41
57:5:145:ILE:HD13	57:5:145:ILE:HA	1.90	0.41
66:AE:47:LYS:HD2	66:AE:77:TYR:O	2.21	0.41
71:AJ:48:LYS:HB3	71:AJ:99:GLU:OE2	2.21	0.41
72:AK:56:PHE:HD1	72:AK:94:HIS:CE1	2.38	0.41
3:D:2824:OMC:HM23	3:D:2824:OMC:H1'	1.86	0.41
7:H:45:ALA:HB3	7:H:183:ILE:HG23	2.02	0.41
13:N:23:ARG:NH2	13:N:41:ILE:O	2.54	0.41
15:P:144:LYS:HE2	15:P:146:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:86:TRP:C	17:R:88:ALA:H	2.29	0.41
28:c:50:LYS:HE3	28:c:50:LYS:HB2	1.84	0.41
38:m:17:LEU:HD23	38:m:17:LEU:HA	1.92	0.41
43:r:79:GLU:OE2	43:r:82:LEU:HG	2.20	0.41
48:w:122:G:H21	53:1:146:THR:HG21	1.84	0.41
48:w:489:A:OP2	48:w:507:G:N2	2.41	0.41
48:w:647:U:H2'	48:w:648:A:C8	2.56	0.41
48:w:1330:G:H4'	48:w:1331:C:H3'	2.01	0.41
48:w:1425:G:O3'	64:AC:33:LYS:NZ	2.35	0.41
48:w:1861:G:H5''	74:AM:3:LYS:HA	2.01	0.41
49:x:140:VAL:HG23	49:x:142:LEU:HB2	2.03	0.41
53:1:99:PHE:CE1	53:1:113:ARG:HG2	2.55	0.41
53:1:209:HIS:CD2	53:1:219:ALA:HB2	2.54	0.41
54:2:35:LEU:HD21	54:2:146:ARG:HD3	2.02	0.41
57:5:157:LYS:HE2	57:5:157:LYS:HB2	1.85	0.41
79:AR:59:LEU:HD13	79:AR:90:TRP:CG	2.55	0.41
3:D:2459:G:H2'	3:D:2461:G:OP2	2.20	0.41
21:V:53:MET:O	21:V:58:ARG:NH1	2.50	0.41
48:w:560:A:N7	58:6:173:VAL:HG11	2.35	0.41
48:w:573:U:H1'	48:w:576:A2M:N7	2.35	0.41
48:w:917:U:O4'	56:4:118:ARG:HD2	2.21	0.41
48:w:1604:G:C6	48:w:1605:G:C4	3.08	0.41
48:w:1630:A:P	66:AE:40:TYR:HB2	2.61	0.41
49:x:157:VAL:O	69:AH:65:SER:HB3	2.20	0.41
57:5:142:SER:O	57:5:146:GLN:HB3	2.20	0.41
57:5:197:PHE:CZ	57:5:201:LYS:HE2	2.55	0.41
64:AC:24:HIS:O	64:AC:68:ILE:HA	2.21	0.41
66:AE:125:HIS:CD2	66:AE:131:VAL:HG11	2.55	0.41
71:AJ:105:PHE:CD1	71:AJ:121:LYS:HB3	2.54	0.41
2:B:30:G:OP1	63:AB:136:THR:HG23	2.20	0.41
2:B:42:U:H2'	2:B:43:U:O4'	2.20	0.41
3:D:1380:G:N2	3:D:1381:U:O4	2.49	0.41
3:D:2780:C:OP1	28:c:134:LYS:NZ	2.41	0.41
3:D:4731:G:H1	3:D:4734:A:N6	2.19	0.41
3:D:4734:A:O2'	3:D:4735:G:OP2	2.35	0.41
6:G:178:PRO:HG2	46:u:26:VAL:HG13	2.03	0.41
22:W:7:GLN:HG3	22:W:41:ILE:HD11	2.01	0.41
47:v:107:ARG:O	47:v:111:ILE:HG12	2.19	0.41
48:w:428:OMU:HM22	58:6:7:TRP:HH2	1.86	0.41
48:w:457:C:H2'	48:w:458:A:C8	2.56	0.41
48:w:1612:G:H5''	66:AE:88:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:63:LYS:O	53:1:67:GLN:HG3	2.21	0.41
54:2:20:PHE:CD2	54:2:23:TRP:HD1	2.37	0.41
57:5:193:LYS:HD3	57:5:193:LYS:HA	1.76	0.41
67:AF:5:THR:HG22	67:AF:6:VAL:N	2.36	0.41
3:D:233:U:O2'	3:D:234:G:H5''	2.21	0.41
3:D:1590:C:H5''	3:D:1591:U:O5'	2.21	0.41
3:D:4862:G:H2'	3:D:4863:G:C8	2.56	0.41
8:I:318:PRO:C	8:I:320:LYS:H	2.29	0.41
21:V:71:LYS:HE3	21:V:71:LYS:HB3	1.89	0.41
22:W:99:MET:O	22:W:103:ARG:HG3	2.20	0.41
28:c:127:LEU:O	28:c:134:LYS:HA	2.20	0.41
36:k:93:PRO:C	36:k:95:LYS:H	2.28	0.41
47:v:32:LEU:O	47:v:33:LYS:HB2	2.21	0.41
48:w:868:G:N7	56:4:115:LYS:HD2	2.36	0.41
48:w:1520:G:H5''	66:AE:136:THR:OG1	2.21	0.41
48:w:1869:A:H2'	74:AM:39:PHE:CD2	2.56	0.41
52:0:81:GLU:OE1	52:0:81:GLU:N	2.53	0.41
62:AA:147:ARG:HA	74:AM:28:ARG:HH11	1.85	0.41
70:AI:18:GLU:OE1	70:AI:65:LEU:HD12	2.21	0.41
79:AR:194:TYR:CE1	79:AR:212:LYS:HB2	2.56	0.41
3:D:184:U:H2'	3:D:189:G:OP1	2.20	0.41
3:D:189:G:H2'	3:D:190:G:H8	1.86	0.41
3:D:1574:G:O2'	3:D:1575:A:P	2.77	0.41
3:D:3784:A:O2'	3:D:3785:A2M:H3'	2.21	0.41
3:D:4612:C:O2	13:N:120:GLU:HG3	2.21	0.41
3:D:4740:G:C4	3:D:4742:G:C8	3.09	0.41
3:D:4967:A:H2'	3:D:4968:A:C8	2.56	0.41
8:I:205:ARG:HA	8:I:205:ARG:HD3	1.85	0.41
13:N:187:VAL:HG12	13:N:188:GLN:N	2.34	0.41
14:O:19:LYS:HE3	14:O:19:LYS:HB2	1.88	0.41
18:S:146:PRO:O	18:S:147:ASP:HB2	2.21	0.41
48:w:1610:G:O5'	66:AE:121:ARG:NH2	2.46	0.41
55:3:20:ASP:OD2	55:3:23:LYS:HG3	2.21	0.41
61:9:119:GLU:O	61:9:123:HIS:ND1	2.52	0.41
79:AR:104:HIS:HE1	79:AR:122:SER:CB	2.34	0.41
3:D:257:C:H2'	3:D:258:G:H8	1.84	0.41
3:D:1574:G:O2'	3:D:1575:A:H8	2.04	0.41
3:D:1604:G:H2'	3:D:1605:G:C8	2.56	0.41
3:D:1881:C:H5'	3:D:2281:U:H1'	2.02	0.41
3:D:2709:C:OP2	22:W:43:LYS:NZ	2.43	0.41
3:D:3663:A:N6	3:D:4168:G:O2'	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4522:G:O2'	3:D:4525:C:OP2	2.26	0.41
3:D:4625:C:O2'	3:D:4626:A:H5'	2.21	0.41
7:H:285:TYR:HA	7:H:363:ILE:HD11	2.02	0.41
8:I:315:LYS:HD2	11:L:168:ALA:HB1	2.02	0.41
9:J:211:LEU:HD23	9:J:211:LEU:HA	1.79	0.41
23:X:71:SER:O	23:X:76:LYS:NZ	2.54	0.41
25:Z:66:SER:HB3	25:Z:69:LYS:HB2	2.03	0.41
29:d:88:GLU:OE2	29:d:88:GLU:N	2.54	0.41
47:v:92:SER:O	47:v:96:MET:HG3	2.21	0.41
48:w:21:U:O2'	48:w:22:A:H5'	2.20	0.41
48:w:485:A:H8	48:w:485:A:OP2	2.03	0.41
48:w:572:PSU:H5'	72:AK:59:GLY:HA2	2.01	0.41
48:w:1016:U:O2	48:w:1016:U:H2'	2.20	0.41
48:w:1445:PSU:H1'	48:w:1580:A:N6	2.36	0.41
48:w:1593:C:O2	67:AF:12:GLN:NE2	2.54	0.41
48:w:1600:G:H2'	48:w:1600:G:N3	2.36	0.41
48:w:1798:C:H2'	48:w:1799:G:O4'	2.21	0.41
52:0:62:LYS:HG3	52:0:62:LYS:O	2.21	0.41
53:1:35:PRO:HD2	53:1:83:PRO:HG2	2.03	0.41
53:1:250:GLU:O	53:1:254:LYS:HG2	2.20	0.41
56:4:21:SER:O	56:4:24:SER:N	2.54	0.41
56:4:37:LYS:O	56:4:39:GLN:NE2	2.50	0.41
56:4:39:GLN:O	56:4:43:LEU:HD13	2.20	0.41
57:5:44:HIS:ND1	57:5:58:LEU:HD11	2.36	0.41
59:7:52:LEU:HD12	59:7:52:LEU:HA	1.92	0.41
61:9:142:GLU:OE1	61:9:142:GLU:HA	2.21	0.41
63:AB:90:VAL:HA	63:AB:107:ILE:HG22	2.03	0.41
65:AD:49:LYS:HE2	65:AD:49:LYS:HB3	1.81	0.41
67:AF:71:GLY:O	67:AF:75:MET:HG2	2.21	0.41
73:AL:62:VAL:N	73:AL:63:PRO:HD2	2.36	0.41
76:AO:34:PHE:C	76:AO:36:ASP:H	2.27	0.41
79:AR:29:ASP:HA	79:AR:45:LEU:HB3	2.01	0.41
79:AR:172:LYS:HG3	79:AR:193:GLY:N	2.36	0.41
79:AR:252:THR:HG21	79:AR:257:LYS:HE3	2.03	0.41
79:AR:259:TRP:CD1	79:AR:266:ILE:HG22	2.55	0.41
3:D:500:G:H2'	3:D:505:G:H8	1.86	0.41
3:D:1175:A:H2	3:D:1185:G:N2	2.18	0.41
3:D:1431:C:H2'	3:D:1432:G:O4'	2.20	0.41
3:D:4620:OMU:HM23	3:D:4620:OMU:H1'	1.90	0.41
3:D:5060:A:O2'	3:D:5061:A:OP1	2.34	0.41
7:H:90:VAL:HG23	7:H:161:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:106:LYS:HD3	8:I:108:TRP:CZ2	2.56	0.41
9:J:217:ASP:HA	9:J:220:LYS:HD3	2.03	0.41
10:K:50:LEU:HD23	10:K:50:LEU:H	1.86	0.41
14:O:32:ARG:O	14:O:33:ILE:C	2.64	0.41
16:Q:59:VAL:HG21	16:Q:73:GLY:HA3	2.01	0.41
18:S:124:ASP:OD1	18:S:125:SER:N	2.49	0.41
25:Z:24:ASP:HB3	25:Z:69:LYS:HD2	2.03	0.41
26:a:85:ARG:HH21	26:a:85:ARG:HG2	1.85	0.41
43:r:104:HIS:CE1	43:r:107:ALA:HB2	2.56	0.41
48:w:5:U:H2'	48:w:6:G:H8	1.86	0.41
48:w:1447:G:OP1	68:AG:87:ARG:NH1	2.45	0.41
48:w:1476:A:O2'	65:AD:3:ARG:NH1	2.45	0.41
49:x:38:ILE:HG13	49:x:39:TYR:N	2.36	0.41
77:AP:12:ARG:HD3	77:AP:12:ARG:HA	1.88	0.41
3:D:151:G:O6	12:M:142:THR:HG23	2.21	0.40
3:D:1332:C:H2'	3:D:1333:A:C8	2.56	0.40
3:D:1408:G:H1'	3:D:1411:C:N4	2.36	0.40
3:D:1553:A:H62	3:D:1574:G:H1'	1.86	0.40
3:D:1742:A:OP2	9:J:10:LYS:HD2	2.21	0.40
3:D:2519:U:O2'	3:D:2530:U:O2	2.38	0.40
3:D:4415:A:H4'	14:O:74:LYS:HE2	2.04	0.40
3:D:4957:C:H2'	3:D:4958:C:O4'	2.21	0.40
9:J:214:GLU:HB3	9:J:215:ASP:H	1.79	0.40
15:P:136:ARG:HD2	15:P:155:HIS:O	2.21	0.40
20:U:4:TYR:OH	20:U:18:ARG:HG3	2.21	0.40
23:X:43:ARG:HD2	23:X:43:ARG:HA	1.79	0.40
24:Y:143:THR:O	24:Y:145:GLY:N	2.52	0.40
29:d:69:LYS:HE2	29:d:69:LYS:HB3	1.73	0.40
47:v:21:ASN:O	47:v:23:GLN:HG2	2.21	0.40
48:w:176:U:H2'	48:w:177:G:H8	1.85	0.40
48:w:824:C:N1	58:6:144:ILE:HD13	2.36	0.40
48:w:880:G:N3	48:w:880:G:H3'	2.36	0.40
48:w:981:A:H2'	48:w:982:G:C8	2.55	0.40
48:w:1403:C:H2'	48:w:1433:C:H42	1.85	0.40
50:y:25:PHE:CD1	62:AA:88:LEU:HD11	2.56	0.40
53:1:181:CYS:O	53:1:192:ILE:HA	2.21	0.40
55:3:50:VAL:CG2	55:3:111:LEU:HB3	2.51	0.40
55:3:63:MET:HE3	55:3:99:GLY:O	2.21	0.40
55:3:138:ALA:HB1	55:3:142:ARG:HH21	1.86	0.40
58:6:65:GLU:HG3	58:6:66:LYS:H	1.86	0.40
61:9:100:LYS:O	61:9:103:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AR:14:HIS:ND1	79:AR:16:GLY:O	2.54	0.40
3:D:2103:G:O2'	3:D:2104:G:H8	2.05	0.40
3:D:2259:G:O2'	3:D:2261:G:N2	2.55	0.40
3:D:2730:U:H2'	3:D:2731:C:C6	2.56	0.40
3:D:4405:G:H5'	14:O:8:CYS:SG	2.61	0.40
4:E:30:C:C2	4:E:48:G:N2	2.89	0.40
8:I:184:TYR:CZ	8:I:225:PRO:HG2	2.57	0.40
11:L:220:MET:C	11:L:222:LYS:H	2.28	0.40
33:h:11:LEU:H	33:h:11:LEU:HD23	1.86	0.40
40:o:32:SER:O	40:o:40:PRO:HG3	2.22	0.40
48:w:1337:4AC:H2'	48:w:1338:G:H8	1.85	0.40
48:w:1459:G:OP2	79:AR:280:LYS:NZ	2.50	0.40
48:w:1597:C:OP1	66:AE:25:LYS:NZ	2.40	0.40
49:x:78:SER:HB2	49:x:87:VAL:HG11	2.03	0.40
62:AA:75:MET:HB3	62:AA:114:SER:HB3	2.03	0.40
63:AB:37:TYR:O	63:AB:42:ARG:NH2	2.53	0.40
68:AG:17:ILE:HG13	68:AG:92:HIS:HB3	2.02	0.40
70:AI:12:LYS:HA	70:AI:12:LYS:HD3	1.94	0.40
70:AI:115:GLU:HB3	70:AI:118:ARG:NH2	2.36	0.40
75:AN:14:GLU:O	75:AN:17:ARG:HG2	2.22	0.40
75:AN:50:ALA:O	75:AN:52:THR:HG22	2.21	0.40
79:AR:131:LEU:H	79:AR:131:LEU:HD23	1.86	0.40
79:AR:178:ASN:O	79:AR:182:CYS:HA	2.21	0.40
2:C:15:G:N2	2:C:21:A:N3	2.69	0.40
3:D:208:A:C2	3:D:233:U:H5''	2.55	0.40
3:D:741:C:H42	3:D:923:C:H42	1.68	0.40
3:D:1194:G:H2'	3:D:1195:G:C8	2.57	0.40
3:D:3710:G:H5'	3:D:3711:A:OP1	2.21	0.40
3:D:4859:C:H5''	3:D:4860:G:N7	2.37	0.40
5:F:86:U:H4'	5:F:87:G:OP1	2.20	0.40
13:N:92:MET:SD	13:N:161:ILE:HD11	2.62	0.40
14:O:208:LYS:HA	14:O:211:VAL:HG12	2.04	0.40
16:Q:128:PRO:HB2	16:Q:130:LYS:O	2.20	0.40
23:X:155:PRO:O	23:X:156:HIS:C	2.64	0.40
48:w:502:C:O3'	53:1:62:LYS:NZ	2.41	0.40
49:x:85:ARG:HD2	65:AD:81:ARG:CD	2.52	0.40
50:y:108:ASP:OD1	50:y:108:ASP:N	2.54	0.40
53:1:92:ILE:HG22	53:1:97:GLU:O	2.21	0.40
54:2:20:PHE:CE1	54:2:50:PRO:HD3	2.56	0.40
58:6:164:PRO:HB3	58:6:170:PRO:HA	2.02	0.40
59:7:57:TYR:HD1	59:7:75:GLY:HA2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:AK:88:LYS:HD2	72:AK:97:TYR:CE2	2.55	0.40
3:D:233:U:O2'	3:D:233:U:O2	2.37	0.40
3:D:2464:C:HO2'	3:D:2465:C:P	2.45	0.40
3:D:4458:C:H2'	3:D:4459:U:C6	2.57	0.40
8:I:150:LEU:HA	8:I:150:LEU:HD12	1.81	0.40
9:J:228:LYS:O	9:J:229:ASN:HB2	2.20	0.40
18:S:119:TYR:OH	18:S:131:GLU:OE2	2.28	0.40
31:f:93:ASN:O	31:f:94:LYS:HE2	2.21	0.40
34:i:36:VAL:HG11	34:i:44:ARG:CD	2.50	0.40
36:k:48:ALA:HB2	36:k:71:TRP:CZ3	2.56	0.40
39:n:44:ILE:HD13	39:n:44:ILE:HA	1.89	0.40
41:p:19:ASP:O	41:p:38:CYS:HA	2.21	0.40
48:w:1558:C:H2'	48:w:1559:C:C6	2.57	0.40
48:w:1601:A:H5'	48:w:1602:U:OP1	2.21	0.40
62:AA:126:ILE:O	74:AM:57:SER:HA	2.21	0.40
68:AG:32:LEU:HD13	68:AG:87:ARG:HG2	2.03	0.40
3:D:1703:C:OP1	8:I:308:LYS:NZ	2.33	0.40
3:D:2631:U:OP2	25:Z:48:LYS:NZ	2.54	0.40
3:D:2711:G:OP1	22:W:39:GLN:NE2	2.55	0.40
3:D:4457:PSU:O4	7:H:252:ALA:HB3	2.22	0.40
7:H:92:TYR:HB2	7:H:159:VAL:HB	2.04	0.40
9:J:41:LYS:HA	9:J:41:LYS:HD2	1.87	0.40
22:W:172:ARG:NE	48:w:909:G:OP1	2.55	0.40
28:c:84:GLU:H	28:c:84:GLU:HG2	1.73	0.40
28:c:100:VAL:HG22	28:c:134:LYS:O	2.21	0.40
33:h:98:ASP:HA	33:h:99:PRO:HD3	1.87	0.40
48:w:958:G:C6	48:w:959:G:C6	3.08	0.40
48:w:1097:G:H4'	49:x:32:PHE:CE1	2.57	0.40
48:w:1454:A:H5''	65:AD:3:ARG:HD2	2.02	0.40
49:x:168:ALA:HB1	49:x:204:TYR:HB3	2.03	0.40
54:2:44:LYS:HA	54:2:44:LYS:HD3	1.95	0.40
57:5:17:LYS:HB2	57:5:17:LYS:HE3	1.83	0.40
57:5:129:LEU:O	57:5:133:GLU:HG2	2.21	0.40
58:6:61:LEU:HD23	58:6:61:LEU:HA	1.80	0.40
62:AA:113:GLN:NE2	74:AM:44:ILE:O	2.55	0.40
71:AJ:94:ILE:HG12	71:AJ:125:VAL:HG21	2.03	0.40
75:AN:33:MET:HE3	75:AN:73:LEU:HD21	2.03	0.40
79:AR:88:ARG:HD2	79:AR:97:THR:HG21	2.02	0.40
79:AR:292:SER:HB2	79:AR:297:THR:HB	2.03	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%)	227 (93%)	18 (7%)	0	100	100
7	H	396/403 (98%)	367 (93%)	29 (7%)	0	100	100
8	I	361/427 (84%)	338 (94%)	23 (6%)	0	100	100
9	J	291/297 (98%)	274 (94%)	17 (6%)	0	100	100
10	K	211/288 (73%)	191 (90%)	20 (10%)	0	100	100
11	L	223/248 (90%)	212 (95%)	11 (5%)	0	100	100
12	M	223/266 (84%)	207 (93%)	16 (7%)	0	100	100
13	N	188/192 (98%)	174 (93%)	14 (7%)	0	100	100
14	O	202/214 (94%)	186 (92%)	16 (8%)	0	100	100
15	P	168/178 (94%)	155 (92%)	13 (8%)	0	100	100
16	Q	206/211 (98%)	190 (92%)	14 (7%)	2 (1%)	12	28
17	R	134/215 (62%)	123 (92%)	11 (8%)	0	100	100
18	S	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
19	T	198/203 (98%)	195 (98%)	3 (2%)	0	100	100
20	U	155/184 (84%)	143 (92%)	12 (8%)	0	100	100
21	V	185/188 (98%)	176 (95%)	9 (5%)	0	100	100
22	W	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
23	X	173/176 (98%)	162 (94%)	11 (6%)	0	100	100
24	Y	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
25	Z	99/128 (77%)	92 (93%)	7 (7%)	0	100	100
26	a	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
27	b	61/157 (39%)	60 (98%)	1 (2%)	0	100	100
28	c	118/156 (76%)	112 (95%)	6 (5%)	0	100	100
29	d	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
30	e	133/136 (98%)	125 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	f	145/148 (98%)	130 (90%)	15 (10%)	0	100	100
32	g	100/159 (63%)	92 (92%)	6 (6%)	2 (2%)	6	14
33	h	95/115 (83%)	94 (99%)	1 (1%)	0	100	100
34	i	105/125 (84%)	101 (96%)	4 (4%)	0	100	100
35	j	126/135 (93%)	123 (98%)	3 (2%)	0	100	100
36	k	107/110 (97%)	97 (91%)	10 (9%)	0	100	100
37	l	110/117 (94%)	101 (92%)	9 (8%)	0	100	100
38	m	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
39	n	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
40	o	84/97 (87%)	79 (94%)	4 (5%)	1 (1%)	10	24
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%)	83 (93%)	6 (7%)	0	100	100
47	v	123/137 (90%)	115 (94%)	8 (6%)	0	100	100
49	x	213/295 (72%)	197 (92%)	15 (7%)	1 (0%)	24	45
50	y	210/264 (80%)	198 (94%)	12 (6%)	0	100	100
51	z	210/293 (72%)	200 (95%)	10 (5%)	0	100	100
52	0	210/243 (86%)	190 (90%)	20 (10%)	0	100	100
53	1	260/263 (99%)	243 (94%)	15 (6%)	2 (1%)	16	34
54	2	185/204 (91%)	171 (92%)	14 (8%)	0	100	100
55	3	235/249 (94%)	228 (97%)	7 (3%)	0	100	100
56	4	185/194 (95%)	166 (90%)	19 (10%)	0	100	100
57	5	204/208 (98%)	186 (91%)	18 (9%)	0	100	100
58	6	180/194 (93%)	171 (95%)	9 (5%)	0	100	100
59	7	94/165 (57%)	88 (94%)	6 (6%)	0	100	100
60	8	138/158 (87%)	127 (92%)	11 (8%)	0	100	100
61	9	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
62	AA	132/151 (87%)	122 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	AB	132/145 (91%)	126 (96%)	6 (4%)	0	100	100
64	AC	140/146 (96%)	129 (92%)	11 (8%)	0	100	100
65	AD	129/135 (96%)	109 (84%)	18 (14%)	2 (2%)	7	18
66	AE	142/152 (93%)	125 (88%)	17 (12%)	0	100	100
67	AF	141/145 (97%)	132 (94%)	9 (6%)	0	100	100
68	AG	100/119 (84%)	94 (94%)	6 (6%)	0	100	100
69	AH	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
70	AI	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
71	AJ	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
72	AK	121/133 (91%)	119 (98%)	2 (2%)	0	100	100
73	AL	70/125 (56%)	66 (94%)	4 (6%)	0	100	100
74	AM	97/115 (84%)	92 (95%)	5 (5%)	0	100	100
75	AN	81/84 (96%)	67 (83%)	13 (16%)	1 (1%)	10	24
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	53/59 (90%)	51 (96%)	2 (4%)	0	100	100
79	AR	311/317 (98%)	270 (87%)	41 (13%)	0	100	100
All	All	10931/12400 (88%)	10208 (93%)	712 (6%)	11 (0%)	49	71

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	48	PRO
32	g	111	ARG
53	1	227	VAL
32	g	110	ALA
65	AD	118	GLN
53	1	228	ILE
16	Q	47	ALA
49	x	12	GLU
65	AD	119	VAL
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%)	89 (99%)	1 (1%)	65	83
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%)	97 (99%)	1 (1%)	68	84
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%)	73 (100%)	0	100	100
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%)	119 (100%)	0	100	100
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	64/103 (62%)	64 (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	45/48 (94%)	45 (100%)	0	100	100
79	AR	272/275 (99%)	272 (100%)	0	100	100
All	All	9499/10553 (90%)	9497 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
25	Z	95	ASN
34	i	18	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
7	H	184	GLN
7	H	245	HIS
8	I	21	ASN
8	I	43	ASN
8	I	61	GLN
8	I	310	HIS
9	J	282	GLN
10	K	191	GLN

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Mol	Chain	Res	Type
10	K	245	GLN
10	K	268	GLN
11	L	80	ASN
13	N	98	HIS
14	O	73	ASN
14	O	177	ASN
15	P	46	GLN
15	P	98	ASN
15	P	104	ASN
16	Q	87	HIS
16	Q	115	GLN
16	Q	149	GLN
16	Q	205	GLN
17	R	66	HIS
17	R	70	GLN
18	S	15	GLN
18	S	87	HIS
18	S	158	HIS
19	T	42	ASN
20	U	10	ASN
21	V	7	HIS
22	W	40	GLN
25	Z	50	ASN
25	Z	116	GLN
29	d	14	ASN
29	d	56	GLN
31	f	60	HIS
31	f	66	ASN
32	g	6	ASN
35	j	107	ASN
37	l	73	HIS
38	m	107	GLN
40	o	66	HIS
42	q	4	HIS
42	q	17	GLN
44	s	22	GLN
45	t	90	HIS
45	t	105	GLN
47	v	30	ASN
49	x	110	ASN
49	x	113	GLN
50	y	118	GLN

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Mol	Chain	Res	Type
50	y	124	HIS
50	y	149	GLN
50	y	186	ASN
51	z	115	GLN
53	1	67	GLN
53	1	188	ASN
53	1	224	ASN
54	2	36	GLN
54	2	83	ASN
54	2	149	GLN
54	2	203	ASN
55	3	81	HIS
55	3	110	ASN
56	4	33	ASN
56	4	73	GLN
56	4	76	GLN
57	5	88	ASN
57	5	165	GLN
58	6	140	GLN
59	7	42	ASN
59	7	50	GLN
59	7	77	GLN
59	7	84	HIS
61	9	36	GLN
62	AA	103	ASN
63	AB	114	HIS
65	AD	93	GLN
66	AE	135	HIS
68	AG	81	GLN
70	AI	15	ASN
70	AI	44	HIS
71	AJ	16	HIS
71	AJ	26	GLN
71	AJ	92	ASN
73	AL	106	GLN
78	AQ	110	GLN
78	AQ	131	ASN
79	AR	56	GLN
79	AR	62	HIS
79	AR	104	HIS
79	AR	143	GLN
79	AR	196	ASN

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Mol	Chain	Res	Type
79	AR	215	GLN
79	AR	226	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	13/14 (92%)	1 (7%)	0
2	B	70/76 (92%)	24 (34%)	1 (1%)
2	C	70/76 (92%)	20 (28%)	0
3	D	3497/5070 (68%)	609 (17%)	26 (0%)
4	E	119/120 (99%)	13 (10%)	0
48	w	1624/1869 (86%)	392 (24%)	0
5	F	155/156 (99%)	25 (16%)	1 (0%)
All	All	5548/7381 (75%)	1084 (19%)	28 (0%)

All (1084) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	19	U
2	B	6	2MG
2	B	7	A
2	B	8	U
2	B	9	A
2	B	11	C
2	B	12	U
2	B	13	C
2	B	19	G
2	B	22	G
2	B	26	M2G
2	B	39	UY1
2	B	46	G7M
2	B	47	H2U
2	B	48	5MC
2	B	49	G
2	B	52	G
2	B	53	G
2	B	54	5MU
2	B	55	PSU
2	B	56	C
2	B	57	G
2	B	58	1MA

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Mol	Chain	Res	Type
2	B	67	C
2	B	76	A
2	C	4	U
2	C	6	2MG
2	C	7	A
2	C	10	2MG
2	C	12	U
2	C	19	G
2	C	24	G
2	C	45	G
2	C	46	G7M
2	C	47	H2U
2	C	48	5MC
2	C	53	G
2	C	54	5MU
2	C	59	U
2	C	61	C
2	C	63	G
2	C	68	G
2	C	71	G
2	C	72	G
2	C	74	C
3	D	2	G
3	D	21	G
3	D	25	A
3	D	39	A
3	D	42	A
3	D	44	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
3	D	98	A
3	D	108	A
3	D	109	G
3	D	110	C
3	D	116	G
3	D	117	C
3	D	119	G

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Mol	Chain	Res	Type
3	D	120	A
3	D	143	C
3	D	144	G
3	D	152	U
3	D	159	C
3	D	171	U
3	D	172	C
3	D	181	C
3	D	183	C
3	D	185	C
3	D	186	G
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	261	G
3	D	265	C
3	D	266	C
3	D	267	G
3	D	269	G
3	D	275	C
3	D	276	C
3	D	278	G
3	D	280	G
3	D	306	A
3	D	315	G
3	D	316	U
3	D	340	C
3	D	344	A
3	D	345	C
3	D	350	C
3	D	386	A
3	D	387	G
3	D	407	A
3	D	410	A
3	D	412	G
3	D	413	G
3	D	432	U

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Mol	Chain	Res	Type
3	D	449	C
3	D	450	G
3	D	452	A
3	D	453	G
3	D	454	U
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	498	C
3	D	499	G
3	D	505	G
3	D	507	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	657	C
3	D	658	C
3	D	659	G
3	D	661	C
3	D	665	C
3	D	667	A
3	D	668	C
3	D	670	G
3	D	673	C
3	D	685	C
3	D	686	A
3	D	687	U
3	D	703	G
3	D	704	C
3	D	731	G
3	D	738	C
3	D	739	G
3	D	740	G

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Mol	Chain	Res	Type
3	D	742	G
3	D	754	U
3	D	760	G
3	D	904	C
3	D	905	C
3	D	906	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	936	C
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	967	C
3	D	970	G
3	D	971	U
3	D	977	C
3	D	982	U
3	D	984	C
3	D	988	C
3	D	989	U
3	D	1071	C
3	D	1075	G
3	D	1082	C
3	D	1083	U
3	D	1094	G
3	D	1168	G
3	D	1171	G
3	D	1172	C

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Mol	Chain	Res	Type
3	D	1173	G
3	D	1178	G
3	D	1179	U
3	D	1180	C
3	D	1181	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	1241	C
3	D	1246	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	1280	C
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

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Mol	Chain	Res	Type
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	1406	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	1415	G
3	D	1417	C
3	D	1420	A
3	D	1421	G
3	D	1439	C
3	D	1441	C
3	D	1442	C
3	D	1443	A
3	D	1452	A
3	D	1482	G
3	D	1483	C
3	D	1497	A
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	1575	A
3	D	1578	U
3	D	1586	G
3	D	1591	U
3	D	1596	U

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Mol	Chain	Res	Type
3	D	1624	G
3	D	1625	OMG
3	D	1631	A
3	D	1633	G
3	D	1634	A
3	D	1638	A
3	D	1640	C
3	D	1641	G
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	1715	C
3	D	1718	C
3	D	1719	A
3	D	1734	G
3	D	1741	G
3	D	1742	A
3	D	1750	G
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
3	D	1804	A
3	D	1810	G
3	D	1821	G
3	D	1822	U
3	D	1836	G
3	D	1837	A

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Mol	Chain	Res	Type
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	1948	G
3	D	1951	G
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	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
3	D	2097	U
3	D	2098	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

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Mol	Chain	Res	Type
3	D	2259	G
3	D	2277	C
3	D	2289	C
3	D	2300	A
3	D	2301	G
3	D	2306	G
3	D	2313	A
3	D	2333	G
3	D	2348	G
3	D	2351	OMC
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	2447	U
3	D	2450	G
3	D	2453	A
3	D	2465	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
3	D	2504	C
3	D	2505	C
3	D	2511	A
3	D	2513	A
3	D	2519	U
3	D	2520	C
3	D	2529	A
3	D	2537	A
3	D	2545	U
3	D	2546	G

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Mol	Chain	Res	Type
3	D	2547	G
3	D	2554	U
3	D	2555	G
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	2675	G
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	2721	G
3	D	2724	G
3	D	2726	G
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
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

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Mol	Chain	Res	Type
3	D	2856	C
3	D	2867	C
3	D	2874	U
3	D	2877	G
3	D	2892	C
3	D	3605	C
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	3750	G
3	D	3756	A
3	D	3757	G
3	D	3758	PSU
3	D	3759	A
3	D	3760	A2M
3	D	3761	C
3	D	3762	PSU
3	D	3766	A
3	D	3772	U
3	D	3773	U
3	D	3774	A
3	D	3777	G
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

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Mol	Chain	Res	Type
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	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	3942	A
3	D	3943	A
3	D	3944	OMG
3	D	4068	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	4112	C
3	D	4113	U
3	D	4114	C
3	D	4115	G
3	D	4116	C
3	D	4119	C
3	D	4122	G
3	D	4127	A
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

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Mol	Chain	Res	Type
3	D	4170	A
3	D	4183	G
3	D	4184	G
3	D	4191	G
3	D	4203	A
3	D	4222	G
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	4306	OMU
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	4405	G
3	D	4422	A
3	D	4424	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

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Mol	Chain	Res	Type
3	D	4513	A
3	D	4519	C
3	D	4524	G
3	D	4548	A
3	D	4554	G
3	D	4560	C
3	D	4567	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	4636	U
3	D	4637	OMG
3	D	4656	A
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
3	D	4732	G
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	4774	C
3	D	4860	G
3	D	4870	G
3	D	4871	C
3	D	4875	G

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Mol	Chain	Res	Type
3	D	4882	U
3	D	4883	C
3	D	4888	U
3	D	4889	G
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	4934	A
3	D	4940	C
3	D	4941	G
3	D	4943	A
3	D	4949	G
3	D	4955	A
3	D	4960	G
3	D	4966	A
3	D	4976	U
3	D	4990	C
3	D	4991	U
3	D	5014	A
3	D	5016	A
3	D	5017	G
3	D	5023	C
3	D	5024	C
3	D	5025	C
3	D	5027	C
3	D	5028	G
3	D	5030	U
3	D	5031	G
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

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Mol	Chain	Res	Type
3	D	5069	U
4	E	7	G
4	E	22	A
4	E	24	C
4	E	47	G
4	E	48	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	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	83	C
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
48	w	2	A
48	w	4	C
48	w	11	A

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Mol	Chain	Res	Type
48	w	17	C
48	w	21	U
48	w	22	A
48	w	33	G
48	w	34	PSU
48	w	41	G
48	w	43	U
48	w	44	U
48	w	45	A
48	w	46	A
48	w	49	C
48	w	52	G
48	w	54	A
48	w	61	A
48	w	66	G
48	w	67	C
48	w	68	A
48	w	69	C
48	w	70	G
48	w	78	C
48	w	79	A
48	w	80	G
48	w	81	U
48	w	83	A
48	w	86	C
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	128	U
48	w	129	C
48	w	130	G
48	w	143	U
48	w	149	A
48	w	155	G
48	w	159	A2M
48	w	160	U
48	w	161	U
48	w	162	C

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Mol	Chain	Res	Type
48	w	163	U
48	w	166	A2M
48	w	171	A
48	w	173	A
48	w	179	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	201	C
48	w	207	G
48	w	211	G
48	w	214	U
48	w	215	G
48	w	226	A
48	w	291	G
48	w	292	A
48	w	293	C
48	w	294	U
48	w	302	A
48	w	310	C
48	w	311	C
48	w	312	G
48	w	313	A
48	w	318	A
48	w	319	C
48	w	332	G
48	w	345	U
48	w	346	C
48	w	347	G
48	w	362	C
48	w	364	A
48	w	368	U
48	w	369	C
48	w	370	G
48	w	380	G
48	w	385	G

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Mol	Chain	Res	Type
48	w	386	C
48	w	400	C
48	w	407	G
48	w	408	A
48	w	409	C
48	w	417	C
48	w	418	A
48	w	421	G
48	w	428	OMU
48	w	441	C
48	w	448	A
48	w	449	A
48	w	450	C
48	w	451	G
48	w	452	G
48	w	464	A
48	w	466	G
48	w	468	A2M
48	w	471	G
48	w	472	C
48	w	474	G
48	w	476	A
48	w	482	G
48	w	485	A
48	w	487	U
48	w	488	U
48	w	489	A
48	w	492	C
48	w	493	A
48	w	495	U
48	w	496	C
48	w	497	C
48	w	498	C
48	w	499	G
48	w	501	C
48	w	507	G
48	w	516	A
48	w	519	A
48	w	523	A
48	w	528	A
48	w	531	A
48	w	532	C

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Mol	Chain	Res	Type
48	w	533	A
48	w	534	G
48	w	549	C
48	w	552	G
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	575	A
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	594	A
48	w	595	U
48	w	596	U
48	w	597	G
48	w	604	A
48	w	605	A
48	w	606	G
48	w	608	C
48	w	612	U
48	w	614	C
48	w	616	A
48	w	617	G
48	w	627	OMU
48	w	628	A
48	w	634	A
48	w	643	A
48	w	655	A
48	w	660	C
48	w	664	A
48	w	668	A2M
48	w	669	A
48	w	671	A
48	w	672	A

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Mol	Chain	Res	Type
48	w	688	U
48	w	810	A
48	w	811	A
48	w	812	A
48	w	821	G
48	w	822	PSU
48	w	830	A
48	w	834	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	847	A
48	w	849	A
48	w	869	A
48	w	870	A
48	w	872	A
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	913	A
48	w	920	A
48	w	922	A
48	w	930	C
48	w	933	G

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Mol	Chain	Res	Type
48	w	934	G
48	w	943	U
48	w	958	G
48	w	970	G
48	w	971	G
48	w	972	A
48	w	990	A
48	w	992	A
48	w	999	G
48	w	1017	U
48	w	1023	A
48	w	1027	A
48	w	1055	A
48	w	1060	A
48	w	1061	U
48	w	1062	A
48	w	1083	A
48	w	1084	A
48	w	1085	C
48	w	1109	C
48	w	1115	U
48	w	1116	C
48	w	1117	C
48	w	1118	C
48	w	1119	A
48	w	1121	G
48	w	1126	G
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

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Mol	Chain	Res	Type
48	w	1243	U
48	w	1251	A
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	1289	U
48	w	1293	A
48	w	1295	A
48	w	1298	G
48	w	1301	A
48	w	1302	G
48	w	1303	C
48	w	1304	U
48	w	1307	U
48	w	1308	U
48	w	1309	C
48	w	1331	C
48	w	1332	A
48	w	1333	U
48	w	1341	C
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	1401	A
48	w	1402	A
48	w	1403	C
48	w	1408	U
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	1447	G
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	1477	U
48	w	1487	A
48	w	1489	A
48	w	1490	OMG
48	w	1497	G
48	w	1498	A
48	w	1508	A
48	w	1509	U
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	1535	U
48	w	1543	U
48	w	1545	A
48	w	1546	G
48	w	1548	G
48	w	1550	G
48	w	1552	G
48	w	1553	C
48	w	1555	U
48	w	1556	A
48	w	1570	G
48	w	1574	C
48	w	1579	A

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Mol	Chain	Res	Type
48	w	1580	A
48	w	1585	U
48	w	1586	U
48	w	1588	A
48	w	1599	U
48	w	1600	G
48	w	1602	U
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	1636	G
48	w	1637	A
48	w	1639	G7M
48	w	1640	A
48	w	1648	G
48	w	1654	G
48	w	1661	A
48	w	1663	A
48	w	1665	G
48	w	1699	A
48	w	1721	U
48	w	1722	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
48	w	1784	G
48	w	1786	U
48	w	1800	A
48	w	1803	U
48	w	1804	OMU
48	w	1813	A
48	w	1824	A
48	w	1829	G

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Mol	Chain	Res	Type
48	w	1831	A
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 (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	48	5MC
3	D	1	C
3	D	385	A
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	1303	A
3	D	1574	G
3	D	1633	G
3	D	1755	C
3	D	2101	C
3	D	2102	G
3	D	2675	G
3	D	3614	G
3	D	3673	C
3	D	3773	U
3	D	4113	U
3	D	4115	G
3	D	4378	A
3	D	4600	G
3	D	4678	G
3	D	4699	U
3	D	4913	G
3	D	5016	A

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Mol	Chain	Res	Type
5	F	86	U

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

222 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G7M	B	46	2	23,26,27	2.84	9 (39%)	35,39,42	1.77	7 (20%)
3	PSU	D	4500	3	18,21,22	1.04	1 (5%)	22,30,33	1.87	4 (18%)
48	OMC	w	462	48	19,22,23	2.98	8 (42%)	26,31,34	0.72	0
48	OMC	w	1391	48	19,22,23	2.96	8 (42%)	26,31,34	0.72	0
3	A2M	D	2363	3,81	22,25,26	1.38	2 (9%)	31,36,39	0.98	3 (9%)
48	OMU	w	627	48	19,22,23	2.91	8 (42%)	26,31,34	1.68	4 (15%)
2	5MU	B	54	2	19,22,23	4.75	5 (26%)	28,32,35	3.62	9 (32%)
3	A2M	D	1534	3,81	22,25,26	1.34	1 (4%)	31,36,39	1.31	6 (19%)
48	4AC	w	1842	48	21,24,25	0.57	0	29,34,37	1.17	4 (13%)
3	OMC	D	3701	3,81	19,22,23	2.85	8 (42%)	26,31,34	0.76	0
48	A2M	w	590	48	22,25,26	1.49	2 (9%)	31,36,39	1.06	2 (6%)
3	OMG	D	1760	3	23,26,27	2.64	8 (34%)	33,38,41	1.94	9 (27%)
48	PSU	w	1347	48	18,21,22	1.01	1 (5%)	22,30,33	1.79	4 (18%)
48	A2M	w	1383	48	22,25,26	1.47	1 (4%)	31,36,39	1.11	3 (9%)
48	OMG	w	601	48	23,26,27	2.59	9 (39%)	33,38,41	1.93	10 (30%)
48	OMU	w	799	48	19,22,23	2.95	8 (42%)	26,31,34	1.67	5 (19%)
3	PSU	D	3695	3	18,21,22	1.02	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	3762	3	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
3	UY1	D	3818	3,81	19,22,23	1.10	1 (5%)	22,31,34	0.93	1 (4%)
48	PSU	w	34	48	18,21,22	1.10	1 (5%)	22,30,33	1.79	4 (18%)
48	OMU	w	172	48	19,22,23	2.90	7 (36%)	26,31,34	1.73	5 (19%)
3	A2M	D	3830	3	22,25,26	1.38	1 (4%)	31,36,39	1.07	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	D	4403	3,81	18,21,22	1.04	1 (5%)	22,30,33	1.84	4 (18%)
3	PSU	D	3758	3	18,21,22	0.96	1 (5%)	22,30,33	1.86	5 (22%)
48	A2M	w	576	48	22,25,26	1.41	2 (9%)	31,36,39	1.05	2 (6%)
3	OMG	D	4618	3	23,26,27	2.54	9 (39%)	33,38,41	1.90	10 (30%)
3	A2M	D	2787	3,81	22,25,26	1.38	1 (4%)	31,36,39	1.04	2 (6%)
2	PSU	B	35	2,1	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
2	2MG	B	6	2	23,26,27	2.60	8 (34%)	32,38,41	2.24	13 (40%)
3	OMC	D	2422	3,81	19,22,23	2.87	8 (42%)	26,31,34	0.72	0
3	OMU	D	4620	3	19,22,23	2.75	6 (31%)	26,31,34	1.79	5 (19%)
48	PSU	w	109	48	18,21,22	1.06	1 (5%)	22,30,33	1.85	5 (22%)
3	PSU	D	1781	3	18,21,22	1.02	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4312	3	18,21,22	1.02	1 (5%)	22,30,33	1.89	5 (22%)
3	OMC	D	2804	3	19,22,23	2.86	8 (42%)	26,31,34	0.68	0
3	PSU	D	5010	3	18,21,22	1.04	1 (5%)	22,30,33	1.85	4 (18%)
2	1MG	C	37	2	22,26,27	2.65	7 (31%)	33,39,42	1.73	8 (24%)
48	OMG	w	509	48	23,26,27	2.58	8 (34%)	33,38,41	1.97	10 (30%)
3	6MZ	D	4220	3	22,25,26	2.81	4 (18%)	30,36,39	2.25	10 (33%)
2	M2G	C	27	2	24,27,28	1.09	2 (8%)	35,40,43	0.87	1 (2%)
3	PSU	D	3715	3	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)
3	OMU	D	4227	3	19,22,23	2.79	6 (31%)	26,31,34	1.78	4 (15%)
48	PSU	w	1625	48	18,21,22	1.08	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	4628	3	18,21,22	1.05	1 (5%)	22,30,33	1.89	4 (18%)
48	PSU	w	815	48	18,21,22	1.08	1 (5%)	22,30,33	1.88	5 (22%)
3	1MA	D	1322	3	21,25,26	0.70	0	31,37,40	0.79	1 (3%)
48	PSU	w	1177	48	18,21,22	1.04	1 (5%)	22,30,33	1.82	4 (18%)
2	PSU	C	55	2	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
3	OMC	D	2365	3,81	19,22,23	2.83	8 (42%)	26,31,34	0.72	0
3	OMG	D	2364	3	23,26,27	2.53	9 (39%)	33,38,41	1.95	10 (30%)
3	A2M	D	4523	3,81	22,25,26	1.45	2 (9%)	31,36,39	1.07	2 (6%)
48	PSU	w	36	48	18,21,22	1.06	1 (5%)	22,30,33	1.81	5 (22%)
2	M2G	B	26	2	24,27,28	1.11	3 (12%)	35,40,43	0.88	0
48	PSU	w	1692	48	18,21,22	1.03	1 (5%)	22,30,33	1.81	4 (18%)
3	A2M	D	1871	3,81	22,25,26	1.44	1 (4%)	31,36,39	1.17	3 (9%)
3	OMC	D	2351	3,81	19,22,23	2.80	7 (36%)	26,31,34	0.83	1 (3%)
3	PSU	D	5001	3,81	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
3	PSU	D	2632	3	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	D	3792	3	23,26,27	2.56	9 (39%)	33,38,41	1.90	9 (27%)
3	OMG	D	4228	3	23,26,27	2.53	9 (39%)	33,38,41	1.97	10 (30%)
3	OMG	D	3627	3	23,26,27	2.56	9 (39%)	33,38,41	1.98	10 (30%)
3	PSU	D	3853	3,81	18,21,22	1.03	1 (5%)	22,30,33	1.77	4 (18%)
48	OMG	w	683	48	23,26,27	2.60	9 (39%)	33,38,41	1.95	9 (27%)
3	OMG	D	3944	3	23,26,27	2.61	8 (34%)	33,38,41	1.92	9 (27%)
48	PSU	w	966	48	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
48	PSU	w	1046	48	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
48	PSU	w	1643	81,48	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)
3	OMU	D	3925	3	19,22,23	2.77	6 (31%)	26,31,34	1.82	5 (19%)
2	UY1	B	39	2	19,22,23	1.19	1 (5%)	22,31,34	0.96	1 (4%)
3	A2M	D	3724	3	22,25,26	1.43	1 (4%)	31,36,39	1.04	1 (3%)
48	PSU	w	866	48	18,21,22	1.07	1 (5%)	22,30,33	1.84	5 (22%)
48	PSU	w	1174	81,48	18,21,22	1.04	1 (5%)	22,30,33	1.77	4 (18%)
48	OMU	w	1442	81,48	19,22,23	2.91	8 (42%)	26,31,34	1.71	5 (19%)
3	OMC	D	2861	3	19,22,23	2.86	8 (42%)	26,31,34	0.67	0
3	OMC	D	4536	3	19,22,23	2.84	8 (42%)	26,31,34	0.72	0
3	PSU	D	4420	3	18,21,22	1.05	1 (5%)	22,30,33	1.84	6 (27%)
3	OMU	D	1773	3	19,22,23	2.96	8 (42%)	26,31,34	1.61	5 (19%)
3	A2M	D	3760	3	22,25,26	1.47	1 (4%)	31,36,39	1.05	1 (3%)
48	OMC	w	1703	81,48	19,22,23	2.94	8 (42%)	26,31,34	0.72	0
48	A2M	w	1678	48	22,25,26	1.48	1 (4%)	31,36,39	0.99	2 (6%)
48	A2M	w	1031	48	22,25,26	1.40	1 (4%)	31,36,39	1.01	2 (6%)
48	PSU	w	1056	48	18,21,22	1.05	1 (5%)	22,30,33	1.82	5 (22%)
48	PSU	w	105	48	18,21,22	1.09	1 (5%)	22,30,33	1.92	5 (22%)
3	OMC	D	1340	3	19,22,23	2.82	8 (42%)	26,31,34	0.70	0
2	5MC	C	48	2	18,22,23	3.83	8 (44%)	26,32,35	1.04	2 (7%)
3	PSU	D	4521	3,81	18,21,22	1.07	2 (11%)	22,30,33	1.88	5 (22%)
3	PSU	D	3920	3,81	18,21,22	1.07	2 (11%)	22,30,33	1.87	4 (18%)
3	PSU	D	4299	3	18,21,22	1.02	1 (5%)	22,30,33	1.87	4 (18%)
3	PSU	D	3734	3	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4361	3	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
48	OMU	w	1804	48	19,22,23	2.90	7 (36%)	26,31,34	1.74	4 (15%)
3	A2M	D	400	3	22,25,26	1.40	1 (4%)	31,36,39	1.03	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	MA6	w	1850	48	23,26,27	1.36	4 (17%)	34,38,41	2.22	11 (32%)
3	OMC	D	3808	3	19,22,23	2.84	8 (42%)	26,31,34	0.74	0
2	1MA	C	58	2	21,25,26	0.91	1 (4%)	31,37,40	0.77	1 (3%)
48	G7M	w	1639	2,48	23,26,27	2.82	8 (34%)	35,39,42	1.80	8 (22%)
48	A2M	w	166	48	22,25,26	1.46	2 (9%)	31,36,39	1.04	2 (6%)
3	PSU	D	3768	3	18,21,22	1.04	1 (5%)	22,30,33	1.75	3 (13%)
3	PSU	D	1862	3	18,21,22	1.03	1 (5%)	22,30,33	1.95	5 (22%)
3	PSU	D	1860	3	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
3	OMC	D	3841	3	19,22,23	2.81	8 (42%)	26,31,34	0.70	0
2	UY1	C	39	2	19,22,23	1.28	2 (10%)	22,31,34	0.95	1 (4%)
3	A2M	D	1524	3	22,25,26	1.48	2 (9%)	31,36,39	1.09	3 (9%)
3	PSU	D	4423	3	18,21,22	1.06	1 (5%)	22,30,33	1.85	4 (18%)
48	OMC	w	517	48	19,22,23	3.01	8 (42%)	26,31,34	0.72	0
48	PSU	w	609	48	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)
48	OMU	w	1326	48	19,22,23	2.89	8 (42%)	26,31,34	1.72	4 (15%)
48	OMG	w	1328	48	23,26,27	2.60	8 (34%)	33,38,41	1.92	9 (27%)
48	PSU	w	119	48	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
48	PSU	w	863	48	18,21,22	1.07	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4431	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
48	PSU	w	686	48	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
3	OMU	D	4306	3	19,22,23	2.72	6 (31%)	26,31,34	1.74	5 (19%)
3	PSU	D	4353	3	18,21,22	1.04	2 (11%)	22,30,33	1.83	4 (18%)
3	PSU	D	4579	3	18,21,22	1.05	2 (11%)	22,30,33	1.84	4 (18%)
3	OMG	D	4637	3	23,26,27	2.55	10 (43%)	33,38,41	1.94	9 (27%)
48	PSU	w	93	48	18,21,22	1.09	1 (5%)	22,30,33	1.75	4 (18%)
48	PSU	w	1004	48	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
48	PSU	w	822	48	18,21,22	1.06	1 (5%)	22,30,33	1.84	4 (18%)
2	56B	C	34	2,80	29,35,36	2.81	10 (34%)	36,52,55	2.35	8 (22%)
48	A2M	w	27	48	22,25,26	1.44	1 (4%)	31,36,39	1.00	2 (6%)
3	PSU	D	3637	3,81	18,21,22	1.05	1 (5%)	22,30,33	1.85	2 (9%)
3	PSU	D	4689	3	18,21,22	1.03	1 (5%)	22,30,33	1.81	4 (18%)
2	H2U	B	47	2	18,21,22	1.03	2 (11%)	21,30,33	0.78	0
3	OMC	D	4456	3	19,22,23	2.84	8 (42%)	26,31,34	0.69	0
48	PSU	w	210	48	18,21,22	1.09	1 (5%)	22,30,33	1.77	4 (18%)
2	5MC	B	48	2	18,22,23	3.82	8 (44%)	26,32,35	1.10	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	D	1677	3,81	18,21,22	1.06	2 (11%)	22,30,33	1.80	4 (18%)
48	PSU	w	814	48	18,21,22	1.06	1 (5%)	22,30,33	1.85	5 (22%)
48	OMG	w	644	48	23,26,27	2.61	8 (34%)	33,38,41	1.94	10 (30%)
2	2MG	B	10	2	23,26,27	2.67	7 (30%)	32,38,41	2.12	9 (28%)
3	OMU	D	2837	3	19,22,23	2.78	6 (31%)	26,31,34	1.88	5 (19%)
3	PSU	D	4442	3	18,21,22	1.05	2 (11%)	22,30,33	1.89	6 (27%)
48	OMU	w	121	48	19,22,23	2.90	8 (42%)	26,31,34	1.67	5 (19%)
48	OMG	w	1490	81,48	23,26,27	2.59	8 (34%)	33,38,41	1.91	9 (27%)
3	A2M	D	3785	3,81	22,25,26	1.41	1 (4%)	31,36,39	1.32	3 (9%)
48	OMU	w	116	48	19,22,23	2.93	8 (42%)	26,31,34	1.69	4 (15%)
48	MA6	w	1851	48	23,26,27	1.29	4 (17%)	34,38,41	2.31	12 (35%)
3	PSU	D	3851	3	18,21,22	1.05	2 (11%)	22,30,33	1.84	4 (18%)
3	5MC	D	4447	3,81	18,22,23	3.63	7 (38%)	26,32,35	1.15	1 (3%)
48	A2M	w	512	48	22,25,26	1.45	1 (4%)	31,36,39	1.09	3 (9%)
48	OMU	w	1288	48	19,22,23	2.96	8 (42%)	26,31,34	1.70	4 (15%)
3	PSU	D	1536	3	18,21,22	1.06	2 (11%)	22,30,33	1.88	4 (18%)
3	5MC	D	3782	3,81	18,22,23	3.59	8 (44%)	26,32,35	1.08	2 (7%)
48	PSU	w	1445	48	18,21,22	1.05	1 (5%)	22,30,33	1.78	5 (22%)
3	OMG	D	2424	3	23,26,27	2.59	9 (39%)	33,38,41	1.92	10 (30%)
2	PSU	B	55	2	18,21,22	1.08	1 (5%)	22,30,33	1.74	6 (27%)
3	OMG	D	4499	2,3	23,26,27	2.58	9 (39%)	33,38,41	1.97	10 (30%)
2	2MG	C	10	2	23,26,27	2.68	7 (30%)	32,38,41	2.22	9 (28%)
3	OMG	D	4392	3	23,26,27	2.54	10 (43%)	33,38,41	1.93	9 (27%)
3	OMG	D	4370	3	23,26,27	2.56	9 (39%)	33,38,41	1.95	9 (27%)
3	PSU	D	1792	3	18,21,22	0.99	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	1744	3,81	18,21,22	1.02	1 (5%)	22,30,33	1.83	4 (18%)
2	PSU	C	35	2,1	18,21,22	1.01	1 (5%)	22,30,33	1.81	5 (22%)
3	A2M	D	398	3	22,25,26	1.41	1 (4%)	31,36,39	1.01	3 (9%)
3	A2M	D	2815	3	22,25,26	1.51	1 (4%)	31,36,39	1.02	3 (9%)
3	UR3	D	4530	3,81	19,22,23	2.64	7 (36%)	26,32,35	1.27	1 (3%)
48	PSU	w	801	48	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)
3	OMG	D	1522	3	23,26,27	2.53	9 (39%)	33,38,41	1.99	10 (30%)
48	PSU	w	1244	48	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
2	G7M	C	46	2	23,26,27	2.83	9 (39%)	35,39,42	1.74	9 (25%)
48	OMU	w	428	48	19,22,23	2.92	8 (42%)	26,31,34	1.72	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	D	3887	3	19,22,23	2.87	8 (42%)	26,31,34	0.78	0
48	PSU	w	1367	48	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
2	5MU	C	54	2	19,22,23	4.73	5 (26%)	28,32,35	3.60	9 (32%)
48	PSU	w	1232	48	18,21,22	1.04	1 (5%)	22,30,33	1.83	5 (22%)
48	PSU	w	218	48	18,21,22	1.08	1 (5%)	22,30,33	1.82	4 (18%)
2	1MA	B	58	2	21,25,26	0.92	1 (4%)	31,37,40	0.76	0
48	PSU	w	649	48	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
48	A2M	w	484	48	22,25,26	1.46	1 (4%)	31,36,39	1.00	3 (9%)
48	A2M	w	668	81,48	22,25,26	1.53	2 (9%)	31,36,39	1.04	3 (9%)
3	PSU	D	4471	3	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
2	2MG	C	6	2	23,26,27	2.67	7 (30%)	32,38,41	2.16	9 (28%)
48	PSU	w	1081	48	18,21,22	1.01	1 (5%)	22,30,33	1.76	5 (22%)
3	PSU	D	1782	3	18,21,22	1.01	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	4532	3	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	4296	3	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
3	OMU	D	4498	3,81	19,22,23	2.77	6 (31%)	26,31,34	1.72	4 (15%)
3	OMG	D	4196	3,81	23,26,27	2.56	9 (39%)	33,38,41	1.91	9 (27%)
3	PSU	D	1683	3,81	18,21,22	1.04	2 (11%)	22,30,33	1.92	5 (22%)
3	PSU	D	4552	3	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
3	PSU	D	3770	3	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
2	1MG	B	37	2	22,26,27	2.65	7 (31%)	33,39,42	1.71	7 (21%)
3	PSU	D	4972	3,81	18,21,22	1.02	1 (5%)	22,30,33	1.88	5 (22%)
48	A2M	w	159	48	22,25,26	1.53	2 (9%)	31,36,39	1.07	3 (9%)
48	A2M	w	468	48	22,25,26	1.58	2 (9%)	31,36,39	1.11	3 (9%)
3	OMU	D	2415	3	19,22,23	2.83	6 (31%)	26,31,34	1.97	6 (23%)
48	PSU	w	681	48	18,21,22	1.04	2 (11%)	22,30,33	1.84	4 (18%)
48	PSU	w	651	48	18,21,22	1.07	1 (5%)	22,30,33	1.83	5 (22%)
48	OMG	w	436	48	23,26,27	2.60	8 (34%)	33,38,41	1.97	9 (27%)
48	PSU	w	1238	48	18,21,22	1.08	1 (5%)	22,30,33	1.73	4 (18%)
3	PSU	D	4457	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	3730	3	18,21,22	1.01	1 (5%)	22,30,33	1.86	5 (22%)
48	4AC	w	1337	48	21,24,25	0.66	0	29,34,37	1.19	4 (13%)
2	H2U	C	47	2	18,21,22	1.08	2 (11%)	21,30,33	1.38	2 (9%)
3	A2M	D	1326	3	22,25,26	1.34	1 (4%)	31,36,39	1.01	2 (6%)
2	M2G	B	27	2	24,27,28	1.14	2 (8%)	35,40,43	0.89	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	D	3764	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
3	OMG	D	1625	3,81	23,26,27	2.59	8 (34%)	33,38,41	1.92	9 (27%)
2	M2G	C	26	2	24,27,28	1.12	2 (8%)	35,40,43	0.84	0
2	56B	B	34	2,80	29,35,36	2.79	10 (34%)	36,52,55	2.31	8 (22%)
48	A2M	w	99	81,48	22,25,26	1.41	1 (4%)	31,36,39	1.03	2 (6%)
48	PSU	w	1045	48	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
48	OMC	w	174	48	19,22,23	3.01	8 (42%)	26,31,34	0.71	0
3	OMG	D	3899	3	23,26,27	2.54	10 (43%)	33,38,41	1.97	10 (30%)
5	OMG	F	75	5	23,26,27	2.57	9 (39%)	33,38,41	1.95	10 (30%)
3	PSU	D	2508	3	18,21,22	1.02	1 (5%)	22,30,33	1.85	5 (22%)
3	PSU	D	4576	3	18,21,22	1.02	1 (5%)	22,30,33	1.85	5 (22%)
3	OMG	D	4623	3	23,26,27	2.53	9 (39%)	33,38,41	1.94	10 (30%)
48	PSU	w	406	48	18,21,22	1.04	1 (5%)	22,30,33	1.85	5 (22%)
48	PSU	w	572	48	18,21,22	1.11	1 (5%)	22,30,33	1.80	5 (22%)
3	A2M	D	3825	3	22,25,26	1.40	1 (4%)	31,36,39	1.05	2 (6%)
3	OMG	D	1316	3	23,26,27	2.55	10 (43%)	33,38,41	1.98	10 (30%)
3	OMG	D	4494	3	23,26,27	2.58	9 (39%)	33,38,41	1.93	9 (27%)
48	6MZ	w	1832	81,48	22,25,26	2.82	4 (18%)	30,36,39	2.20	9 (30%)
3	A2M	D	2401	3	22,25,26	1.40	1 (4%)	31,36,39	1.01	2 (6%)
3	OMG	D	3744	3	23,26,27	2.57	9 (39%)	33,38,41	1.96	10 (30%)
48	B8N	w	1248	48	24,29,30	0.82	0	29,42,45	0.94	2 (6%)
3	OMC	D	2824	3	19,22,23	2.88	8 (42%)	26,31,34	0.70	0
3	PSU	D	3639	3	18,21,22	1.03	2 (11%)	22,30,33	1.85	4 (18%)
3	A2M	D	3718	3	22,25,26	1.40	1 (4%)	31,36,39	1.01	2 (6%)
3	PSU	D	4293	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G7M	B	46	2	-	2/7/25/26	0/3/3/3
3	PSU	D	4500	3	-	5/7/25/26	0/2/2/2
48	OMC	w	462	48	-	0/9/27/28	0/2/2/2
48	OMC	w	1391	48	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	D	2363	3,81	-	0/9/27/28	0/3/3/3
48	OMU	w	627	48	-	8/9/27/28	0/2/2/2
2	5MU	B	54	2	-	2/7/25/26	0/2/2/2
3	A2M	D	1534	3,81	-	3/9/27/28	0/3/3/3
48	4AC	w	1842	48	-	0/11/29/30	0/2/2/2
3	OMC	D	3701	3,81	-	4/9/27/28	0/2/2/2
48	A2M	w	590	48	-	2/9/27/28	0/3/3/3
3	OMG	D	1760	3	-	2/9/27/28	0/3/3/3
48	PSU	w	1347	48	-	0/7/25/26	0/2/2/2
48	A2M	w	1383	48	-	0/9/27/28	0/3/3/3
48	OMG	w	601	48	-	0/9/27/28	0/3/3/3
48	OMU	w	799	48	-	3/9/27/28	0/2/2/2
3	PSU	D	3695	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3762	3	-	2/7/25/26	0/2/2/2
3	UY1	D	3818	3,81	-	4/9/27/28	0/2/2/2
48	PSU	w	34	48	-	3/7/25/26	0/2/2/2
48	OMU	w	172	48	-	0/9/27/28	0/2/2/2
3	A2M	D	3830	3	-	0/9/27/28	0/3/3/3
3	PSU	D	4403	3,81	-	0/7/25/26	0/2/2/2
3	PSU	D	3758	3	-	2/7/25/26	0/2/2/2
48	A2M	w	576	48	-	2/9/27/28	0/3/3/3
3	OMG	D	4618	3	-	0/9/27/28	0/3/3/3
3	A2M	D	2787	3,81	-	3/9/27/28	0/3/3/3
2	PSU	B	35	2,1	-	0/7/25/26	0/2/2/2
2	2MG	B	6	2	-	0/9/27/28	0/3/3/3
3	OMC	D	2422	3,81	-	1/9/27/28	0/2/2/2
3	OMU	D	4620	3	-	0/9/27/28	0/2/2/2
48	PSU	w	109	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1781	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4312	3	-	0/7/25/26	0/2/2/2
3	OMC	D	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	D	5010	3	-	0/7/25/26	0/2/2/2
2	1MG	C	37	2	-	0/7/25/26	0/3/3/3
48	OMG	w	509	48	-	1/9/27/28	0/3/3/3
3	6MZ	D	4220	3	-	0/9/27/28	0/3/3/3
2	M2G	C	27	2	-	0/11/29/30	0/3/3/3
3	PSU	D	3715	3	-	2/7/25/26	0/2/2/2
3	OMU	D	4227	3	-	0/9/27/28	0/2/2/2
48	PSU	w	1625	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	D	4628	3	-	0/7/25/26	0/2/2/2
48	PSU	w	815	48	-	0/7/25/26	0/2/2/2
3	1MA	D	1322	3	-	2/7/25/26	0/3/3/3
48	PSU	w	1177	48	-	0/7/25/26	0/2/2/2
2	PSU	C	55	2	-	2/7/25/26	0/2/2/2
3	OMC	D	2365	3,81	-	0/9/27/28	0/2/2/2
3	OMG	D	2364	3	-	2/9/27/28	0/3/3/3
3	A2M	D	4523	3,81	-	0/9/27/28	0/3/3/3
48	PSU	w	36	48	-	0/7/25/26	0/2/2/2
2	M2G	B	26	2	-	2/11/29/30	0/3/3/3
48	PSU	w	1692	48	-	0/7/25/26	0/2/2/2
3	A2M	D	1871	3,81	-	0/9/27/28	0/3/3/3
3	OMC	D	2351	3,81	-	2/9/27/28	0/2/2/2
3	PSU	D	5001	3,81	-	0/7/25/26	0/2/2/2
3	PSU	D	2632	3	-	0/7/25/26	0/2/2/2
3	OMG	D	3792	3	-	1/9/27/28	0/3/3/3
3	OMG	D	4228	3	-	0/9/27/28	0/3/3/3
3	OMG	D	3627	3	-	0/9/27/28	0/3/3/3
3	PSU	D	3853	3,81	-	0/7/25/26	0/2/2/2
48	OMG	w	683	48	-	0/9/27/28	0/3/3/3
3	OMG	D	3944	3	-	3/9/27/28	0/3/3/3
48	PSU	w	966	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1046	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1643	81,48	-	0/7/25/26	0/2/2/2
3	OMU	D	3925	3	-	1/9/27/28	0/2/2/2
2	UY1	B	39	2	-	2/9/27/28	0/2/2/2
3	A2M	D	3724	3	-	1/9/27/28	0/3/3/3
48	PSU	w	866	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1174	81,48	-	0/7/25/26	0/2/2/2
48	OMU	w	1442	81,48	-	1/9/27/28	0/2/2/2
3	OMC	D	2861	3	-	0/9/27/28	0/2/2/2
3	OMC	D	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4420	3	-	0/7/25/26	0/2/2/2
3	OMU	D	1773	3	-	1/9/27/28	0/2/2/2
3	A2M	D	3760	3	-	0/9/27/28	0/3/3/3
48	OMC	w	1703	81,48	-	2/9/27/28	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	PSU	w	1056	48	-	0/7/25/26	0/2/2/2
48	PSU	w	105	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	D	1340	3	-	0/9/27/28	0/2/2/2
2	5MC	C	48	2	-	2/7/25/26	0/2/2/2
3	PSU	D	4521	3,81	-	2/7/25/26	0/2/2/2
3	PSU	D	3920	3,81	-	0/7/25/26	0/2/2/2
3	PSU	D	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3734	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4361	3	-	0/7/25/26	0/2/2/2
48	OMU	w	1804	48	-	2/9/27/28	0/2/2/2
3	A2M	D	400	3	-	0/9/27/28	0/3/3/3
48	MA6	w	1850	48	-	0/11/29/30	0/3/3/3
3	OMC	D	3808	3	-	0/9/27/28	0/2/2/2
2	1MA	C	58	2	-	0/7/25/26	0/3/3/3
48	G7M	w	1639	2,48	-	2/7/25/26	0/3/3/3
48	A2M	w	166	48	-	3/9/27/28	0/3/3/3
3	PSU	D	3768	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1860	3	-	0/7/25/26	0/2/2/2
3	OMC	D	3841	3	-	0/9/27/28	0/2/2/2
2	UY1	C	39	2	-	0/9/27/28	0/2/2/2
3	A2M	D	1524	3	-	1/9/27/28	0/3/3/3
3	PSU	D	4423	3	-	0/7/25/26	0/2/2/2
48	OMC	w	517	48	-	1/9/27/28	0/2/2/2
48	PSU	w	609	48	-	0/7/25/26	0/2/2/2
48	OMU	w	1326	48	-	3/9/27/28	0/2/2/2
48	OMG	w	1328	48	-	0/9/27/28	0/3/3/3
48	PSU	w	119	48	-	1/7/25/26	0/2/2/2
48	PSU	w	863	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4431	3	-	0/7/25/26	0/2/2/2
48	PSU	w	686	48	-	0/7/25/26	0/2/2/2
3	OMU	D	4306	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4579	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	93	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1004	48	-	0/7/25/26	0/2/2/2
48	PSU	w	822	48	-	2/7/25/26	0/2/2/2
2	56B	C	34	2,80	-	2/12/43/44	0/4/4/4
48	A2M	w	27	48	-	0/9/27/28	0/3/3/3
3	PSU	D	3637	3,81	-	0/7/25/26	0/2/2/2
3	PSU	D	4689	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	H2U	B	47	2	-	3/7/38/39	0/2/2/2
3	OMC	D	4456	3	-	0/9/27/28	0/2/2/2
48	PSU	w	210	48	-	0/7/25/26	0/2/2/2
2	5MC	B	48	2	-	3/7/25/26	0/2/2/2
3	PSU	D	1677	3,81	-	3/7/25/26	0/2/2/2
48	PSU	w	814	48	-	0/7/25/26	0/2/2/2
48	OMG	w	644	48	-	3/9/27/28	0/3/3/3
2	2MG	B	10	2	-	0/9/27/28	0/3/3/3
3	OMU	D	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4442	3	-	0/7/25/26	0/2/2/2
48	OMU	w	121	48	-	0/9/27/28	0/2/2/2
48	OMG	w	1490	81,48	-	4/9/27/28	0/3/3/3
3	A2M	D	3785	3,81	-	3/9/27/28	0/3/3/3
48	OMU	w	116	48	-	0/9/27/28	0/2/2/2
48	MA6	w	1851	48	-	2/11/29/30	0/3/3/3
3	PSU	D	3851	3	-	0/7/25/26	0/2/2/2
3	5MC	D	4447	3,81	-	4/7/25/26	0/2/2/2
48	A2M	w	512	48	-	2/9/27/28	0/3/3/3
48	OMU	w	1288	48	-	1/9/27/28	0/2/2/2
3	PSU	D	1536	3	-	0/7/25/26	0/2/2/2
3	5MC	D	3782	3,81	-	0/7/25/26	0/2/2/2
48	PSU	w	1445	48	-	0/7/25/26	0/2/2/2
3	OMG	D	2424	3	-	2/9/27/28	0/3/3/3
2	PSU	B	55	2	-	2/7/25/26	0/2/2/2
3	OMG	D	4499	2,3	-	0/9/27/28	0/3/3/3
2	2MG	C	10	2	-	0/9/27/28	0/3/3/3
3	OMG	D	4392	3	-	0/9/27/28	0/3/3/3
3	OMG	D	4370	3	-	0/9/27/28	0/3/3/3
3	PSU	D	1792	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1744	3,81	-	0/7/25/26	0/2/2/2
2	PSU	C	35	2,1	-	0/7/25/26	0/2/2/2
3	A2M	D	398	3	-	0/9/27/28	0/3/3/3
3	A2M	D	2815	3	-	2/9/27/28	0/3/3/3
3	UR3	D	4530	3,81	-	0/7/25/26	0/2/2/2
48	PSU	w	801	48	-	0/7/25/26	0/2/2/2
3	OMG	D	1522	3	-	0/9/27/28	0/3/3/3
48	PSU	w	1244	48	-	0/7/25/26	0/2/2/2
2	G7M	C	46	2	-	2/7/25/26	0/3/3/3
48	OMU	w	428	48	-	7/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	D	3887	3	-	1/9/27/28	0/2/2/2
48	PSU	w	1367	48	-	0/7/25/26	0/2/2/2
2	5MU	C	54	2	-	2/7/25/26	0/2/2/2
48	PSU	w	1232	48	-	0/7/25/26	0/2/2/2
48	PSU	w	218	48	-	0/7/25/26	0/2/2/2
2	1MA	B	58	2	-	2/7/25/26	0/3/3/3
48	PSU	w	649	48	-	0/7/25/26	0/2/2/2
48	A2M	w	484	48	-	0/9/27/28	0/3/3/3
48	A2M	w	668	81,48	-	3/9/27/28	0/3/3/3
3	PSU	D	4471	3	-	0/7/25/26	0/2/2/2
2	2MG	C	6	2	-	3/9/27/28	0/3/3/3
48	PSU	w	1081	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1782	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4296	3	-	0/7/25/26	0/2/2/2
3	OMU	D	4498	3,81	-	0/9/27/28	0/2/2/2
3	OMG	D	4196	3,81	-	0/9/27/28	0/3/3/3
3	PSU	D	1683	3,81	-	0/7/25/26	0/2/2/2
3	PSU	D	4552	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3770	3	-	0/7/25/26	0/2/2/2
2	1MG	B	37	2	-	1/7/25/26	0/3/3/3
3	PSU	D	4972	3,81	-	0/7/25/26	0/2/2/2
48	A2M	w	159	48	-	2/9/27/28	0/3/3/3
48	A2M	w	468	48	-	2/9/27/28	0/3/3/3
3	OMU	D	2415	3	-	1/9/27/28	0/2/2/2
48	PSU	w	681	48	-	0/7/25/26	0/2/2/2
48	PSU	w	651	48	-	0/7/25/26	0/2/2/2
48	OMG	w	436	48	-	0/9/27/28	0/3/3/3
48	PSU	w	1238	48	-	2/7/25/26	0/2/2/2
3	PSU	D	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3730	3	-	0/7/25/26	0/2/2/2
48	4AC	w	1337	48	-	0/11/29/30	0/2/2/2
2	H2U	C	47	2	-	3/7/38/39	0/2/2/2
3	A2M	D	1326	3	-	1/9/27/28	0/3/3/3
2	M2G	B	27	2	-	0/11/29/30	0/3/3/3
3	PSU	D	3764	3	-	0/7/25/26	0/2/2/2
3	OMG	D	1625	3,81	-	0/9/27/28	0/3/3/3
2	M2G	C	26	2	-	0/11/29/30	0/3/3/3
2	56B	B	34	2,80	-	3/12/43/44	0/4/4/4
48	A2M	w	99	81,48	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	w	1045	48	-	0/7/25/26	0/2/2/2
48	OMC	w	174	48	-	0/9/27/28	0/2/2/2
3	OMG	D	3899	3	-	0/9/27/28	0/3/3/3
5	OMG	F	75	5	-	1/9/27/28	0/3/3/3
3	PSU	D	2508	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4576	3	-	0/7/25/26	0/2/2/2
3	OMG	D	4623	3	-	0/9/27/28	0/3/3/3
48	PSU	w	406	48	-	0/7/25/26	0/2/2/2
48	PSU	w	572	48	-	0/7/25/26	0/2/2/2
3	A2M	D	3825	3	-	0/9/27/28	0/3/3/3
3	OMG	D	1316	3	-	0/9/27/28	0/3/3/3
3	OMG	D	4494	3	-	0/9/27/28	0/3/3/3
48	6MZ	w	1832	81,48	-	2/9/27/28	0/3/3/3
3	A2M	D	2401	3	-	0/9/27/28	0/3/3/3
3	OMG	D	3744	3	-	0/9/27/28	0/3/3/3
48	B8N	w	1248	48	-	4/16/34/35	0/2/2/2
3	OMC	D	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	D	3639	3	-	0/7/25/26	0/2/2/2
3	A2M	D	3718	3	-	0/9/27/28	0/3/3/3
3	PSU	D	4293	3	-	0/7/25/26	0/2/2/2

All (832) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	1832	6MZ	C6-N6	12.19	1.47	1.34
3	D	4220	6MZ	C6-N6	12.03	1.47	1.34
2	B	54	5MU	C6-N1	11.03	1.56	1.38
2	C	54	5MU	C6-N1	10.87	1.56	1.38
2	B	54	5MU	C2-N1	10.70	1.55	1.38
2	C	54	5MU	C2-N1	10.70	1.55	1.38
2	C	48	5MC	C6-C5	9.59	1.50	1.34
3	D	4447	5MC	C6-C5	9.45	1.50	1.34
2	B	48	5MC	C6-C5	9.44	1.50	1.34
2	C	54	5MU	C4-C5	9.29	1.60	1.44
2	B	54	5MU	C4-C5	9.20	1.60	1.44
3	D	3782	5MC	C6-C5	9.05	1.49	1.34
2	C	10	2MG	C2-N3	7.77	1.46	1.31
2	C	6	2MG	C2-N3	7.76	1.46	1.31
2	B	10	2MG	C2-N3	7.75	1.46	1.31
2	B	48	5MC	C4-N3	7.47	1.46	1.34
2	C	48	5MC	C4-N3	7.36	1.46	1.34
3	D	1760	OMG	C4-N3	7.36	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	2MG	C2-N3	7.34	1.46	1.31
3	D	3944	OMG	C4-N3	7.32	1.51	1.34
2	C	54	5MU	C4-N3	-7.29	1.25	1.38
3	D	1773	OMU	C2-N1	7.28	1.50	1.38
48	w	644	OMG	C4-N3	7.27	1.51	1.34
48	w	436	OMG	C4-N3	7.27	1.51	1.34
48	w	1328	OMG	C4-N3	7.26	1.51	1.34
48	w	1490	OMG	C4-N3	7.24	1.51	1.34
48	w	683	OMG	C4-N3	7.22	1.51	1.34
48	w	509	OMG	C4-N3	7.21	1.51	1.34
48	w	1288	OMU	C2-N1	7.21	1.50	1.38
2	B	54	5MU	C4-N3	-7.21	1.25	1.38
48	w	601	OMG	C4-N3	7.20	1.51	1.34
3	D	1625	OMG	C4-N3	7.19	1.51	1.34
3	D	4494	OMG	C4-N3	7.12	1.51	1.34
3	D	4370	OMG	C4-N3	7.12	1.51	1.34
48	w	116	OMU	C2-N1	7.12	1.49	1.38
3	D	3744	OMG	C4-N3	7.11	1.51	1.34
5	F	75	OMG	C4-N3	7.10	1.51	1.34
3	D	4499	OMG	C4-N3	7.08	1.51	1.34
48	w	799	OMU	C2-N1	7.08	1.49	1.38
3	D	3792	OMG	C4-N3	7.07	1.51	1.34
3	D	2424	OMG	C4-N3	7.07	1.51	1.34
3	D	4196	OMG	C4-N3	7.07	1.51	1.34
3	D	4618	OMG	C4-N3	7.05	1.51	1.34
3	D	3627	OMG	C4-N3	7.03	1.51	1.34
3	D	4637	OMG	C4-N3	7.03	1.51	1.34
3	D	4228	OMG	C4-N3	7.00	1.50	1.34
3	D	4392	OMG	C4-N3	7.00	1.50	1.34
48	w	627	OMU	C2-N1	7.00	1.49	1.38
48	w	428	OMU	C2-N1	6.98	1.49	1.38
48	w	1442	OMU	C2-N1	6.96	1.49	1.38
3	D	2364	OMG	C4-N3	6.96	1.50	1.34
3	D	4623	OMG	C4-N3	6.95	1.50	1.34
3	D	3899	OMG	C4-N3	6.95	1.50	1.34
48	w	172	OMU	C2-N1	6.94	1.49	1.38
3	D	1522	OMG	C4-N3	6.92	1.50	1.34
3	D	3782	5MC	C4-N3	6.91	1.45	1.34
48	w	1804	OMU	C2-N1	6.91	1.49	1.38
2	C	34	56B	C14-C13	6.90	1.52	1.32
48	w	121	OMU	C2-N1	6.89	1.49	1.38
2	B	34	56B	C14-C13	6.86	1.52	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	1326	OMU	C2-N1	6.85	1.49	1.38
3	D	1316	OMG	C4-N3	6.85	1.50	1.34
3	D	2415	OMU	C2-N1	6.81	1.49	1.38
2	B	54	5MU	C6-C5	6.76	1.45	1.34
3	D	4227	OMU	C2-N1	6.73	1.49	1.38
48	w	799	OMU	C2-N3	6.71	1.49	1.38
3	D	1773	OMU	C2-N3	6.66	1.49	1.38
3	D	4530	UR3	C2-N1	6.64	1.48	1.38
2	C	10	2MG	C4-N3	6.64	1.50	1.34
2	C	54	5MU	C6-C5	6.64	1.45	1.34
48	w	1288	OMU	C2-N3	6.63	1.49	1.38
3	D	4447	5MC	C4-N3	6.61	1.45	1.34
3	D	3925	OMU	C2-N1	6.61	1.49	1.38
2	C	6	2MG	C4-N3	6.60	1.49	1.34
48	w	428	OMU	C2-N3	6.60	1.49	1.38
2	B	10	2MG	C4-N3	6.59	1.49	1.34
2	B	46	G7M	C4-N3	6.58	1.49	1.34
48	w	627	OMU	C2-N3	6.57	1.49	1.38
48	w	172	OMU	C2-N3	6.57	1.49	1.38
2	B	48	5MC	C2-N3	6.57	1.49	1.36
2	C	46	G7M	C2-N2	6.56	1.49	1.34
2	C	46	G7M	C4-N3	6.55	1.49	1.34
3	D	4498	OMU	C2-N1	6.54	1.48	1.38
48	w	1326	OMU	C2-N3	6.54	1.49	1.38
2	C	48	5MC	C2-N3	6.54	1.49	1.36
48	w	1804	OMU	C2-N3	6.54	1.49	1.38
48	w	1442	OMU	C2-N3	6.54	1.49	1.38
48	w	121	OMU	C2-N3	6.53	1.49	1.38
48	w	116	OMU	C2-N3	6.53	1.49	1.38
48	w	1639	G7M	C4-N3	6.50	1.49	1.34
2	B	46	G7M	C2-N2	6.50	1.49	1.34
48	w	1639	G7M	C2-N2	6.49	1.49	1.34
3	D	2837	OMU	C2-N1	6.47	1.48	1.38
2	B	37	1MG	C2-N3	6.47	1.46	1.34
2	C	37	1MG	C2-N3	6.46	1.46	1.34
3	D	4620	OMU	C2-N1	6.33	1.48	1.38
48	w	517	OMC	C2-N3	6.33	1.49	1.36
48	w	174	OMC	C2-N3	6.32	1.49	1.36
3	D	2837	OMU	C2-N3	6.31	1.49	1.38
2	B	37	1MG	C4-N3	6.30	1.49	1.34
2	C	37	1MG	C4-N3	6.27	1.49	1.34
2	B	6	2MG	C4-N3	6.25	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	462	OMC	C2-N3	6.25	1.49	1.36
3	D	4306	OMU	C2-N1	6.24	1.48	1.38
3	D	2415	OMU	C2-N3	6.22	1.49	1.38
2	C	37	1MG	C2-N2	6.20	1.45	1.34
48	w	1391	OMC	C2-N3	6.20	1.48	1.36
2	C	34	56B	C4-N3	6.19	1.49	1.34
2	B	37	1MG	C2-N2	6.19	1.45	1.34
2	B	34	56B	C4-N3	6.18	1.49	1.34
3	D	4620	OMU	C2-N3	6.14	1.48	1.38
3	D	3782	5MC	C2-N3	6.14	1.48	1.36
3	D	4227	OMU	C2-N3	6.11	1.48	1.38
3	D	4498	OMU	C2-N3	6.09	1.48	1.38
3	D	3925	OMU	C2-N3	6.08	1.48	1.38
3	D	2861	OMC	C2-N3	6.07	1.48	1.36
48	w	1703	OMC	C2-N3	6.06	1.48	1.36
48	w	174	OMC	C6-C5	6.05	1.49	1.35
3	D	4306	OMU	C2-N3	6.05	1.48	1.38
3	D	3887	OMC	C2-N3	6.04	1.48	1.36
3	D	2422	OMC	C2-N3	6.03	1.48	1.36
48	w	462	OMC	C6-C5	6.00	1.49	1.35
3	D	2824	OMC	C2-N3	5.99	1.48	1.36
3	D	4530	UR3	C6-C5	5.99	1.49	1.35
48	w	517	OMC	C6-C5	5.98	1.48	1.35
3	D	2804	OMC	C2-N3	5.98	1.48	1.36
48	w	1391	OMC	C6-C5	5.98	1.48	1.35
48	w	1703	OMC	C6-C5	5.97	1.48	1.35
3	D	4536	OMC	C2-N3	5.96	1.48	1.36
3	D	4447	5MC	C2-N3	5.95	1.48	1.36
3	D	2365	OMC	C2-N3	5.94	1.48	1.36
3	D	3701	OMC	C6-C5	5.93	1.48	1.35
3	D	3701	OMC	C2-N3	5.91	1.48	1.36
3	D	1340	OMC	C2-N3	5.88	1.48	1.36
3	D	3808	OMC	C2-N3	5.88	1.48	1.36
2	B	46	G7M	C2-N3	5.87	1.47	1.33
3	D	4456	OMC	C2-N3	5.87	1.48	1.36
3	D	1773	OMU	C6-C5	5.86	1.48	1.35
2	C	46	G7M	C2-N3	5.86	1.47	1.33
3	D	2351	OMC	C2-N3	5.85	1.48	1.36
48	w	172	OMU	C6-C5	5.85	1.48	1.35
48	w	1288	OMU	C6-C5	5.85	1.48	1.35
3	D	2422	OMC	C6-C5	5.84	1.48	1.35
48	w	121	OMU	C6-C5	5.84	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3841	OMC	C2-N3	5.84	1.48	1.36
48	w	116	OMU	C6-C5	5.83	1.48	1.35
48	w	428	OMU	C6-C5	5.83	1.48	1.35
3	D	2861	OMC	C6-C5	5.82	1.48	1.35
3	D	2824	OMC	C6-C5	5.82	1.48	1.35
48	w	799	OMU	C6-C5	5.82	1.48	1.35
3	D	3841	OMC	C6-C5	5.81	1.48	1.35
3	D	4456	OMC	C6-C5	5.81	1.48	1.35
48	w	1639	G7M	C2-N3	5.80	1.47	1.33
48	w	1442	OMU	C6-C5	5.80	1.48	1.35
3	D	4536	OMC	C6-C5	5.79	1.48	1.35
3	D	3887	OMC	C6-C5	5.78	1.48	1.35
3	D	3808	OMC	C6-C5	5.78	1.48	1.35
48	w	1326	OMU	C6-C5	5.77	1.48	1.35
3	D	2365	OMC	C6-C5	5.77	1.48	1.35
3	D	2804	OMC	C6-C5	5.76	1.48	1.35
48	w	627	OMU	C6-C5	5.76	1.48	1.35
3	D	1340	OMC	C6-C5	5.73	1.48	1.35
48	w	1804	OMU	C6-C5	5.71	1.48	1.35
3	D	2415	OMU	C6-C5	5.71	1.48	1.35
3	D	2351	OMC	C6-C5	5.65	1.48	1.35
3	D	2815	A2M	O5'-C5'	-5.61	1.31	1.44
3	D	4306	OMU	C6-C5	5.60	1.48	1.35
3	D	4498	OMU	C6-C5	5.59	1.48	1.35
3	D	4227	OMU	C6-C5	5.58	1.48	1.35
3	D	4620	OMU	C6-C5	5.58	1.48	1.35
3	D	1760	OMG	C2-N3	5.57	1.46	1.33
2	B	34	56B	C11-C10	5.56	1.62	1.54
2	C	34	56B	C2-N3	5.55	1.46	1.33
2	C	34	56B	C11-C10	5.55	1.62	1.54
2	B	34	56B	C2-N3	5.54	1.46	1.33
3	D	3925	OMU	C6-C5	5.54	1.47	1.35
3	D	2837	OMU	C6-C5	5.53	1.47	1.35
48	w	1328	OMG	C2-N3	5.51	1.46	1.33
48	w	644	OMG	C2-N3	5.51	1.46	1.33
3	D	1625	OMG	C2-N3	5.43	1.46	1.33
48	w	509	OMG	C2-N3	5.42	1.46	1.33
48	w	436	OMG	C2-N3	5.40	1.46	1.33
3	D	3944	OMG	C2-N3	5.39	1.46	1.33
48	w	601	OMG	C2-N3	5.38	1.46	1.33
48	w	683	OMG	C2-N3	5.38	1.46	1.33
3	D	3785	A2M	O5'-C5'	-5.36	1.31	1.44

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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
48	w	1490	OMG	C2-N3	5.34	1.46	1.33
3	D	2424	OMG	C2-N3	5.33	1.46	1.33
3	D	4370	OMG	C2-N3	5.30	1.46	1.33
3	D	3792	OMG	C2-N3	5.29	1.45	1.33
3	D	4196	OMG	C2-N3	5.28	1.45	1.33
3	D	3744	OMG	C2-N3	5.27	1.45	1.33
2	C	48	5MC	C6-N1	5.24	1.47	1.38
48	w	468	A2M	O5'-C5'	-5.24	1.31	1.44
5	F	75	OMG	C2-N3	5.24	1.45	1.33
48	w	668	A2M	O5'-C5'	-5.23	1.32	1.44
2	C	10	2MG	C2-N1	5.22	1.45	1.36
2	B	6	2MG	C2-N1	5.21	1.45	1.36
48	w	517	OMC	C4-N3	5.21	1.45	1.34
2	B	10	2MG	C2-N1	5.21	1.45	1.36
3	D	4637	OMG	C2-N3	5.21	1.45	1.33
3	D	4499	OMG	C2-N3	5.21	1.45	1.33
3	D	1760	OMG	C2-N2	5.18	1.46	1.34
3	D	3627	OMG	C2-N3	5.17	1.45	1.33
3	D	4392	OMG	C2-N3	5.16	1.45	1.33
2	B	48	5MC	C6-N1	5.15	1.46	1.38
3	D	4618	OMG	C2-N3	5.15	1.45	1.33
2	C	6	2MG	C2-N1	5.13	1.44	1.36
48	w	644	OMG	C2-N2	5.13	1.46	1.34
48	w	1328	OMG	C2-N2	5.13	1.46	1.34
3	D	3944	OMG	C2-N2	5.13	1.46	1.34
3	D	2787	A2M	O5'-C5'	-5.13	1.32	1.44
48	w	462	OMC	C4-N3	5.12	1.44	1.34
3	D	4623	OMG	C2-N3	5.12	1.45	1.33
48	w	683	OMG	C2-N2	5.11	1.46	1.34
3	D	1524	A2M	O5'-C5'	-5.11	1.32	1.44
3	D	4228	OMG	C2-N3	5.11	1.45	1.33
48	w	1490	OMG	C2-N2	5.11	1.46	1.34
3	D	1316	OMG	C2-N3	5.11	1.45	1.33
48	w	436	OMG	C2-N2	5.10	1.46	1.34
48	w	174	OMC	C4-N3	5.10	1.44	1.34
3	D	3825	A2M	O5'-C5'	-5.09	1.32	1.44
3	D	3899	OMG	C2-N3	5.09	1.45	1.33
3	D	1522	OMG	C2-N3	5.09	1.45	1.33
3	D	2424	OMG	C2-N2	5.09	1.46	1.34
48	w	601	OMG	C2-N2	5.08	1.46	1.34
3	D	2364	OMG	C2-N3	5.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1871	A2M	O5'-C5'	-5.05	1.32	1.44
3	D	1625	OMG	C2-N2	5.01	1.46	1.34
48	w	509	OMG	C2-N2	5.00	1.46	1.34
3	D	4499	OMG	C2-N2	5.00	1.46	1.34
5	F	75	OMG	C2-N2	5.00	1.46	1.34
48	w	512	A2M	O5'-C5'	-4.99	1.32	1.44
48	w	1391	OMC	C4-N3	4.99	1.44	1.34
3	D	3830	A2M	O5'-C5'	-4.97	1.32	1.44
3	D	4447	5MC	C6-N1	4.97	1.46	1.38
3	D	4494	OMG	C2-N2	4.97	1.46	1.34
3	D	3627	OMG	C2-N2	4.96	1.46	1.34
3	D	2401	A2M	O5'-C5'	-4.96	1.32	1.44
48	w	1703	OMC	C4-N3	4.95	1.44	1.34
3	D	4370	OMG	C2-N2	4.95	1.46	1.34
3	D	3744	OMG	C2-N2	4.95	1.46	1.34
48	w	159	A2M	O5'-C5'	-4.94	1.32	1.44
3	D	4618	OMG	C2-N2	4.94	1.45	1.34
3	D	3792	OMG	C2-N2	4.92	1.45	1.34
48	w	174	OMC	C4-N4	4.92	1.45	1.33
3	D	400	A2M	O5'-C5'	-4.91	1.32	1.44
48	w	517	OMC	C4-N4	4.91	1.45	1.33
3	D	4196	OMG	C2-N2	4.91	1.45	1.34
3	D	398	A2M	O5'-C5'	-4.90	1.32	1.44
3	D	4623	OMG	C2-N2	4.90	1.45	1.34
48	w	1031	A2M	O5'-C5'	-4.90	1.32	1.44
3	D	3718	A2M	O5'-C5'	-4.89	1.32	1.44
3	D	1326	A2M	O5'-C5'	-4.89	1.32	1.44
3	D	4523	A2M	O5'-C5'	-4.89	1.32	1.44
48	w	1391	OMC	C4-N4	4.88	1.45	1.33
3	D	1316	OMG	C2-N2	4.88	1.45	1.34
3	D	2364	OMG	C2-N2	4.87	1.45	1.34
48	w	462	OMC	C4-N4	4.86	1.45	1.33
3	D	3899	OMG	C2-N2	4.85	1.45	1.34
3	D	4228	OMG	C2-N2	4.85	1.45	1.34
48	w	1383	A2M	O5'-C5'	-4.85	1.32	1.44
3	D	3724	A2M	O5'-C5'	-4.85	1.32	1.44
3	D	1522	OMG	C2-N2	4.84	1.45	1.34
48	w	1703	OMC	C4-N4	4.83	1.45	1.33
3	D	2824	OMC	C4-N3	4.83	1.44	1.34
3	D	4637	OMG	C2-N2	4.83	1.45	1.34
3	D	4392	OMG	C2-N2	4.82	1.45	1.34
3	D	2804	OMC	C4-N3	4.81	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3887	OMC	C4-N3	4.81	1.44	1.34
3	D	2363	A2M	O5'-C5'	-4.80	1.33	1.44
48	w	484	A2M	O5'-C5'	-4.76	1.33	1.44
3	D	2861	OMC	C4-N3	4.75	1.44	1.34
3	D	1340	OMC	C4-N3	4.75	1.44	1.34
3	D	4530	UR3	C2-N3	4.74	1.48	1.39
3	D	2422	OMC	C4-N3	4.72	1.44	1.34
3	D	3701	OMC	C4-N3	4.72	1.44	1.34
3	D	2861	OMC	C4-N4	4.71	1.45	1.33
3	D	3808	OMC	C4-N4	4.71	1.45	1.33
3	D	2422	OMC	C4-N4	4.71	1.45	1.33
3	D	1340	OMC	C4-N4	4.71	1.45	1.33
3	D	3782	5MC	C6-N1	4.71	1.46	1.38
3	D	4536	OMC	C4-N3	4.70	1.44	1.34
48	w	27	A2M	O5'-C5'	-4.70	1.33	1.44
3	D	2365	OMC	C4-N3	4.70	1.44	1.34
3	D	2804	OMC	C4-N4	4.69	1.45	1.33
3	D	2824	OMC	C4-N4	4.69	1.45	1.33
3	D	3701	OMC	C4-N4	4.69	1.45	1.33
2	C	34	56B	C2-N2	4.69	1.45	1.34
3	D	4456	OMC	C4-N3	4.69	1.44	1.34
3	D	3808	OMC	C4-N3	4.68	1.43	1.34
3	D	3887	OMC	C4-N4	4.68	1.44	1.33
48	w	99	A2M	O5'-C5'	-4.68	1.33	1.44
3	D	4536	OMC	C4-N4	4.68	1.44	1.33
48	w	1678	A2M	O5'-C5'	-4.67	1.33	1.44
3	D	2365	OMC	C4-N4	4.67	1.44	1.33
3	D	3760	A2M	O5'-C5'	-4.66	1.33	1.44
3	D	4456	OMC	C4-N4	4.66	1.44	1.33
2	B	34	56B	C2-N2	4.64	1.45	1.34
3	D	3841	OMC	C4-N4	4.62	1.44	1.33
3	D	2351	OMC	C4-N3	4.57	1.43	1.34
3	D	1534	A2M	O5'-C5'	-4.57	1.33	1.44
3	D	2351	OMC	C4-N4	4.56	1.44	1.33
48	w	1639	G7M	C5-N7	-4.53	1.33	1.39
3	D	3841	OMC	C4-N3	4.53	1.43	1.34
48	w	576	A2M	O5'-C5'	-4.50	1.33	1.44
48	w	166	A2M	O5'-C5'	-4.49	1.33	1.44
48	w	590	A2M	O5'-C5'	-4.44	1.33	1.44
48	w	174	OMC	C2-N1	4.43	1.49	1.40
48	w	517	OMC	C2-N1	4.41	1.49	1.40
2	B	48	5MC	C2-N1	4.38	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	462	OMC	C2-N1	4.36	1.49	1.40
48	w	1391	OMC	C2-N1	4.36	1.49	1.40
2	C	48	5MC	C2-N1	4.30	1.49	1.40
48	w	1703	OMC	C2-N1	4.26	1.49	1.40
2	C	48	5MC	C4-N4	4.18	1.45	1.34
2	B	46	G7M	C5-N7	-4.17	1.34	1.39
3	D	2824	OMC	C2-N1	4.16	1.49	1.40
2	B	48	5MC	C4-N4	4.15	1.44	1.34
3	D	2804	OMC	C2-N1	4.14	1.49	1.40
3	D	2422	OMC	C2-N1	4.14	1.49	1.40
3	D	2351	OMC	C2-N1	4.13	1.49	1.40
2	C	34	56B	C5-C6	4.12	1.53	1.44
3	D	3808	OMC	C2-N1	4.09	1.48	1.40
3	D	3887	OMC	C2-N1	4.09	1.48	1.40
2	B	34	56B	C5-C6	4.06	1.53	1.44
2	C	46	G7M	C5-C6	4.05	1.54	1.43
2	C	46	G7M	C5-N7	-4.02	1.34	1.39
3	D	2861	OMC	C2-N1	4.00	1.48	1.40
3	D	3782	5MC	C2-N1	3.97	1.48	1.40
3	D	4456	OMC	C2-N1	3.97	1.48	1.40
3	D	2365	OMC	C2-N1	3.95	1.48	1.40
3	D	4536	OMC	C2-N1	3.95	1.48	1.40
3	D	3701	OMC	C2-N1	3.95	1.48	1.40
3	D	3841	OMC	C2-N1	3.95	1.48	1.40
3	D	4447	5MC	C4-N4	3.94	1.44	1.34
3	D	3782	5MC	C4-N4	3.94	1.44	1.34
2	B	46	G7M	C5-C6	3.93	1.54	1.43
3	D	1340	OMC	C2-N1	3.91	1.48	1.40
2	C	39	UY1	C2-N1	3.83	1.41	1.36
3	D	4447	5MC	C2-N1	3.80	1.48	1.40
48	w	1639	G7M	C5-C6	3.75	1.53	1.43
48	w	210	PSU	C6-C5	3.59	1.39	1.35
48	w	799	OMU	C4-N3	3.55	1.44	1.38
48	w	627	OMU	C4-N3	3.53	1.44	1.38
48	w	1288	OMU	C4-N3	3.52	1.44	1.38
2	B	55	PSU	C6-C5	3.51	1.39	1.35
48	w	609	PSU	C6-C5	3.50	1.39	1.35
48	w	218	PSU	C6-C5	3.49	1.39	1.35
48	w	93	PSU	C6-C5	3.49	1.39	1.35
2	C	55	PSU	C6-C5	3.49	1.39	1.35
2	B	39	UY1	C2-N1	3.48	1.41	1.36
48	w	1804	OMU	C4-N3	3.48	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	572	PSU	C6-C5	3.48	1.39	1.35
48	w	801	PSU	C6-C5	3.47	1.39	1.35
3	D	1773	OMU	C4-N3	3.45	1.44	1.38
48	w	34	PSU	C6-C5	3.45	1.39	1.35
48	w	428	OMU	C4-N3	3.43	1.44	1.38
48	w	1625	PSU	C6-C5	3.42	1.39	1.35
48	w	1442	OMU	C4-N3	3.41	1.44	1.38
48	w	1238	PSU	C6-C5	3.41	1.39	1.35
48	w	815	PSU	C6-C5	3.39	1.39	1.35
48	w	866	PSU	C6-C5	3.39	1.39	1.35
48	w	119	PSU	C6-C5	3.38	1.39	1.35
48	w	686	PSU	C6-C5	3.38	1.39	1.35
48	w	121	OMU	C4-N3	3.38	1.44	1.38
48	w	105	PSU	C6-C5	3.37	1.39	1.35
48	w	172	OMU	C4-N3	3.37	1.44	1.38
48	w	822	PSU	C6-C5	3.37	1.39	1.35
48	w	863	PSU	C6-C5	3.36	1.39	1.35
48	w	116	OMU	C4-N3	3.35	1.44	1.38
3	D	3762	PSU	C6-C5	3.34	1.39	1.35
48	w	1244	PSU	C6-C5	3.34	1.39	1.35
48	w	1326	OMU	C4-N3	3.33	1.44	1.38
48	w	966	PSU	C6-C5	3.31	1.39	1.35
48	w	109	PSU	C6-C5	3.30	1.39	1.35
48	w	1445	PSU	C6-C5	3.30	1.39	1.35
48	w	36	PSU	C6-C5	3.30	1.39	1.35
3	D	3770	PSU	C6-C5	3.27	1.39	1.35
48	w	651	PSU	C6-C5	3.27	1.39	1.35
3	D	4392	OMG	C5-N7	-3.26	1.32	1.39
3	D	3734	PSU	C6-C5	3.26	1.39	1.35
48	w	814	PSU	C6-C5	3.24	1.39	1.35
3	D	1316	OMG	C5-N7	-3.24	1.32	1.39
48	w	1056	PSU	C6-C5	3.24	1.39	1.35
3	D	3768	PSU	C6-C5	3.24	1.39	1.35
3	D	4494	OMG	C5-N7	-3.23	1.32	1.39
3	D	3715	PSU	C6-C5	3.23	1.39	1.35
48	w	1004	PSU	C6-C5	3.23	1.39	1.35
3	D	3818	UY1	C2-N1	3.21	1.41	1.36
3	D	3792	OMG	C5-N7	-3.21	1.32	1.39
48	w	517	OMC	C6-N1	3.21	1.45	1.38
48	w	174	OMC	C6-N1	3.21	1.45	1.38
3	D	4420	PSU	C6-C5	3.20	1.39	1.35
48	w	1177	PSU	C6-C5	3.19	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1625	OMG	C5-N7	-3.18	1.32	1.39
48	w	1643	PSU	C6-C5	3.18	1.39	1.35
2	B	35	PSU	C6-C5	3.18	1.39	1.35
3	D	4500	PSU	C6-C5	3.17	1.39	1.35
48	w	1367	PSU	C6-C5	3.17	1.39	1.35
48	w	649	PSU	C6-C5	3.17	1.39	1.35
3	D	4196	OMG	C5-N7	-3.17	1.32	1.39
48	w	1232	PSU	C6-C5	3.16	1.39	1.35
48	w	1045	PSU	C6-C5	3.16	1.39	1.35
48	w	462	OMC	C6-N1	3.14	1.45	1.38
2	B	37	1MG	C5-C6	3.14	1.53	1.45
3	D	4370	OMG	C5-N7	-3.13	1.33	1.39
3	D	1522	OMG	C5-N7	-3.13	1.33	1.39
3	D	2415	OMU	C4-N3	3.13	1.44	1.38
3	D	4637	OMG	C5-N7	-3.12	1.33	1.39
3	D	2424	OMG	C5-N7	-3.12	1.33	1.39
3	D	3899	OMG	C5-N7	-3.12	1.33	1.39
48	w	1703	OMC	C6-N1	3.11	1.45	1.38
48	w	1391	OMC	C6-N1	3.11	1.45	1.38
3	D	3627	OMG	C5-N7	-3.11	1.33	1.39
48	w	1046	PSU	C6-C5	3.11	1.38	1.35
48	w	1347	PSU	C6-C5	3.11	1.38	1.35
48	w	1692	PSU	C6-C5	3.10	1.38	1.35
3	D	4499	OMG	C5-N7	-3.09	1.33	1.39
3	D	5010	PSU	C6-C5	3.08	1.38	1.35
3	D	4456	OMC	O2-C2	-3.08	1.18	1.23
48	w	1490	OMG	C5-N7	-3.08	1.33	1.39
3	D	4423	PSU	C6-C5	3.08	1.38	1.35
48	w	1174	PSU	C6-C5	3.07	1.38	1.35
3	D	4392	OMG	O6-C6	-3.07	1.17	1.23
5	F	75	OMG	C5-N7	-3.07	1.33	1.39
2	C	35	PSU	C6-C5	3.06	1.38	1.35
3	D	1522	OMG	O6-C6	-3.06	1.17	1.23
3	D	4623	OMG	C5-N7	-3.06	1.33	1.39
2	C	34	56B	C11-C12	3.06	1.58	1.53
3	D	2351	OMC	O2-C2	-3.06	1.18	1.23
3	D	1860	PSU	C6-C5	3.05	1.38	1.35
3	D	3764	PSU	C6-C5	3.05	1.38	1.35
3	D	4620	OMU	O2-C2	-3.05	1.17	1.23
48	w	406	PSU	C6-C5	3.05	1.38	1.35
3	D	4536	OMC	O2-C2	-3.05	1.18	1.23
3	D	4498	OMU	C4-N3	3.04	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	37	1MG	C5-C6	3.04	1.53	1.45
2	B	37	1MG	C5-N7	-3.04	1.33	1.39
2	C	37	1MG	C5-N7	-3.04	1.33	1.39
3	D	3841	OMC	O2-C2	-3.03	1.18	1.23
3	D	4618	OMG	C5-N7	-3.03	1.33	1.39
3	D	2364	OMG	O6-C6	-3.03	1.17	1.23
3	D	3925	OMU	O2-C2	-3.03	1.17	1.23
3	D	3899	OMG	O6-C6	-3.03	1.17	1.23
48	w	1850	MA6	C8-N9	-3.03	1.32	1.37
3	D	2364	OMG	C5-N7	-3.03	1.33	1.39
3	D	2632	PSU	C6-C5	3.03	1.38	1.35
3	D	4228	OMG	C5-N7	-3.02	1.33	1.39
3	D	1316	OMG	O6-C6	-3.02	1.17	1.23
3	D	3744	OMG	C5-N7	-3.02	1.33	1.39
3	D	4306	OMU	O2-C2	-3.02	1.17	1.23
3	D	2837	OMU	O4-C4	-3.02	1.18	1.24
48	w	1081	PSU	C6-C5	3.01	1.38	1.35
2	C	46	G7M	C6-N1	3.01	1.44	1.38
3	D	4628	PSU	C6-C5	3.01	1.38	1.35
3	D	2804	OMC	C6-N1	3.01	1.45	1.38
3	D	4228	OMG	O6-C6	-3.00	1.17	1.23
3	D	4296	PSU	C6-C5	3.00	1.38	1.35
3	D	3925	OMU	O4-C4	-3.00	1.18	1.24
3	D	3627	OMG	O6-C6	-2.99	1.17	1.23
3	D	4552	PSU	C6-C5	2.99	1.38	1.35
3	D	3887	OMC	C6-N1	2.99	1.45	1.38
48	w	1851	MA6	C5-C4	-2.99	1.33	1.39
2	C	46	G7M	C2-N1	2.98	1.45	1.37
48	w	683	OMG	C5-N7	-2.98	1.33	1.39
3	D	2837	OMU	C4-N3	2.98	1.43	1.38
3	D	1340	OMC	O2-C2	-2.98	1.18	1.23
3	D	4494	OMG	O6-C6	-2.98	1.17	1.23
3	D	2422	OMC	C6-N1	2.97	1.45	1.38
3	D	2824	OMC	O2-C2	-2.97	1.18	1.23
3	D	4521	PSU	C6-C5	2.97	1.38	1.35
3	D	2824	OMC	C6-N1	2.97	1.45	1.38
3	D	3744	OMG	O6-C6	-2.97	1.17	1.23
3	D	4623	OMG	O6-C6	-2.97	1.17	1.23
3	D	4620	OMU	C4-N3	2.96	1.43	1.38
48	w	1850	MA6	C6-N6	2.96	1.45	1.36
3	D	2861	OMC	O2-C2	-2.96	1.18	1.23
3	D	2365	OMC	O2-C2	-2.96	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4227	OMU	C4-N3	2.96	1.43	1.38
3	D	1781	PSU	C6-C5	2.96	1.38	1.35
3	D	3887	OMC	O2-C2	-2.96	1.18	1.23
3	D	4456	OMC	C6-N1	2.96	1.45	1.38
3	D	3808	OMC	O2-C2	-2.96	1.18	1.23
3	D	5001	PSU	C6-C5	2.96	1.38	1.35
2	B	46	G7M	C6-N1	2.95	1.44	1.38
2	B	46	G7M	C2-N1	2.95	1.45	1.37
3	D	4361	PSU	C6-C5	2.95	1.38	1.35
3	D	4637	OMG	O6-C6	-2.95	1.18	1.23
3	D	3853	PSU	C6-C5	2.94	1.38	1.35
3	D	4498	OMU	O2-C2	-2.94	1.17	1.23
3	D	4431	PSU	C6-C5	2.94	1.38	1.35
48	w	1639	G7M	C2-N1	2.94	1.44	1.37
3	D	4620	OMU	O4-C4	-2.94	1.18	1.24
3	D	2422	OMC	O2-C2	-2.93	1.18	1.23
48	w	1328	OMG	C5-C6	2.93	1.55	1.44
2	C	10	2MG	C5-N7	-2.93	1.33	1.39
3	D	4227	OMU	O4-C4	-2.93	1.18	1.24
3	D	1744	PSU	C6-C5	2.93	1.38	1.35
3	D	3944	OMG	C5-N7	-2.92	1.33	1.39
3	D	4471	PSU	C6-C5	2.92	1.38	1.35
3	D	4196	OMG	O6-C6	-2.92	1.18	1.23
3	D	2861	OMC	C6-N1	2.92	1.45	1.38
3	D	1862	PSU	C6-C5	2.92	1.38	1.35
2	B	34	56B	C11-C12	2.92	1.58	1.53
48	w	436	OMG	C5-N7	-2.92	1.33	1.39
3	D	3925	OMU	C4-N3	2.92	1.43	1.38
3	D	2351	OMC	C6-N1	2.92	1.45	1.38
3	D	4499	OMG	O6-C6	-2.91	1.18	1.23
3	D	3792	OMG	O6-C6	-2.91	1.18	1.23
3	D	4370	OMG	O6-C6	-2.91	1.18	1.23
3	D	4442	PSU	C6-C5	2.91	1.38	1.35
3	D	2365	OMC	C6-N1	2.91	1.45	1.38
3	D	3730	PSU	C6-C5	2.90	1.38	1.35
3	D	4498	OMU	O4-C4	-2.90	1.18	1.24
3	D	3701	OMC	C6-N1	2.90	1.45	1.38
3	D	1760	OMG	C5-C6	2.90	1.55	1.44
3	D	3808	OMC	C6-N1	2.90	1.45	1.38
3	D	4293	PSU	C6-C5	2.89	1.38	1.35
3	D	4306	OMU	O4-C4	-2.89	1.18	1.24
3	D	4972	PSU	C6-C5	2.89	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2837	OMU	O2-C2	-2.89	1.17	1.23
3	D	4532	PSU	C6-C5	2.89	1.38	1.35
3	D	4306	OMU	C4-N3	2.89	1.43	1.38
3	D	4353	PSU	C6-C5	2.89	1.38	1.35
3	D	3944	OMG	C5-C6	2.88	1.55	1.44
3	D	4536	OMC	C6-N1	2.88	1.44	1.38
3	D	4618	OMG	O6-C6	-2.88	1.18	1.23
48	w	681	PSU	C6-C5	2.87	1.38	1.35
48	w	644	OMG	C5-C6	2.87	1.55	1.44
3	D	2804	OMC	O2-C2	-2.87	1.18	1.23
3	D	3920	PSU	C6-C5	2.87	1.38	1.35
3	D	1625	OMG	O6-C6	-2.87	1.18	1.23
3	D	2415	OMU	O4-C4	-2.87	1.18	1.24
48	w	436	OMG	C5-C6	2.86	1.55	1.44
3	D	4689	PSU	C6-C5	2.86	1.38	1.35
48	w	1703	OMC	O2-C2	-2.86	1.18	1.23
3	D	4579	PSU	C6-C5	2.86	1.38	1.35
48	w	509	OMG	C5-C6	2.86	1.55	1.44
3	D	3841	OMC	C6-N1	2.86	1.44	1.38
3	D	3701	OMC	O2-C2	-2.86	1.18	1.23
3	D	4227	OMU	O2-C2	-2.86	1.17	1.23
48	w	601	OMG	C5-N7	-2.85	1.33	1.39
3	D	1792	PSU	C6-C5	2.85	1.38	1.35
48	w	1639	G7M	C6-N1	2.85	1.44	1.38
48	w	509	OMG	C5-N7	-2.84	1.33	1.39
3	D	2424	OMG	O6-C6	-2.84	1.18	1.23
3	D	1340	OMC	C6-N1	2.84	1.44	1.38
2	B	10	2MG	C5-N7	-2.84	1.33	1.39
48	w	1851	MA6	C6-N6	2.84	1.45	1.36
3	D	4457	PSU	C6-C5	2.83	1.38	1.35
2	C	58	1MA	C2-N1	2.83	1.41	1.35
3	D	4576	PSU	C6-C5	2.83	1.38	1.35
48	w	644	OMG	C5-N7	-2.82	1.33	1.39
5	F	75	OMG	O6-C6	-2.82	1.18	1.23
3	D	3637	PSU	C6-C5	2.82	1.38	1.35
2	C	6	2MG	C5-N7	-2.82	1.33	1.39
48	w	1328	OMG	C5-N7	-2.81	1.33	1.39
2	C	47	H2U	C2-N3	-2.81	1.33	1.38
3	D	4403	PSU	C6-C5	2.81	1.38	1.35
3	D	1760	OMG	C5-N7	-2.81	1.33	1.39
48	w	601	OMG	C5-C6	2.81	1.54	1.44
3	D	4312	PSU	C6-C5	2.81	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1760	OMG	C6-N1	2.81	1.44	1.38
48	w	1850	MA6	C5-C4	-2.80	1.33	1.39
3	D	3695	PSU	C6-C5	2.80	1.38	1.35
3	D	2415	OMU	O2-C2	-2.80	1.17	1.23
3	D	2508	PSU	C6-C5	2.80	1.38	1.35
2	B	58	1MA	C2-N1	2.80	1.41	1.35
48	w	683	OMG	C5-C6	2.79	1.54	1.44
3	D	4530	UR3	C6-N1	2.79	1.44	1.38
48	w	509	OMG	O6-C6	-2.78	1.18	1.23
48	w	601	OMG	O6-C6	-2.78	1.18	1.23
2	B	27	M2G	C6-N1	2.78	1.44	1.38
48	w	683	OMG	O6-C6	-2.77	1.18	1.23
3	D	4299	PSU	C6-C5	2.77	1.38	1.35
3	D	1782	PSU	C6-C5	2.76	1.38	1.35
5	F	75	OMG	C5-C6	2.76	1.54	1.44
2	C	34	56B	C2-N1	2.76	1.44	1.37
48	w	436	OMG	O6-C6	-2.76	1.18	1.23
3	D	3851	PSU	C6-C5	2.75	1.38	1.35
2	B	27	M2G	C2-N2	2.75	1.40	1.35
3	D	3744	OMG	C5-C6	2.75	1.54	1.44
2	C	26	M2G	C2-N2	2.75	1.40	1.35
48	w	1490	OMG	O6-C6	-2.75	1.18	1.23
48	w	1490	OMG	C5-C6	2.74	1.54	1.44
2	B	6	2MG	C5-C6	2.74	1.54	1.44
3	D	4618	OMG	C5-C6	2.74	1.54	1.44
3	D	4220	6MZ	C5-C4	-2.74	1.33	1.39
3	D	3944	OMG	C6-N1	2.73	1.43	1.38
48	w	1850	MA6	C5-N7	-2.73	1.33	1.39
3	D	4447	5MC	O2-C2	-2.73	1.18	1.23
48	w	174	OMC	O2-C2	-2.73	1.18	1.23
3	D	3792	OMG	C5-C6	2.72	1.54	1.44
48	w	116	OMU	O4-C4	-2.72	1.19	1.24
3	D	4499	OMG	C5-C6	2.72	1.54	1.44
48	w	644	OMG	O6-C6	-2.72	1.18	1.23
3	D	2364	OMG	C5-C6	2.72	1.54	1.44
3	D	2424	OMG	C5-C6	2.71	1.54	1.44
48	w	1326	OMU	O4-C4	-2.71	1.19	1.24
3	D	4637	OMG	C5-C6	2.71	1.54	1.44
2	C	47	H2U	C4-N3	-2.70	1.33	1.37
3	D	1625	OMG	C5-C6	2.70	1.54	1.44
2	B	6	2MG	C6-N1	2.70	1.43	1.38
48	w	1442	OMU	O4-C4	-2.70	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	1804	OMU	O4-C4	-2.70	1.19	1.24
48	w	1391	OMC	O2-C2	-2.70	1.18	1.23
3	D	4228	OMG	C5-C6	2.69	1.54	1.44
2	B	34	56B	C2-N1	2.69	1.44	1.37
48	w	1804	OMU	O2-C2	-2.69	1.18	1.23
48	w	517	OMC	O2-C2	-2.69	1.18	1.23
48	w	428	OMU	O4-C4	-2.69	1.19	1.24
3	D	3627	OMG	C5-C6	2.68	1.54	1.44
3	D	4196	OMG	C5-C6	2.68	1.54	1.44
48	w	1326	OMU	O2-C2	-2.68	1.18	1.23
48	w	462	OMC	O2-C2	-2.68	1.18	1.23
48	w	644	OMG	C6-N1	2.68	1.43	1.38
48	w	1442	OMU	O2-C2	-2.67	1.18	1.23
3	D	4623	OMG	C5-C6	2.67	1.54	1.44
48	w	121	OMU	O2-C2	-2.67	1.18	1.23
2	C	6	2MG	C5-C6	2.67	1.54	1.44
2	B	47	H2U	C2-N3	-2.67	1.33	1.38
48	w	172	OMU	O4-C4	-2.67	1.19	1.24
3	D	3899	OMG	C5-C6	2.67	1.54	1.44
3	D	4392	OMG	C5-C6	2.67	1.54	1.44
3	D	1683	PSU	C6-C5	2.66	1.38	1.35
3	D	1536	PSU	C6-C5	2.66	1.38	1.35
48	w	121	OMU	O4-C4	-2.66	1.19	1.24
3	D	4494	OMG	C5-C6	2.66	1.54	1.44
48	w	627	OMU	O4-C4	-2.66	1.19	1.24
3	D	1760	OMG	O6-C6	-2.65	1.18	1.23
3	D	3944	OMG	O6-C6	-2.65	1.18	1.23
3	D	3758	PSU	C6-C5	2.65	1.38	1.35
3	D	4370	OMG	C5-C6	2.64	1.54	1.44
48	w	428	OMU	O2-C2	-2.64	1.18	1.23
48	w	1328	OMG	C6-N1	2.64	1.43	1.38
48	w	683	OMG	C6-N1	2.64	1.43	1.38
48	w	1328	OMG	O6-C6	-2.63	1.18	1.23
3	D	1760	OMG	C2-N1	2.63	1.44	1.37
48	w	799	OMU	O4-C4	-2.63	1.19	1.24
48	w	668	A2M	O4'-C4'	-2.63	1.39	1.45
48	w	601	OMG	C6-N1	2.63	1.43	1.38
2	B	34	56B	O6-C6	-2.63	1.18	1.23
48	w	116	OMU	O2-C2	-2.63	1.18	1.23
3	D	1677	PSU	C6-C5	2.62	1.38	1.35
2	C	10	2MG	C5-C6	2.61	1.54	1.44
48	w	172	OMU	O2-C2	-2.61	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	627	OMU	O2-C2	-2.61	1.18	1.23
48	w	1288	OMU	O4-C4	-2.61	1.19	1.24
3	D	1522	OMG	C5-C6	2.61	1.54	1.44
2	B	26	M2G	C2-N2	2.60	1.40	1.35
2	B	6	2MG	C5-N7	-2.59	1.34	1.39
2	B	10	2MG	C5-C6	2.59	1.54	1.44
2	C	34	56B	O6-C6	-2.59	1.18	1.23
2	C	27	M2G	C2-N2	2.59	1.40	1.35
2	C	26	M2G	C6-N1	2.59	1.43	1.38
48	w	509	OMG	C6-N1	2.58	1.43	1.38
48	w	1639	G7M	O6-C6	-2.58	1.18	1.23
3	D	3944	OMG	C2-N1	2.58	1.44	1.37
3	D	1316	OMG	C5-C6	2.57	1.54	1.44
3	D	2424	OMG	C6-N1	2.55	1.43	1.38
3	D	1773	OMU	O4-C4	-2.55	1.19	1.24
3	D	3639	PSU	C6-C5	2.55	1.38	1.35
48	w	1490	OMG	C6-N1	2.55	1.43	1.38
48	w	799	OMU	O2-C2	-2.55	1.18	1.23
3	D	1773	OMU	O2-C2	-2.54	1.18	1.23
48	w	1832	6MZ	C5-C4	-2.53	1.34	1.39
48	w	1288	OMU	O2-C2	-2.53	1.18	1.23
48	w	644	OMG	C2-N1	2.53	1.43	1.37
48	w	462	OMC	C5-C4	2.52	1.48	1.42
48	w	174	OMC	C5-C4	2.52	1.48	1.42
48	w	1851	MA6	C5-N7	-2.52	1.34	1.39
48	w	436	OMG	C6-N1	2.52	1.43	1.38
2	B	47	H2U	C4-N3	-2.52	1.33	1.37
2	C	6	2MG	C6-N1	2.52	1.43	1.38
2	B	10	2MG	C6-N1	2.51	1.43	1.38
48	w	517	OMC	C5-C4	2.51	1.48	1.42
3	D	4499	OMG	C6-N1	2.50	1.43	1.38
5	F	75	OMG	C6-N1	2.50	1.43	1.38
2	C	10	2MG	C6-N1	2.50	1.43	1.38
48	w	1328	OMG	C2-N1	2.49	1.43	1.37
48	w	436	OMG	C2-N1	2.48	1.43	1.37
3	D	2363	A2M	O4'-C4'	-2.47	1.39	1.45
2	B	46	G7M	O6-C6	-2.47	1.18	1.23
48	w	1851	MA6	C8-N9	-2.46	1.33	1.37
48	w	601	OMG	C2-N1	2.46	1.43	1.37
48	w	683	OMG	C2-N1	2.45	1.43	1.37
48	w	509	OMG	C2-N1	2.45	1.43	1.37
3	D	3744	OMG	C6-N1	2.42	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1316	OMG	C4-N9	-2.42	1.31	1.38
48	w	1391	OMC	C5-C4	2.41	1.48	1.42
2	C	34	56B	C6-N1	2.41	1.43	1.38
3	D	4530	UR3	O4-C4	-2.41	1.18	1.23
48	w	1703	OMC	C5-C4	2.41	1.48	1.42
3	D	2424	OMG	C2-N1	2.40	1.43	1.37
2	C	27	M2G	C6-N1	2.39	1.43	1.38
3	D	4618	OMG	C6-N1	2.39	1.43	1.38
3	D	3782	5MC	O2-C2	-2.38	1.19	1.23
3	D	4196	OMG	C6-N1	2.38	1.43	1.38
3	D	1625	OMG	C6-N1	2.38	1.43	1.38
48	w	1490	OMG	C2-N1	2.38	1.43	1.37
2	B	26	M2G	C6-N1	2.36	1.43	1.38
3	D	3899	OMG	C6-N1	2.36	1.43	1.38
2	B	34	56B	C6-N1	2.36	1.43	1.38
3	D	3627	OMG	C6-N1	2.36	1.43	1.38
3	D	4618	OMG	C2-N1	2.36	1.43	1.37
3	D	4499	OMG	C2-N1	2.35	1.43	1.37
3	D	4228	OMG	C6-N1	2.34	1.43	1.38
5	F	75	OMG	C2-N1	2.33	1.43	1.37
3	D	2364	OMG	C6-N1	2.32	1.43	1.38
2	C	48	5MC	CM5-C5	2.32	1.56	1.50
2	C	46	G7M	O6-C6	-2.32	1.19	1.23
3	D	4637	OMG	C6-N1	2.32	1.43	1.38
3	D	4370	OMG	C6-N1	2.32	1.43	1.38
3	D	1524	A2M	O4'-C4'	-2.31	1.39	1.45
3	D	3792	OMG	C6-N1	2.31	1.43	1.38
3	D	3701	OMC	C5-C4	2.31	1.48	1.42
3	D	1316	OMG	C6-N1	2.30	1.43	1.38
3	D	4530	UR3	O2-C2	-2.30	1.18	1.22
3	D	4220	6MZ	C8-N9	-2.30	1.33	1.37
3	D	1522	OMG	C4-N9	-2.29	1.32	1.38
3	D	3744	OMG	C2-N1	2.29	1.43	1.37
3	D	4494	OMG	C6-N1	2.29	1.43	1.38
3	D	4623	OMG	C4-N9	-2.28	1.32	1.38
3	D	4623	OMG	C6-N1	2.28	1.43	1.38
3	D	2824	OMC	C5-C4	2.28	1.48	1.42
3	D	1625	OMG	C2-N1	2.28	1.43	1.37
3	D	4196	OMG	C2-N1	2.28	1.43	1.37
3	D	1522	OMG	C6-N1	2.27	1.43	1.38
3	D	3808	OMC	C5-C4	2.26	1.48	1.42
2	C	10	2MG	O6-C6	-2.26	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	48	5MC	CM5-C5	2.26	1.56	1.50
3	D	4623	OMG	C2-N1	2.26	1.43	1.37
3	D	3899	OMG	C4-N9	-2.25	1.32	1.38
2	C	48	5MC	O2-C2	-2.25	1.19	1.23
3	D	4494	OMG	C2-N1	2.25	1.43	1.37
2	B	46	G7M	C8-N7	2.25	1.37	1.33
2	B	10	2MG	O6-C6	-2.24	1.19	1.23
3	D	2422	OMC	C5-C4	2.24	1.48	1.42
3	D	2364	OMG	C4-N9	-2.24	1.32	1.38
3	D	4228	OMG	C2-N1	2.24	1.43	1.37
3	D	4392	OMG	C6-N1	2.23	1.43	1.38
3	D	3627	OMG	C2-N1	2.23	1.43	1.37
3	D	3899	OMG	C2-N1	2.23	1.43	1.37
2	B	48	5MC	O2-C2	-2.23	1.19	1.23
3	D	4228	OMG	C4-N9	-2.22	1.32	1.38
3	D	4499	OMG	C4-N9	-2.22	1.32	1.38
3	D	2861	OMC	C5-C4	2.21	1.48	1.42
3	D	3887	OMC	C5-C4	2.21	1.48	1.42
3	D	4456	OMC	C5-C4	2.21	1.48	1.42
3	D	3841	OMC	C5-C4	2.21	1.48	1.42
3	D	4392	OMG	C2-N1	2.20	1.43	1.37
3	D	3792	OMG	C2-N1	2.20	1.43	1.37
3	D	1316	OMG	C2-N1	2.20	1.43	1.37
3	D	2804	OMC	C5-C4	2.18	1.47	1.42
3	D	3627	OMG	C4-N9	-2.18	1.32	1.38
2	C	37	1MG	O6-C6	-2.18	1.18	1.23
3	D	4370	OMG	C2-N1	2.18	1.43	1.37
3	D	2424	OMG	C4-N9	-2.18	1.32	1.38
3	D	2364	OMG	C2-N1	2.18	1.43	1.37
2	C	6	2MG	O6-C6	-2.17	1.19	1.23
2	B	6	2MG	C4-N9	-2.17	1.32	1.38
3	D	4536	OMC	C5-C4	2.17	1.47	1.42
2	B	6	2MG	O6-C6	-2.17	1.19	1.23
3	D	4220	6MZ	C5-N7	-2.17	1.34	1.39
2	C	46	G7M	C8-N7	2.16	1.36	1.33
3	D	2365	OMC	C5-C4	2.16	1.47	1.42
3	D	4392	OMG	C4-N9	-2.16	1.32	1.38
3	D	4637	OMG	C2-N1	2.15	1.43	1.37
3	D	4637	OMG	C4-N9	-2.15	1.32	1.38
3	D	1522	OMG	C2-N1	2.15	1.43	1.37
3	D	1536	PSU	C4-C5	-2.14	1.38	1.44
2	B	37	1MG	O6-C6	-2.13	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3744	OMG	C4-N9	-2.13	1.32	1.38
2	C	37	1MG	C4-N9	-2.13	1.32	1.38
48	w	799	OMU	C6-N1	2.13	1.43	1.38
3	D	1773	OMU	C6-N1	2.13	1.43	1.38
3	D	4618	OMG	C4-N9	-2.12	1.32	1.38
48	w	590	A2M	C5-C4	2.12	1.43	1.39
48	w	121	OMU	C5-C4	2.12	1.48	1.43
3	D	4370	OMG	C4-N9	-2.11	1.32	1.38
3	D	1316	OMG	C8-N9	-2.11	1.32	1.37
3	D	4196	OMG	C4-N9	-2.11	1.32	1.38
5	F	75	OMG	C4-N9	-2.11	1.32	1.38
48	w	1288	OMU	C5-C4	2.10	1.48	1.43
2	C	39	UY1	C4-N3	2.10	1.42	1.38
2	B	26	M2G	C8-N9	2.10	1.42	1.37
3	D	3792	OMG	C4-N9	-2.10	1.32	1.38
3	D	1340	OMC	C5-C4	2.09	1.47	1.42
3	D	3639	PSU	C4-C5	-2.09	1.38	1.44
2	B	37	1MG	C4-N9	-2.09	1.32	1.38
48	w	172	OMU	C5-C4	2.09	1.48	1.43
3	D	4530	UR3	C5-C4	2.09	1.49	1.43
48	w	1832	6MZ	C8-N9	-2.09	1.33	1.37
48	w	166	A2M	C5-C4	2.08	1.42	1.39
3	D	4494	OMG	C4-N9	-2.08	1.32	1.38
3	D	4392	OMG	C8-N9	-2.07	1.32	1.37
3	D	1773	OMU	C5-C4	2.07	1.48	1.43
48	w	1288	OMU	C6-N1	2.07	1.43	1.38
48	w	428	OMU	C5-C4	2.07	1.48	1.43
48	w	116	OMU	C6-N1	2.06	1.43	1.38
3	D	1683	PSU	C4-C5	-2.06	1.38	1.44
48	w	1442	OMU	C5-C4	2.05	1.48	1.43
3	D	3851	PSU	C4-C5	-2.05	1.38	1.44
3	D	3899	OMG	C8-N9	-2.05	1.33	1.37
48	w	799	OMU	C5-C4	2.05	1.48	1.43
48	w	1326	OMU	C6-N1	2.05	1.42	1.38
48	w	601	OMG	C4-N9	-2.04	1.32	1.38
3	D	4523	A2M	O4'-C4'	-2.04	1.40	1.45
48	w	576	A2M	C5-C4	2.04	1.42	1.39
48	w	627	OMU	C6-N1	2.04	1.42	1.38
48	w	116	OMU	C5-C4	2.04	1.48	1.43
48	w	121	OMU	C6-N1	2.04	1.42	1.38
3	D	4637	OMG	C8-N9	-2.03	1.33	1.37
48	w	1832	6MZ	C5-N7	-2.03	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	627	OMU	C5-C4	2.03	1.48	1.43
48	w	159	A2M	C5-C4	2.02	1.42	1.39
48	w	1442	OMU	C6-N1	2.02	1.42	1.38
3	D	4442	PSU	O4'-C1'	-2.02	1.41	1.43
48	w	428	OMU	C6-N1	2.01	1.42	1.38
3	D	3782	5MC	CM5-C5	2.01	1.55	1.50
3	D	4579	PSU	C4-C5	-2.01	1.38	1.44
48	w	1804	OMU	C5-C4	2.01	1.48	1.43
48	w	683	OMG	C4-N9	-2.01	1.32	1.38
3	D	3920	PSU	C4-C5	-2.01	1.38	1.44
48	w	1326	OMU	C5-C4	2.01	1.48	1.43
3	D	4353	PSU	C4-C5	-2.00	1.38	1.44
3	D	4521	PSU	C4-C5	-2.00	1.38	1.44
48	w	681	PSU	C4-C5	-2.00	1.38	1.44
3	D	1677	PSU	O4'-C1'	-2.00	1.41	1.43
48	w	468	A2M	C5-C4	2.00	1.42	1.39

All (1000) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	5MU	C5-C4-N3	12.25	125.76	115.31
2	C	54	5MU	C5-C4-N3	12.01	125.57	115.31
2	B	54	5MU	C5-C6-N1	-10.01	113.04	123.34
2	C	54	5MU	C5-C6-N1	-9.97	113.08	123.34
2	C	34	56B	C1'-N9-C4	-7.62	103.86	126.50
2	B	34	56B	C1'-N9-C4	-7.39	104.54	126.50
2	C	10	2MG	C2-N3-C4	6.73	120.39	112.04
2	C	6	2MG	C2-N3-C4	6.51	120.12	112.04
2	B	6	2MG	C2-N3-C4	6.39	119.96	112.04
2	B	10	2MG	C2-N3-C4	6.16	119.68	112.04
2	C	34	56B	C5-C4-N3	-6.08	120.40	127.52
2	B	34	56B	C5-C4-N3	-6.08	120.41	127.52
48	w	1851	MA6	N1-C2-N3	-5.84	119.47	128.60
48	w	1850	MA6	N1-C2-N3	-5.82	119.49	128.60
3	D	2415	OMU	C4-N3-C2	-5.81	118.92	126.58
3	D	4220	6MZ	N1-C2-N3	-5.76	119.60	128.60
3	D	2837	OMU	C4-N3-C2	-5.71	119.05	126.58
3	D	4227	OMU	C4-N3-C2	-5.63	119.15	126.58
48	w	1832	6MZ	N1-C2-N3	-5.63	119.80	128.60
3	D	3925	OMU	C4-N3-C2	-5.60	119.20	126.58
2	C	10	2MG	C5-C4-N3	-5.49	119.55	128.46
3	D	4498	OMU	C4-N3-C2	-5.40	119.46	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4620	OMU	C4-N3-C2	-5.37	119.49	126.58
3	D	1625	OMG	C5-C4-N3	-5.37	119.75	128.46
48	w	172	OMU	C4-N3-C2	-5.36	119.51	126.58
2	B	54	5MU	O4-C4-C5	-5.36	118.69	124.90
3	D	4306	OMU	C4-N3-C2	-5.34	119.53	126.58
48	w	428	OMU	C4-N3-C2	-5.32	119.56	126.58
48	w	1804	OMU	C4-N3-C2	-5.31	119.58	126.58
48	w	1442	OMU	C4-N3-C2	-5.30	119.59	126.58
3	D	3792	OMG	C5-C4-N3	-5.29	119.88	128.46
48	w	436	OMG	C5-C4-N3	-5.26	119.92	128.46
3	D	4494	OMG	C5-C4-N3	-5.23	119.97	128.46
3	D	3944	OMG	C5-C4-N3	-5.22	119.99	128.46
48	w	1490	OMG	C5-C4-N3	-5.22	119.99	128.46
3	D	4196	OMG	C5-C4-N3	-5.21	120.01	128.46
3	D	4392	OMG	C5-C4-N3	-5.20	120.03	128.46
2	C	6	2MG	C5-C4-N3	-5.19	120.03	128.46
48	w	121	OMU	C4-N3-C2	-5.19	119.73	126.58
48	w	627	OMU	C4-N3-C2	-5.19	119.74	126.58
48	w	1326	OMU	C4-N3-C2	-5.16	119.77	126.58
48	w	116	OMU	C4-N3-C2	-5.15	119.79	126.58
48	w	1288	OMU	C4-N3-C2	-5.15	119.79	126.58
3	D	4370	OMG	C5-C4-N3	-5.12	120.15	128.46
48	w	509	OMG	C5-C4-N3	-5.10	120.19	128.46
48	w	1328	OMG	C5-C4-N3	-5.10	120.19	128.46
48	w	683	OMG	C5-C4-N3	-5.09	120.20	128.46
3	D	4637	OMG	C5-C4-N3	-5.09	120.21	128.46
48	w	799	OMU	C4-N3-C2	-5.07	119.89	126.58
5	F	75	OMG	C5-C4-N3	-5.07	120.24	128.46
3	D	1760	OMG	C5-C4-N3	-5.06	120.26	128.46
3	D	3744	OMG	C5-C4-N3	-5.04	120.28	128.46
3	D	3899	OMG	C5-C4-N3	-5.04	120.28	128.46
3	D	3627	OMG	C5-C4-N3	-5.02	120.32	128.46
3	D	1316	OMG	C5-C4-N3	-5.01	120.34	128.46
3	D	1862	PSU	N1-C2-N3	5.00	120.80	115.13
3	D	4618	OMG	C5-C4-N3	-4.98	120.38	128.46
3	D	2424	OMG	C5-C4-N3	-4.97	120.41	128.46
3	D	2364	OMG	C5-C4-N3	-4.96	120.41	128.46
48	w	1832	6MZ	C5-C4-N3	-4.96	120.27	126.75
3	D	1683	PSU	N1-C2-N3	4.96	120.75	115.13
3	D	4628	PSU	N1-C2-N3	4.96	120.75	115.13
2	C	54	5MU	O4-C4-C5	-4.95	119.16	124.90
2	C	47	H2U	C4-N3-C2	-4.95	121.69	125.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4499	OMG	C5-C4-N3	-4.93	120.46	128.46
3	D	4521	PSU	C4-N3-C2	-4.93	119.23	126.34
48	w	644	OMG	C5-C4-N3	-4.93	120.47	128.46
48	w	601	OMG	C5-C4-N3	-4.92	120.47	128.46
3	D	3637	PSU	C4-N3-C2	-4.92	119.26	126.34
3	D	1862	PSU	C4-N3-C2	-4.91	119.26	126.34
3	D	1677	PSU	C4-N3-C2	-4.91	119.27	126.34
48	w	105	PSU	N1-C2-N3	4.89	120.67	115.13
48	w	681	PSU	C4-N3-C2	-4.89	119.29	126.34
3	D	4312	PSU	C4-N3-C2	-4.89	119.30	126.34
2	B	10	2MG	C5-C4-N3	-4.89	120.53	128.46
2	B	54	5MU	C4-N3-C2	-4.87	121.04	127.35
48	w	815	PSU	C4-N3-C2	-4.87	119.32	126.34
3	D	4972	PSU	C4-N3-C2	-4.87	119.33	126.34
3	D	4228	OMG	C5-C4-N3	-4.86	120.57	128.46
3	D	4299	PSU	N1-C2-N3	4.86	120.64	115.13
3	D	4312	PSU	N1-C2-N3	4.85	120.62	115.13
3	D	1683	PSU	C4-N3-C2	-4.84	119.37	126.34
3	D	3758	PSU	C4-N3-C2	-4.84	119.37	126.34
48	w	814	PSU	C4-N3-C2	-4.83	119.38	126.34
3	D	1536	PSU	N1-C2-N3	4.82	120.59	115.13
2	B	37	1MG	C5-C4-N3	-4.82	120.64	128.46
3	D	1522	OMG	C5-C4-N3	-4.82	120.64	128.46
3	D	4500	PSU	C4-N3-C2	-4.82	119.40	126.34
3	D	3920	PSU	N1-C2-N3	4.82	120.59	115.13
3	D	4442	PSU	N1-C2-N3	4.80	120.57	115.13
3	D	3695	PSU	C4-N3-C2	-4.80	119.42	126.34
3	D	4972	PSU	N1-C2-N3	4.80	120.57	115.13
3	D	3639	PSU	C4-N3-C2	-4.80	119.42	126.34
3	D	1782	PSU	C4-N3-C2	-4.80	119.42	126.34
3	D	4530	UR3	C4-N3-C2	-4.80	120.04	124.56
3	D	1773	OMU	C4-N3-C2	-4.80	120.25	126.58
3	D	5010	PSU	C4-N3-C2	-4.80	119.42	126.34
3	D	4521	PSU	N1-C2-N3	4.80	120.56	115.13
2	B	35	PSU	C4-N3-C2	-4.79	119.43	126.34
3	D	2508	PSU	C4-N3-C2	-4.79	119.43	126.34
3	D	3730	PSU	C4-N3-C2	-4.79	119.43	126.34
3	D	4442	PSU	C4-N3-C2	-4.79	119.43	126.34
48	w	822	PSU	C4-N3-C2	-4.79	119.44	126.34
3	D	5001	PSU	C4-N3-C2	-4.79	119.44	126.34
2	C	37	1MG	C5-C4-N3	-4.78	120.70	128.46
3	D	3920	PSU	C4-N3-C2	-4.78	119.45	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4403	PSU	C4-N3-C2	-4.78	119.45	126.34
3	D	4220	6MZ	C5-C4-N3	-4.78	120.52	126.75
3	D	4576	PSU	C4-N3-C2	-4.78	119.46	126.34
3	D	4623	OMG	C5-C4-N3	-4.77	120.72	128.46
3	D	1536	PSU	C4-N3-C2	-4.77	119.46	126.34
48	w	649	PSU	C4-N3-C2	-4.77	119.47	126.34
3	D	4353	PSU	C4-N3-C2	-4.77	119.47	126.34
3	D	4552	PSU	N1-C2-N3	4.76	120.53	115.13
3	D	4500	PSU	N1-C2-N3	4.76	120.52	115.13
3	D	4220	6MZ	N9-C8-N7	-4.76	107.40	113.91
3	D	3851	PSU	C4-N3-C2	-4.76	119.48	126.34
3	D	3637	PSU	N1-C2-N3	4.76	120.52	115.13
3	D	4299	PSU	C4-N3-C2	-4.75	119.49	126.34
3	D	4579	PSU	C4-N3-C2	-4.75	119.49	126.34
3	D	3851	PSU	N1-C2-N3	4.75	120.51	115.13
3	D	4403	PSU	N1-C2-N3	4.74	120.50	115.13
48	w	1367	PSU	C4-N3-C2	-4.74	119.50	126.34
3	D	1792	PSU	C4-N3-C2	-4.74	119.51	126.34
48	w	218	PSU	C4-N3-C2	-4.74	119.51	126.34
48	w	1177	PSU	C4-N3-C2	-4.74	119.51	126.34
3	D	4579	PSU	N1-C2-N3	4.74	120.50	115.13
3	D	4689	PSU	C4-N3-C2	-4.73	119.52	126.34
2	C	54	5MU	C4-N3-C2	-4.72	121.24	127.35
48	w	1045	PSU	C4-N3-C2	-4.72	119.54	126.34
48	w	1851	MA6	C5-C4-N3	-4.72	120.59	126.75
3	D	1744	PSU	C4-N3-C2	-4.72	119.54	126.34
3	D	2508	PSU	N1-C2-N3	4.72	120.47	115.13
3	D	1781	PSU	C4-N3-C2	-4.71	119.55	126.34
3	D	4296	PSU	N1-C2-N3	4.71	120.47	115.13
3	D	4423	PSU	N1-C2-N3	4.71	120.47	115.13
3	D	1744	PSU	N1-C2-N3	4.71	120.47	115.13
48	w	651	PSU	C4-N3-C2	-4.71	119.55	126.34
3	D	4628	PSU	C4-N3-C2	-4.70	119.56	126.34
48	w	109	PSU	N1-C2-N3	4.70	120.46	115.13
48	w	863	PSU	C4-N3-C2	-4.70	119.56	126.34
48	w	1056	PSU	N1-C2-N3	4.70	120.45	115.13
3	D	4361	PSU	C4-N3-C2	-4.70	119.57	126.34
2	C	35	PSU	C4-N3-C2	-4.69	119.58	126.34
3	D	1860	PSU	C4-N3-C2	-4.69	119.58	126.34
48	w	686	PSU	C4-N3-C2	-4.69	119.58	126.34
3	D	2632	PSU	C4-N3-C2	-4.69	119.58	126.34
48	w	105	PSU	C4-N3-C2	-4.68	119.59	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1850	MA6	C5-C4-N3	-4.68	120.64	126.75
48	w	406	PSU	C4-N3-C2	-4.68	119.60	126.34
48	w	866	PSU	C4-N3-C2	-4.68	119.60	126.34
3	D	4423	PSU	C4-N3-C2	-4.68	119.60	126.34
3	D	5010	PSU	N1-C2-N3	4.68	120.43	115.13
3	D	4457	PSU	C4-N3-C2	-4.67	119.61	126.34
48	w	1625	PSU	C4-N3-C2	-4.67	119.61	126.34
48	w	109	PSU	C4-N3-C2	-4.67	119.61	126.34
3	D	3715	PSU	C4-N3-C2	-4.67	119.61	126.34
3	D	4532	PSU	C4-N3-C2	-4.67	119.61	126.34
48	w	1692	PSU	C4-N3-C2	-4.67	119.62	126.34
3	D	4552	PSU	C4-N3-C2	-4.67	119.62	126.34
3	D	4576	PSU	N1-C2-N3	4.66	120.41	115.13
48	w	406	PSU	N1-C2-N3	4.66	120.41	115.13
3	D	3639	PSU	N1-C2-N3	4.65	120.40	115.13
48	w	1177	PSU	N1-C2-N3	4.65	120.40	115.13
48	w	815	PSU	N1-C2-N3	4.65	120.40	115.13
48	w	686	PSU	N1-C2-N3	4.65	120.40	115.13
3	D	3764	PSU	C4-N3-C2	-4.65	119.64	126.34
3	D	3768	PSU	C4-N3-C2	-4.65	119.64	126.34
3	D	1677	PSU	N1-C2-N3	4.65	120.40	115.13
3	D	4353	PSU	N1-C2-N3	4.65	120.40	115.13
3	D	4420	PSU	C4-N3-C2	-4.65	119.64	126.34
3	D	4293	PSU	C4-N3-C2	-4.64	119.65	126.34
3	D	1792	PSU	N1-C2-N3	4.64	120.39	115.13
48	w	1643	PSU	N1-C2-N3	4.64	120.39	115.13
48	w	1367	PSU	N1-C2-N3	4.64	120.39	115.13
48	w	866	PSU	N1-C2-N3	4.64	120.38	115.13
48	w	1004	PSU	C4-N3-C2	-4.64	119.66	126.34
48	w	1232	PSU	C4-N3-C2	-4.63	119.66	126.34
48	w	1174	PSU	C4-N3-C2	-4.63	119.67	126.34
3	D	4457	PSU	N1-C2-N3	4.63	120.37	115.13
3	D	4532	PSU	N1-C2-N3	4.62	120.37	115.13
3	D	1860	PSU	N1-C2-N3	4.62	120.37	115.13
48	w	1850	MA6	C2-N1-C6	4.62	122.66	111.75
48	w	1692	PSU	N1-C2-N3	4.62	120.36	115.13
3	D	4431	PSU	C4-N3-C2	-4.62	119.69	126.34
3	D	4293	PSU	N1-C2-N3	4.62	120.36	115.13
48	w	218	PSU	N1-C2-N3	4.62	120.36	115.13
3	D	4296	PSU	C4-N3-C2	-4.61	119.69	126.34
3	D	2632	PSU	N1-C2-N3	4.61	120.36	115.13
3	D	3853	PSU	C4-N3-C2	-4.61	119.69	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1347	PSU	C4-N3-C2	-4.61	119.69	126.34
3	D	3715	PSU	N1-C2-N3	4.61	120.35	115.13
3	D	3730	PSU	N1-C2-N3	4.61	120.35	115.13
48	w	1232	PSU	N1-C2-N3	4.60	120.35	115.13
48	w	36	PSU	C4-N3-C2	-4.60	119.71	126.34
48	w	1244	PSU	C4-N3-C2	-4.60	119.71	126.34
3	D	1781	PSU	N1-C2-N3	4.60	120.34	115.13
3	D	4689	PSU	N1-C2-N3	4.60	120.34	115.13
3	D	5001	PSU	N1-C2-N3	4.59	120.33	115.13
48	w	814	PSU	N1-C2-N3	4.59	120.33	115.13
48	w	572	PSU	C4-N3-C2	-4.59	119.72	126.34
48	w	863	PSU	N1-C2-N3	4.59	120.33	115.13
48	w	1625	PSU	N1-C2-N3	4.59	120.33	115.13
3	D	3758	PSU	N1-C2-N3	4.59	120.33	115.13
48	w	651	PSU	N1-C2-N3	4.58	120.32	115.13
3	D	3853	PSU	N1-C2-N3	4.58	120.32	115.13
48	w	1832	6MZ	N9-C8-N7	-4.58	107.65	113.91
2	B	35	PSU	N1-C2-N3	4.57	120.31	115.13
48	w	1851	MA6	N9-C8-N7	-4.57	107.66	113.91
48	w	1004	PSU	N1-C2-N3	4.57	120.31	115.13
48	w	210	PSU	C4-N3-C2	-4.57	119.76	126.34
3	D	1782	PSU	N1-C2-N3	4.57	120.30	115.13
48	w	34	PSU	N1-C2-N3	4.56	120.30	115.13
48	w	649	PSU	N1-C2-N3	4.56	120.30	115.13
3	D	3734	PSU	N1-C2-N3	4.56	120.30	115.13
48	w	1643	PSU	C4-N3-C2	-4.56	119.77	126.34
48	w	36	PSU	N1-C2-N3	4.56	120.29	115.13
3	D	4361	PSU	N1-C2-N3	4.55	120.29	115.13
48	w	681	PSU	N1-C2-N3	4.55	120.28	115.13
3	D	3695	PSU	N1-C2-N3	4.55	120.28	115.13
3	D	3770	PSU	N1-C2-N3	4.55	120.28	115.13
3	D	4420	PSU	N1-C2-N3	4.54	120.28	115.13
48	w	822	PSU	N1-C2-N3	4.54	120.28	115.13
48	w	572	PSU	N1-C2-N3	4.54	120.28	115.13
3	D	3762	PSU	C4-N3-C2	-4.54	119.79	126.34
3	D	4431	PSU	N1-C2-N3	4.53	120.27	115.13
48	w	966	PSU	C4-N3-C2	-4.53	119.81	126.34
2	C	55	PSU	C4-N3-C2	-4.53	119.81	126.34
48	w	1046	PSU	N1-C2-N3	4.53	120.26	115.13
3	D	3734	PSU	C4-N3-C2	-4.53	119.81	126.34
48	w	119	PSU	C4-N3-C2	-4.53	119.81	126.34
2	C	10	2MG	C2-N1-C6	-4.52	119.27	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4471	PSU	C4-N3-C2	-4.52	119.82	126.34
48	w	119	PSU	N1-C2-N3	4.51	120.24	115.13
3	D	3762	PSU	N1-C2-N3	4.51	120.24	115.13
2	B	54	5MU	N3-C2-N1	4.51	120.87	114.89
2	B	55	PSU	N1-C2-N3	4.51	120.24	115.13
48	w	1174	PSU	N1-C2-N3	4.51	120.24	115.13
48	w	609	PSU	C4-N3-C2	-4.51	119.85	126.34
48	w	801	PSU	C4-N3-C2	-4.50	119.85	126.34
48	w	1056	PSU	C4-N3-C2	-4.50	119.85	126.34
3	D	3764	PSU	N1-C2-N3	4.50	120.23	115.13
48	w	1046	PSU	C4-N3-C2	-4.50	119.86	126.34
2	C	35	PSU	N1-C2-N3	4.49	120.22	115.13
48	w	1445	PSU	N1-C2-N3	4.49	120.22	115.13
2	C	55	PSU	N1-C2-N3	4.49	120.22	115.13
3	D	4471	PSU	N1-C2-N3	4.49	120.22	115.13
48	w	1045	PSU	N1-C2-N3	4.48	120.21	115.13
48	w	93	PSU	N1-C2-N3	4.48	120.21	115.13
2	B	6	2MG	C5-C4-N3	-4.48	121.19	128.46
2	B	46	G7M	C2-N3-C4	4.47	120.27	112.30
48	w	801	PSU	N1-C2-N3	4.47	120.19	115.13
48	w	1238	PSU	N1-C2-N3	4.47	120.19	115.13
48	w	210	PSU	N1-C2-N3	4.46	120.19	115.13
48	w	1347	PSU	N1-C2-N3	4.46	120.18	115.13
2	C	54	5MU	N3-C2-N1	4.46	120.81	114.89
48	w	93	PSU	C4-N3-C2	-4.45	119.92	126.34
48	w	966	PSU	N1-C2-N3	4.45	120.17	115.13
48	w	1081	PSU	C4-N3-C2	-4.45	119.93	126.34
48	w	1244	PSU	N1-C2-N3	4.44	120.17	115.13
48	w	1238	PSU	C4-N3-C2	-4.44	119.94	126.34
2	C	46	G7M	C2-N3-C4	4.44	120.20	112.30
48	w	1490	OMG	C2-N3-C4	4.44	120.20	112.30
3	D	2364	OMG	C2-N3-C4	4.43	120.19	112.30
48	w	1851	MA6	C2-N1-C6	4.41	122.17	111.75
3	D	3770	PSU	C4-N3-C2	-4.41	119.99	126.34
48	w	609	PSU	N1-C2-N3	4.41	120.12	115.13
3	D	3768	PSU	N1-C2-N3	4.40	120.12	115.13
48	w	1850	MA6	C4-C5-C6	4.39	120.80	115.88
48	w	1445	PSU	C4-N3-C2	-4.39	120.01	126.34
48	w	1081	PSU	N1-C2-N3	4.39	120.10	115.13
3	D	3627	OMG	C2-N3-C4	4.38	120.09	112.30
3	D	3944	OMG	C2-N3-C4	4.37	120.09	112.30
48	w	436	OMG	C2-N3-C4	4.36	120.07	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	34	56B	C2-N3-C4	4.36	120.07	112.30
3	D	3744	OMG	C2-N3-C4	4.36	120.07	112.30
48	w	683	OMG	C2-N3-C4	4.36	120.07	112.30
3	D	4392	OMG	C2-N3-C4	4.36	120.06	112.30
3	D	3899	OMG	C2-N3-C4	4.35	120.05	112.30
48	w	1639	G7M	C2-N3-C4	4.34	120.04	112.30
5	F	75	OMG	C2-N3-C4	4.34	120.04	112.30
3	D	4499	OMG	C2-N3-C4	4.34	120.03	112.30
3	D	4196	OMG	C2-N3-C4	4.34	120.03	112.30
2	C	6	2MG	C2-N1-C6	-4.33	119.49	124.48
2	B	6	2MG	C2-N1-C6	-4.32	119.50	124.48
3	D	4370	OMG	C2-N3-C4	4.31	119.98	112.30
3	D	1625	OMG	C2-N3-C4	4.30	119.97	112.30
48	w	34	PSU	C4-N3-C2	-4.30	120.14	126.34
3	D	4228	OMG	C2-N3-C4	4.29	119.95	112.30
48	w	601	OMG	C2-N3-C4	4.29	119.94	112.30
3	D	3792	OMG	C2-N3-C4	4.28	119.92	112.30
2	B	55	PSU	C4-N3-C2	-4.28	120.17	126.34
3	D	4494	OMG	C2-N3-C4	4.27	119.91	112.30
3	D	1760	OMG	C2-N3-C4	4.27	119.90	112.30
3	D	1316	OMG	C2-N3-C4	4.27	119.90	112.30
3	D	1522	OMG	C2-N3-C4	4.26	119.89	112.30
2	B	34	56B	C2-N3-C4	4.26	119.89	112.30
3	D	2424	OMG	C2-N3-C4	4.26	119.89	112.30
3	D	4618	OMG	C2-N3-C4	4.24	119.85	112.30
48	w	1328	OMG	C2-N3-C4	4.23	119.84	112.30
48	w	509	OMG	C2-N3-C4	4.22	119.82	112.30
3	D	4637	OMG	C2-N3-C4	4.21	119.80	112.30
48	w	644	OMG	C2-N3-C4	4.20	119.78	112.30
3	D	2415	OMU	N3-C2-N1	4.19	120.46	114.89
3	D	2837	OMU	N3-C2-N1	4.18	120.44	114.89
2	B	46	G7M	C5-C4-N3	-4.16	120.18	128.15
2	B	10	2MG	C2-N1-C6	-4.14	119.71	124.48
3	D	4623	OMG	C2-N3-C4	4.11	119.62	112.30
48	w	1639	G7M	C5-C4-N3	-4.10	120.28	128.15
2	C	34	56B	C7-C5-C4	-4.08	107.93	112.66
2	B	46	G7M	C5-C6-N1	4.08	120.31	111.79
2	C	46	G7M	C5-C4-N3	-4.08	120.33	128.15
3	D	4620	OMU	N3-C2-N1	4.07	120.30	114.89
3	D	3925	OMU	N3-C2-N1	4.04	120.25	114.89
48	w	1851	MA6	C4-C5-C6	4.03	120.39	115.88
2	B	34	56B	C7-C5-C4	-4.02	108.00	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	54	5MU	C5M-C5-C6	-4.01	117.50	122.85
3	D	4306	OMU	N3-C2-N1	3.98	120.17	114.89
48	w	1639	G7M	C5-C6-N1	3.95	120.04	111.79
3	D	4447	5MC	C5-C6-N1	-3.95	119.28	123.34
3	D	4498	OMU	N3-C2-N1	3.93	120.10	114.89
48	w	172	OMU	N3-C2-N1	3.90	120.07	114.89
2	C	54	5MU	C5M-C5-C4	3.89	123.05	118.77
2	C	46	G7M	C5-C6-N1	3.88	119.89	111.79
3	D	4227	OMU	N3-C2-N1	3.86	120.02	114.89
48	w	121	OMU	N3-C2-N1	3.82	119.96	114.89
48	w	116	OMU	N3-C2-N1	3.80	119.94	114.89
48	w	1442	OMU	N3-C2-N1	3.80	119.93	114.89
3	D	4220	6MZ	C5-N7-C8	3.78	108.88	103.51
48	w	1850	MA6	N9-C8-N7	-3.78	108.75	113.91
48	w	1326	OMU	N3-C2-N1	3.77	119.89	114.89
3	D	1625	OMG	N9-C4-N3	3.76	133.49	125.94
48	w	428	OMU	N3-C2-N1	3.73	119.85	114.89
3	D	4227	OMU	C5-C4-N3	3.73	120.42	114.84
48	w	1804	OMU	N3-C2-N1	3.69	119.79	114.89
48	w	1851	MA6	C5-N7-C8	3.68	108.74	103.51
48	w	799	OMU	N3-C2-N1	3.68	119.78	114.89
2	C	10	2MG	N9-C4-N3	3.68	133.33	125.94
3	D	3792	OMG	N9-C4-N3	3.68	133.32	125.94
2	C	34	56B	C7-C8-N9	-3.66	107.47	111.06
3	D	1522	OMG	N9-C8-N7	-3.63	106.56	113.39
3	D	4220	6MZ	C2-N3-C4	3.62	120.30	111.75
48	w	1337	4AC	O7-C7-N4	3.60	127.65	121.82
48	w	1288	OMU	N3-C2-N1	3.59	119.66	114.89
3	D	2415	OMU	C5-C4-N3	3.59	120.21	114.84
3	D	3944	OMG	N9-C4-N3	3.59	133.14	125.94
3	D	4196	OMG	N9-C4-N3	3.58	133.12	125.94
48	w	1832	6MZ	C2-N3-C4	3.57	120.19	111.75
3	D	4494	OMG	N9-C4-N3	3.57	133.10	125.94
3	D	4623	OMG	N9-C8-N7	-3.57	106.67	113.39
2	B	34	56B	C7-C8-N9	-3.57	107.56	111.06
3	D	4499	OMG	N9-C8-N7	-3.56	106.69	113.39
3	D	1773	OMU	N3-C2-N1	3.56	119.61	114.89
3	D	4370	OMG	N9-C4-N3	3.55	133.07	125.94
2	B	6	2MG	N9-C8-N7	-3.54	106.72	113.39
3	D	2837	OMU	C5-C4-N3	3.54	120.13	114.84
3	D	4392	OMG	N9-C4-N3	3.53	133.03	125.94
3	D	4228	OMG	N9-C8-N7	-3.53	106.75	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	627	OMU	N3-C2-N1	3.52	119.57	114.89
48	w	436	OMG	N9-C4-N3	3.52	133.02	125.94
48	w	1832	6MZ	C4-C5-C6	3.52	119.54	116.81
48	w	644	OMG	N9-C8-N7	-3.52	106.77	113.39
3	D	3925	OMU	C5-C4-N3	3.52	120.10	114.84
48	w	1490	OMG	N9-C4-N3	3.51	132.99	125.94
2	B	37	1MG	C2-N3-C4	3.51	119.87	111.98
48	w	509	OMG	N9-C8-N7	-3.50	106.79	113.39
3	D	1760	OMG	N9-C4-N3	3.50	132.97	125.94
2	C	37	1MG	C2-N3-C4	3.50	119.85	111.98
3	D	3782	5MC	C5-C6-N1	-3.49	119.75	123.34
3	D	4637	OMG	N9-C4-N3	3.49	132.94	125.94
2	B	54	5MU	C5M-C5-C6	-3.47	118.22	122.85
48	w	683	OMG	N9-C4-N3	3.46	132.88	125.94
48	w	1842	4AC	O7-C7-N4	3.46	127.42	121.82
48	w	1328	OMG	N9-C8-N7	-3.45	106.90	113.39
3	D	4498	OMU	C5-C4-N3	3.44	119.99	114.84
48	w	1804	OMU	C5-C4-N3	3.44	119.99	114.84
48	w	509	OMG	N9-C4-N3	3.44	132.85	125.94
48	w	1328	OMG	N9-C4-N3	3.44	132.84	125.94
48	w	601	OMG	N9-C8-N7	-3.44	106.92	113.39
3	D	4370	OMG	N9-C8-N7	-3.43	106.92	113.39
3	D	4637	OMG	N9-C8-N7	-3.43	106.94	113.39
3	D	2364	OMG	N9-C8-N7	-3.43	106.94	113.39
48	w	436	OMG	N9-C8-N7	-3.42	106.94	113.39
3	D	1760	OMG	N9-C8-N7	-3.42	106.95	113.39
48	w	683	OMG	N9-C8-N7	-3.42	106.95	113.39
3	D	3744	OMG	N9-C8-N7	-3.42	106.95	113.39
5	F	75	OMG	N9-C8-N7	-3.41	106.96	113.39
3	D	1316	OMG	N9-C8-N7	-3.40	106.98	113.39
48	w	627	OMU	C5-C4-N3	3.40	119.93	114.84
48	w	1639	G7M	O6-C6-C5	-3.40	120.39	128.06
3	D	3899	OMG	N9-C8-N7	-3.40	107.00	113.39
48	w	1851	MA6	C2-N3-C4	3.38	119.73	111.75
48	w	1832	6MZ	C5-N7-C8	3.38	108.31	103.51
48	w	1442	OMU	C5-C4-N3	3.38	119.89	114.84
3	D	3627	OMG	N9-C8-N7	-3.37	107.05	113.39
48	w	428	OMU	C5-C4-N3	3.36	119.87	114.84
48	w	34	PSU	O2-C2-N1	-3.36	119.09	122.79
3	D	2424	OMG	N9-C8-N7	-3.36	107.06	113.39
2	C	6	2MG	N9-C4-N3	3.35	132.67	125.94
48	w	172	OMU	C5-C4-N3	3.35	119.85	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	46	G7M	O6-C6-C5	-3.34	120.52	128.06
48	w	1288	OMU	C5-C4-N3	3.34	119.83	114.84
3	D	4306	OMU	C5-C4-N3	3.33	119.82	114.84
5	F	75	OMG	N9-C4-N3	3.33	132.62	125.94
3	D	4620	OMU	C5-C4-N3	3.32	119.81	114.84
48	w	1326	OMU	C5-C4-N3	3.32	119.81	114.84
2	C	34	56B	C9-N10-C10	-3.32	106.12	113.35
2	B	34	56B	N9-C4-N3	3.32	132.60	125.94
48	w	116	OMU	C5-C4-N3	3.31	119.79	114.84
48	w	644	OMG	N9-C4-N3	3.31	132.58	125.94
3	D	3899	OMG	N9-C4-N3	3.30	132.57	125.94
3	D	1522	OMG	C1'-N9-C4	-3.30	116.71	126.50
48	w	121	OMU	C5-C4-N3	3.29	119.77	114.84
3	D	1625	OMG	N9-C8-N7	-3.29	107.19	113.39
3	D	2424	OMG	N9-C4-N3	3.29	132.55	125.94
3	D	4494	OMG	N9-C8-N7	-3.29	107.20	113.39
3	D	4618	OMG	N9-C8-N7	-3.28	107.21	113.39
3	D	3744	OMG	N9-C4-N3	3.28	132.52	125.94
3	D	4499	OMG	N9-C4-N3	3.28	132.52	125.94
48	w	601	OMG	N9-C4-N3	3.27	132.51	125.94
3	D	3944	OMG	N9-C8-N7	-3.27	107.23	113.39
2	C	46	G7M	O6-C6-C5	-3.27	120.68	128.06
48	w	799	OMU	C5-C4-N3	3.27	119.73	114.84
2	C	37	1MG	N9-C8-N7	-3.26	107.24	113.39
2	C	34	56B	N9-C4-N3	3.26	132.49	125.94
3	D	4392	OMG	N9-C8-N7	-3.26	107.25	113.39
2	B	54	5MU	C5M-C5-C4	3.26	122.35	118.77
2	B	10	2MG	N9-C8-N7	-3.25	107.27	113.39
3	D	3792	OMG	N9-C8-N7	-3.25	107.27	113.39
3	D	1316	OMG	N9-C4-N3	3.25	132.46	125.94
3	D	3627	OMG	N9-C4-N3	3.25	132.46	125.94
3	D	1316	OMG	C2-N1-C6	-3.24	119.20	125.10
3	D	2364	OMG	N9-C4-N3	3.23	132.43	125.94
48	w	1850	MA6	C2-N3-C4	3.23	119.39	111.75
2	B	10	2MG	N9-C4-N3	3.23	132.42	125.94
3	D	4196	OMG	N9-C8-N7	-3.23	107.31	113.39
3	D	4196	OMG	C2-N1-C6	-3.23	119.22	125.10
3	D	4637	OMG	C2-N1-C6	-3.23	119.22	125.10
3	D	3785	A2M	C2'-C1'-N9	-3.22	108.10	113.53
3	D	4228	OMG	C1'-N9-C4	-3.21	116.96	126.50
3	D	4618	OMG	N9-C4-N3	3.21	132.38	125.94
3	D	4220	6MZ	C4-C5-N7	-3.20	106.72	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	48	5MC	C5-C6-N1	-3.20	120.05	123.34
48	w	1850	MA6	C5-N7-C8	3.20	108.06	103.51
48	w	509	OMG	C2-N1-C6	-3.19	119.28	125.10
3	D	1625	OMG	C2-N1-C6	-3.19	119.28	125.10
3	D	4392	OMG	C2-N1-C6	-3.17	119.31	125.10
2	B	37	1MG	N9-C8-N7	-3.17	107.42	113.39
3	D	4228	OMG	N9-C4-N3	3.17	132.30	125.94
3	D	4623	OMG	N9-C4-N3	3.17	132.29	125.94
48	w	1639	G7M	N9-C4-N3	3.16	132.29	125.94
2	B	46	G7M	C2-N1-C6	-3.16	119.34	125.10
3	D	1522	OMG	C2-N1-C6	-3.15	119.35	125.10
3	D	2424	OMG	C2-N1-C6	-3.15	119.36	125.10
3	D	1522	OMG	N9-C4-N3	3.14	132.25	125.94
3	D	1773	OMU	C5-C4-N3	3.14	119.54	114.84
3	D	4623	OMG	C1'-N9-C4	-3.12	117.23	126.50
2	B	46	G7M	N9-C4-N3	3.11	132.19	125.94
2	C	6	2MG	N9-C8-N7	-3.11	107.53	113.39
3	D	3899	OMG	C2-N1-C6	-3.11	119.43	125.10
3	D	4494	OMG	C2-N1-C6	-3.11	119.43	125.10
48	w	1490	OMG	N9-C8-N7	-3.09	107.56	113.39
3	D	3627	OMG	C2-N1-C6	-3.09	119.46	125.10
5	F	75	OMG	C2-N1-C6	-3.09	119.47	125.10
48	w	436	OMG	C2-N1-C6	-3.09	119.47	125.10
3	D	4499	OMG	C1'-N9-C4	-3.08	117.34	126.50
2	B	48	5MC	C5-C6-N1	-3.08	120.17	123.34
3	D	2364	OMG	C2-N1-C6	-3.08	119.49	125.10
48	w	1851	MA6	C4-C5-N7	-3.07	106.87	110.62
3	D	3944	OMG	C2-N1-C6	-3.06	119.52	125.10
3	D	3744	OMG	C2-N1-C6	-3.06	119.53	125.10
3	D	4370	OMG	C2-N1-C6	-3.05	119.53	125.10
3	D	3627	OMG	C1'-N9-C4	-3.05	117.44	126.50
3	D	4228	OMG	C2-N1-C6	-3.05	119.55	125.10
3	D	3792	OMG	C2-N1-C6	-3.04	119.55	125.10
3	D	2837	OMU	O4-C4-C5	-3.04	119.81	125.16
48	w	683	OMG	C2-N1-C6	-3.04	119.56	125.10
48	w	1639	G7M	C2-N1-C6	-3.04	119.56	125.10
3	D	4499	OMG	C2-N1-C6	-3.03	119.57	125.10
3	D	1760	OMG	C2-N1-C6	-3.02	119.58	125.10
48	w	644	OMG	C1'-N9-C4	-3.02	117.55	126.50
3	D	4220	6MZ	C4-C5-C6	3.01	119.14	116.81
48	w	1328	OMG	C2-N1-C6	-3.00	119.62	125.10
3	D	4618	OMG	C2-N1-C6	-3.00	119.62	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	601	OMG	C2-N1-C6	-3.00	119.62	125.10
48	w	644	OMG	C2-N1-C6	-2.99	119.64	125.10
2	C	46	G7M	C2-N1-C6	-2.99	119.65	125.10
2	B	34	56B	C2-N1-C6	-2.99	119.66	125.10
48	w	627	OMU	O4-C4-C5	-2.97	119.93	125.16
3	D	3925	OMU	O4-C4-C5	-2.97	119.94	125.16
48	w	1804	OMU	O4-C4-C5	-2.97	119.94	125.16
2	C	10	2MG	N9-C8-N7	-2.97	107.80	113.39
2	C	34	56B	C2-N1-C6	-2.97	119.69	125.10
2	C	37	1MG	C1'-N9-C8	-2.97	118.25	126.70
3	D	4623	OMG	C2-N1-C6	-2.96	119.70	125.10
3	D	3899	OMG	C1'-N9-C4	-2.95	117.73	126.50
48	w	601	OMG	C1'-N9-C4	-2.95	117.75	126.50
3	D	3744	OMG	C1'-N9-C4	-2.94	117.77	126.50
2	C	37	1MG	N9-C4-N3	2.93	131.83	125.94
3	D	2364	OMG	C1'-N9-C4	-2.93	117.80	126.50
3	D	1316	OMG	C1'-N9-C4	-2.93	117.81	126.50
2	C	46	G7M	N9-C4-N3	2.93	131.82	125.94
48	w	1288	OMU	O4-C4-C5	-2.92	120.03	125.16
48	w	509	OMG	C1'-N9-C4	-2.91	117.86	126.50
3	D	4628	PSU	O2-C2-N1	-2.91	119.59	122.79
48	w	799	OMU	O4-C4-C5	-2.91	120.05	125.16
48	w	428	OMU	O4-C4-C5	-2.91	120.05	125.16
3	D	2424	OMG	C1'-N9-C4	-2.90	117.88	126.50
3	D	1522	OMG	C5-C6-N1	2.89	120.53	113.19
3	D	3730	PSU	O2-C2-N1	-2.88	119.62	122.79
5	F	75	OMG	C1'-N9-C4	-2.88	117.95	126.50
3	D	1683	PSU	O2-C2-N1	-2.88	119.62	122.79
48	w	1442	OMU	O4-C4-C5	-2.87	120.11	125.16
48	w	1056	PSU	O2-C2-N1	-2.86	119.64	122.79
48	w	1850	MA6	C4-C5-N7	-2.86	107.13	110.62
3	D	4423	PSU	O2-C2-N1	-2.85	119.65	122.79
3	D	3734	PSU	O2-C2-N1	-2.85	119.66	122.79
3	D	2364	OMG	C5-C6-N1	2.84	120.41	113.19
3	D	4227	OMU	O4-C4-C5	-2.84	120.16	125.16
48	w	686	PSU	O2-C2-N1	-2.84	119.66	122.79
2	B	37	1MG	N9-C4-N3	2.84	131.64	125.94
3	D	3920	PSU	O2-C2-N1	-2.84	119.67	122.79
3	D	4196	OMG	C5-C6-N1	2.83	120.39	113.19
3	D	3627	OMG	C5-C6-N1	2.83	120.39	113.19
3	D	3762	PSU	O2-C2-N1	-2.83	119.67	122.79
48	w	1232	PSU	O2-C2-N1	-2.83	119.67	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1490	OMG	C2-N1-C6	-2.83	119.94	125.10
2	B	6	2MG	CM2-N2-C2	-2.83	117.62	123.86
3	D	4392	OMG	C5-C6-N1	2.83	120.37	113.19
3	D	1316	OMG	C5-C6-N1	2.81	120.34	113.19
48	w	116	OMU	O4-C4-C5	-2.81	120.21	125.16
3	D	4637	OMG	C5-C6-N1	2.81	120.33	113.19
3	D	4370	OMG	C5-C6-N1	2.81	120.33	113.19
3	D	3744	OMG	C5-C6-N1	2.81	120.33	113.19
48	w	1832	6MZ	N3-C4-N9	2.81	131.72	127.08
3	D	4228	OMG	C5-C6-N1	2.81	120.33	113.19
3	D	4370	OMG	C1'-N9-C4	-2.80	118.17	126.50
48	w	1326	OMU	O4-C4-C5	-2.80	120.23	125.16
48	w	105	PSU	C6-C5-C4	2.80	120.16	118.20
3	D	4618	OMG	C1'-N9-C4	-2.80	118.19	126.50
48	w	1081	PSU	O2-C2-N1	-2.80	119.71	122.79
2	B	6	2MG	C1'-N9-C4	-2.79	118.20	126.50
3	D	4420	PSU	O2-C2-N1	-2.79	119.72	122.79
3	D	1625	OMG	C5-C6-N1	2.79	120.28	113.19
3	D	4500	PSU	O2-C2-N1	-2.79	119.72	122.79
48	w	172	OMU	O4-C4-C5	-2.79	120.26	125.16
48	w	406	PSU	O2-C2-N1	-2.79	119.72	122.79
3	D	2415	OMU	O4-C4-C5	-2.79	120.26	125.16
3	D	2424	OMG	C5-C6-N1	2.78	120.25	113.19
3	D	4494	OMG	C5-C6-N1	2.78	120.25	113.19
3	D	4628	PSU	C6-N1-C2	-2.78	119.84	122.68
3	D	3899	OMG	C5-C6-N1	2.77	120.23	113.19
2	C	10	2MG	C5-C6-N1	2.77	120.22	113.19
3	D	4499	OMG	C5-C6-N1	2.77	120.22	113.19
3	D	1534	A2M	O4'-C1'-N9	-2.77	102.61	108.06
3	D	1744	PSU	O2-C2-N1	-2.76	119.75	122.79
48	w	601	OMG	C5-C6-N1	2.76	120.21	113.19
48	w	1851	MA6	N1-C6-N6	-2.76	114.06	117.08
48	w	509	OMG	C5-C6-N1	2.76	120.20	113.19
5	F	75	OMG	C5-C6-N1	2.76	120.19	113.19
3	D	4296	PSU	O2-C2-N1	-2.75	119.76	122.79
48	w	683	OMG	C5-C6-N1	2.75	120.17	113.19
3	D	4620	OMU	O4-C4-C5	-2.75	120.33	125.16
3	D	1862	PSU	O2-C2-N1	-2.75	119.77	122.79
3	D	4442	PSU	O2-C2-N1	-2.74	119.77	122.79
48	w	109	PSU	O2-C2-N1	-2.74	119.77	122.79
3	D	1871	A2M	C2'-C1'-N9	-2.74	108.92	113.53
3	D	4498	OMU	O4-C4-C5	-2.74	120.35	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1860	PSU	O2-C2-N1	-2.74	119.78	122.79
48	w	436	OMG	C1'-N9-C4	-2.73	118.38	126.50
2	C	55	PSU	O2-C2-N1	-2.73	119.78	122.79
48	w	436	OMG	C5-C6-N1	2.73	120.13	113.19
3	D	1534	A2M	C3'-C2'-C1'	-2.73	97.76	102.89
48	w	1639	G7M	CN7-N7-C5	2.73	130.16	126.77
3	D	1536	PSU	O2-C2-N1	-2.73	119.79	122.79
3	D	4312	PSU	O2-C2-N1	-2.73	119.79	122.79
3	D	4972	PSU	O2-C2-N1	-2.73	119.79	122.79
2	C	6	2MG	C5-C6-N1	2.72	120.10	113.19
3	D	4637	OMG	C1'-N9-C4	-2.72	118.42	126.50
48	w	644	OMG	C5-C6-N1	2.72	120.09	113.19
48	w	572	PSU	O2-C2-N1	-2.72	119.80	122.79
2	B	6	2MG	C5-C6-N1	2.71	120.08	113.19
3	D	4306	OMU	O4-C4-C5	-2.71	120.39	125.16
2	C	10	2MG	O6-C6-C5	-2.71	119.41	126.60
3	D	1760	OMG	C5-C6-N1	2.71	120.07	113.19
48	w	1004	PSU	O2-C2-N1	-2.70	119.82	122.79
48	w	683	OMG	C1'-N9-C4	-2.69	118.51	126.50
3	D	4623	OMG	C5-C6-N1	2.69	120.02	113.19
3	D	3770	PSU	O2-C2-N1	-2.69	119.83	122.79
48	w	119	PSU	O2-C2-N1	-2.69	119.83	122.79
3	D	3944	OMG	C5-C6-N1	2.69	120.01	113.19
48	w	866	PSU	O2-C2-N1	-2.68	119.84	122.79
3	D	4220	6MZ	C5-C4-N9	2.68	108.90	105.78
3	D	4618	OMG	C5-C6-N1	2.68	120.00	113.19
2	B	37	1MG	C1'-N9-C8	-2.68	119.06	126.70
2	B	34	56B	C9-N10-C10	-2.68	107.52	113.35
48	w	1328	OMG	C1'-N9-C4	-2.68	118.54	126.50
3	D	3639	PSU	O2-C2-N1	-2.68	119.84	122.79
48	w	1445	PSU	O2-C2-N1	-2.68	119.84	122.79
3	D	1773	OMU	O4-C4-C5	-2.67	120.47	125.16
48	w	1692	PSU	O2-C2-N1	-2.67	119.85	122.79
3	D	4576	PSU	O2-C2-N1	-2.66	119.86	122.79
3	D	3792	OMG	C5-C6-N1	2.66	119.96	113.19
2	C	35	PSU	O2-C2-N1	-2.66	119.86	122.79
3	D	4299	PSU	O2-C2-N1	-2.66	119.86	122.79
3	D	3758	PSU	O2-C2-N1	-2.66	119.86	122.79
48	w	121	OMU	O4-C4-C5	-2.66	120.49	125.16
3	D	1316	OMG	O6-C6-C5	-2.66	119.56	126.60
48	w	1490	OMG	C5-C6-N1	2.65	119.93	113.19
48	w	1328	OMG	C5-C6-N1	2.65	119.92	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	649	PSU	O2-C2-N1	-2.65	119.87	122.79
2	B	10	2MG	C5-C6-N1	2.65	119.92	113.19
48	w	863	PSU	O2-C2-N1	-2.64	119.88	122.79
48	w	1625	PSU	O2-C2-N1	-2.64	119.88	122.79
48	w	93	PSU	O2-C2-N1	-2.64	119.88	122.79
3	D	1677	PSU	O2-C2-N1	-2.63	119.89	122.79
48	w	1643	PSU	O2-C2-N1	-2.63	119.90	122.79
3	D	1760	OMG	C1'-N9-C4	-2.63	118.70	126.50
3	D	1781	PSU	O2-C2-N1	-2.62	119.90	122.79
3	D	1534	A2M	O2'-C2'-C1'	2.62	114.20	109.08
3	D	1522	OMG	O6-C6-C5	-2.62	119.65	126.60
3	D	2424	OMG	O6-C6-C5	-2.62	119.66	126.60
3	D	3764	PSU	O2-C2-N1	-2.62	119.91	122.79
2	C	37	1MG	C5-C6-N1	2.62	119.96	114.91
3	D	4196	OMG	O6-C6-C5	-2.61	119.69	126.60
48	w	34	PSU	C6-N1-C2	-2.61	120.02	122.68
2	B	54	5MU	O2-C2-N1	-2.60	119.33	122.79
48	w	815	PSU	O2-C2-N1	-2.60	119.93	122.79
3	D	3695	PSU	O2-C2-N1	-2.60	119.93	122.79
2	B	37	1MG	C5-C6-N1	2.60	119.93	114.91
3	D	4392	OMG	C1'-N9-C4	-2.59	118.80	126.50
3	D	3899	OMG	O6-C6-C5	-2.59	119.73	126.60
3	D	1625	OMG	O6-C6-C5	-2.59	119.73	126.60
2	B	35	PSU	O2-C2-N1	-2.59	119.94	122.79
3	D	4499	OMG	O6-C6-C5	-2.58	119.74	126.60
3	D	3715	PSU	O2-C2-N1	-2.58	119.95	122.79
48	w	822	PSU	O2-C2-N1	-2.58	119.95	122.79
3	D	4370	OMG	O6-C6-C5	-2.58	119.75	126.60
48	w	609	PSU	O2-C2-N1	-2.58	119.95	122.79
5	F	75	OMG	O6-C6-C5	-2.58	119.76	126.60
2	B	10	2MG	O6-C6-C5	-2.58	119.77	126.60
48	w	36	PSU	O2-C2-N1	-2.57	119.96	122.79
3	D	4637	OMG	O6-C6-C5	-2.57	119.78	126.60
48	w	1177	PSU	O2-C2-N1	-2.57	119.96	122.79
3	D	4392	OMG	O6-C6-C5	-2.57	119.79	126.60
48	w	966	PSU	O2-C2-N1	-2.57	119.97	122.79
3	D	4403	PSU	O2-C2-N1	-2.56	119.97	122.79
3	D	4431	PSU	O2-C2-N1	-2.56	119.97	122.79
48	w	1056	PSU	C6-N1-C2	-2.56	120.06	122.68
3	D	4689	PSU	O2-C2-N1	-2.56	119.97	122.79
48	w	1490	OMG	O6-C6-C5	-2.56	119.81	126.60
3	D	2632	PSU	O2-C2-N1	-2.56	119.97	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1347	PSU	O2-C2-N1	-2.55	119.98	122.79
48	w	210	PSU	O2-C2-N1	-2.55	119.98	122.79
3	D	1536	PSU	C6-N1-C2	-2.55	120.07	122.68
3	D	2508	PSU	O2-C2-N1	-2.55	119.98	122.79
3	D	4552	PSU	O2-C2-N1	-2.55	119.98	122.79
3	D	3768	PSU	O2-C2-N1	-2.55	119.98	122.79
3	D	4494	OMG	O6-C6-C5	-2.55	119.84	126.60
48	w	814	PSU	O2-C2-N1	-2.55	119.99	122.79
48	w	1244	PSU	O2-C2-N1	-2.55	119.99	122.79
48	w	509	OMG	O6-C6-C5	-2.55	119.85	126.60
3	D	5010	PSU	O2-C2-N1	-2.54	119.99	122.79
3	D	4579	PSU	O2-C2-N1	-2.54	119.99	122.79
48	w	801	PSU	O2-C2-N1	-2.54	120.00	122.79
3	D	2364	OMG	O6-C6-C5	-2.53	119.88	126.60
48	w	683	OMG	O6-C6-C5	-2.53	119.88	126.60
48	w	1367	PSU	O2-C2-N1	-2.53	120.00	122.79
48	w	1490	OMG	C1'-N9-C4	-2.53	118.97	126.50
3	D	3792	OMG	O6-C6-C5	-2.53	119.88	126.60
2	C	6	2MG	O6-C6-C5	-2.53	119.88	126.60
3	D	3627	OMG	O6-C6-C5	-2.53	119.88	126.60
48	w	105	PSU	C6-N1-C2	-2.53	120.10	122.68
48	w	1046	PSU	O2-C2-N1	-2.53	120.01	122.79
2	C	54	5MU	O4-C4-N3	-2.53	115.28	120.12
48	w	601	OMG	O6-C6-C5	-2.53	119.90	126.60
48	w	1238	PSU	O2-C2-N1	-2.52	120.01	122.79
3	D	4532	PSU	O2-C2-N1	-2.52	120.02	122.79
3	D	3944	OMG	O6-C6-C5	-2.52	119.92	126.60
3	D	1760	OMG	O6-C6-C5	-2.51	119.93	126.60
3	D	1683	PSU	C6-N1-C2	-2.51	120.12	122.68
3	D	4494	OMG	C1'-N9-C4	-2.51	119.06	126.50
3	D	4228	OMG	O6-C6-C5	-2.51	119.95	126.60
3	D	3851	PSU	O2-C2-N1	-2.50	120.04	122.79
3	D	4353	PSU	O2-C2-N1	-2.49	120.05	122.79
3	D	3853	PSU	O2-C2-N1	-2.49	120.05	122.79
48	w	1337	4AC	CM7-C7-N4	-2.49	110.98	115.29
48	w	105	PSU	O2-C2-N1	-2.49	120.05	122.79
2	B	6	2MG	N1-C2-N3	-2.49	120.11	123.95
48	w	1643	PSU	C6-N1-C2	-2.49	120.14	122.68
3	D	4620	OMU	O2-C2-N1	-2.48	119.48	122.79
2	C	46	G7M	CN7-N7-C5	2.48	129.85	126.77
48	w	1832	6MZ	C4-N9-C8	2.48	108.42	105.73
3	D	4299	PSU	C6-N1-C2	-2.48	120.15	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	644	OMG	O6-C6-C5	-2.48	120.02	126.60
48	w	1851	MA6	C5-C4-N9	2.47	108.66	105.78
48	w	1832	6MZ	C4-C5-N7	-2.47	107.61	110.62
48	w	681	PSU	O2-C2-N1	-2.47	120.07	122.79
3	D	3770	PSU	C6-N1-C2	-2.47	120.16	122.68
3	D	4293	PSU	O2-C2-N1	-2.47	120.08	122.79
3	D	3744	OMG	O6-C6-C5	-2.46	120.07	126.60
48	w	218	PSU	O2-C2-N1	-2.46	120.08	122.79
3	D	2837	OMU	O2-C2-N1	-2.46	119.52	122.79
3	D	4457	PSU	C6-N1-C2	-2.45	120.17	122.68
48	w	1174	PSU	O2-C2-N1	-2.45	120.09	122.79
2	B	6	2MG	O6-C6-C5	-2.45	120.10	126.60
3	D	4623	OMG	O6-C6-C5	-2.45	120.11	126.60
3	D	4618	OMG	O6-C6-C5	-2.44	120.12	126.60
3	D	3782	5MC	CM5-C5-C6	-2.44	119.59	122.85
3	D	3920	PSU	C6-N1-C2	-2.44	120.19	122.68
3	D	4423	PSU	C6-N1-C2	-2.44	120.19	122.68
2	B	55	PSU	C6-N1-C2	-2.43	120.20	122.68
3	D	4361	PSU	O2-C2-N1	-2.42	120.12	122.79
3	D	4552	PSU	C6-N1-C2	-2.42	120.21	122.68
3	D	1782	PSU	O2-C2-N1	-2.42	120.13	122.79
3	D	3944	OMG	C1'-N9-C4	-2.42	119.32	126.50
2	C	6	2MG	N1-C2-N3	-2.42	120.21	123.95
48	w	436	OMG	O6-C6-C5	-2.42	120.19	126.60
48	w	815	PSU	C6-C5-C4	2.42	119.89	118.20
2	C	10	2MG	N1-C2-N3	-2.42	120.22	123.95
2	B	10	2MG	N1-C2-N3	-2.41	120.22	123.95
3	D	4196	OMG	C1'-N9-C4	-2.41	119.33	126.50
48	w	1842	4AC	C5-C4-N4	-2.41	118.73	122.92
3	D	4457	PSU	O2-C2-N1	-2.41	120.14	122.79
3	D	3851	PSU	C6-N1-C2	-2.40	120.22	122.68
3	D	1522	OMG	C1'-N9-C8	2.40	133.53	126.70
2	C	54	5MU	O2-C2-N1	-2.40	119.60	122.79
3	D	1862	PSU	C6-C5-C4	2.39	119.87	118.20
2	B	6	2MG	C8-N7-C5	2.39	108.57	104.24
48	w	1046	PSU	C6-N1-C2	-2.39	120.24	122.68
2	B	54	5MU	O4-C4-N3	-2.38	115.55	120.12
48	w	93	PSU	C6-N1-C2	-2.38	120.25	122.68
3	D	4442	PSU	C6-N1-C2	-2.38	120.25	122.68
3	D	4293	PSU	C6-N1-C2	-2.37	120.26	122.68
3	D	1744	PSU	C6-N1-C2	-2.37	120.26	122.68
3	D	3734	PSU	C6-N1-C2	-2.37	120.26	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	109	PSU	C6-N1-C2	-2.37	120.26	122.68
48	w	119	PSU	C6-N1-C2	-2.37	120.26	122.68
3	D	4579	PSU	C6-N1-C2	-2.37	120.26	122.68
48	w	406	PSU	C6-N1-C2	-2.37	120.26	122.68
3	D	2815	A2M	N3-C4-N9	2.36	130.98	127.08
48	w	1328	OMG	O6-C6-C5	-2.36	120.33	126.60
48	w	1045	PSU	O2-C2-N1	-2.36	120.19	122.79
48	w	1337	4AC	C5-C4-N4	-2.36	118.82	122.92
48	w	651	PSU	O2-C2-N1	-2.35	120.20	122.79
3	D	1860	PSU	C6-N1-C2	-2.35	120.28	122.68
3	D	4296	PSU	C6-N1-C2	-2.35	120.28	122.68
3	D	1862	PSU	C6-N1-C2	-2.35	120.28	122.68
2	B	6	2MG	N9-C4-N3	2.35	130.65	125.94
3	D	2415	OMU	O3'-C3'-C2'	2.34	117.82	111.17
3	D	4228	OMG	C1'-N9-C8	2.34	133.36	126.70
48	w	436	OMG	C8-N7-C5	2.34	108.47	104.24
3	D	3792	OMG	C1'-N9-C4	-2.33	119.57	126.50
48	w	1238	PSU	C6-N1-C2	-2.33	120.30	122.68
3	D	4420	PSU	O4'-C1'-C2'	2.33	108.43	105.14
3	D	4521	PSU	O2-C2-N1	-2.33	120.23	122.79
3	D	1524	A2M	N3-C4-N9	2.33	130.92	127.08
48	w	1850	MA6	N3-C4-N9	2.33	130.92	127.08
3	D	5001	PSU	O2-C2-N1	-2.33	120.23	122.79
48	w	1445	PSU	C6-N1-C2	-2.32	120.31	122.68
2	B	46	G7M	CN7-N7-C5	2.32	129.65	126.77
3	D	4431	PSU	C6-N1-C2	-2.32	120.31	122.68
48	w	509	OMG	C8-N7-C5	2.31	108.43	104.24
48	w	1328	OMG	C8-N7-C5	2.31	108.43	104.24
48	w	1004	PSU	C6-N1-C2	-2.31	120.32	122.68
2	B	48	5MC	CM5-C5-C6	-2.31	119.76	122.85
3	D	3853	PSU	C6-N1-C2	-2.31	120.32	122.68
3	D	4471	PSU	O2-C2-N1	-2.31	120.25	122.79
3	D	4403	PSU	C6-N1-C2	-2.31	120.33	122.68
48	w	484	A2M	N3-C4-N9	2.31	130.88	127.08
3	D	4972	PSU	C6-N1-C2	-2.30	120.33	122.68
3	D	4532	PSU	C6-N1-C2	-2.30	120.33	122.68
48	w	468	A2M	C2'-C1'-N9	-2.30	109.65	113.53
3	D	4471	PSU	C6-N1-C2	-2.30	120.33	122.68
48	w	1692	PSU	C6-N1-C2	-2.30	120.33	122.68
48	w	1842	4AC	C4-N3-C2	-2.29	117.00	120.12
48	w	36	PSU	C6-N1-C2	-2.29	120.34	122.68
48	w	644	OMG	C8-N7-C5	2.29	108.38	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1850	MA6	C5-C4-N9	2.29	108.44	105.78
3	D	3627	OMG	C1'-N9-C8	2.29	133.20	126.70
48	w	686	PSU	C6-N1-C2	-2.28	120.35	122.68
48	w	1383	A2M	C2'-C1'-N9	-2.28	109.69	113.53
3	D	4499	OMG	C8-N7-C5	2.27	108.35	104.24
3	D	2787	A2M	C2-N1-C6	-2.27	114.87	118.77
3	D	3785	A2M	C2-N1-C6	-2.27	114.87	118.77
48	w	1081	PSU	C6-N1-C2	-2.27	120.36	122.68
3	D	1625	OMG	C1'-N9-C4	-2.27	119.77	126.50
48	w	468	A2M	N3-C4-N9	2.26	130.81	127.08
3	D	3715	PSU	C6-N1-C2	-2.26	120.37	122.68
48	w	866	PSU	C6-N1-C2	-2.26	120.37	122.68
48	w	1842	4AC	CM7-C7-N4	-2.26	111.39	115.29
48	w	572	PSU	C6-N1-C2	-2.26	120.37	122.68
2	C	47	H2U	O4-C4-N3	2.26	123.86	120.28
3	D	1522	OMG	C8-N7-C5	2.26	108.32	104.24
48	w	609	PSU	C6-N1-C2	-2.25	120.38	122.68
3	D	1773	OMU	C1'-N1-C2	2.25	121.65	117.57
3	D	3730	PSU	C6-C5-C4	2.25	119.77	118.20
2	C	39	UY1	O4-C4-N3	-2.24	115.82	120.12
3	D	1760	OMG	C8-N7-C5	2.24	108.29	104.24
48	w	166	A2M	N3-C4-N9	2.24	130.77	127.08
48	w	1232	PSU	C6-N1-C2	-2.24	120.39	122.68
3	D	4228	OMG	C8-N7-C5	2.24	108.29	104.24
3	D	3639	PSU	C6-N1-C2	-2.24	120.40	122.68
3	D	4521	PSU	C6-N1-C2	-2.23	120.40	122.68
2	C	46	G7M	CN7-N7-C8	-2.23	121.39	124.84
3	D	2632	PSU	C6-N1-C2	-2.23	120.40	122.68
3	D	3762	PSU	C6-N1-C2	-2.23	120.40	122.68
3	D	1326	A2M	N3-C4-N9	2.23	130.76	127.08
48	w	683	OMG	C8-N7-C5	2.23	108.28	104.24
48	w	966	PSU	C6-N1-C2	-2.23	120.40	122.68
48	w	1678	A2M	N3-C4-N9	2.23	130.76	127.08
5	F	75	OMG	C8-N7-C5	2.23	108.27	104.24
3	D	3744	OMG	C8-N7-C5	2.23	108.27	104.24
48	w	668	A2M	N3-C4-N9	2.23	130.75	127.08
3	D	4353	PSU	C6-N1-C2	-2.23	120.41	122.68
3	D	4361	PSU	C6-N1-C2	-2.23	120.41	122.68
48	w	801	PSU	C6-N1-C2	-2.22	120.41	122.68
48	w	1445	PSU	C6-C5-C4	2.22	119.75	118.20
3	D	4623	OMG	C8-N7-C5	2.22	108.27	104.24
48	w	590	A2M	N3-C4-N9	2.22	130.75	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	55	PSU	C6-N1-C2	-2.22	120.41	122.68
3	D	4306	OMU	O2-C2-N1	-2.22	119.83	122.79
48	w	1851	MA6	N3-C4-N9	2.22	130.74	127.08
3	D	1871	A2M	C3'-C2'-C1'	-2.22	98.71	102.89
3	D	5010	PSU	C6-N1-C2	-2.22	120.41	122.68
3	D	400	A2M	N3-C4-N9	2.22	130.74	127.08
3	D	2401	A2M	N3-C4-N9	2.22	130.74	127.08
48	w	1174	PSU	C6-N1-C2	-2.22	120.42	122.68
48	w	172	OMU	O2-C2-N1	-2.22	119.84	122.79
3	D	1524	A2M	C2-N1-C6	-2.22	114.96	118.77
3	D	4500	PSU	C6-N1-C2	-2.22	120.42	122.68
3	D	4689	PSU	C6-N1-C2	-2.21	120.42	122.68
3	D	3785	A2M	N3-C4-N9	2.21	130.72	127.08
3	D	2363	A2M	C2-N1-C6	-2.21	114.97	118.77
3	D	2508	PSU	C6-N1-C2	-2.21	120.43	122.68
3	D	1792	PSU	O2-C2-N1	-2.21	120.36	122.79
48	w	863	PSU	C6-N1-C2	-2.21	120.43	122.68
3	D	4523	A2M	C2-N1-C6	-2.20	114.98	118.77
48	w	512	A2M	N3-C4-N9	2.20	130.71	127.08
3	D	398	A2M	N3-C4-N9	2.20	130.71	127.08
3	D	4623	OMG	C1'-N9-C8	2.20	132.96	126.70
3	D	1534	A2M	N3-C4-N9	2.20	130.71	127.08
2	B	39	UY1	O4-C4-N3	-2.20	115.90	120.12
48	w	1177	PSU	C6-N1-C2	-2.20	120.44	122.68
48	w	814	PSU	C6-C5-C4	2.20	119.73	118.20
3	D	4312	PSU	C6-N1-C2	-2.19	120.44	122.68
3	D	1534	A2M	C2-N1-C6	-2.19	115.00	118.77
48	w	99	A2M	N3-C4-N9	2.19	130.69	127.08
3	D	2815	A2M	C5-C4-N3	-2.19	123.90	126.75
3	D	4220	6MZ	C4-N9-C8	2.19	108.10	105.73
2	C	6	2MG	C8-N7-C5	2.19	108.20	104.24
3	D	2415	OMU	O2-C2-N1	-2.18	119.88	122.79
48	w	601	OMG	C8-N7-C5	2.18	108.19	104.24
48	w	651	PSU	C6-C5-C4	2.18	119.72	118.20
48	w	1367	PSU	C6-C5-C4	2.18	119.72	118.20
3	D	4499	OMG	C1'-N9-C8	2.18	132.90	126.70
48	w	1081	PSU	O4'-C1'-C2'	2.18	108.22	105.14
48	w	36	PSU	C6-C5-C4	2.18	119.72	118.20
3	D	3818	UY1	O4-C4-N3	-2.18	115.95	120.12
2	B	10	2MG	C8-N7-C5	2.18	108.18	104.24
48	w	1031	A2M	N3-C4-N9	2.17	130.66	127.08
3	D	3825	A2M	N3-C4-N9	2.17	130.66	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3758	PSU	C6-N1-C2	-2.17	120.46	122.68
3	D	3944	OMG	C8-N7-C5	2.17	108.17	104.24
3	D	4576	PSU	C6-N1-C2	-2.17	120.46	122.68
2	B	37	1MG	C8-N7-C5	2.17	108.17	104.24
3	D	4420	PSU	C6-N1-C2	-2.17	120.47	122.68
3	D	3830	A2M	N3-C4-N9	2.17	130.66	127.08
3	D	4370	OMG	C8-N7-C5	2.17	108.16	104.24
48	w	576	A2M	N3-C4-N9	2.16	130.65	127.08
2	C	37	1MG	C8-N7-C5	2.16	108.16	104.24
2	C	48	5MC	CM5-C5-C6	-2.16	119.96	122.85
3	D	4637	OMG	C8-N7-C5	2.16	108.16	104.24
2	B	55	PSU	C6-C5-C4	2.16	119.71	118.20
3	D	1781	PSU	C6-N1-C2	-2.16	120.47	122.68
48	w	166	A2M	C2-N1-C6	-2.16	115.06	118.77
48	w	822	PSU	O4'-C1'-C2'	2.16	108.19	105.14
3	D	2815	A2M	C2-N1-C6	-2.16	115.06	118.77
48	w	406	PSU	C6-C5-C4	2.16	119.71	118.20
3	D	2364	OMG	C8-N7-C5	2.15	108.14	104.24
48	w	1244	PSU	C6-N1-C2	-2.15	120.48	122.68
3	D	4576	PSU	C6-C5-C4	2.15	119.70	118.20
48	w	866	PSU	C6-C5-C4	2.15	119.70	118.20
48	w	1851	MA6	C4-N9-C8	2.15	108.06	105.73
3	D	4442	PSU	O4'-C1'-C2'	2.15	108.17	105.14
3	D	4392	OMG	C8-N7-C5	2.15	108.13	104.24
3	D	4494	OMG	C8-N7-C5	2.15	108.13	104.24
3	D	400	A2M	C2-N1-C6	-2.15	115.08	118.77
48	w	651	PSU	C6-N1-C2	-2.15	120.49	122.68
3	D	4523	A2M	N3-C4-N9	2.14	130.62	127.08
48	w	1678	A2M	C2-N1-C6	-2.14	115.09	118.77
3	D	3760	A2M	N3-C4-N9	2.14	130.61	127.08
3	D	3744	OMG	C1'-N9-C8	2.14	132.79	126.70
3	D	3764	PSU	C6-N1-C2	-2.14	120.50	122.68
3	D	1625	OMG	C8-N7-C5	2.14	108.11	104.24
48	w	159	A2M	N3-C4-N9	2.14	130.60	127.08
3	D	3899	OMG	C8-N7-C5	2.14	108.11	104.24
3	D	3730	PSU	C6-N1-C2	-2.14	120.50	122.68
48	w	484	A2M	C2-N1-C6	-2.13	115.11	118.77
48	w	1347	PSU	C6-N1-C2	-2.13	120.51	122.68
3	D	1677	PSU	C6-C5-C4	2.13	119.69	118.20
48	w	1383	A2M	C3'-C2'-C1'	-2.13	98.89	102.89
3	D	3627	OMG	C8-N7-C5	2.13	108.09	104.24
48	w	1367	PSU	C6-N1-C2	-2.13	120.51	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	159	A2M	C2-N1-C6	-2.13	115.12	118.77
48	w	644	OMG	C1'-N9-C8	2.12	132.74	126.70
3	D	4220	6MZ	N3-C4-N9	2.12	130.58	127.08
3	D	1782	PSU	C6-N1-C2	-2.12	120.51	122.68
3	D	3899	OMG	C1'-N9-C8	2.12	132.74	126.70
3	D	1524	A2M	C5-C4-N3	-2.12	123.98	126.75
48	w	649	PSU	C6-C5-C4	2.12	119.68	118.20
3	D	1534	A2M	C5-C4-N3	-2.12	123.98	126.75
3	D	3695	PSU	C6-N1-C2	-2.12	120.52	122.68
3	D	4442	PSU	C6-C5-C4	2.12	119.68	118.20
3	D	1322	1MA	C6-C5-N7	-2.11	128.35	132.20
3	D	2401	A2M	C2-N1-C6	-2.11	115.14	118.77
48	w	210	PSU	C6-N1-C2	-2.11	120.52	122.68
3	D	1316	OMG	C8-N7-C5	2.11	108.06	104.24
3	D	3718	A2M	N3-C4-N9	2.11	130.56	127.08
48	w	1248	B8N	O4'-C1'-C2'	2.11	108.12	105.14
48	w	27	A2M	N3-C4-N9	2.11	130.56	127.08
2	C	35	PSU	C6-N1-C2	-2.11	120.53	122.68
3	D	1792	PSU	C6-N1-C2	-2.11	120.53	122.68
3	D	2363	A2M	N3-C4-N9	2.11	130.55	127.08
3	D	2424	OMG	C8-N7-C5	2.10	108.05	104.24
2	B	6	2MG	C4-C5-N7	-2.10	107.39	110.72
3	D	2364	OMG	C1'-N9-C8	2.10	132.69	126.70
3	D	3792	OMG	C8-N7-C5	2.10	108.05	104.24
3	D	2424	OMG	C1'-N9-C8	2.10	132.68	126.70
3	D	4618	OMG	C8-N7-C5	2.10	108.05	104.24
3	D	3825	A2M	C2-N1-C6	-2.10	115.16	118.77
3	D	1316	OMG	C1'-N9-C8	2.10	132.68	126.70
48	w	468	A2M	C2-N1-C6	-2.10	115.16	118.77
2	C	10	2MG	C8-N7-C5	2.10	108.04	104.24
48	w	109	PSU	C6-C5-C4	2.10	119.67	118.20
3	D	1326	A2M	C2-N1-C6	-2.10	115.16	118.77
3	D	5001	PSU	C6-N1-C2	-2.10	120.54	122.68
48	w	218	PSU	C6-N1-C2	-2.10	120.54	122.68
48	w	814	PSU	C6-N1-C2	-2.10	120.54	122.68
48	w	1248	B8N	C32-C33-C34	-2.10	105.31	110.30
48	w	601	OMG	C1'-N9-C8	2.10	132.66	126.70
2	C	37	1MG	C1'-N9-C4	2.10	132.73	126.50
48	w	121	OMU	O2-C2-N1	-2.09	120.00	122.79
48	w	159	A2M	C2'-C1'-N9	-2.09	110.01	113.53
48	w	649	PSU	C6-N1-C2	-2.09	120.55	122.68
2	C	27	M2G	O6-C6-N1	-2.09	116.11	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	668	A2M	C2-N1-C6	-2.09	115.19	118.77
2	B	6	2MG	C1'-N9-C8	2.08	132.63	126.70
2	B	35	PSU	C6-C5-C4	2.08	119.65	118.20
48	w	1232	PSU	C6-C5-C4	2.08	119.65	118.20
3	D	2787	A2M	N3-C4-N9	2.08	130.50	127.08
48	w	1850	MA6	N1-C6-N6	-2.07	114.82	117.08
2	B	35	PSU	C6-N1-C2	-2.07	120.57	122.68
5	F	75	OMG	C1'-N9-C8	2.07	132.58	126.70
48	w	1625	PSU	C6-N1-C2	-2.07	120.57	122.68
48	w	99	A2M	C2-N1-C6	-2.06	115.22	118.77
48	w	428	OMU	O2-C2-N1	-2.06	120.04	122.79
2	C	58	1MA	C6-C5-N7	-2.06	128.45	132.20
3	D	1683	PSU	C6-C5-C4	2.06	119.64	118.20
2	C	35	PSU	C6-C5-C4	2.06	119.64	118.20
3	D	4618	OMG	C1'-N9-C8	2.06	132.55	126.70
3	D	398	A2M	C2-N1-C6	-2.06	115.24	118.77
3	D	3718	A2M	C2-N1-C6	-2.06	115.24	118.77
48	w	512	A2M	C2-N1-C6	-2.06	115.24	118.77
48	w	681	PSU	C6-N1-C2	-2.06	120.58	122.68
48	w	27	A2M	C2-N1-C6	-2.05	115.24	118.77
2	B	55	PSU	O2-C2-N1	-2.05	120.53	122.79
48	w	590	A2M	C2-N1-C6	-2.05	115.25	118.77
48	w	799	OMU	O2-C2-N1	-2.05	120.06	122.79
3	D	3758	PSU	C6-C5-C4	2.04	119.62	118.20
48	w	1639	G7M	CN7-N7-C8	-2.04	121.69	124.84
3	D	2363	A2M	C5-C4-N3	-2.04	124.09	126.75
3	D	4196	OMG	C8-N7-C5	2.03	107.92	104.24
3	D	1871	A2M	N3-C4-N9	2.03	130.43	127.08
48	w	1490	OMG	C8-N7-C5	2.03	107.92	104.24
2	C	46	G7M	N9-C8-N7	-2.03	107.19	112.21
48	w	509	OMG	C1'-N9-C8	2.03	132.47	126.70
3	D	4312	PSU	C6-C5-C4	2.03	119.61	118.20
48	w	576	A2M	C2-N1-C6	-2.03	115.29	118.77
3	D	3724	A2M	N3-C4-N9	2.02	130.42	127.08
48	w	1442	OMU	O2-C2-N1	-2.02	120.10	122.79
48	w	1045	PSU	C6-N1-C2	-2.02	120.61	122.68
48	w	815	PSU	C6-N1-C2	-2.02	120.62	122.68
48	w	1031	A2M	C2-N1-C6	-2.02	115.30	118.77
48	w	1383	A2M	N3-C4-N9	2.02	130.41	127.08
3	D	398	A2M	C5-C4-N3	-2.02	124.12	126.75
48	w	512	A2M	C2'-C1'-N9	-2.02	110.13	113.53
3	D	3925	OMU	O2-C2-N1	-2.02	120.10	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1056	PSU	C6-C5-C4	2.02	119.61	118.20
3	D	2351	OMC	O2-C2-N3	-2.02	119.05	122.33
3	D	4972	PSU	C6-C5-C4	2.02	119.61	118.20
48	w	572	PSU	C6-C5-C4	2.01	119.61	118.20
48	w	668	A2M	C5-C4-N3	-2.01	124.13	126.75
48	w	1337	4AC	C5-C4-N3	2.01	125.83	122.59
3	D	4420	PSU	C6-C5-C4	2.01	119.60	118.20
2	B	55	PSU	O4'-C1'-C2'	2.00	107.97	105.14
48	w	484	A2M	C5-C4-N3	-2.00	124.14	126.75
2	B	27	M2G	O6-C6-N1	-2.00	116.28	120.12
3	D	4521	PSU	O4'-C1'-C2'	2.00	107.97	105.14
3	D	2508	PSU	C6-C5-C4	2.00	119.60	118.20

There are no chirality outliers.

All (174) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	26	M2G	C3'-C4'-C5'-O5'
2	B	34	56B	C11-C10-N10-C9
2	B	39	UY1	C3'-C4'-C5'-O5'
2	B	39	UY1	O4'-C4'-C5'-O5'
2	C	46	G7M	C3'-C4'-C5'-O5'
2	B	47	H2U	C3'-C4'-C5'-O5'
2	C	47	H2U	O4'-C4'-C5'-O5'
2	B	48	5MC	O4'-C4'-C5'-O5'
2	B	48	5MC	C3'-C4'-C5'-O5'
2	C	54	5MU	O4'-C4'-C5'-O5'
2	B	58	1MA	O4'-C4'-C5'-O5'
3	D	1534	A2M	C1'-C2'-O2'-CM'
3	D	1760	OMG	C3'-C4'-C5'-O5'
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	C3'-C4'-C5'-O5'
3	D	3724	A2M	C1'-C2'-O2'-CM'
3	D	3762	PSU	C3'-C4'-C5'-O5'
3	D	3785	A2M	O4'-C4'-C5'-O5'
3	D	3818	UY1	C3'-C4'-C5'-O5'
3	D	3925	OMU	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

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Mol	Chain	Res	Type	Atoms
5	F	75	OMG	C1'-C2'-O2'-CM2
48	w	34	PSU	C3'-C4'-C5'-O5'
48	w	159	A2M	C3'-C4'-C5'-O5'
48	w	428	OMU	C2'-C1'-N1-C2
48	w	428	OMU	C2'-C1'-N1-C6
48	w	428	OMU	C1'-C2'-O2'-CM2
48	w	468	A2M	O4'-C4'-C5'-O5'
48	w	468	A2M	C3'-C4'-C5'-O5'
48	w	509	OMG	C1'-C2'-O2'-CM2
48	w	517	OMC	C1'-C2'-O2'-CM2
48	w	576	A2M	C3'-C4'-C5'-O5'
48	w	644	OMG	C3'-C4'-C5'-O5'
48	w	799	OMU	C1'-C2'-O2'-CM2
48	w	799	OMU	O4'-C4'-C5'-O5'
48	w	1248	B8N	C31-C32-C33-C34
48	w	1248	B8N	C31-C32-C33-N34
48	w	1442	OMU	C1'-C2'-O2'-CM2
48	w	1490	OMG	C1'-C2'-O2'-CM2
48	w	1678	A2M	C1'-C2'-O2'-CM'
48	w	1804	OMU	C3'-C4'-C5'-O5'
48	w	1832	6MZ	C5-C6-N6-C9
48	w	1832	6MZ	N1-C6-N6-C9
48	w	1851	MA6	O4'-C4'-C5'-O5'
2	C	6	2MG	O4'-C4'-C5'-O5'
2	C	46	G7M	O4'-C4'-C5'-O5'
2	C	54	5MU	C3'-C4'-C5'-O5'
2	B	58	1MA	C3'-C4'-C5'-O5'
3	D	1534	A2M	O4'-C4'-C5'-O5'
3	D	2364	OMG	O4'-C4'-C5'-O5'
3	D	2815	A2M	O4'-C4'-C5'-O5'
3	D	3762	PSU	O4'-C4'-C5'-O5'
3	D	3785	A2M	C3'-C4'-C5'-O5'
3	D	3818	UY1	O4'-C4'-C5'-O5'
48	w	159	A2M	O4'-C4'-C5'-O5'
48	w	166	A2M	O4'-C4'-C5'-O5'
48	w	166	A2M	C3'-C4'-C5'-O5'
48	w	428	OMU	C3'-C4'-C5'-O5'
48	w	627	OMU	O4'-C4'-C5'-O5'
48	w	668	A2M	O4'-C4'-C5'-O5'
48	w	668	A2M	C3'-C4'-C5'-O5'
48	w	1851	MA6	C3'-C4'-C5'-O5'
2	C	6	2MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	47	H2U	O4'-C4'-C5'-O5'
2	C	47	H2U	C3'-C4'-C5'-O5'
3	D	1760	OMG	O4'-C4'-C5'-O5'
48	w	34	PSU	O4'-C4'-C5'-O5'
48	w	99	A2M	O4'-C4'-C5'-O5'
48	w	428	OMU	O4'-C4'-C5'-O5'
48	w	512	A2M	C3'-C4'-C5'-O5'
48	w	576	A2M	O4'-C4'-C5'-O5'
48	w	799	OMU	C3'-C4'-C5'-O5'
48	w	1238	PSU	C3'-C4'-C5'-O5'
48	w	1238	PSU	O4'-C4'-C5'-O5'
48	w	1639	G7M	O4'-C4'-C5'-O5'
48	w	1639	G7M	C3'-C4'-C5'-O5'
48	w	1804	OMU	O4'-C4'-C5'-O5'
3	D	3701	OMC	C2'-C1'-N1-C6
3	D	4447	5MC	C2'-C1'-N1-C6
3	D	2364	OMG	C3'-C4'-C5'-O5'
3	D	3944	OMG	C3'-C4'-C5'-O5'
3	D	4447	5MC	C2'-C1'-N1-C2
2	B	26	M2G	O4'-C4'-C5'-O5'
2	B	54	5MU	C3'-C4'-C5'-O5'
2	C	55	PSU	C3'-C4'-C5'-O5'
2	C	48	5MC	C3'-C4'-C5'-O5'
2	B	54	5MU	O4'-C4'-C5'-O5'
3	D	1677	PSU	O4'-C4'-C5'-O5'
3	D	3944	OMG	O4'-C4'-C5'-O5'
48	w	512	A2M	O4'-C4'-C5'-O5'
48	w	644	OMG	O4'-C4'-C5'-O5'
48	w	1490	OMG	O4'-C4'-C5'-O5'
48	w	1703	OMC	O4'-C4'-C5'-O5'
2	C	55	PSU	O4'-C4'-C5'-O5'
48	w	1490	OMG	C3'-C4'-C5'-O5'
3	D	3701	OMC	C2'-C1'-N1-C2
48	w	1490	OMG	C4'-C5'-O5'-P
48	w	627	OMU	C2'-C1'-N1-C6
48	w	1248	B8N	N34-C33-C34-O36
2	C	34	56B	O4'-C4'-C5'-O5'
48	w	590	A2M	C3'-C4'-C5'-O5'
48	w	627	OMU	C3'-C4'-C5'-O5'
48	w	822	PSU	O4'-C4'-C5'-O5'
48	w	1248	B8N	N34-C33-C34-O35
3	D	3701	OMC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
3	D	2787	A2M	C2'-C1'-N9-C8
48	w	590	A2M	O4'-C4'-C5'-O5'
48	w	627	OMU	C1'-C2'-O2'-CM2
3	D	4447	5MC	O4'-C1'-N1-C2
3	D	4500	PSU	C4'-C5'-O5'-P
48	w	644	OMG	C4'-C5'-O5'-P
2	B	46	G7M	C3'-C4'-C5'-O5'
3	D	1677	PSU	C3'-C4'-C5'-O5'
3	D	4447	5MC	O4'-C1'-N1-C6
2	B	55	PSU	C4'-C5'-O5'-P
3	D	3944	OMG	C4'-C5'-O5'-P
2	B	48	5MC	C4'-C5'-O5'-P
3	D	3701	OMC	O4'-C1'-N1-C2
48	w	428	OMU	O4'-C1'-N1-C2
2	C	34	56B	C3'-C4'-C5'-O5'
48	w	428	OMU	O4'-C1'-N1-C6
2	C	6	2MG	C4'-C5'-O5'-P
48	w	166	A2M	C4'-C5'-O5'-P
48	w	627	OMU	O4'-C1'-N1-C6
48	w	1326	OMU	O4'-C1'-N1-C6
48	w	627	OMU	C3'-C2'-O2'-CM2
2	C	47	H2U	C4'-C5'-O5'-P
2	C	48	5MC	C4'-C5'-O5'-P
3	D	1534	A2M	C4'-C5'-O5'-P
2	B	34	56B	C14-C10-N10-C9
3	D	2787	A2M	C2'-C1'-N9-C4
48	w	34	PSU	C4'-C5'-O5'-P
48	w	627	OMU	O4'-C1'-N1-C2
48	w	1326	OMU	O4'-C1'-N1-C2
2	B	34	56B	C8-C7-C9-N10
3	D	3715	PSU	O4'-C1'-C5-C4
3	D	3758	PSU	O4'-C1'-C5-C4
3	D	3818	UY1	O4'-C1'-C5-C4
3	D	4500	PSU	O4'-C1'-C5-C4
3	D	4521	PSU	O4'-C1'-C5-C4
48	w	627	OMU	C2'-C1'-N1-C2
3	D	1322	1MA	C2'-C1'-N9-C8
3	D	1322	1MA	C2'-C1'-N9-C4
2	B	46	G7M	O4'-C4'-C5'-O5'
48	w	99	A2M	C3'-C4'-C5'-O5'
48	w	119	PSU	C3'-C4'-C5'-O5'
3	D	1524	A2M	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
3	D	2351	OMC	C2'-C1'-N1-C2
2	B	37	1MG	O4'-C4'-C5'-O5'
48	w	822	PSU	C3'-C4'-C5'-O5'
48	w	1703	OMC	C3'-C4'-C5'-O5'
3	D	3792	OMG	C1'-C2'-O2'-CM2
48	w	1326	OMU	C2'-C1'-N1-C2
3	D	2787	A2M	O4'-C1'-N9-C8
3	D	1677	PSU	O4'-C1'-C5-C6
3	D	3715	PSU	O4'-C1'-C5-C6
3	D	3758	PSU	O4'-C1'-C5-C6
3	D	3818	UY1	O4'-C1'-C5-C6
3	D	4500	PSU	O4'-C1'-C5-C6
3	D	4521	PSU	O4'-C1'-C5-C6
3	D	1773	OMU	C2'-C1'-N1-C2
2	B	47	H2U	C4'-C5'-O5'-P
3	D	3887	OMC	C4'-C5'-O5'-P
2	B	55	PSU	C3'-C4'-C5'-O5'
3	D	2422	OMC	O4'-C4'-C5'-O5'
3	D	1326	A2M	C3'-C4'-C5'-O5'
3	D	2351	OMC	O4'-C4'-C5'-O5'
48	w	1288	OMU	C2'-C1'-N1-C2
3	D	3785	A2M	C2'-C1'-N9-C8
48	w	668	A2M	C2'-C1'-N9-C8

There are no ring outliers.

60 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	w	1391	OMC	1	0
3	D	2363	A2M	1	0
48	w	627	OMU	1	0
2	B	54	5MU	2	0
3	D	1534	A2M	1	0
48	w	1842	4AC	1	0
3	D	1760	OMG	1	0
48	w	601	OMG	1	0
48	w	799	OMU	2	0
3	D	3818	UY1	1	0
48	w	576	A2M	1	0
3	D	4620	OMU	2	0
3	D	4220	6MZ	1	0
3	D	2364	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	26	M2G	1	0
48	w	1692	PSU	1	0
3	D	2351	OMC	2	0
48	w	683	OMG	1	0
3	D	3925	OMU	1	0
3	D	3724	A2M	1	0
3	D	4420	PSU	1	0
3	D	1773	OMU	3	0
48	w	1678	A2M	1	0
3	D	1340	OMC	1	0
48	w	1850	MA6	1	0
48	w	1639	G7M	2	0
48	w	166	A2M	2	0
3	D	3768	PSU	1	0
48	w	517	OMC	2	0
48	w	686	PSU	1	0
3	D	4637	OMG	2	0
48	w	93	PSU	1	0
48	w	27	A2M	1	0
48	w	644	OMG	1	0
48	w	1490	OMG	3	0
3	D	3785	A2M	1	0
48	w	116	OMU	2	0
3	D	4447	5MC	1	0
48	w	512	A2M	1	0
48	w	1288	OMU	1	0
48	w	1445	PSU	1	0
2	B	55	PSU	3	0
3	D	4392	OMG	1	0
3	D	398	A2M	1	0
3	D	2815	A2M	1	0
2	C	46	G7M	2	0
48	w	428	OMU	2	0
3	D	2415	OMU	1	0
48	w	436	OMG	1	0
3	D	4457	PSU	1	0
48	w	1337	4AC	1	0
2	C	47	H2U	2	0
3	D	1326	A2M	1	0
2	C	26	M2G	2	0
5	F	75	OMG	1	0
3	D	4623	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	w	572	PSU	1	0
3	D	4494	OMG	1	0
3	D	2824	OMC	1	0
3	D	3718	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 528 ligands modelled in this entry, 526 are monoatomic - leaving 2 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
80	GAL	C	101	2	11,11,12	1.96	3 (27%)	15,15,17	1.82	6 (40%)
80	GAL	B	101	2	11,11,12	1.89	2 (18%)	15,15,17	1.99	6 (40%)

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
80	GAL	C	101	2	-	2/2/19/22	0/1/1/1
80	GAL	B	101	2	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B	101	GAL	O5-C1	-3.65	1.37	1.43
80	C	101	GAL	O5-C1	-3.34	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	C	101	GAL	C2-C3	3.09	1.57	1.52
80	B	101	GAL	C2-C3	2.80	1.56	1.52
80	C	101	GAL	C4-C5	2.40	1.58	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	C	101	GAL	O2-C2-C3	-3.37	103.39	110.14
80	B	101	GAL	O4-C4-C5	-3.33	101.04	109.30
80	B	101	GAL	O2-C2-C3	-3.26	103.61	110.14
80	B	101	GAL	C6-C5-C4	-3.16	105.60	113.00
80	B	101	GAL	C2-C3-C4	-2.65	106.31	110.89
80	C	101	GAL	O4-C4-C5	-2.62	102.80	109.30
80	C	101	GAL	C2-C3-C4	-2.60	106.40	110.89
80	B	101	GAL	C1-C2-C3	-2.52	106.57	109.67
80	C	101	GAL	O3-C3-C4	-2.33	104.97	110.35
80	C	101	GAL	C1-C2-C3	-2.15	107.02	109.67
80	B	101	GAL	O3-C3-C4	-2.10	105.49	110.35
80	C	101	GAL	C6-C5-C4	-2.06	108.18	113.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

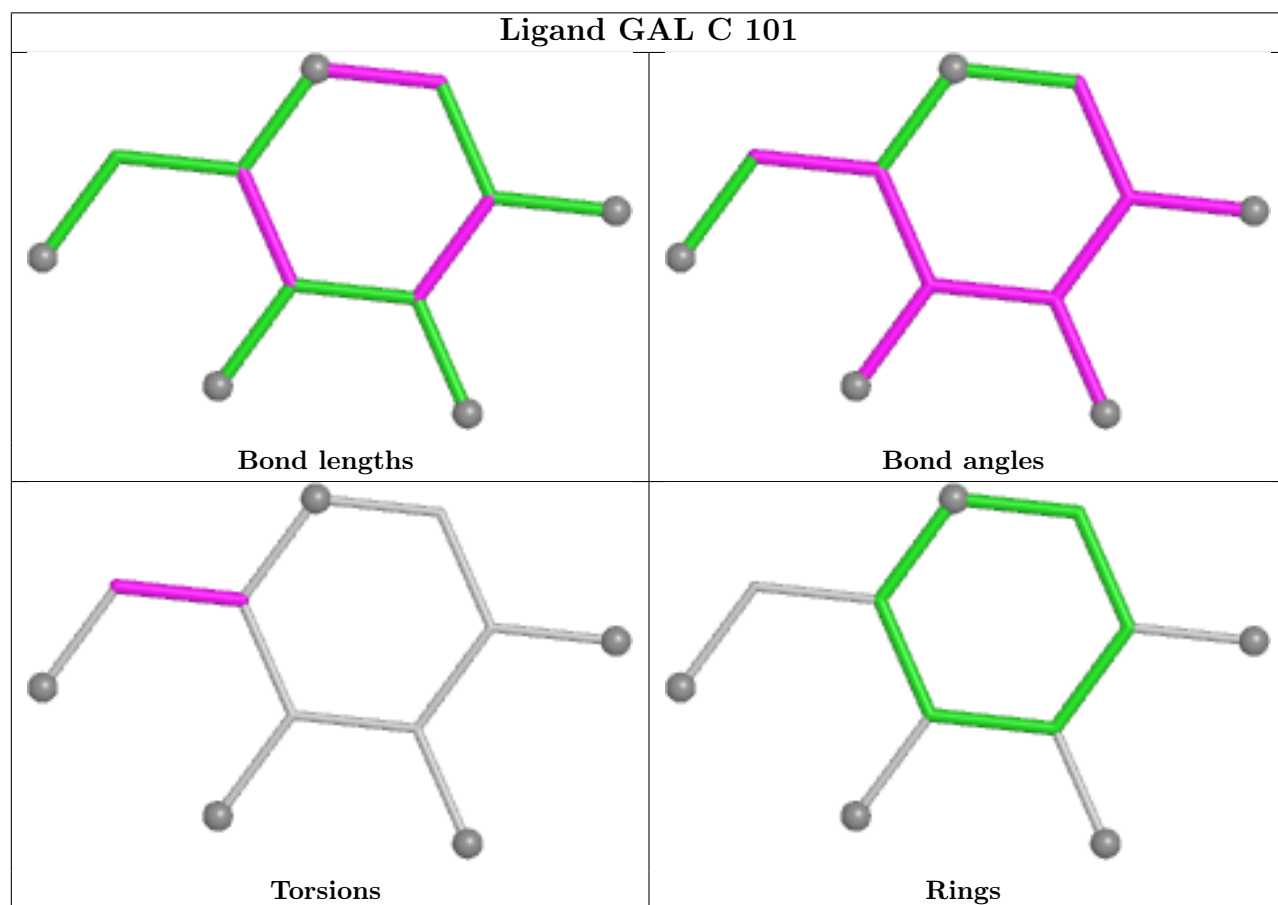
Mol	Chain	Res	Type	Atoms
80	C	101	GAL	O5-C5-C6-O6
80	C	101	GAL	C4-C5-C6-O6
80	B	101	GAL	O5-C5-C6-O6
80	B	101	GAL	C4-C5-C6-O6

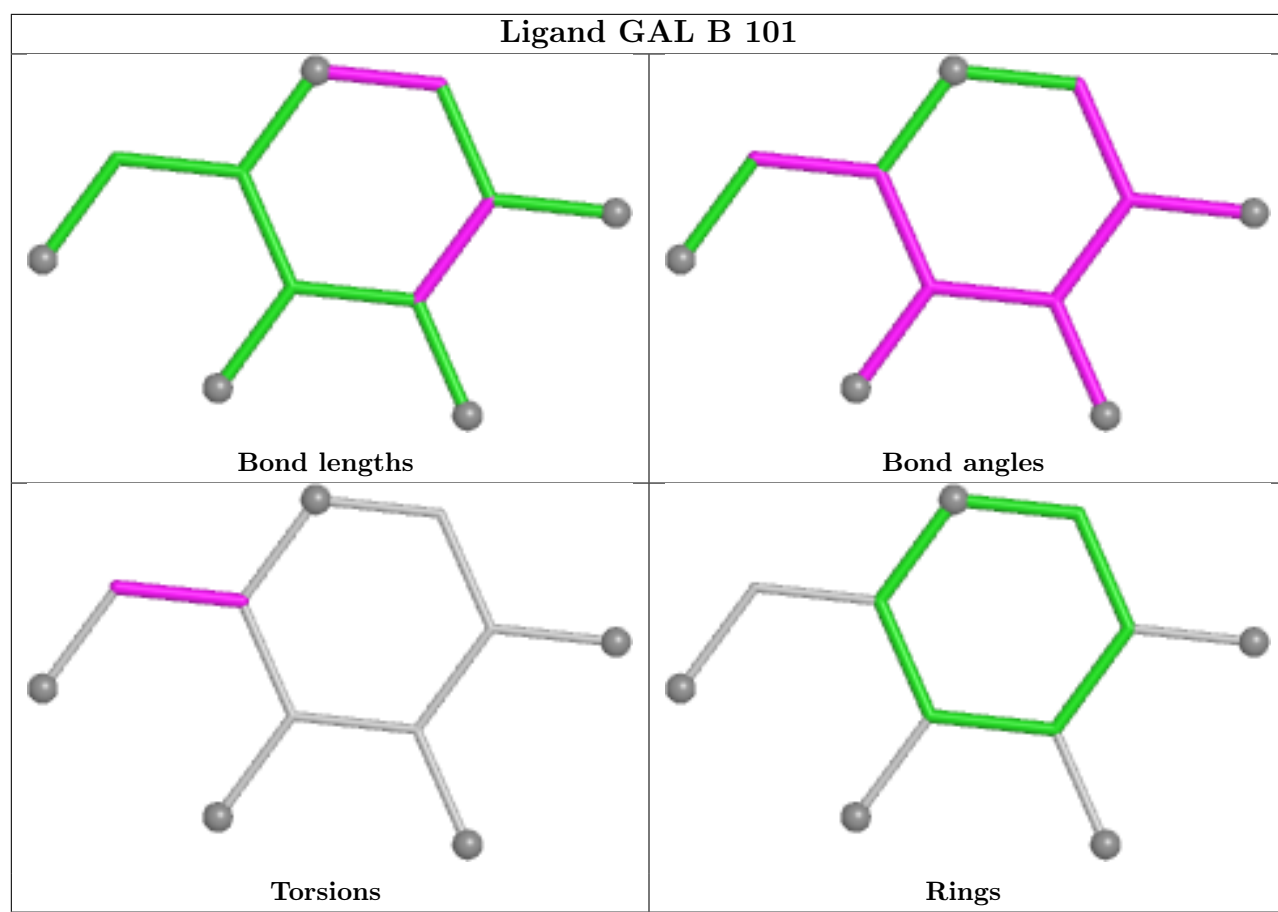
There are no ring outliers.

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.

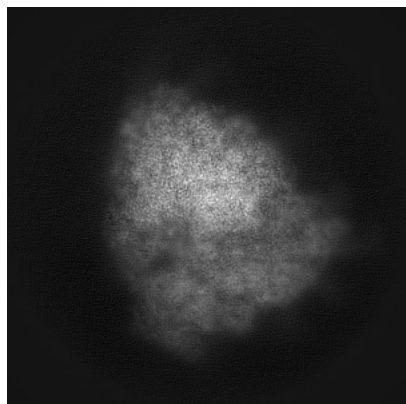
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36181. These allow visual inspection of the internal detail of the map and identification of artifacts.

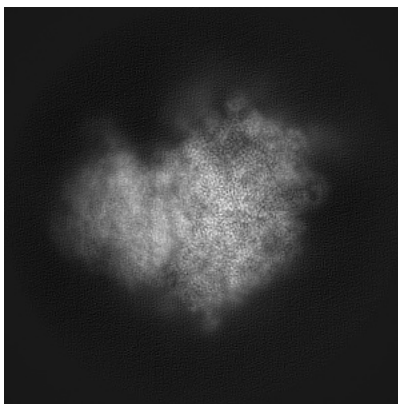
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

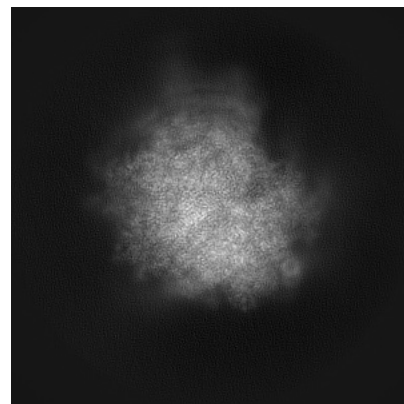
6.1.1 Primary map



X

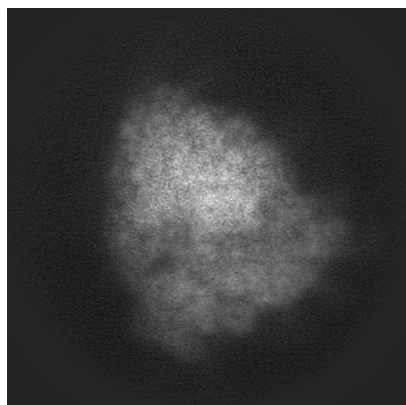


Y

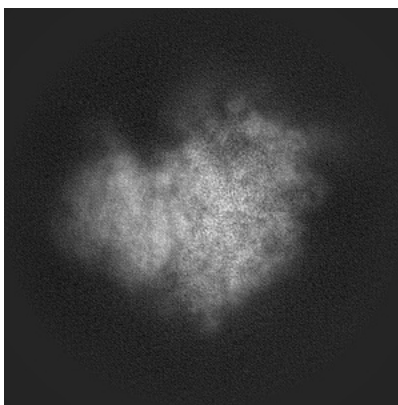


Z

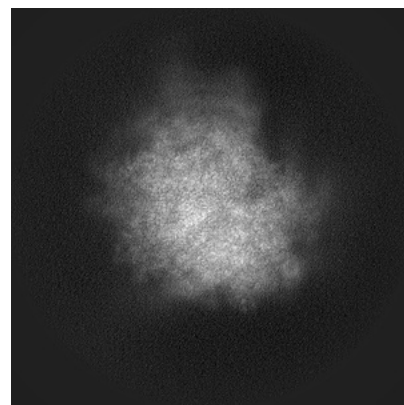
6.1.2 Raw map



X



Y

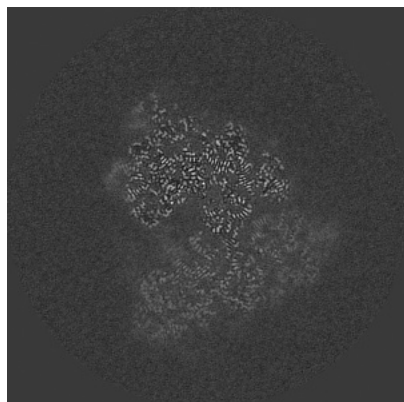


Z

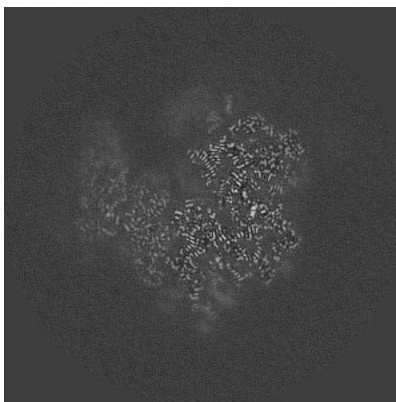
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

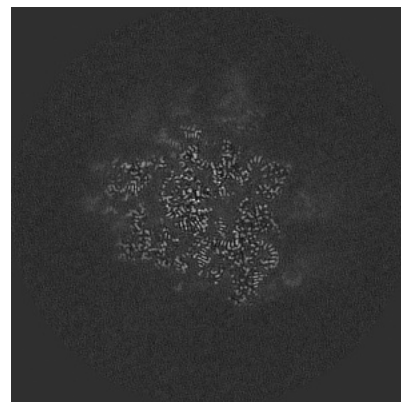
6.2.1 Primary map



X Index: 265

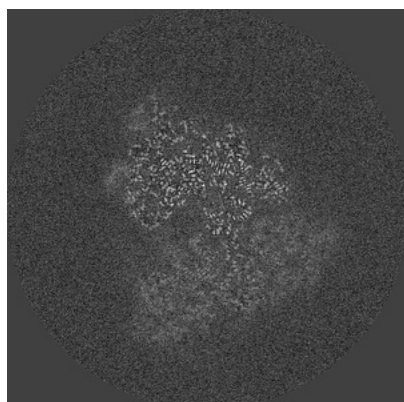


Y Index: 265

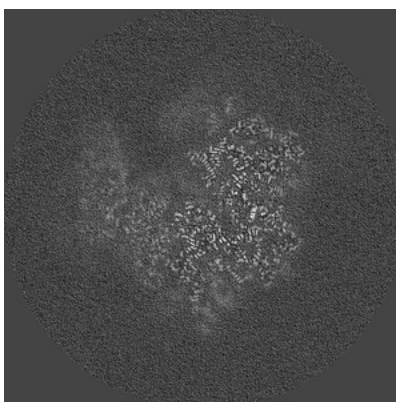


Z Index: 265

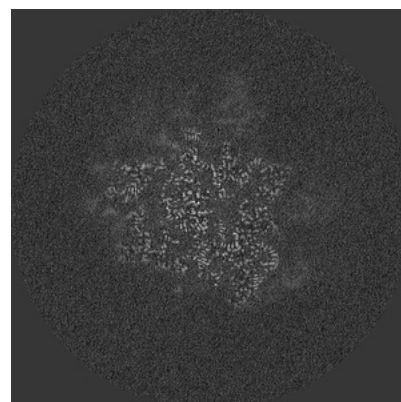
6.2.2 Raw map



X Index: 265



Y Index: 265

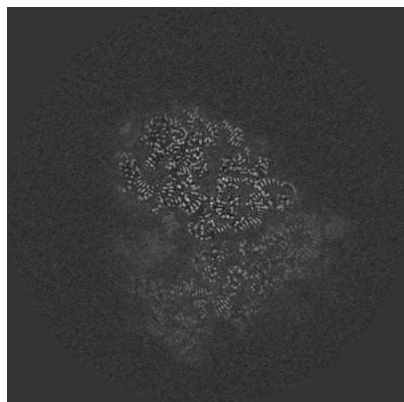


Z Index: 265

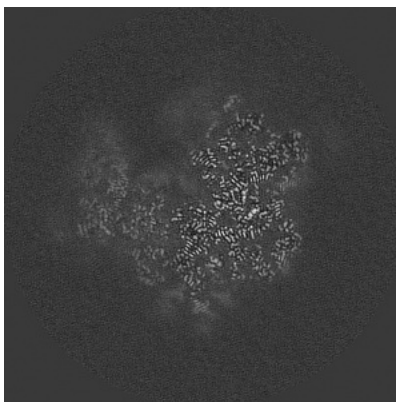
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

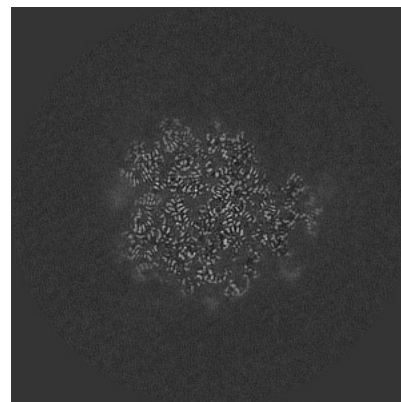
6.3.1 Primary map



X Index: 245

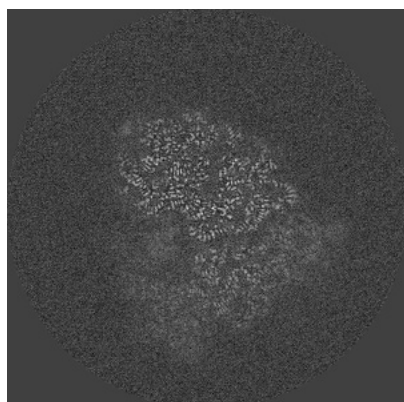


Y Index: 261

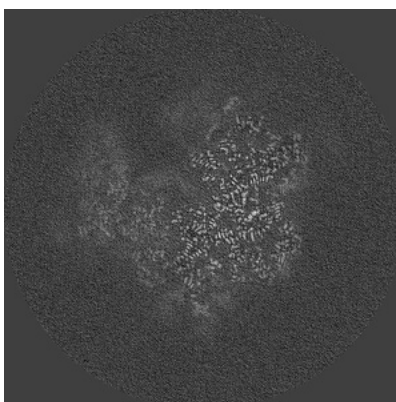


Z Index: 302

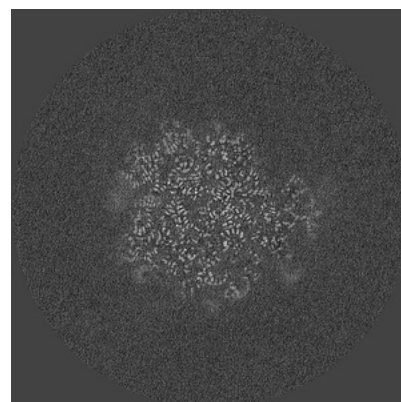
6.3.2 Raw map



X Index: 248



Y Index: 261

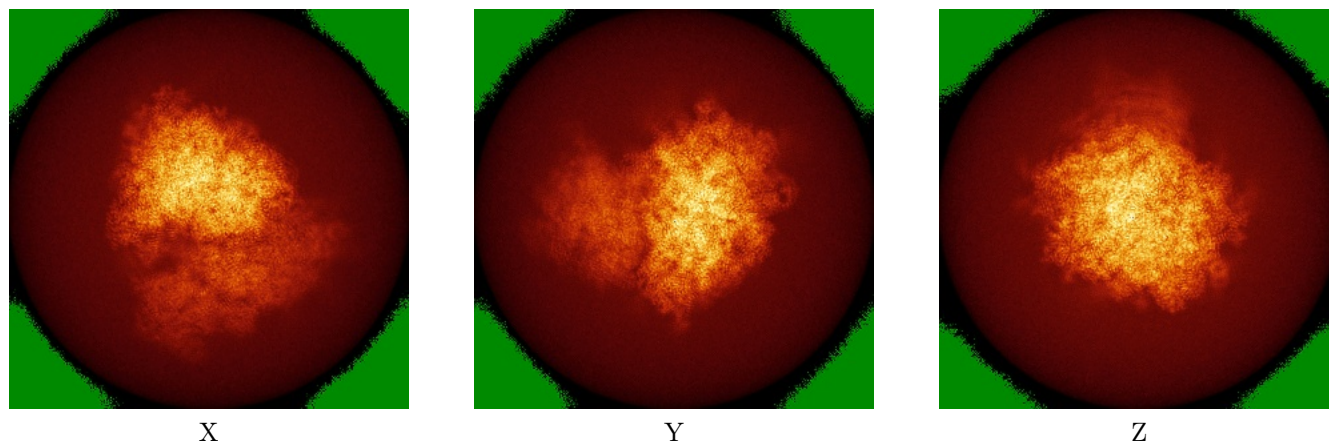


Z Index: 302

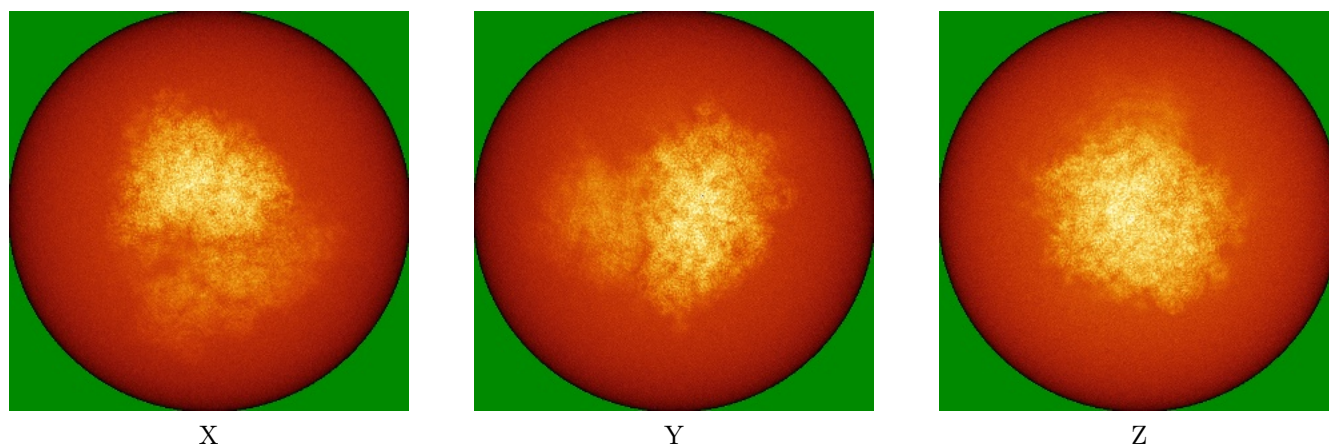
The images above show the largest variance slices of the map in three orthogonal directions.

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



X



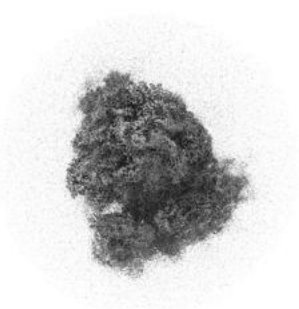
Y



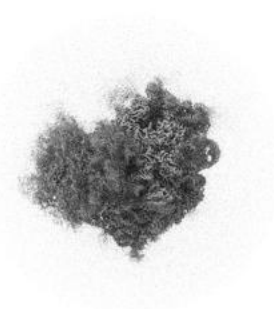
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0183. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

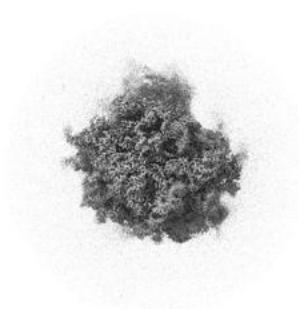
6.5.2 Raw map



X



Y



Z

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

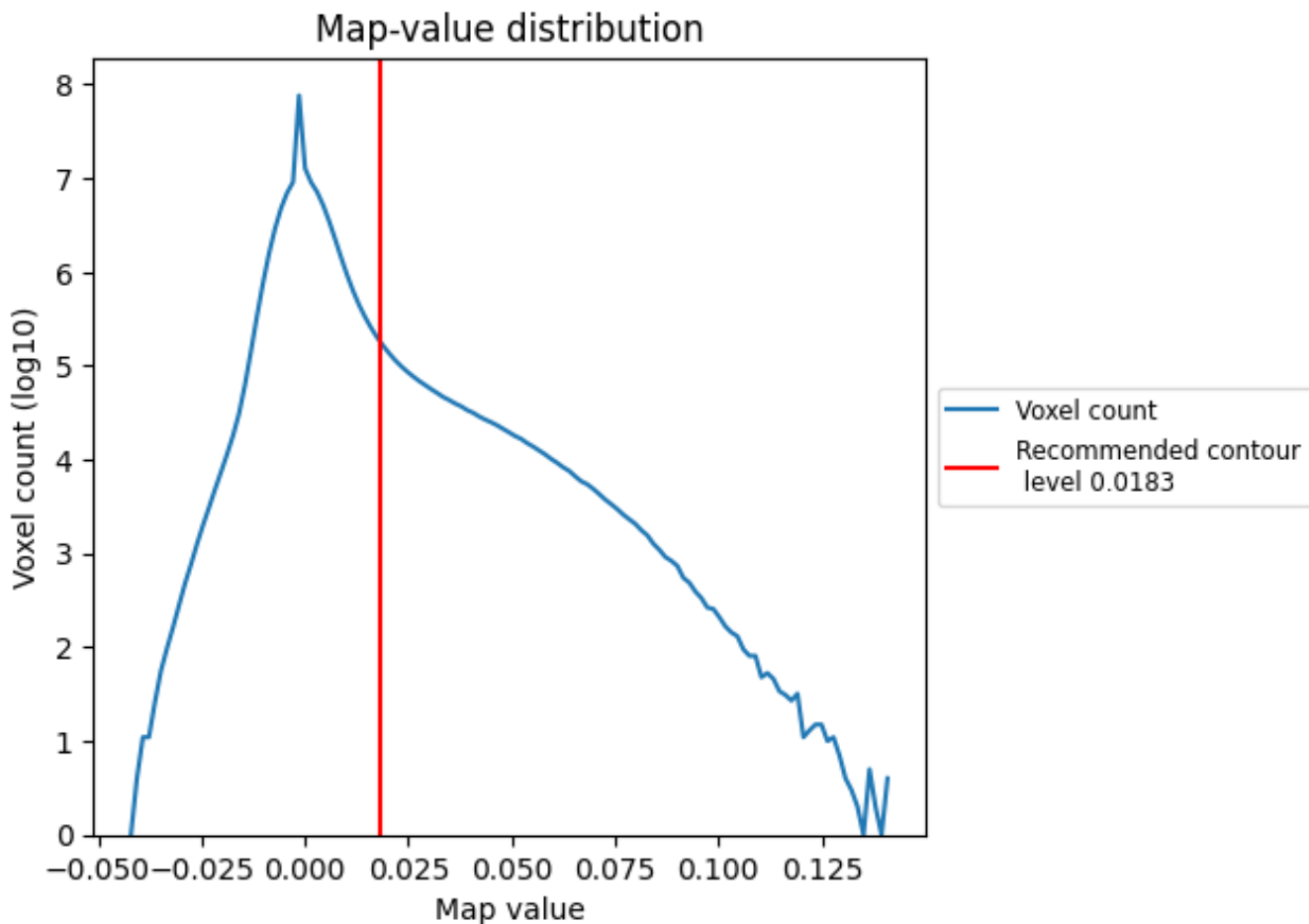
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

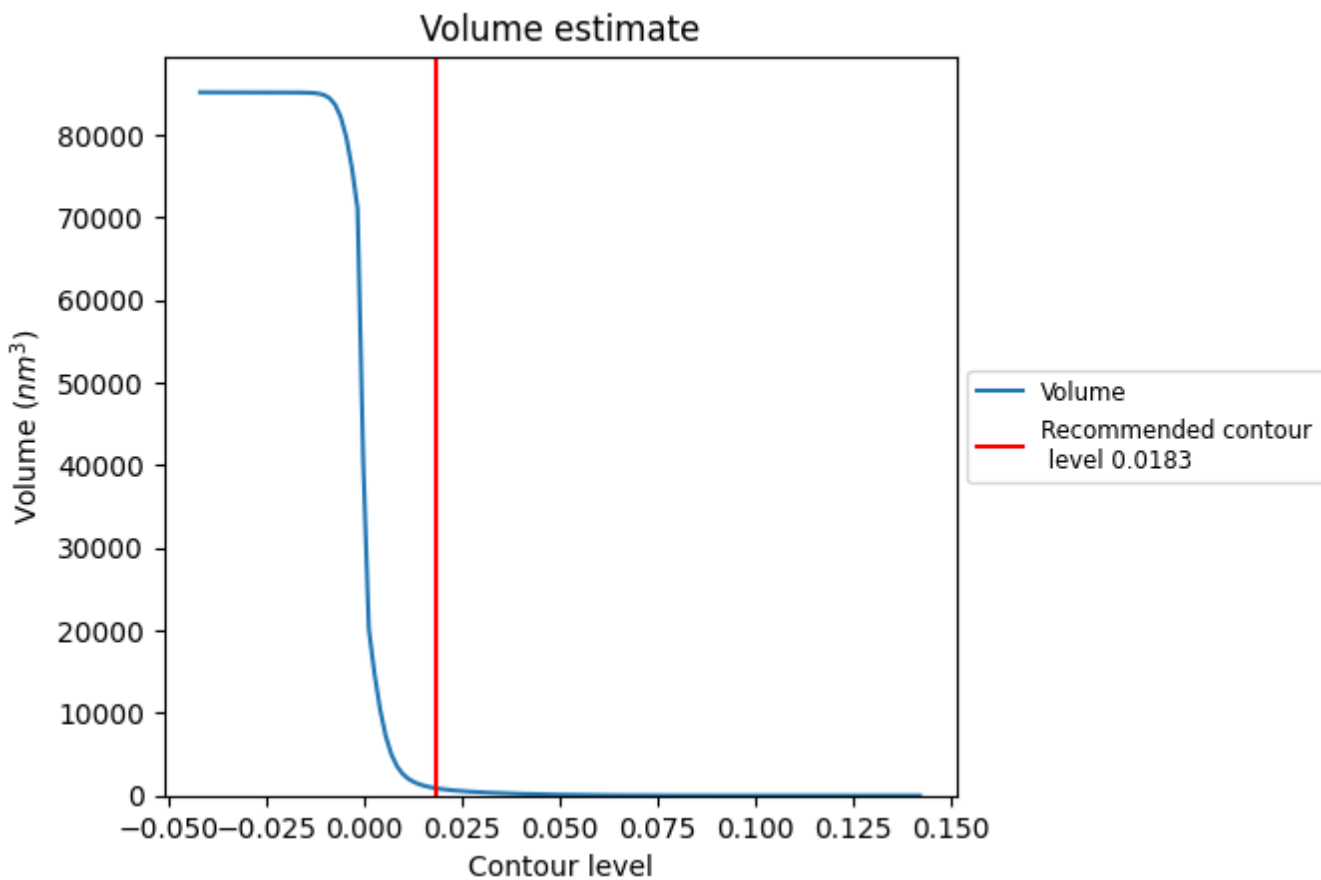
This section contains the results of statistical analysis of the map.

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.

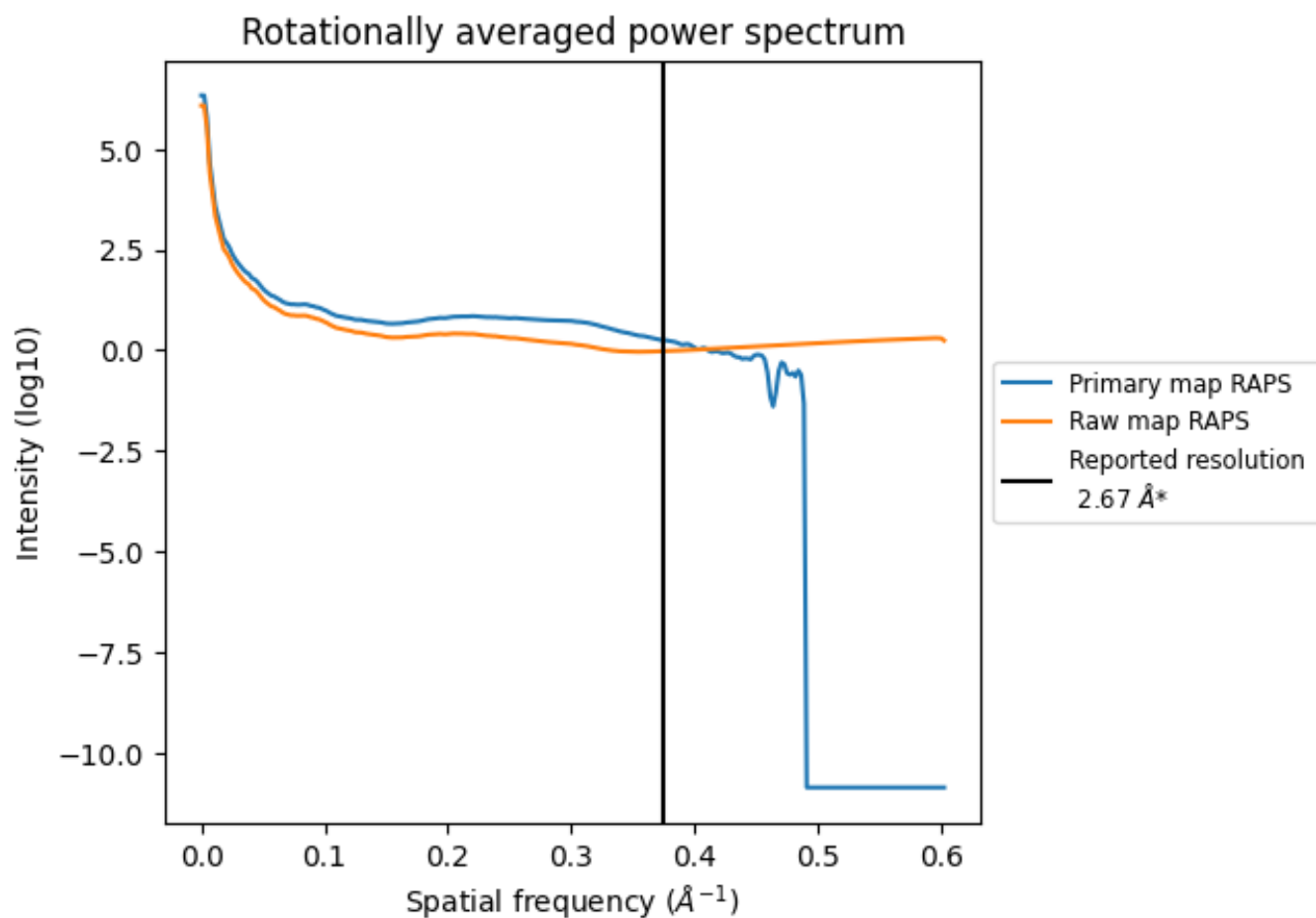
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 889 nm^3 ; this corresponds to an approximate mass of 803 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](#)

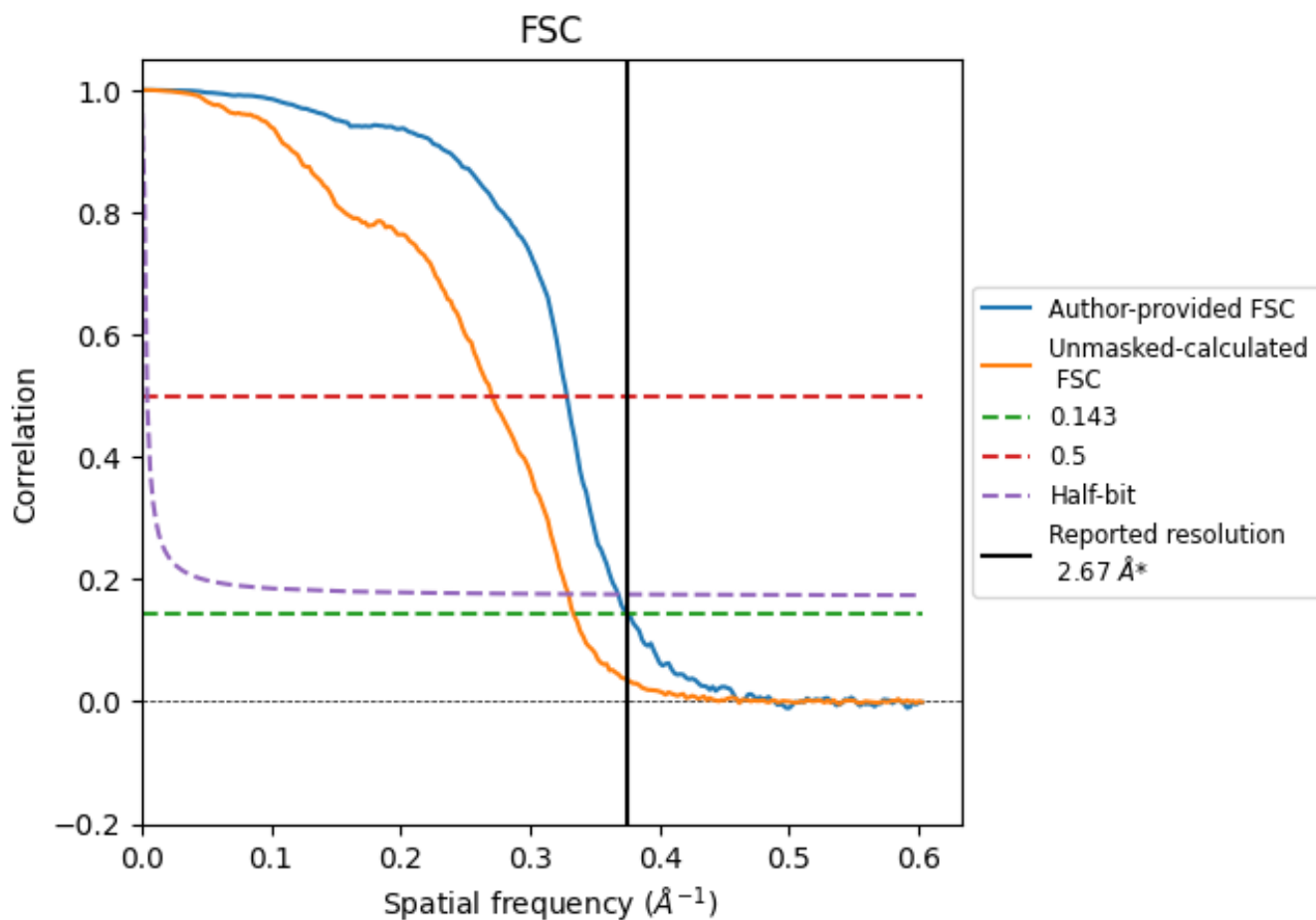


*Reported resolution corresponds to spatial frequency of 0.375 Å⁻¹

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 0.375 Å⁻¹

8.2 Resolution estimates [i](#)

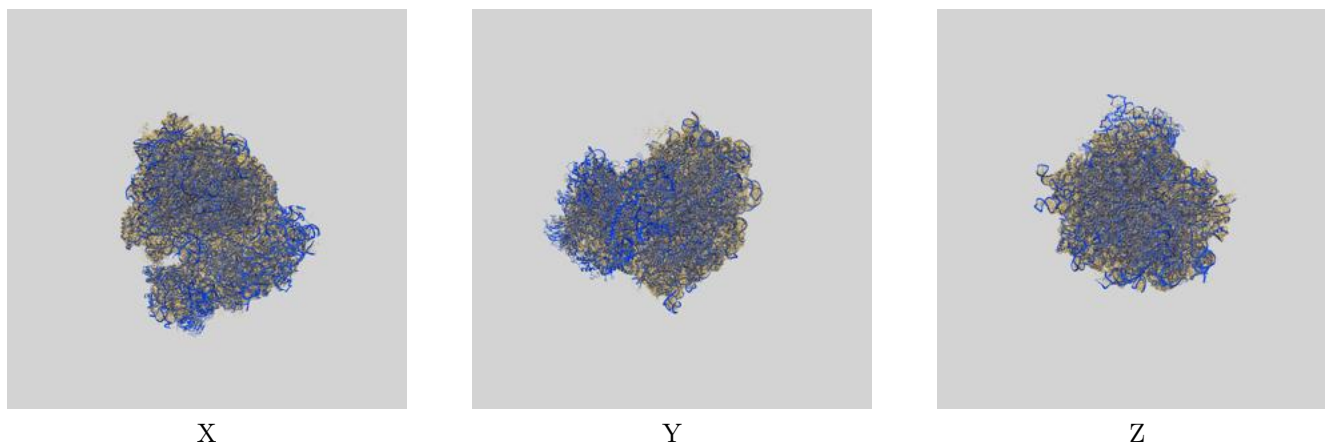
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.66	3.05	2.72
Unmasked-calculated*	3.00	3.70	3.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 2.67 by more than 10 %

9 Map-model fit [i](#)

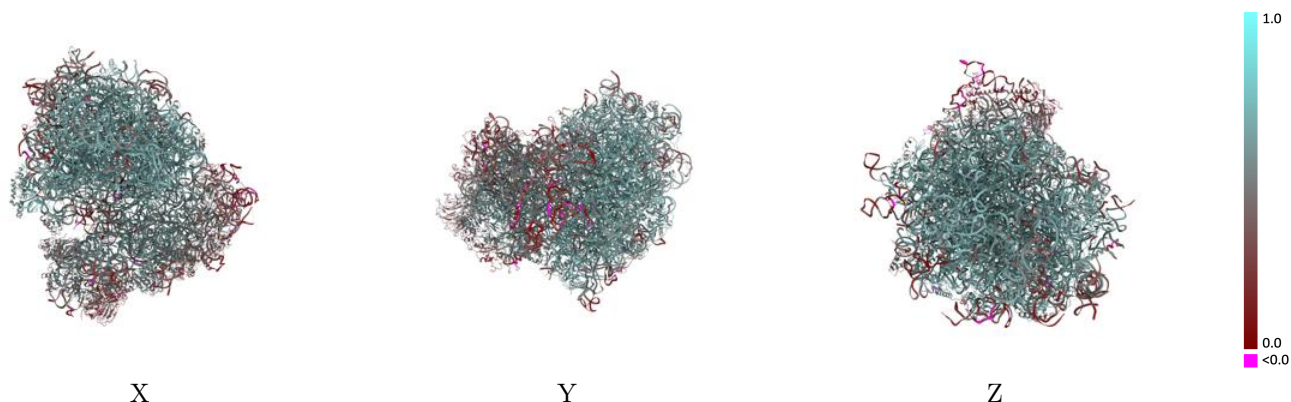
This section contains information regarding the fit between EMDB map EMD-36181 and PDB model 8JDM. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



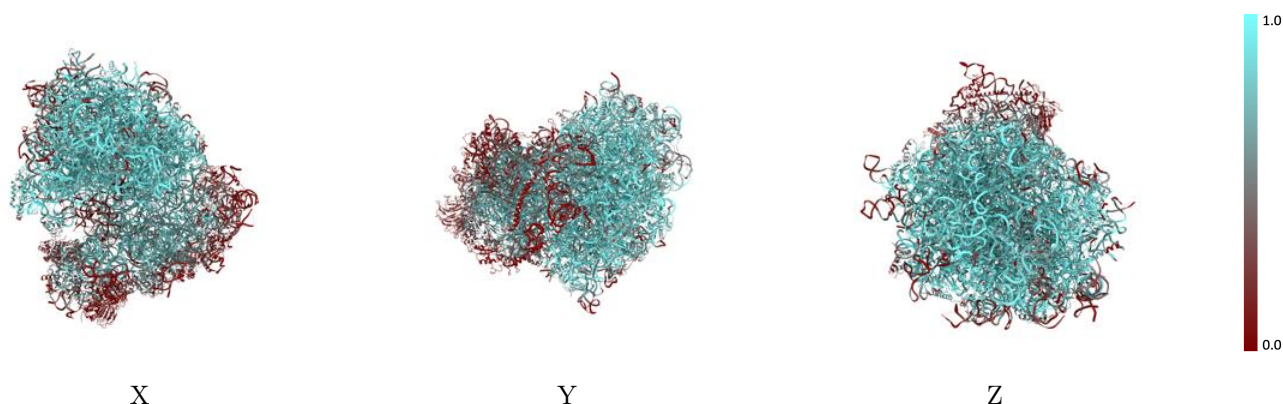
The images above show the 3D surface view of the map at the recommended contour level 0.0183 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



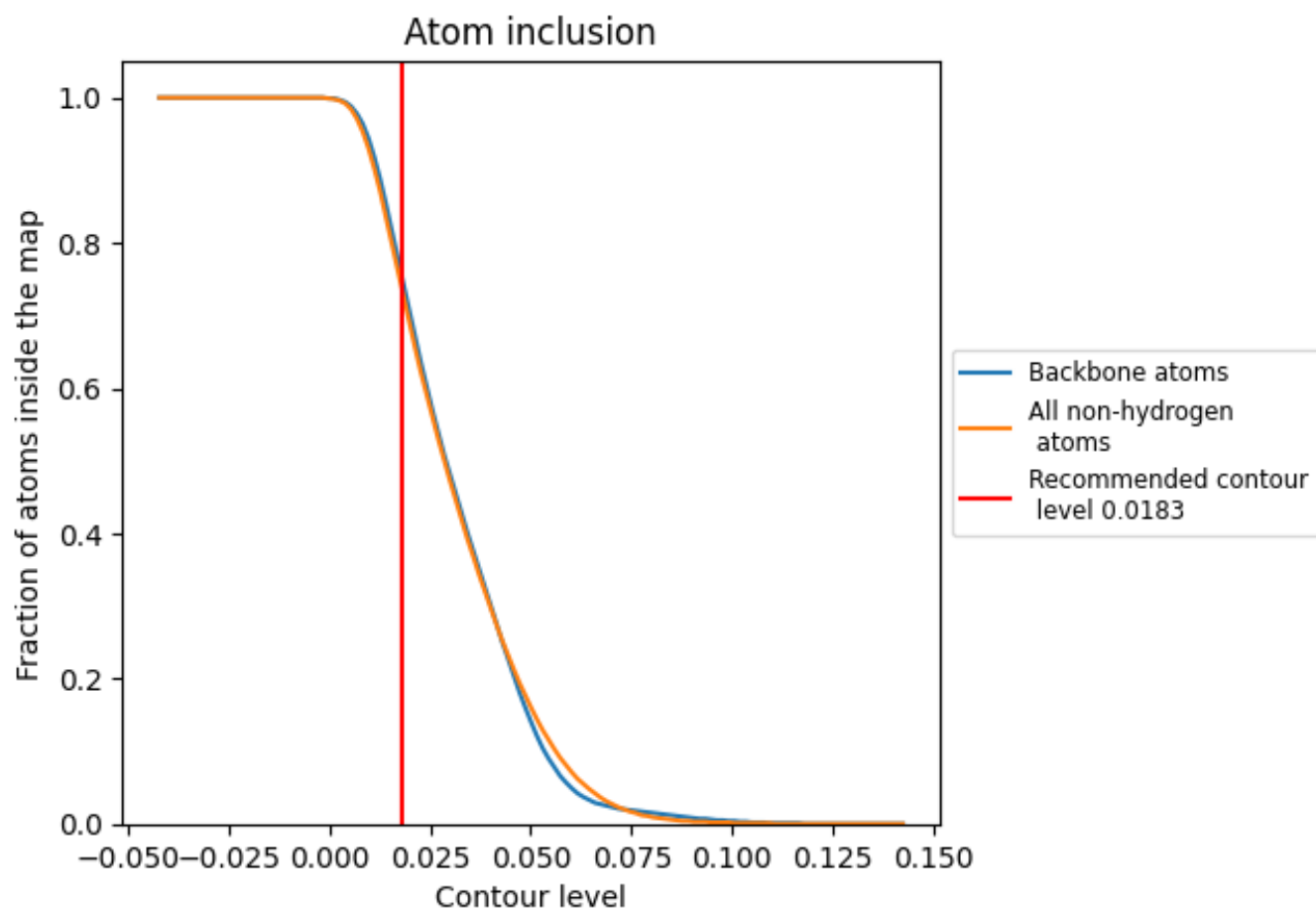
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0183).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0183) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.5570
0	 0.2850	 0.4030
1	 0.2820	 0.4000
2	 0.3330	 0.4450
3	 0.1340	 0.2970
4	 0.1880	 0.3550
5	 0.2830	 0.3820
6	 0.3140	 0.4030
7	 0.1250	 0.3230
8	 0.5370	 0.5070
9	 0.5530	 0.5220
A	 0.6390	 0.4810
AA	 0.6000	 0.5160
AB	 0.3450	 0.4440
AC	 0.3380	 0.4510
AD	 0.2440	 0.3960
AE	 0.3440	 0.4500
AF	 0.3400	 0.4600
AG	 0.2430	 0.3470
AH	 0.4820	 0.5120
AI	 0.6960	 0.5720
AJ	 0.6390	 0.5460
AK	 0.1460	 0.3490
AL	 0.1360	 0.3880
AM	 0.6730	 0.5470
AN	 0.3770	 0.4270
AO	 0.2780	 0.4160
AP	 0.6050	 0.5410
AQ	 0.2670	 0.3780
AR	 0.0550	 0.2820
B	 0.4160	 0.3640
C	 0.2080	 0.3570
D	 0.8570	 0.5990
E	 0.9720	 0.6550
F	 0.9020	 0.6160











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Chain	Atom inclusion	Q-score
G	0.9470	0.6630
H	0.8740	0.6410
I	0.8890	0.6290
J	0.7820	0.5920
K	0.7550	0.5800
L	0.8980	0.6460
M	0.6930	0.5620
N	0.8040	0.6070
O	0.8480	0.6130
P	0.6540	0.5270
Q	0.7910	0.5920
R	0.8300	0.6060
S	0.9580	0.6670
T	0.9120	0.6530
U	0.8800	0.6420
V	0.9340	0.6560
W	0.7500	0.5740
X	0.9140	0.6490
Y	0.8550	0.6230
Z	0.5770	0.5140
a	0.8900	0.6460
b	0.8490	0.6200
c	0.8160	0.6050
d	0.8150	0.6020
e	0.7800	0.5940
f	0.9070	0.6490
g	0.7090	0.5380
h	0.7780	0.5940
i	0.8200	0.6110
j	0.9180	0.6600
k	0.9310	0.6540
l	0.8330	0.6120
m	0.8070	0.6050
n	0.7430	0.5910
o	0.9450	0.6600
p	0.6440	0.5400
q	0.9120	0.6390
r	0.8630	0.6290
s	0.8440	0.6250
t	0.7940	0.5960
u	0.8840	0.6480
v	0.8860	0.6240

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Chain	Atom inclusion	Q-score
w	 0.6900	 0.5140
x	 0.4430	 0.5020
y	 0.4980	 0.5220
z	 0.6020	 0.5380