



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 07:06 PM JST

PDB ID : 8JDK / pdb_00008jdk
EMDB ID : EMD-36179
Title : Structure of the Human cytoplasmic Ribosome with human tRNA
Asp(ManQ34) and mRNA(GAU)
Authors : Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.
Deposited on : 2023-05-14
Resolution : 2.26 Å(reported)
Based on initial model : 6Y0G

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

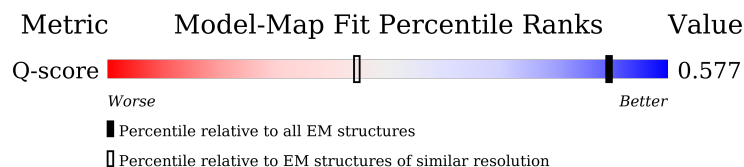
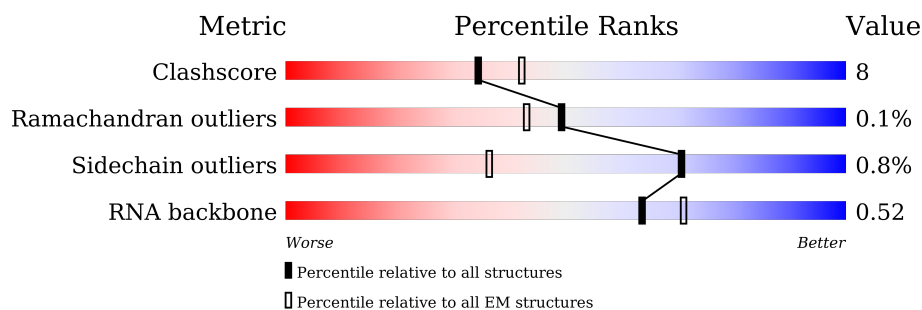
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.26 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.



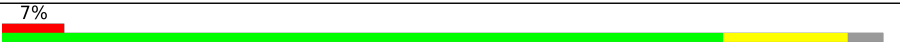
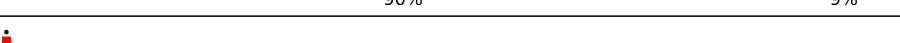
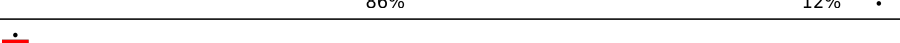
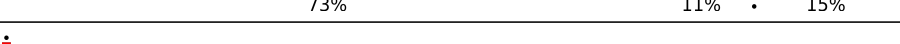
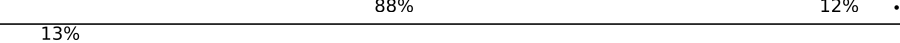
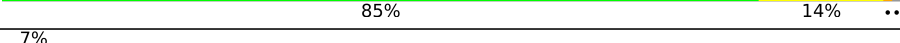
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3535 (1.76 - 2.76)

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	75	
2	C	75	

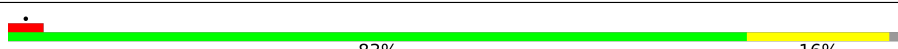
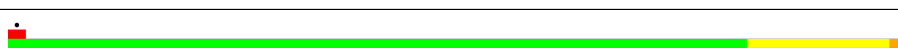
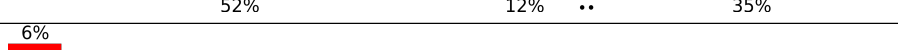
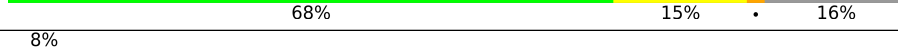
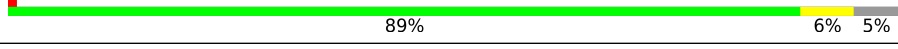
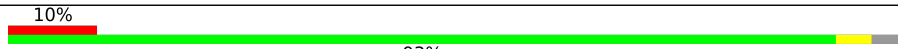
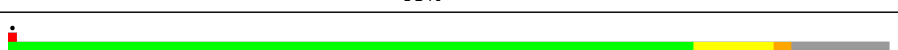
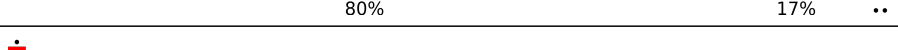
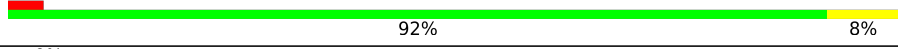
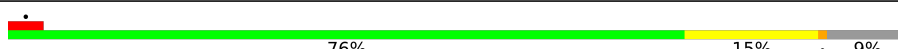
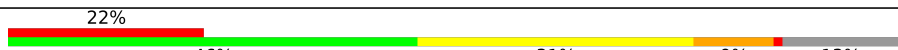
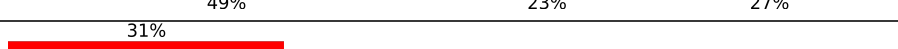
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Mol	Chain	Length	Quality of chain
3	D	5070	
4	E	120	
5	F	156	
6	G	257	
7	H	403	
8	I	427	
9	J	297	
10	K	288	
11	L	248	
12	M	266	
13	N	192	
14	O	214	
15	P	178	
16	Q	211	
17	R	215	
18	S	204	
19	T	203	
20	U	184	
21	V	188	
22	W	196	
23	X	176	
24	Y	160	
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	
54	2	204	
55	3	249	
56	4	194	
57	5	208	
58	6	194	
59	7	165	
60	8	158	
61	9	151	
62	AA	151	
63	AB	145	
64	AC	146	
65	AD	135	
66	AE	152	
67	AF	145	
68	AG	119	
69	AH	83	
70	AI	130	
71	AJ	143	
72	AK	133	
73	AL	125	
74	AM	115	
75	AN	84	
76	AO	69	
77	AP	56	

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Mol	Chain	Length	Quality of chain
78	AQ	59	85% 71% 24% • •
79	AR	317	98% 53% 45% ••

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 209567 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
1	A	14	Total	C	N	O	P	0	0
			303	135	55	99	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	75	Total	C	N	O	P	0	0
			1612	726	283	529	74		
2	C	75	Total	C	N	O	P	0	0
			1612	726	283	529	74		

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

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

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

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

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

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

- 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
20	U	157	Total	C	N	O	S	0	0
			1273	797	246	221	9		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

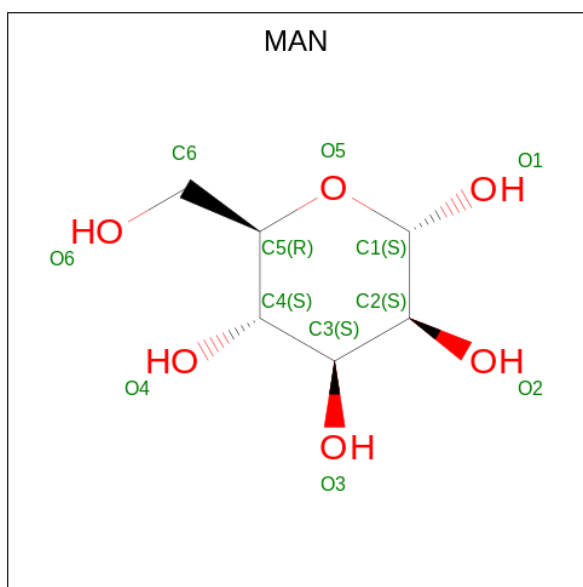
Mol	Chain	Residues	Atoms		AltConf
80	A	1	Total	Mg	0
			1	1	
80	D	397	Total	Mg	0
			397	397	
80	E	10	Total	Mg	0
			10	10	
80	F	7	Total	Mg	0
			7	7	
80	G	2	Total	Mg	0
			2	2	
80	H	2	Total	Mg	0
			2	2	
80	I	1	Total	Mg	0
			1	1	
80	N	1	Total	Mg	0
			1	1	
80	O	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
80	S	1	Total 1	Mg 1	0
80	U	2	Total 2	Mg 2	0
80	V	2	Total 2	Mg 2	0
80	X	1	Total 1	Mg 1	0
80	a	1	Total 1	Mg 1	0
80	g	1	Total 1	Mg 1	0
80	j	1	Total 1	Mg 1	0
80	k	1	Total 1	Mg 1	0
80	l	1	Total 1	Mg 1	0
80	u	1	Total 1	Mg 1	0
80	w	102	Total 102	Mg 102	0
80	2	1	Total 1	Mg 1	0
80	AF	1	Total 1	Mg 1	0
80	AM	1	Total 1	Mg 1	0

- Molecule 81 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



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

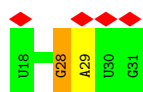
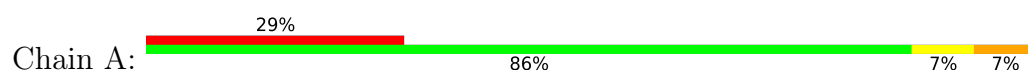
- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

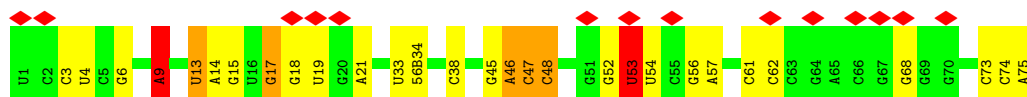
3 Residue-property plots [i](#)

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

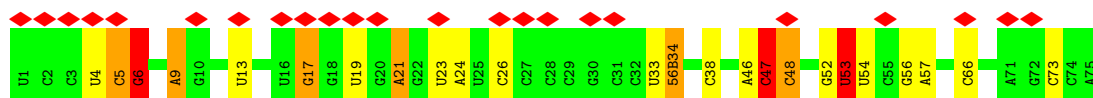
• Molecule 1: mRNA



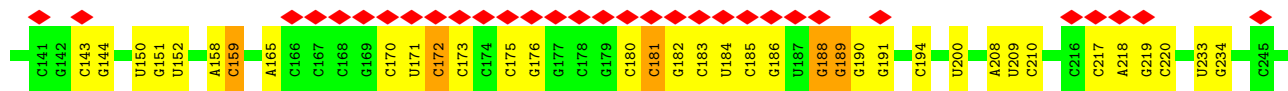
• Molecule 2: tRNA (Asp)



• Molecule 2: tRNA (Asp)



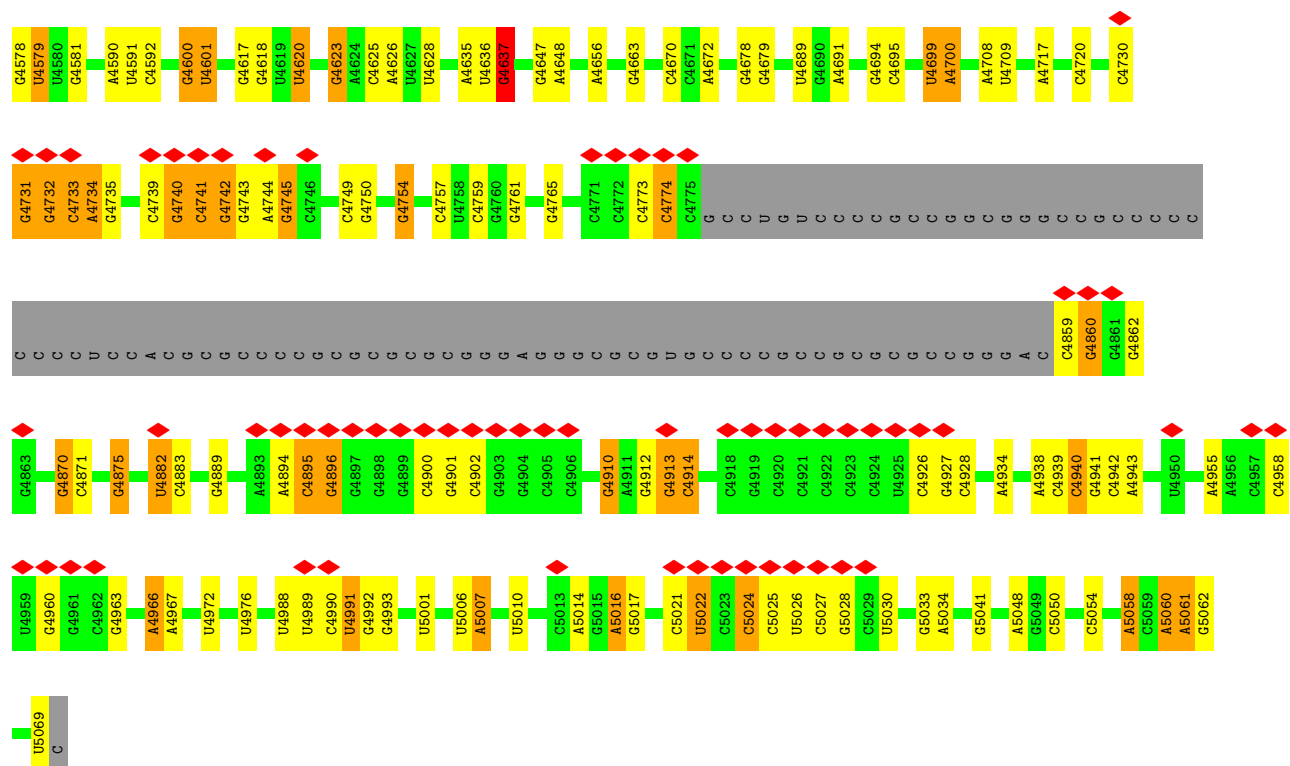
• Molecule 3: 28S ribosomal RNA



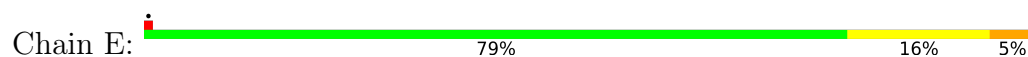




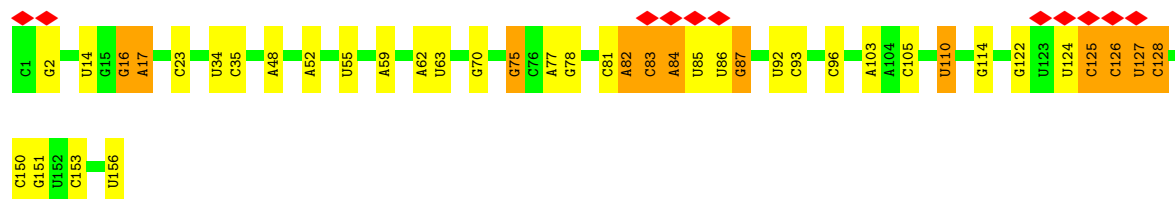
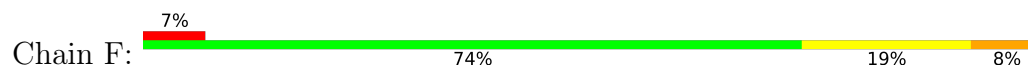




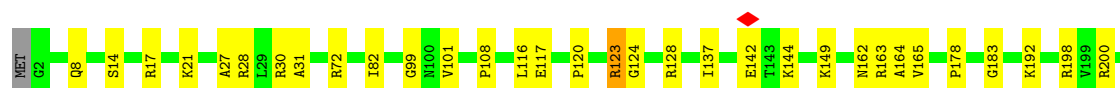
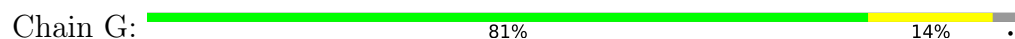
• Molecule 4: 5S ribosomal RNA



• Molecule 5: 5.8S ribosomal RNA

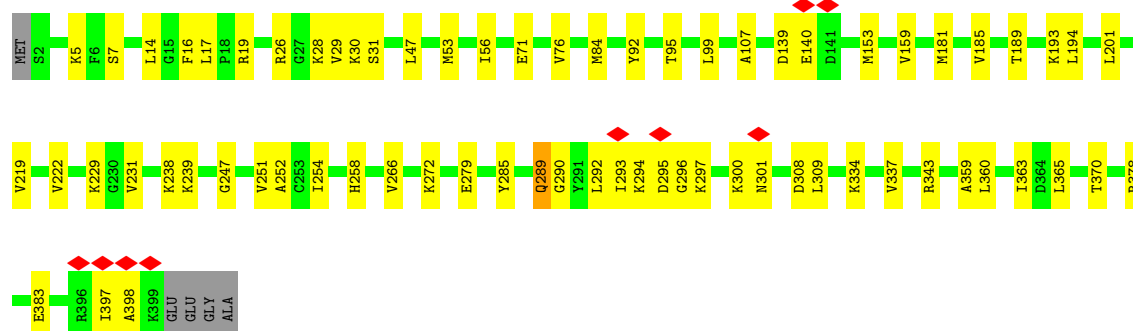


• Molecule 6: 60S ribosomal protein L8



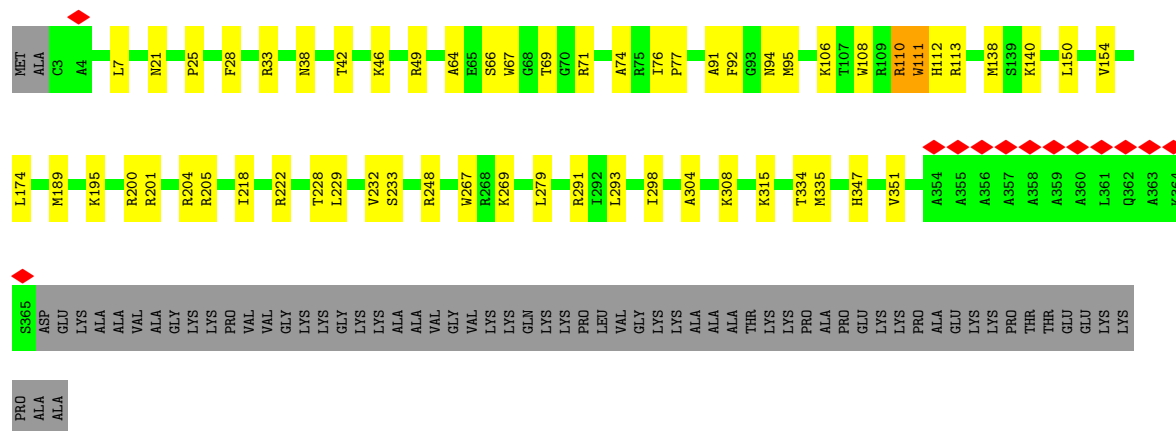
- Molecule 7: 60S ribosomal protein L3

Chain H: 81% 17%

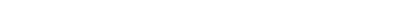


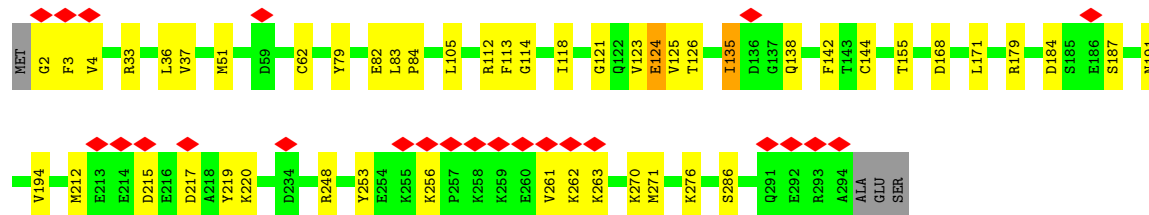
- Molecule 8: 60S ribosomal protein L4

Chain I: 71% 13% 15%

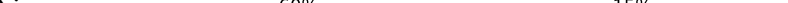


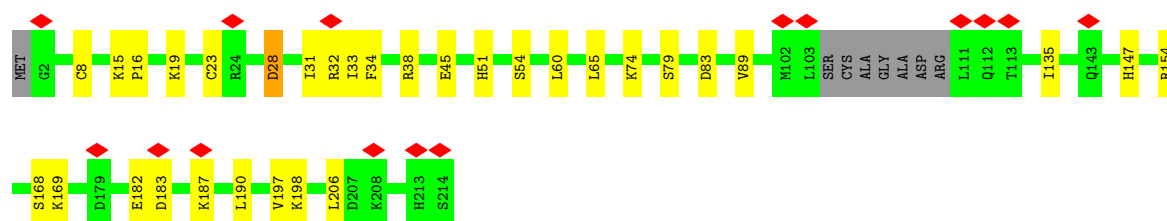
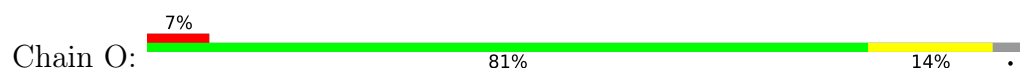
- Molecule 9: 60S ribosomal protein L5

Chain J:  8% 82% 16%

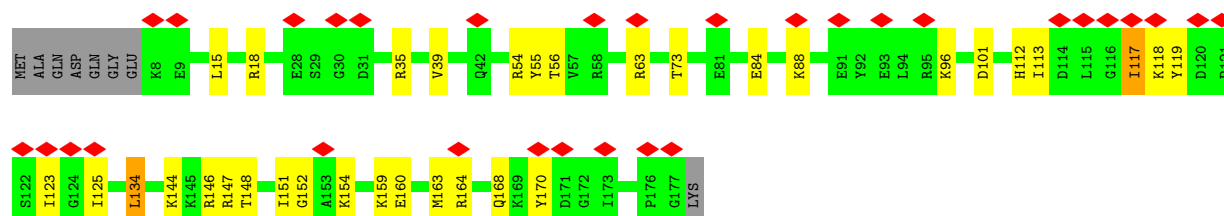
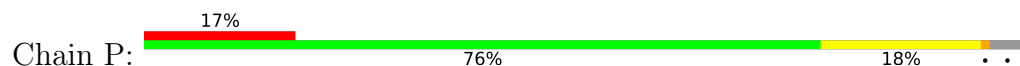


- Molecule 10: 60S ribosomal protein L6

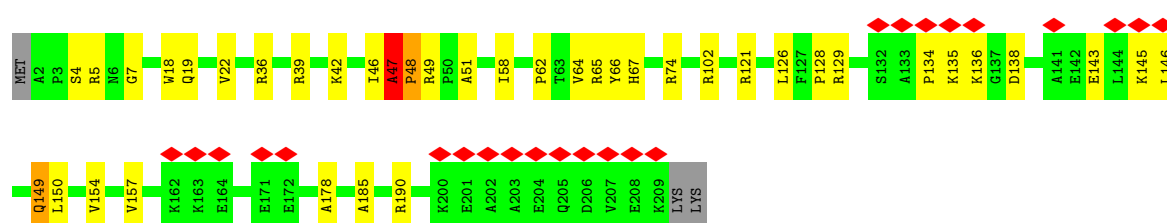
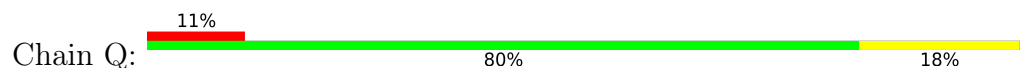
Chain K: 



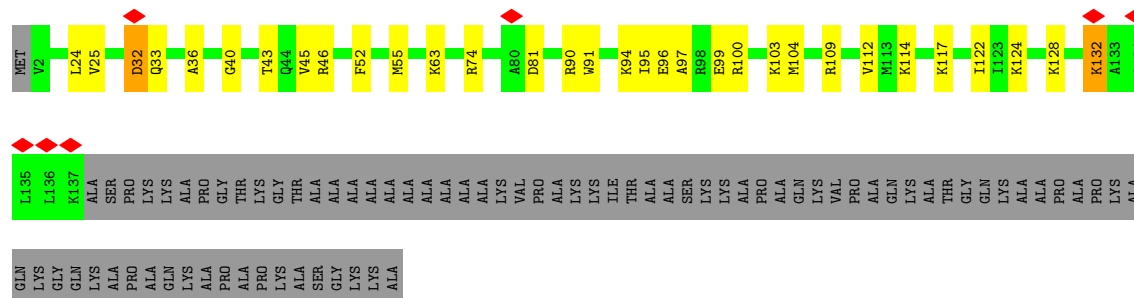
- Molecule 15: 60S ribosomal protein L11



- Molecule 16: 60S ribosomal protein L13



- Molecule 17: 60S ribosomal protein L14

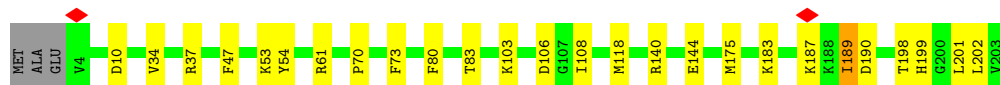
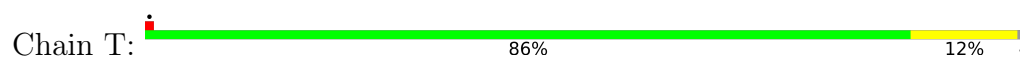


- Molecule 18: 60S ribosomal protein L15

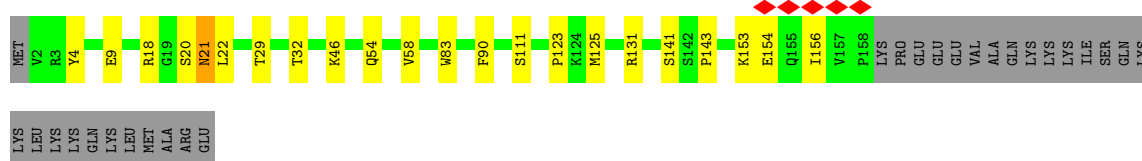




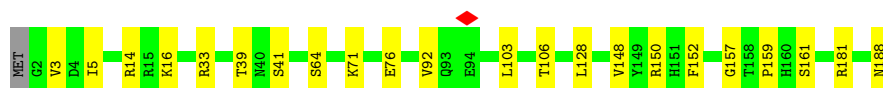
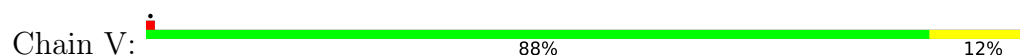
- Molecule 19: 60S ribosomal protein L13a



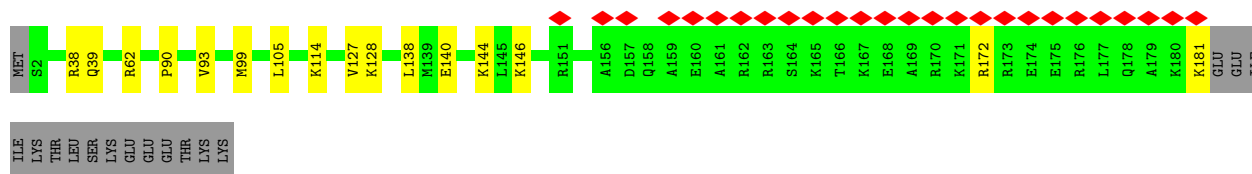
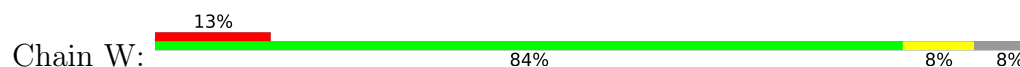
- Molecule 20: 60S ribosomal protein L17



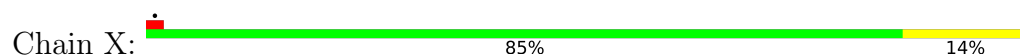
- Molecule 21: 60S ribosomal protein L18



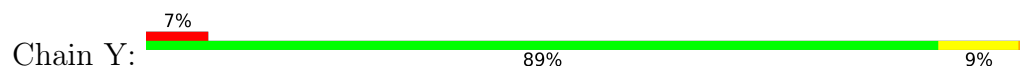
- Molecule 22: 60S ribosomal protein L19



- Molecule 23: 60S ribosomal protein L18a



- Molecule 24: 60S ribosomal protein L21



ILE
GLU
LYS
MET
GLN
GLU

- Molecule 30: 60S ribosomal protein L27

Chain e:  83% 16% .

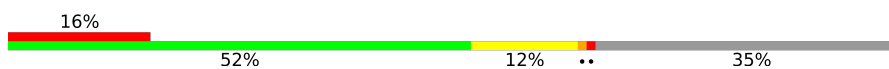


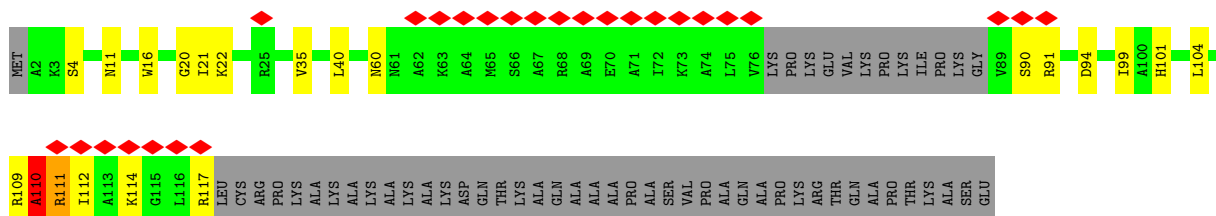
- Molecule 31: 60S ribosomal protein L27a

Chain f:  83% 16% ..



- Molecule 32: 60S ribosomal protein L29

Chain g:  16% 52% 12% .. 35%



- Molecule 33: 60S ribosomal protein L30

Chain h:  6% 68% 15% . 16%



- Molecule 34: 60S ribosomal protein L31

Chain i:  8% 74% 11% 14%

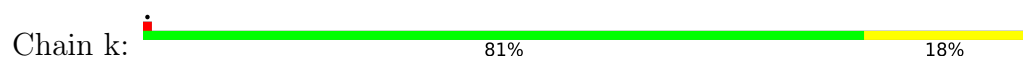


- Molecule 35: 60S ribosomal protein L32

Chain j:  89% 6% 5%



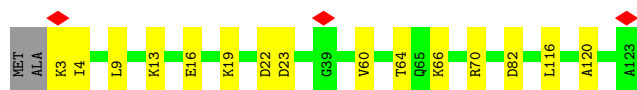
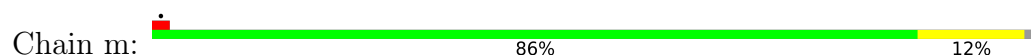
- Molecule 36: 60S ribosomal protein L35a



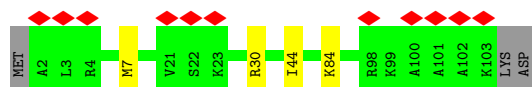
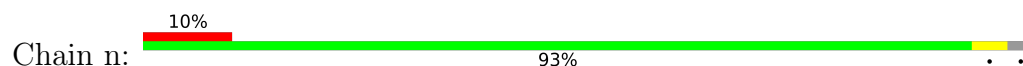
- Molecule 37: 60S ribosomal protein L34



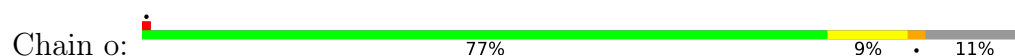
- Molecule 38: 60S ribosomal protein L35



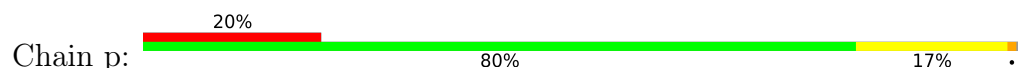
- Molecule 39: 60S ribosomal protein L36



- Molecule 40: 60S ribosomal protein L37



- Molecule 41: 60S ribosomal protein L38



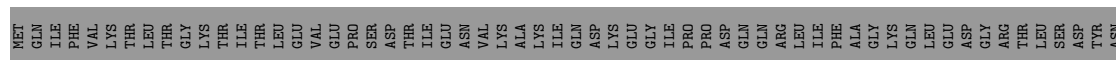
- Molecule 42: 60S ribosomal protein L39

Chain q:  75% 22%



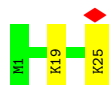
- Molecule 43: Ubiquitin-60S ribosomal protein L40

Chain r:  33% 8% 59%



- Molecule 44: 60S ribosomal protein L41

Chain s:  92% 8%



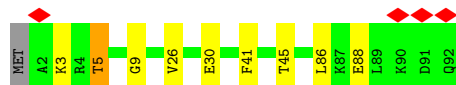
- Molecule 45: 60S ribosomal protein L36a

Chain t:  9% 77% 22%



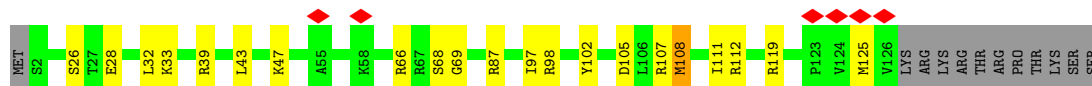
- Molecule 46: 60S ribosomal protein L37a

Chain u:  89% 9%



- Molecule 47: 60S ribosomal protein L28

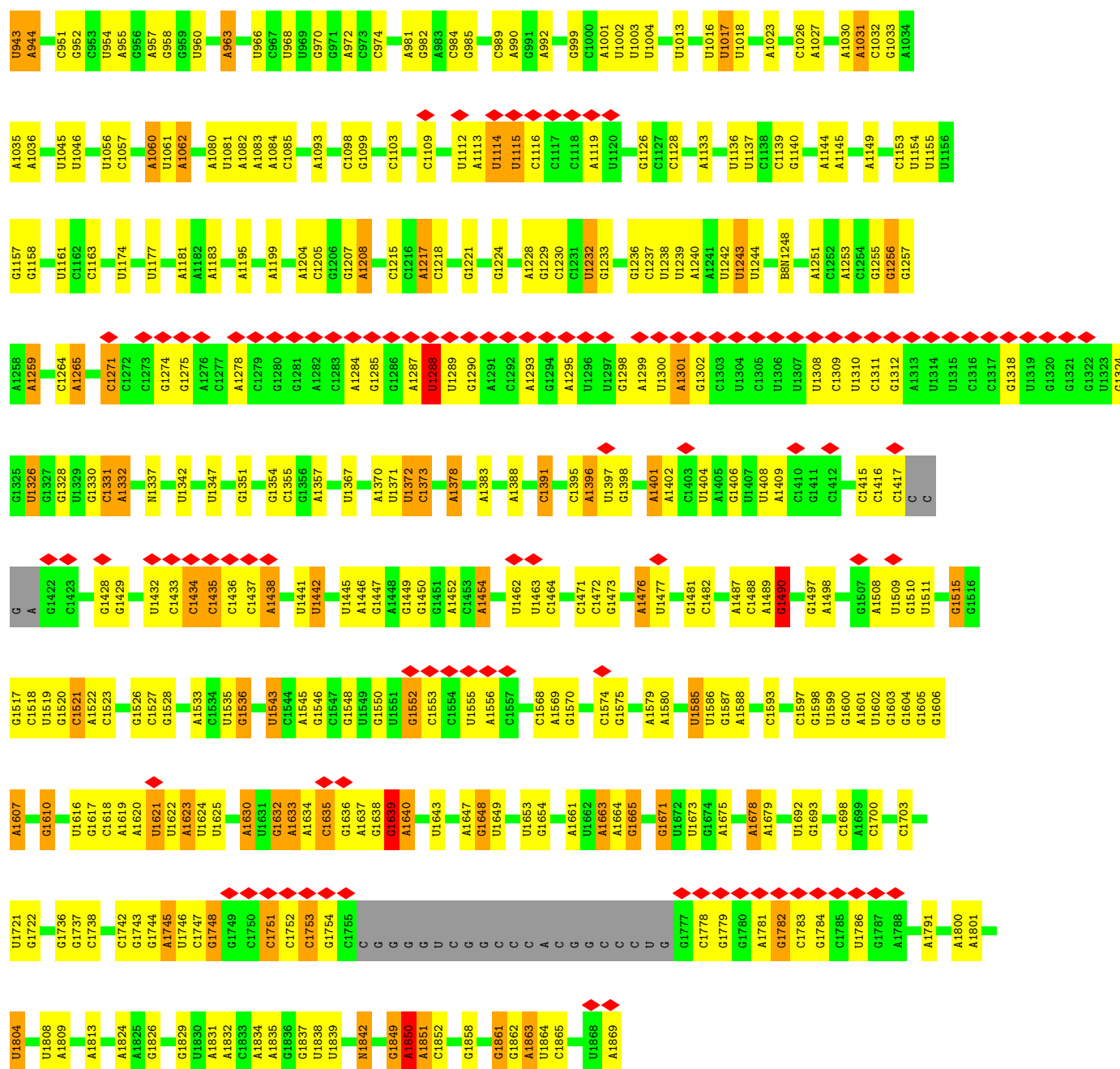
Chain v:  76% 15% 9%



- Molecule 48: 18S ribosomal RNA

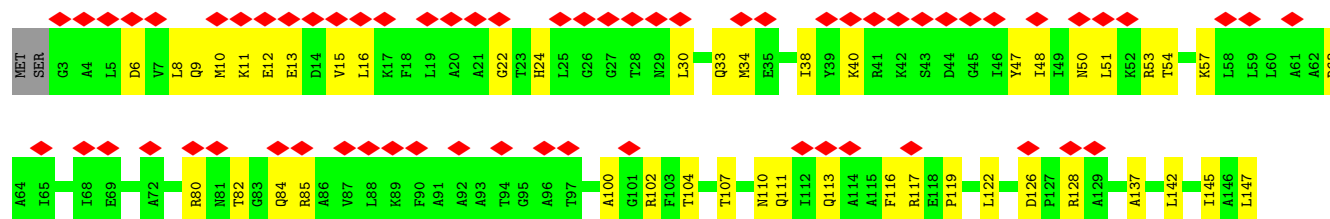
Chain w:  22% 46% 31% 9% 13%



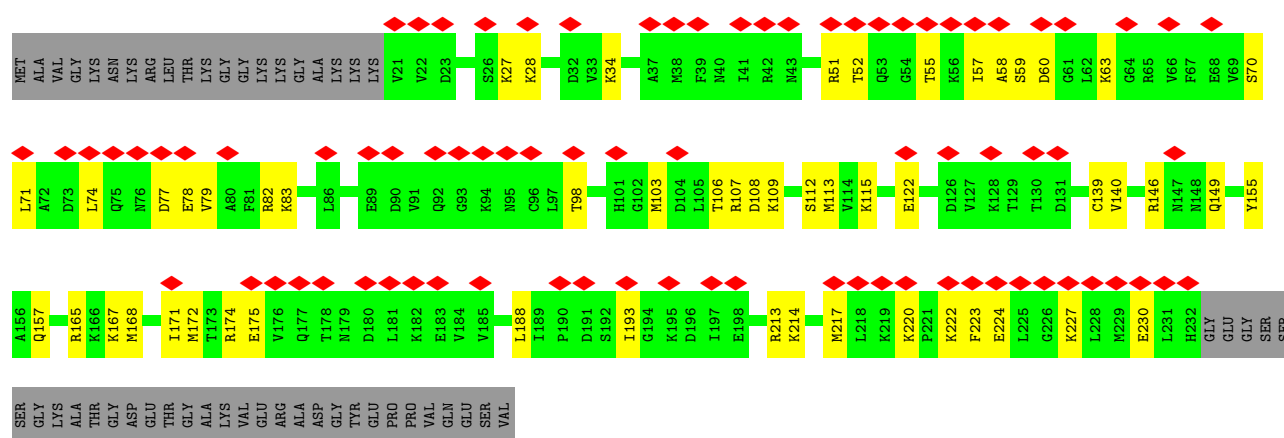


• Molecule 49: 40S ribosomal protein SA

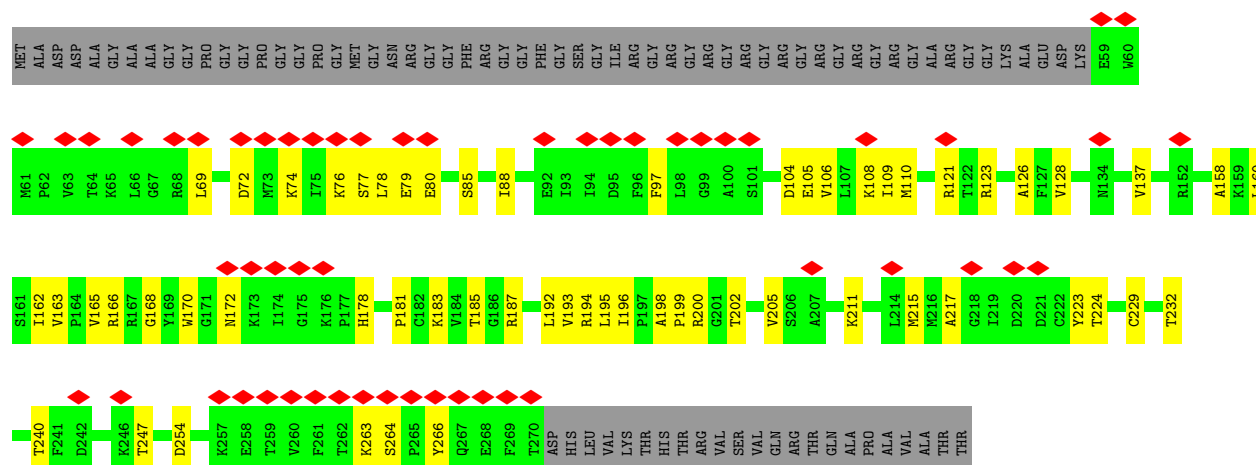
Chain x:



- Molecule 50: 40S ribosomal protein S3a



- Molecule 51: 40S ribosomal protein S2

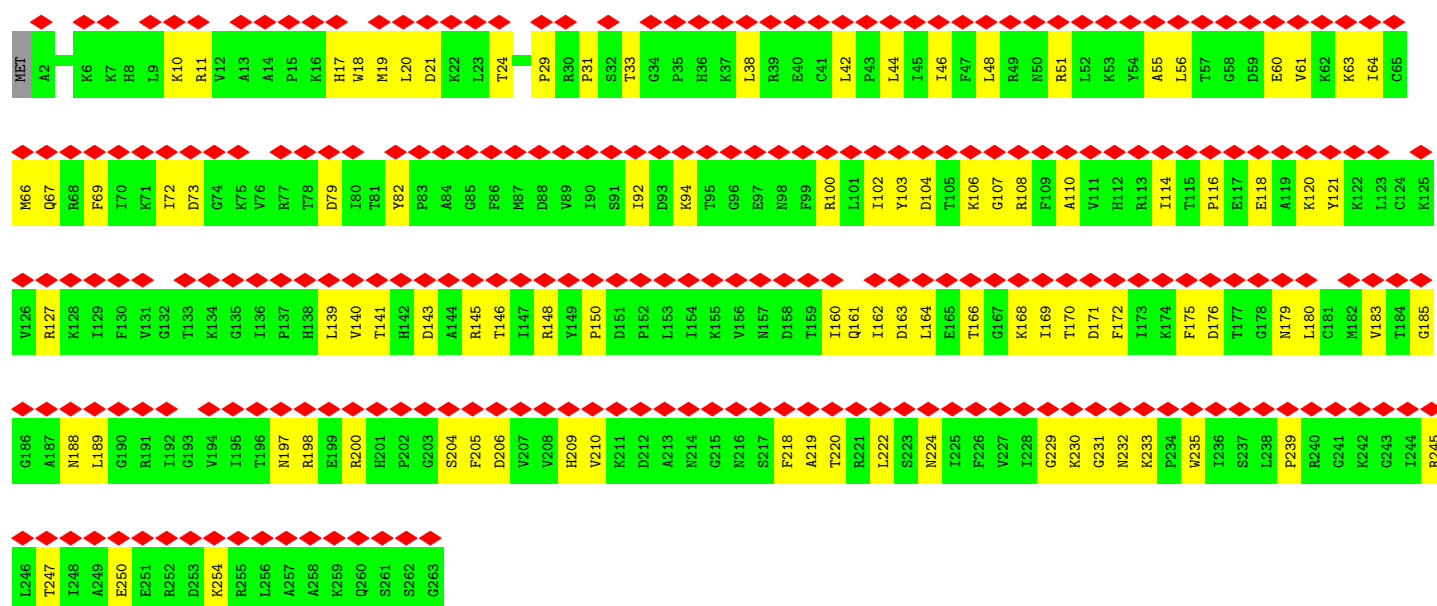
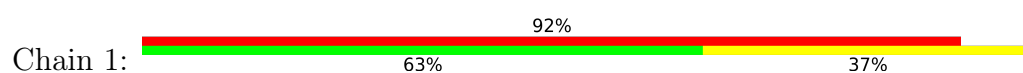


- Molecule 52: 40S ribosomal protein S3

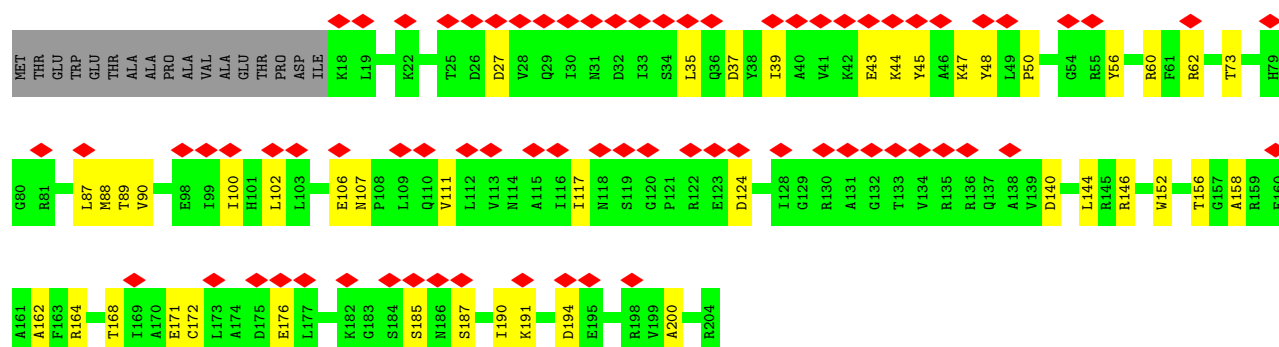
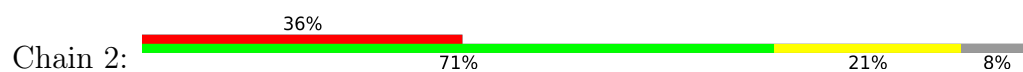




• Molecule 53: 40S ribosomal protein S4, X isoform



• Molecule 54: 40S ribosomal protein S5



Chain 3:

R183	G123	F61	M1
V184	L124	P62	K2
L185	T125	M63	L3
Q186	D126	N64	N4
H187	T127	Q65	I5
K188	T128	G66	S6
R189	V129	V67	F7
R190	P130	L68	P8
R191	R131	T69	A9
I192	R132	H70	T10
A193	L133	G71	G11
L194	G134	R72	C12
K195	P135	V73	Q13
K196	K136	L76	K14
Q197	R137	L77	L15
R198	A138	S78	I16
T199	S139	K79	E17
K200	R140	G80	V18
K201	I141	H81	D19
N202	R142	S82	D20
K203	K143	C83	R22
E204	L144	Y84	K23
E205	F145	R85	L24
A206	N146	P86	R25
A207	L147	R87	T26
E208	S148	R88	F27
Y209	K149	E91	Y28
A210	E150	R92	E29
K211	D151	K93	K30
L212	D152	E94	R31
L213	V153	K96	M32
A214	R154	S96	A33
K215	Q155	V97	T34
R216	Y156	R98	E35
N217	V157	G99	V36
K218	V158	C100	A37
E219	R159	I101	A38
A220	K160	V102	D39
K221	P161	D103	A40
E222	L162	A104	L41
K223	N163	N105	Q42
R224	K164	L106	E43
Q225	E165	S107	E44
E226	G166	V108	W45
Q227	K167	L109	K46
T228	K168	N110	G47
A229	P169	L111	Y48
K230	R170	V112	V49
R231	T171	I113	V50
R232	K172	V114	R51
R233	A173	K115	I52
L234	P174	K116	S53
S235	K175	G117	G54
S236	I176	E118	G55
L237	Q177	K119	N56
ARG	R178	I121	D120
ALA	L179	P122	D57
SER	V180		K58
THR	T181		Q59
SER			G60

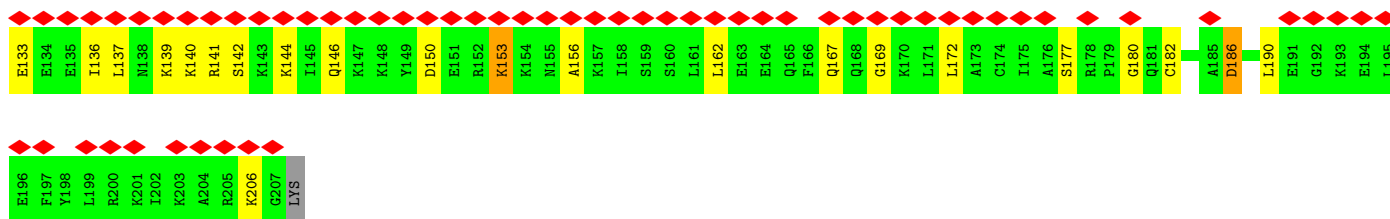
Chain 4:

Amino Acid
MET
PHE
SER
SER
SER
SER
ALA
K7
I8
V9
K10
P11
N12
G13
E14
K15
P16
D17
E18
F19
E20
S21
G22
I23
S24
Q25
A26
L27
L28
E29
L30
E31
M32
N33
S34
D35
L36
K37
A38
Q39
L40
R41
E42
L43
N44
I45
T46
A47
A48
K49
E50
I51
E52
V53
G54
G55
G56
R57
K58
A59
I60
I61
I62
F63
V64
P65
V66
P67
Q68
L69
K70
S71
F72
Q73
K74
I75
Q76
V77
R78
L79
V80
R81
E82
L83
E84
K85
K86
F87
S88
G89
K90
H91
V92
V93
F94
I95
A96
Q97
R98
R99
I100
L101
P102
K103
P104
T105
R106
K107
S108
R109
T110
K111
M112
K113
Q114
K115
R118
T121
T122
I123
A124
V125
H126
D127
A128
I129
L130
E131
D132
L133
V134
F135
P136
S137
E138
I139
V140
G141
K142
R143
I144
K147
L148
D149
G150
S151
R152
L153
I154
K155
V156
H157
L158
D159
K160
A161
Q162
Q163
M164
M165
V166
E167
H168
K169
V170
E171
T172
F173
S174
G175
V176
V177
K178
K179
L180
T181
G182
K183
D184
V185
M186
F187
E188
F189
P190
E191
F192
Q193
LEU

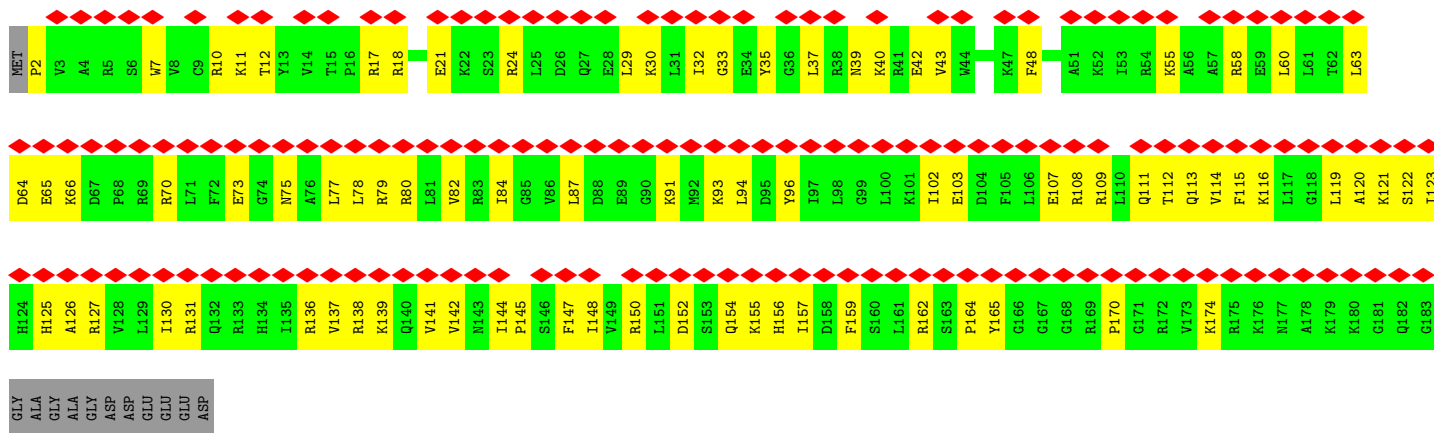
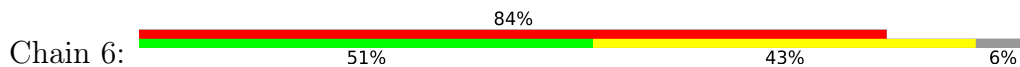
Chain 5:

63% 65% 33% ..

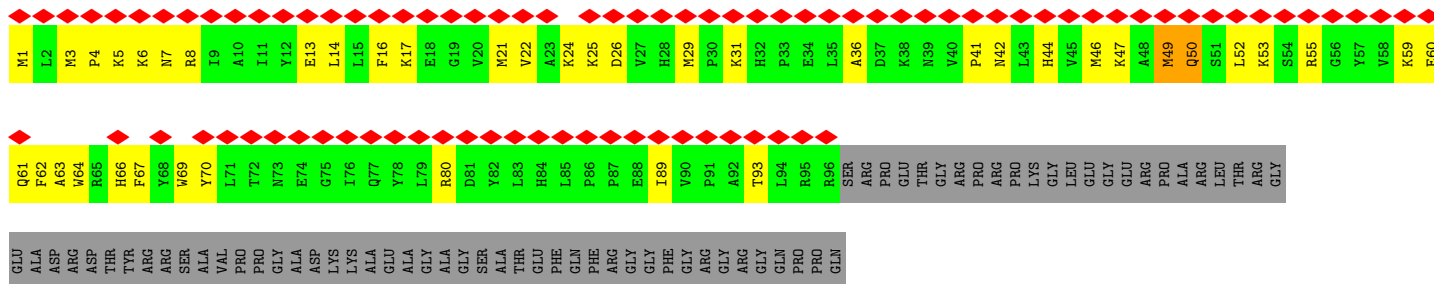
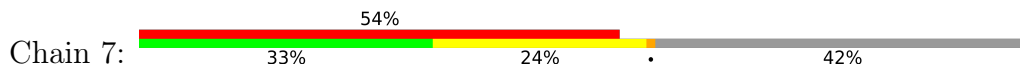
Chain 5: MET G2 I3 S4 R5 D6 N7 W8 H9 R10 R11 R12 R13 R14 T14 G15 G16 K19 P20 Y21 H22 K23 R24 R25 E28 A34 N35 T36 K37 T38 G39 P40 P41 R41 R42 R43 V46 R47 V48 R49 G50 G51 N52 N53 R56 A57 L58 R59 L60 D61 V62 G63 N64 F65 S66 A67 G68 S69 E70 C71 C72 T73 R74 K75 R76 R77 I78 R79 D80 D81 V81 V82 Y83 N84 A85 S86 N87 N88 E89 L90 L91 V91 R92 T93 K94 T95 L96 C100 I101 V102 L103 I104 D105 Y109 R110 Q111 W112 Y113 E114 S115 H116 Y117 A118 L119 P120 L121 G122 K123 K124 K125 G126 A127 K128 L129 T130 P131 L132



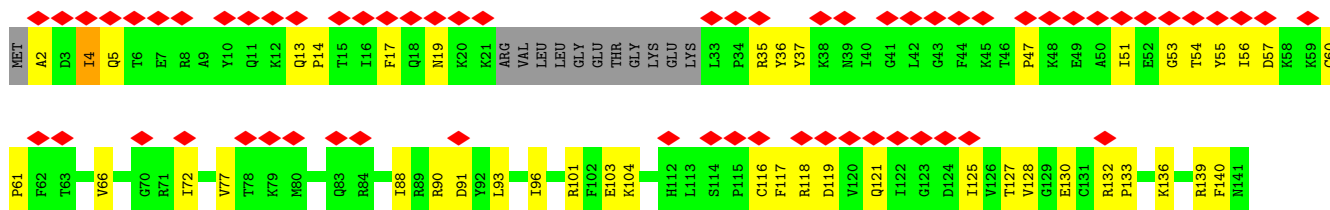
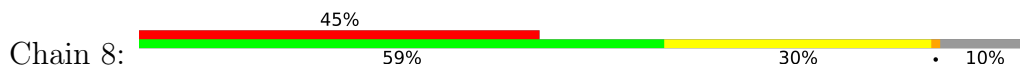
• Molecule 58: 40S ribosomal protein S9



• Molecule 59: 40S ribosomal protein S10

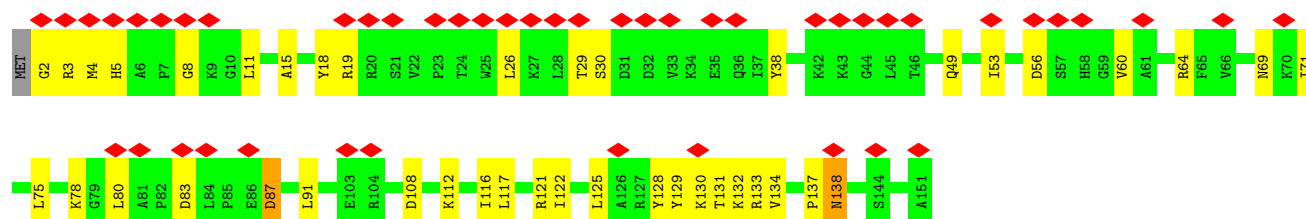


• Molecule 60: 40S ribosomal protein S11

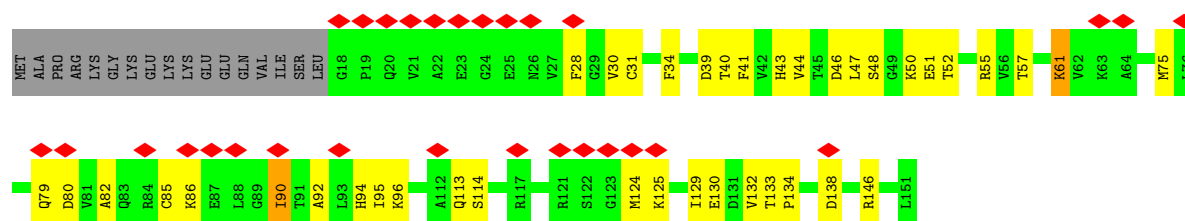




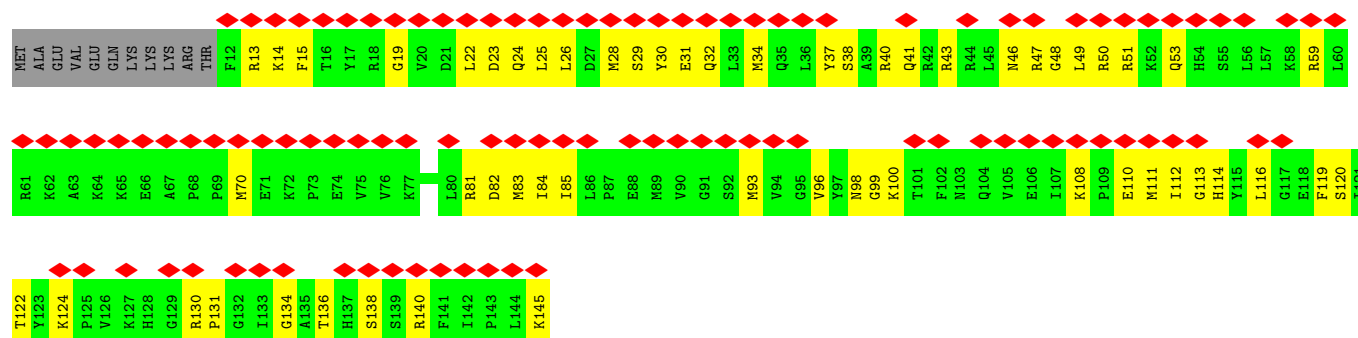
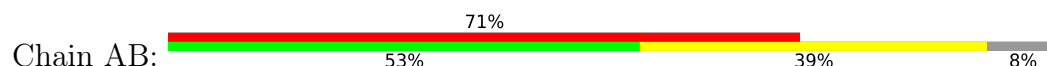
• Molecule 61: 40S ribosomal protein S13



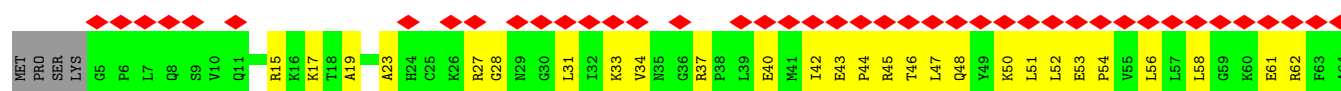
• Molecule 62: 40S ribosomal protein S14



• Molecule 63: 40S ribosomal protein S15

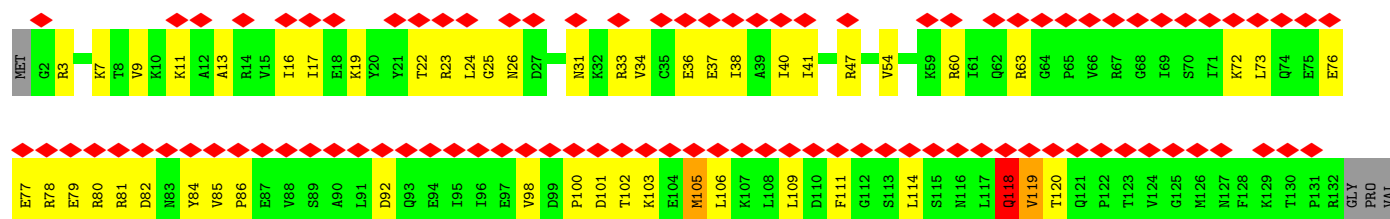
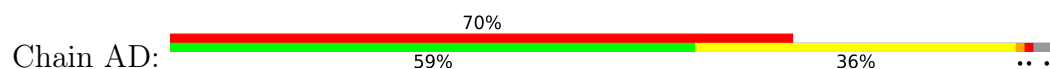


• Molecule 64: 40S ribosomal protein S16

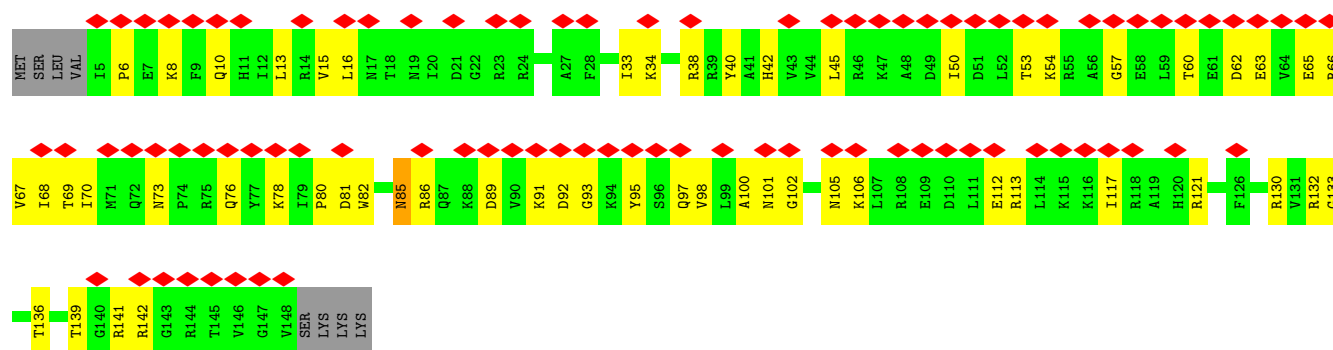




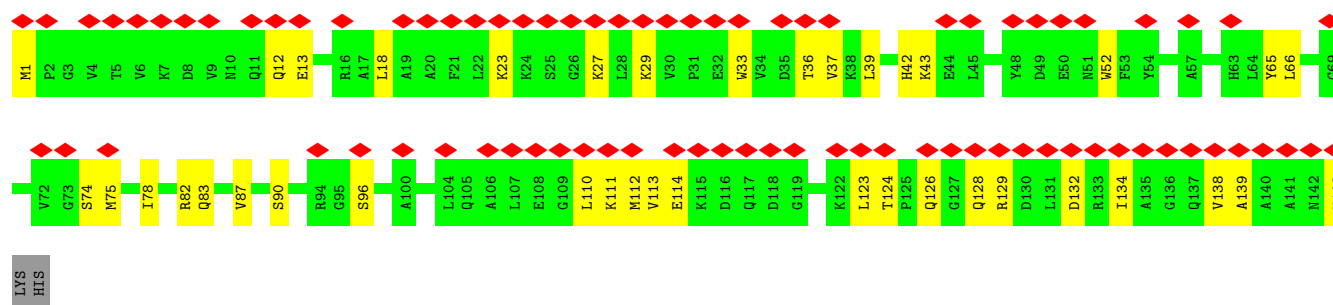
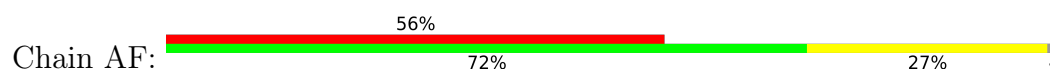
- Molecule 65: 40S ribosomal protein S17



- Molecule 66: 40S ribosomal protein S18

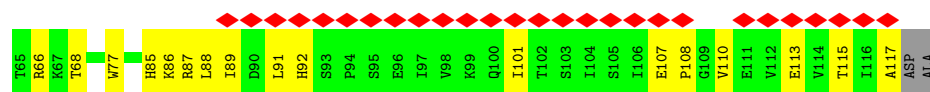


- Molecule 67: 40S ribosomal protein S19

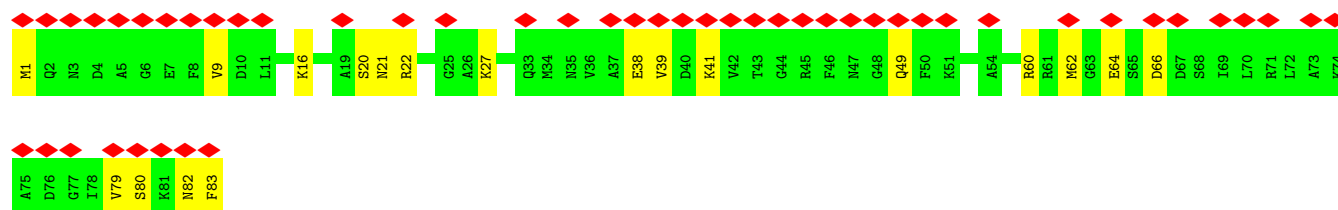
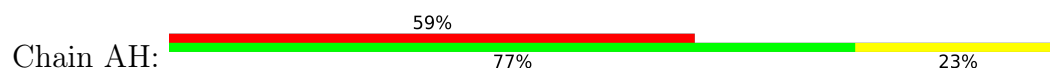


- Molecule 68: 40S ribosomal protein S20

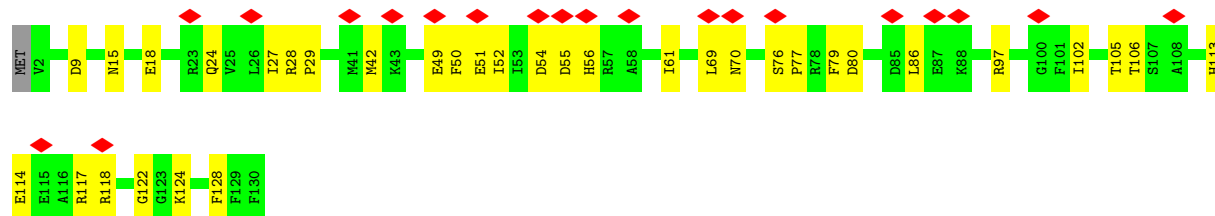
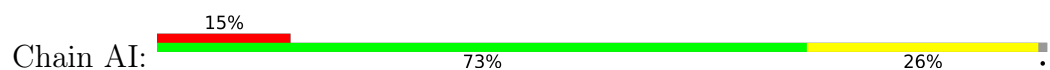




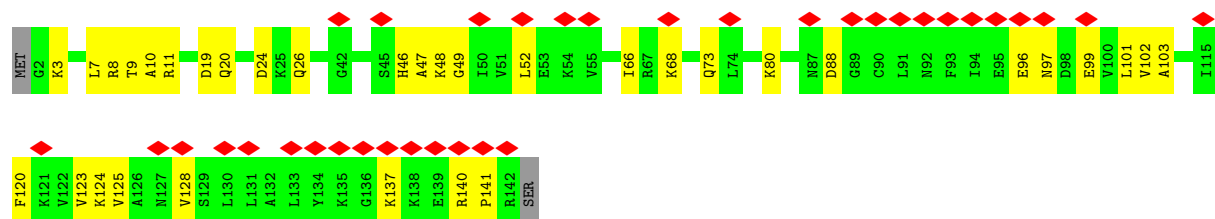
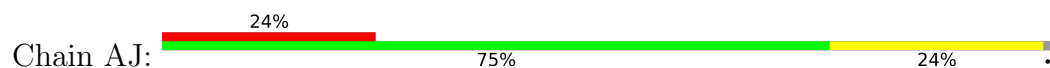
- Molecule 69: 40S ribosomal protein S21



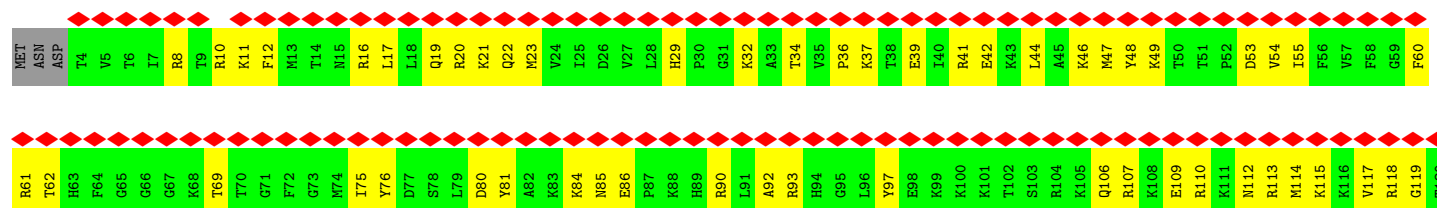
- Molecule 70: 40S ribosomal protein S15a

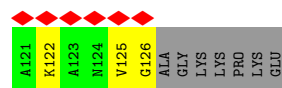


- Molecule 71: 40S ribosomal protein S23

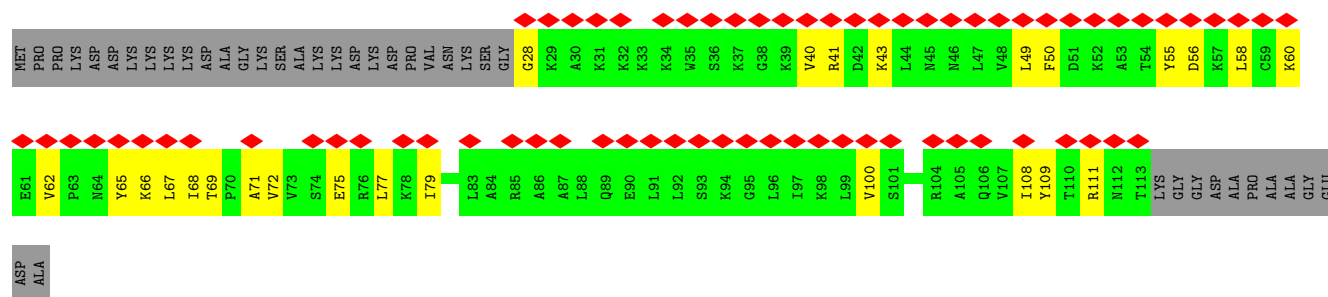


- Molecule 72: 40S ribosomal protein S24

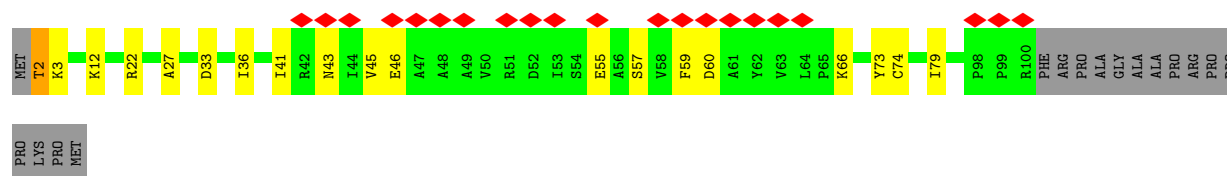
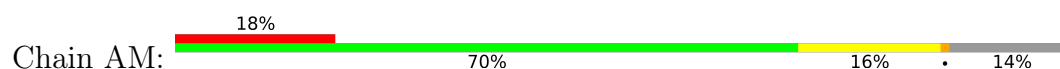




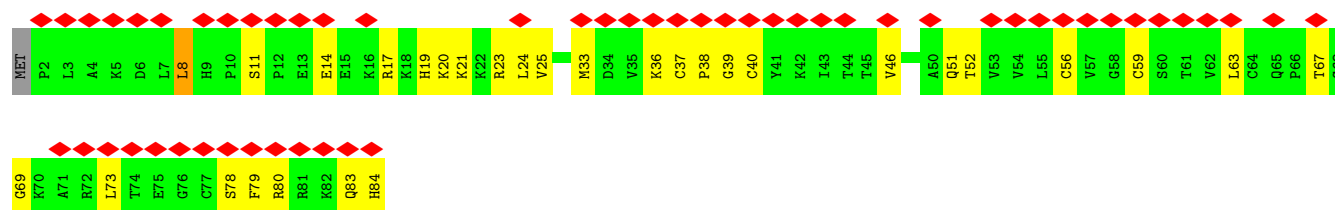
- Molecule 73: 40S ribosomal protein S25



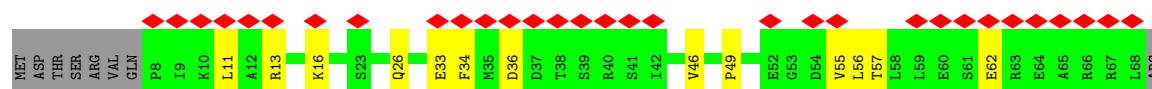
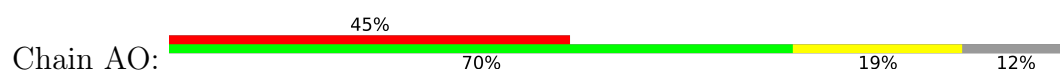
- Molecule 74: 40S ribosomal protein S26



- Molecule 75: 40S ribosomal protein S27

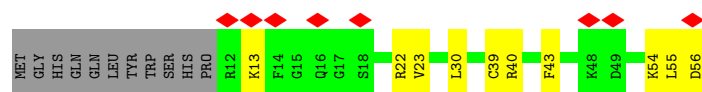


- Molecule 76: 40S ribosomal protein S28

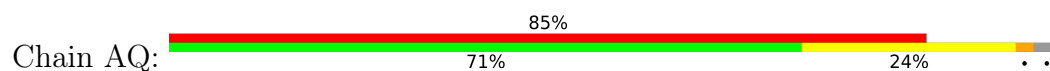


- Molecule 77: 40S ribosomal protein S29

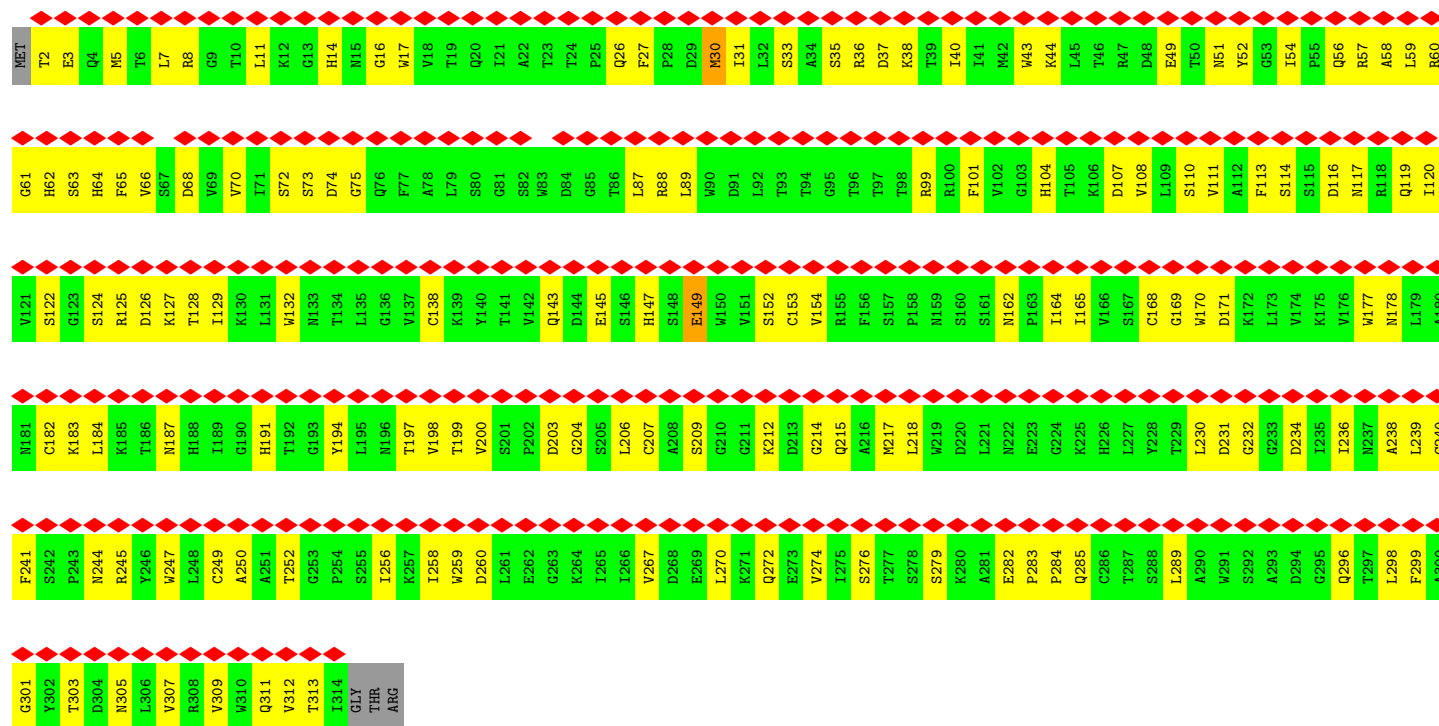




- Molecule 78: 40S ribosomal protein S30



- Molecule 79: Receptor of activated protein C kinase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224907	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	0.217	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0197	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: 5MC, UR3, PSU, 5MU, B8N, 6MZ, 2MG, 56B, H2U, MG, MA6, A2M, OMU, 4AC, OMG, OMC, UY1, MAN, ZN, G7M, 1MA

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	0.24	0/339	0.22	0/527
2	B	0.19	0/1525	0.21	0/2375
2	C	0.15	0/1525	0.21	0/2375
3	D	0.39	1/81567 (0.0%)	0.31	6/127232 (0.0%)
4	E	0.37	0/2858	0.27	0/4455
5	F	0.38	0/3675	0.29	0/5725
6	G	0.37	0/1929	0.51	0/2586
7	H	0.36	0/3279	0.48	0/4388
8	I	0.38	0/2938	0.48	0/3946
9	J	0.30	0/2425	0.45	0/3248
10	K	0.29	0/1785	0.48	0/2394
11	L	0.37	0/1905	0.46	0/2539
12	M	0.31	0/1863	0.49	2/2510 (0.1%)
13	N	0.30	0/1537	0.45	0/2066
14	O	0.29	0/1699	0.45	0/2270
15	P	0.24	0/1385	0.41	0/1852
16	Q	0.33	0/1713	0.46	0/2293
17	R	0.30	0/1142	0.43	0/1527
18	S	0.40	0/1746	0.45	0/2338
19	T	0.38	0/1673	0.47	0/2238
20	U	0.37	0/1300	0.47	0/1746
21	V	0.39	0/1537	0.52	0/2052
22	W	0.32	0/1524	0.44	0/2013
23	X	0.36	0/1493	0.44	0/2003
24	Y	0.34	0/1326	0.44	0/1770
25	Z	0.23	0/835	0.43	0/1122
26	a	0.34	0/993	0.46	0/1332
27	b	0.32	0/541	0.40	0/720
28	c	0.32	0/998	0.42	0/1340
29	d	0.35	0/1132	0.47	0/1504
30	e	0.31	0/1130	0.42	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.39	0/1191	0.46	0/1591
32	g	0.29	0/844	0.54	0/1115
33	h	0.30	0/765	0.39	0/1027
34	i	0.34	0/903	0.42	0/1216
35	j	0.38	0/1071	0.44	0/1429
36	k	0.39	0/895	0.55	0/1198
37	l	0.34	0/898	0.49	1/1197 (0.1%)
38	m	0.32	0/1018	0.38	0/1344
39	n	0.27	0/843	0.41	0/1115
40	o	0.39	0/720	0.52	0/952
41	p	0.27	0/575	0.47	0/761
42	q	0.36	0/454	0.47	0/599
43	r	0.25	0/435	0.43	0/575
44	s	0.34	0/240	0.46	0/305
45	t	0.34	0/876	0.52	0/1156
46	u	0.34	0/718	0.42	0/953
47	v	0.37	0/1017	0.48	0/1364
48	w	0.25	2/37158 (0.0%)	0.27	0/57908
49	x	0.21	0/1732	0.44	0/2355
50	y	0.19	0/1752	0.41	0/2345
51	z	0.20	0/1668	0.44	0/2254
52	0	0.18	0/1672	0.39	0/2250
53	1	0.15	0/2112	0.38	0/2842
54	2	0.19	0/1485	0.43	0/1998
55	3	0.15	0/1940	0.42	0/2583
56	4	0.17	0/1533	0.45	0/2053
57	5	0.16	0/1703	0.42	0/2275
58	6	0.19	0/1531	0.48	0/2045
59	7	0.19	0/834	0.46	0/1125
60	8	0.21	0/1170	0.49	2/1568 (0.1%)
61	9	0.21	0/1232	0.41	0/1656
62	AA	0.23	0/1015	0.51	0/1361
63	AB	0.18	0/1126	0.47	0/1505
64	AC	0.22	0/1146	0.51	0/1534
65	AD	0.29	0/1071	0.60	0/1438
66	AE	0.21	0/1187	0.55	0/1593
67	AF	0.20	0/1130	0.49	0/1515
68	AG	0.21	0/809	0.49	0/1087
69	AH	0.21	0/643	0.45	0/860
70	AI	0.25	0/1051	0.44	0/1406
71	AJ	0.19	0/1116	0.40	0/1490
72	AK	0.16	0/1019	0.44	0/1355
73	AL	0.18	0/688	0.42	0/921

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	AM	0.25	0/805	0.47	0/1079
75	AN	0.19	0/657	0.47	0/883
76	AO	0.20	0/481	0.56	0/643
77	AP	0.26	0/375	0.53	0/492
78	AQ	0.18	0/458	0.48	0/602
79	AR	0.17	0/2493	0.48	1/3394 (0.0%)
All	All	0.33	3/219572 (0.0%)	0.37	12/322305 (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
9	J	0	1
10	K	0	1
11	L	0	1
16	Q	0	1
17	R	0	1
20	U	0	1
21	V	0	1
24	Y	0	2
29	d	0	1
32	g	0	1
40	o	0	1
53	l	0	1
65	AD	0	1
78	AQ	0	1
79	AR	0	1
All	All	0	22

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	576	A2M	O3'-P	5.14	1.61	1.56
3	D	3785	A2M	O3'-P	5.07	1.61	1.56
48	w	484	A2M	O3'-P	5.05	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2101	C	OP1-P-OP2	-13.17	80.08	119.60
3	D	2100	A	OP2-P-O3'	-12.05	71.84	108.00
3	D	2101	C	O5'-P-OP1	-10.42	76.74	108.00
3	D	2100	A	OP1-P-O3'	9.24	135.72	108.00
3	D	2101	C	O5'-P-OP2	7.39	130.17	108.00
60	8	14	PRO	CA-N-CD	-6.50	102.90	112.00
60	8	4	ILE	N-CA-C	-5.67	108.33	113.71
79	AR	30	MET	CB-CG-SD	5.59	129.49	112.70
12	M	206	GLN	CA-CB-CG	5.46	125.03	114.10
3	D	2100	A	O3'-P-O5'	-5.41	95.88	104.00
37	l	53	LEU	N-CA-C	5.27	117.60	111.02
12	M	165	GLU	N-CA-C	-5.05	101.72	108.34

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	1	66	MET	Peptide
65	AD	118	GLN	Peptide
78	AQ	81	ARG	Peptide
79	AR	149	GLU	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
9	J	124	GLU	Peptide
10	K	130	LYS	Peptide
11	L	163	ASN	Peptide
16	Q	47	ALA	Peptide
17	R	32	ASP	Peptide
20	U	131	ARG	Peptide
21	V	159	PRO	Peptide
24	Y	135	PRO	Peptide
24	Y	80	VAL	Peptide
29	d	108	ARG	Peptide
32	g	110	ALA	Peptide
40	o	39	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	303	0	150	2	0
2	B	1612	0	814	10	0
2	C	1612	0	814	8	0
3	D	75336	0	38154	452	0
4	E	2558	0	1296	10	0
5	F	3315	0	1685	24	0
6	G	1891	0	1986	29	0
7	H	3211	0	3356	52	0
8	I	2884	0	3060	44	0
9	J	2379	0	2408	37	0
10	K	1751	0	1905	38	0
11	L	1870	0	1996	19	0
12	M	1832	0	1962	32	0
13	N	1518	0	1601	31	0
14	O	1660	0	1692	24	0
15	P	1362	0	1399	29	0
16	Q	1682	0	1792	36	0
17	R	1120	0	1187	27	0
18	S	1701	0	1749	19	0
19	T	1641	0	1788	21	0
20	U	1273	0	1304	15	0
21	V	1513	0	1628	16	0
22	W	1508	0	1664	12	0
23	X	1453	0	1490	20	0
24	Y	1298	0	1366	14	0
25	Z	821	0	839	22	0
26	a	979	0	1039	11	0
27	b	528	0	541	5	0
28	c	981	0	1062	10	0
29	d	1115	0	1205	21	0
30	e	1107	0	1182	15	0
31	f	1162	0	1213	21	0
32	g	832	0	883	15	0
33	h	755	0	791	14	0
34	i	888	0	930	9	0
35	j	1053	0	1147	6	0
36	k	876	0	912	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	l	888	0	981	14	0
38	m	1010	0	1143	11	0
39	n	832	0	917	4	0
40	o	705	0	737	8	0
41	p	569	0	637	8	0
42	q	444	0	483	9	0
43	r	429	0	466	8	0
44	s	239	0	289	2	0
45	t	862	0	930	17	0
46	u	708	0	756	8	0
47	v	1002	0	1068	16	0
48	w	34933	0	17694	449	0
49	x	1695	0	1690	54	0
50	y	1725	0	1800	40	0
51	z	1633	0	1716	43	0
52	0	1646	0	1734	50	0
53	1	2070	0	2166	81	0
54	2	1464	0	1505	34	0
55	3	1917	0	2078	89	0
56	4	1510	0	1606	56	0
57	5	1674	0	1739	56	0
58	6	1506	0	1618	75	0
59	7	810	0	836	39	0
60	8	1150	0	1199	40	0
61	9	1208	0	1294	34	0
62	AA	1002	0	1023	31	0
63	AB	1103	0	1156	51	0
64	AC	1128	0	1195	52	0
65	AD	1057	0	1110	47	0
66	AE	1169	0	1198	44	0
67	AF	1111	0	1144	31	0
68	AG	799	0	850	35	0
69	AH	636	0	637	21	0
70	AI	1034	0	1080	34	0
71	AJ	1098	0	1167	27	0
72	AK	1002	0	1067	52	0
73	AL	680	0	744	20	0
74	AM	792	0	842	17	0
75	AN	643	0	650	26	0
76	AO	479	0	507	12	0
77	AP	370	0	373	12	0
78	AQ	452	0	494	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	AR	2436	0	2393	112	0
80	2	1	0	0	0	0
80	A	1	0	0	0	0
80	AF	1	0	0	0	0
80	AM	1	0	0	0	0
80	D	397	0	0	0	0
80	E	10	0	0	0	0
80	F	7	0	0	0	0
80	G	2	0	0	0	0
80	H	2	0	0	0	0
80	I	1	0	0	0	0
80	N	1	0	0	0	0
80	O	1	0	0	0	0
80	S	1	0	0	0	0
80	U	2	0	0	0	0
80	V	2	0	0	0	0
80	X	1	0	0	0	0
80	a	1	0	0	0	0
80	g	1	0	0	0	0
80	j	1	0	0	0	0
80	k	1	0	0	0	0
80	l	1	0	0	0	0
80	u	1	0	0	0	0
80	w	102	0	0	0	0
81	B	11	0	9	0	0
81	C	11	0	10	0	0
82	AM	1	0	0	0	0
82	AP	1	0	0	0	0
82	o	1	0	0	0	0
82	r	1	0	0	0	0
82	t	1	0	0	0	0
82	u	1	0	0	0	0
All	All	209567	0	154721	2601	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (2601) 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:4092:G:H21	3:D:4093:G:H1	1.06	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1303:A:N6	3:D:2316:G:N7	2.15	0.94
64:AC:43:GLU:HG2	64:AC:44:PRO:HD3	1.50	0.90
3:D:453:G:N1	3:D:1293:G:N7	2.22	0.88
3:D:3751:G:H21	3:D:3775:A:H8	1.24	0.85
13:N:106:GLN:NE2	13:N:113:GLU:OE2	2.11	0.84
66:AE:92:ASP:OD1	66:AE:93:GLY:N	2.09	0.83
57:5:87:ASN:HB3	57:5:90:LEU:HG	1.60	0.83
3:D:4494:OMG:HM21	26:a:22:VAL:HG11	1.61	0.82
6:G:117:GLU:HB2	6:G:162:ASN:HB2	1.61	0.82
48:w:616:A:O2'	78:AQ:81:ARG:NH1	2.12	0.82
52:0:101:GLN:HG3	52:0:126:ILE:HD11	1.61	0.81
48:w:1396:A:O2'	48:w:1398:G:N7	2.13	0.81
36:k:109:ARG:HG3	36:k:110:ILE:HD12	1.62	0.81
48:w:1060:A:O2'	48:w:1062:A:N7	2.13	0.81
59:7:25:LYS:HA	59:7:46:MET:HE1	1.62	0.80
48:w:925:G:H1	48:w:1017:U:H3	1.29	0.80
48:w:33:G:H1	48:w:522:A:H8	1.30	0.80
48:w:952:G:H21	62:AA:52:THR:HG21	1.46	0.80
48:w:830:A:OP2	48:w:846:G:N2	2.13	0.80
79:AR:51:ASN:OD1	79:AR:52:TYR:N	2.15	0.80
46:u:5:THR:HG21	46:u:9:GLY:H	1.44	0.80
48:w:1003:U:H5''	50:y:165:ARG:HH22	1.46	0.79
3:D:1656:U:OP2	31:f:26:ARG:NH2	2.15	0.79
59:7:4:PRO:HB2	59:7:6:LYS:HE3	1.65	0.79
79:AR:14:HIS:CE1	79:AR:35:SER:HB2	2.17	0.78
31:f:17:HIS:O	31:f:19:HIS:N	2.16	0.78
1:A:28:G:H1	48:w:1331:C:H42	1.31	0.78
3:D:478:G:OP1	47:v:66:ARG:NH2	2.17	0.78
48:w:1649:U:H3	48:w:1675:A:H2	1.32	0.78
5:F:55:U:H3	5:F:62:A:H2	1.32	0.78
74:AM:43:ASN:HB2	74:AM:46:GLU:HG3	1.64	0.78
48:w:643:A:OP1	58:6:39:ASN:ND2	2.16	0.78
62:AA:86:LYS:HA	62:AA:86:LYS:HE3	1.66	0.78
51:z:263:LYS:HE2	51:z:263:LYS:HA	1.64	0.77
72:AK:20:ARG:NH1	72:AK:85:ASN:O	2.17	0.77
7:H:254:ILE:HG23	7:H:266:VAL:HG11	1.65	0.77
3:D:4882:U:OP1	17:R:117:LYS:NZ	2.18	0.77
79:AR:35:SER:OG	79:AR:37:ASP:OD1	2.02	0.77
32:g:110:ALA:O	32:g:112:ILE:N	2.15	0.77
33:h:51:ASN:O	33:h:51:ASN:ND2	2.18	0.77
3:D:963:G:H22	3:D:2093:A:H61	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1701:A:H5'	3:D:2096:G:H22	1.48	0.76
48:w:50:A:OP2	48:w:472:C:N4	2.16	0.76
3:D:3689:G:O2'	3:D:3818:UY1:OP2	2.04	0.76
56:4:31:GLU:HB2	56:4:41:ARG:HH11	1.51	0.76
78:AQ:113:ARG:HB2	78:AQ:113:ARG:HH11	1.51	0.76
6:G:30:ARG:O	6:G:163:ARG:NH2	2.19	0.76
9:J:271:MET:HE2	9:J:276:LYS:HG3	1.68	0.76
48:w:1271:C:H42	48:w:1511:U:H3	1.34	0.76
62:AA:92:ALA:HB2	62:AA:125:LYS:HB2	1.68	0.76
66:AE:101:ASN:O	66:AE:105:ASN:ND2	2.19	0.76
3:D:1:C:H42	5:F:156:U:H3	1.34	0.76
47:v:26:SER:OG	47:v:28:GLU:OE1	2.01	0.76
3:D:184:U:O2	3:D:253:G:N2	2.17	0.76
3:D:496:G:H2'	3:D:497:G:H8	1.50	0.76
48:w:1745:A:H1'	55:3:66:GLY:HA2	1.66	0.76
48:w:446:G:OP2	57:5:47:ARG:NH2	2.20	0.75
14:O:79:SER:OG	14:O:147:HIS:ND1	2.19	0.75
50:y:165:ARG:HA	50:y:168:MET:HB2	1.68	0.75
3:D:4742:G:N2	3:D:4958:C:O2	2.19	0.75
14:O:38:ARG:HD3	14:O:83:ASP:HB2	1.68	0.75
48:w:1488:C:O2'	48:w:1490:OMG:OP2	2.03	0.75
3:D:2487:G:H22	3:D:2492:C:H1'	1.52	0.75
66:AE:16:LEU:HD13	66:AE:68:ILE:HD11	1.69	0.75
79:AR:26:GLN:NE2	79:AR:73:SER:O	2.19	0.75
3:D:188:G:N2	3:D:190:G:O6	2.19	0.74
57:5:57:ALA:H	57:5:180:GLY:HA2	1.53	0.74
59:7:44:HIS:HA	59:7:47:LYS:HE3	1.69	0.74
62:AA:85:CYS:HB3	62:AA:90:ILE:HB	1.69	0.74
48:w:483:C:H5''	71:AJ:48:LYS:HD2	1.69	0.74
48:w:525:A:H2'	48:w:526:A:H8	1.52	0.74
48:w:96:C:O2	48:w:473:A:O2'	2.05	0.74
48:w:429:C:O2'	48:w:811:A:N1	2.21	0.74
25:Z:65:ARG:HH11	25:Z:65:ARG:HG2	1.53	0.74
50:y:107:ARG:NH2	62:AA:133:THR:O	2.21	0.74
3:D:1391:A:OP1	21:V:181:ARG:NH1	2.19	0.74
3:D:1952:G:H4'	23:X:93:MET:HG2	1.70	0.74
19:T:187:LYS:HA	19:T:187:LYS:HE2	1.69	0.74
49:x:80:ARG:NH2	49:x:165:ASN:O	2.20	0.73
3:D:496:G:N2	3:D:658:C:O2	2.15	0.73
48:w:345:U:O2	53:1:33:THR:OG1	2.06	0.73
48:w:1535:U:O2'	54:2:88:MET:SD	2.46	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AD:103:LYS:NZ	65:AD:118:GLN:O	2.21	0.73
3:D:453:G:N2	3:D:1293:G:O6	2.20	0.73
8:I:110:ARG:O	8:I:113:ARG:NH1	2.21	0.73
55:3:54:GLY:HA2	55:3:63:MET:HE2	1.71	0.73
56:4:27:LEU:HA	56:4:30:LEU:HD23	1.70	0.73
55:3:20:ASP:OD1	55:3:22:ARG:NH1	2.22	0.72
56:4:144:ILE:HG22	56:4:154:ILE:HG12	1.72	0.72
3:D:516:C:N4	3:D:645:G:O6	2.19	0.72
63:AB:93:MET:HA	63:AB:93:MET:HE3	1.70	0.72
75:AN:36:LYS:HE2	75:AN:36:LYS:HA	1.71	0.72
3:D:2562:G:N2	3:D:2565:A:OP2	2.23	0.72
48:w:1289:U:H3	48:w:1310:U:H3	1.38	0.72
63:AB:130:ARG:HA	63:AB:130:ARG:HE	1.55	0.72
64:AC:118:THR:HG23	64:AC:119:LEU:H	1.55	0.72
9:J:263:LYS:HE2	9:J:263:LYS:HA	1.72	0.72
75:AN:67:THR:HG22	75:AN:69:GLY:H	1.54	0.71
19:T:37:ARG:HD2	19:T:108:ILE:HD11	1.72	0.71
64:AC:43:GLU:HG2	64:AC:44:PRO:CD	2.20	0.71
3:D:3937:C:H1'	18:S:125:SER:HB2	1.72	0.71
48:w:1834:A:H2	48:w:1837:G:H1	1.37	0.71
62:AA:30:VAL:HG12	62:AA:94:HIS:HB2	1.73	0.71
50:y:57:ILE:HG13	50:y:58:ALA:H	1.54	0.71
3:D:4635:A:H2	3:D:4663:G:H21	1.37	0.71
49:x:10:MET:HE3	49:x:15:VAL:HG12	1.72	0.71
3:D:2658:G:N2	3:D:2676:A:OP2	2.20	0.71
48:w:918:U:OP2	61:9:64:ARG:NH1	2.23	0.71
3:D:4993:G:H1	3:D:5058:A:H61	1.38	0.71
69:AH:38:GLU:OE1	69:AH:38:GLU:N	2.24	0.71
79:AR:249:CYS:HA	79:AR:258:ILE:HA	1.72	0.71
9:J:184:ASP:OD2	9:J:187:SER:OG	2.09	0.71
48:w:561:A:H61	48:w:590:A2M:H2	1.55	0.71
48:w:851:C:H5''	48:w:852:G:H5'	1.71	0.71
48:w:943:U:OP1	50:y:214:LYS:NZ	2.23	0.71
3:D:4940:C:OP2	10:K:219:LYS:NZ	2.21	0.71
37:l:107:LEU:O	37:l:110:GLN:NE2	2.23	0.71
56:4:127:ASP:OD1	56:4:142:LYS:NZ	2.24	0.71
3:D:2469:C:H5	3:D:2471:G:H1	1.38	0.70
8:I:195:LYS:HB2	8:I:200:ARG:HD2	1.74	0.70
68:AG:26:SER:HB3	68:AG:32:LEU:HD21	1.73	0.70
55:3:182:PRO:HA	55:3:185:LEU:HD12	1.74	0.70
64:AC:107:GLU:OE2	64:AC:107:GLU:N	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:158:A:H2'	48:w:159:A2M:H8	1.74	0.70
3:D:182:G:N2	3:D:255:C:O2	2.25	0.70
63:AB:48:GLY:O	63:AB:50:ARG:NH1	2.25	0.69
65:AD:106:LEU:HD23	65:AD:109:LEU:HD12	1.73	0.69
58:6:152:ASP:O	58:6:155:LYS:NZ	2.26	0.69
47:v:125:MET:HA	47:v:125:MET:HE3	1.74	0.69
49:x:198:MET:HE2	65:AD:85:VAL:HG12	1.75	0.69
53:1:100:ARG:NH2	53:1:121:TYR:O	2.25	0.69
54:2:87:LEU:HD11	64:AC:47:LEU:HD22	1.73	0.69
5:F:82:A:N7	29:d:50:ARG:NH2	2.40	0.69
3:D:505:G:H1	3:D:653:U:H3	1.40	0.69
79:AR:279:SER:HB2	79:AR:282:GLU:HB2	1.71	0.69
48:w:29:G:OP1	71:AJ:124:LYS:NZ	2.25	0.69
48:w:928:G:H1	48:w:1013:U:H3	1.38	0.69
79:AR:111:VAL:HG12	79:AR:122:SER:HA	1.75	0.69
3:D:4094:G:N1	3:D:4114:C:O2	2.13	0.69
4:E:110:G:OP1	9:J:270:LYS:NZ	2.25	0.69
48:w:153:G:N3	55:3:13:GLN:NE2	2.40	0.69
48:w:511:U:H2'	48:w:512:A2M:H8	1.75	0.69
68:AG:49:LYS:H	68:AG:92:HIS:CE1	2.10	0.69
48:w:489:A:OP2	48:w:507:G:N2	2.26	0.68
48:w:1858:G:OP2	62:AA:146:ARG:NH2	2.25	0.68
3:D:496:G:H2'	3:D:497:G:C8	2.28	0.68
3:D:4635:A:H8	3:D:5048:A:H61	1.40	0.68
68:AG:30:LYS:HA	68:AG:30:LYS:HE3	1.74	0.68
73:AL:50:PHE:HZ	73:AL:58:LEU:HD13	1.58	0.68
3:D:1761:G:H1	3:D:1771:U:H3	1.41	0.68
3:D:2711:G:OP1	22:W:39:GLN:NE2	2.25	0.68
3:D:4092:G:N3	3:D:4093:G:N2	2.34	0.68
55:3:45:TRP:O	55:3:46:LYS:NZ	2.26	0.68
15:P:56:THR:HG23	15:P:63:ARG:HA	1.76	0.68
25:Z:28:PRO:HB2	25:Z:34:MET:HG2	1.76	0.68
48:w:974:C:HO2'	62:AA:43:HIS:HD1	1.42	0.68
48:w:1161:U:O4	71:AJ:3:LYS:NZ	2.26	0.68
3:D:1364:U:OP2	16:Q:36:ARG:NH2	2.27	0.68
8:I:201:ARG:HH11	8:I:201:ARG:HG2	1.58	0.68
66:AE:136:THR:HA	66:AE:139:THR:HG23	1.75	0.68
15:P:63:ARG:NH2	45:t:106:PHE:O	2.27	0.68
29:d:66:GLN:CD	29:d:66:GLN:H	2.02	0.68
48:w:924:G:N2	61:9:87:ASP:OD2	2.25	0.68
56:4:37:LYS:O	56:4:39:GLN:NE2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:492:U:O2	3:D:663:G:N2	2.27	0.68
56:4:12:ASN:ND2	56:4:14:GLU:O	2.27	0.68
73:AL:100:VAL:HB	73:AL:108:ILE:HG13	1.76	0.67
79:AR:107:ASP:OD2	79:AR:125:ARG:NH1	2.25	0.67
3:D:4942:C:H5''	10:K:155:GLY:HA2	1.75	0.67
3:D:2474:G:N2	3:D:2502:G:O2'	2.28	0.67
48:w:568:C:H42	48:w:582:C:H42	1.43	0.67
64:AC:97:GLN:HE21	64:AC:105:LYS:HE3	1.59	0.67
61:9:56:ASP:OD2	75:AN:52:THR:OG1	2.09	0.67
18:S:138:PHE:HA	18:S:143:ARG:HD2	1.76	0.67
48:w:531:A:N6	48:w:552:G:O6	2.27	0.67
54:2:27:ASP:OD2	54:2:107:ASN:ND2	2.27	0.67
65:AD:73:LEU:O	65:AD:77:GLU:HB2	1.95	0.67
69:AH:41:LYS:HE2	69:AH:41:LYS:H	1.60	0.67
3:D:2755:A:OP1	30:e:65:ARG:NH1	2.27	0.67
48:w:868:G:H21	56:4:111:LYS:HD2	1.59	0.67
64:AC:52:LEU:HB3	64:AC:56:LEU:HD13	1.75	0.67
10:K:46:ARG:HG3	10:K:62:MET:HE1	1.77	0.67
56:4:36:LEU:HD21	56:4:40:LEU:HD23	1.75	0.67
64:AC:118:THR:C	64:AC:120:LEU:H	2.02	0.67
55:3:49:VAL:HG12	55:3:115:LYS:HB3	1.75	0.67
66:AE:45:LEU:HD12	66:AE:50:ILE:HD12	1.75	0.66
13:N:14:GLU:CD	13:N:14:GLU:H	2.03	0.66
56:4:42:GLU:HG2	56:4:43:LEU:HD12	1.76	0.66
79:AR:120:ILE:HB	79:AR:132:TRP:HB2	1.76	0.66
48:w:579:C:N3	72:AK:61:ARG:NH2	2.42	0.66
51:z:166:ARG:HB3	51:z:247:THR:HG22	1.77	0.66
63:AB:70:MET:HA	63:AB:70:MET:HE3	1.76	0.66
48:w:571:U:O2'	72:AK:60:PHE:O	2.14	0.66
48:w:1597:C:H4'	48:w:1603:G:C6	2.31	0.66
63:AB:41:GLN:HG3	63:AB:84:ILE:HD13	1.78	0.66
63:AB:134:GLY:HA2	63:AB:140:ARG:HG3	1.75	0.66
72:AK:90:ARG:HA	72:AK:93:ARG:HD2	1.77	0.66
53:1:168:LYS:HE3	53:1:169:ILE:H	1.60	0.66
16:Q:46:ILE:HD11	16:Q:51:ALA:HA	1.76	0.66
48:w:1736:G:H2'	48:w:1737:G:C8	2.31	0.66
50:y:175:GLU:OE1	50:y:175:GLU:N	2.28	0.66
52:0:37:VAL:HG12	52:0:50:ILE:HA	1.78	0.66
60:8:35:ARG:NH2	60:8:55:TYR:O	2.29	0.66
60:8:103:GLU:HG3	71:AJ:11:ARG:HB3	1.76	0.66
68:AG:63:ILE:HD11	77:AP:43:PHE:CE2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:222:LYS:HB3	11:L:231:GLY:HA2	1.77	0.66
15:P:118:LYS:NZ	66:AE:10:GLN:OE1	2.29	0.66
48:w:525:A:OP2	78:AQ:99:LYS:NZ	2.29	0.66
48:w:570:C:H4'	72:AK:36:PRO:HG3	1.78	0.66
55:3:183:ARG:HA	55:3:186:GLN:HE21	1.61	0.66
56:4:15:LYS:H	56:4:15:LYS:HE2	1.60	0.66
3:D:2562:G:O2'	3:D:2565:A:N6	2.28	0.66
64:AC:31:LEU:HD11	64:AC:33:LYS:HE2	1.76	0.66
3:D:375:G:OP2	40:o:52:LYS:NZ	2.26	0.65
3:D:937:U:OP1	17:R:46:ARG:NH1	2.28	0.65
3:D:1772:C:H2'	3:D:1773:OMU:H6	1.78	0.65
51:z:121:ARG:HH22	51:z:123:ARG:HD3	1.61	0.65
55:3:87:ARG:N	55:3:91:GLU:OE1	2.26	0.65
63:AB:38:SER:OG	63:AB:41:GLN:OE1	2.13	0.65
50:y:109:LYS:NZ	50:y:113:MET:SD	2.69	0.65
52:0:40:ARG:NH1	68:AG:107:GLU:O	2.29	0.65
66:AE:8:LYS:HD2	66:AE:8:LYS:H	1.61	0.65
73:AL:40:VAL:HG23	73:AL:41:ARG:H	1.61	0.65
3:D:2601:A:N6	3:D:2744:A:OP2	2.29	0.65
7:H:231:VAL:HG11	7:H:251:VAL:HG23	1.79	0.65
8:I:49:ARG:HH11	8:I:111:TRP:HB3	1.62	0.65
58:6:159:PHE:CE2	58:6:165:TYR:HB3	2.31	0.65
60:8:91:ASP:OD1	60:8:104:LYS:NZ	2.25	0.65
68:AG:56:MET:HG3	68:AG:86:LYS:HD2	1.79	0.65
71:AJ:96:GLU:HG3	71:AJ:97:ASN:OD1	1.96	0.65
79:AR:184:LEU:HD21	79:AR:187:ASN:HD21	1.62	0.65
48:w:155:G:N2	55:3:56:ASN:OD1	2.26	0.65
56:4:31:GLU:HB2	56:4:41:ARG:NH1	2.11	0.65
3:D:2578:G:N7	30:e:17:ARG:NH1	2.44	0.65
49:x:38:ILE:HD11	49:x:47:TYR:HB3	1.79	0.65
3:D:3651:A:OP2	6:G:200:ARG:NH1	2.30	0.64
63:AB:53:GLN:HB3	63:AB:83:MET:HE2	1.79	0.64
48:w:1781:A:O2'	48:w:1782:G:N7	2.28	0.64
58:6:136:ARG:NH1	58:6:159:PHE:O	2.31	0.64
3:D:4740:G:H1'	3:D:4742:G:H5''	1.78	0.64
30:e:51:ARG:HB2	30:e:65:ARG:HG2	1.79	0.64
16:Q:4:SER:O	31:f:44:ASN:ND2	2.30	0.64
3:D:515:C:H4'	3:D:516:C:OP1	1.96	0.64
3:D:4754:G:N7	10:K:279:ASN:HB2	2.11	0.64
8:I:140:LYS:O	8:I:204:ARG:NH1	2.30	0.64
48:w:1520:G:O2'	48:w:1521:C:OP1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AR:147:HIS:HB2	79:AR:171:ASP:HB2	1.80	0.64
3:D:662:C:H2'	3:D:663:G:C4	2.33	0.64
53:1:161:GLN:NE2	53:1:170:THR:OG1	2.31	0.64
54:2:100:ILE:HG21	54:2:111:VAL:HG11	1.78	0.64
3:D:1362:G:OP1	16:Q:39:ARG:NH2	2.30	0.64
60:8:4:ILE:HG23	60:8:5:GLN:HG2	1.79	0.64
61:9:19:ARG:NH1	75:AN:84:HIS:OXT	2.29	0.64
70:AI:97:ARG:HH21	70:AI:97:ARG:HG3	1.62	0.64
4:E:13:A:OP1	4:E:109:U:O2'	2.16	0.64
16:Q:178:ALA:N	31:f:134:GLU:OE1	2.29	0.64
52:0:23:GLU:OE2	52:0:27:ARG:NH2	2.31	0.64
55:3:136:LYS:HG3	55:3:174:PRO:HB2	1.79	0.64
79:AR:108:VAL:HA	79:AR:124:SER:HA	1.78	0.64
3:D:4623:OMG:N2	7:H:279:GLU:OE2	2.31	0.64
3:D:4875:G:H2'	23:X:169:THR:HG22	1.78	0.64
9:J:142:PHE:HE1	9:J:171:LEU:HD22	1.62	0.64
38:m:13:LYS:NZ	38:m:16:GLU:OE2	2.29	0.64
48:w:1354:G:N2	48:w:1357:A:OP2	2.30	0.63
48:w:1751:C:H42	48:w:1782:G:H1	1.44	0.63
55:3:85:ARG:O	55:3:87:ARG:NH1	2.31	0.63
75:AN:36:LYS:N	75:AN:78:SER:OG	2.28	0.63
48:w:156:G:OP1	55:3:2:LYS:NZ	2.31	0.63
48:w:382:C:H2'	48:w:383:G:H8	1.62	0.63
3:D:1409:C:H41	3:D:1411:C:H1'	1.63	0.63
17:R:81:ASP:N	17:R:81:ASP:OD2	2.31	0.63
48:w:1372:U:O2'	48:w:1373:C:O5'	2.15	0.63
54:2:168:THR:N	54:2:171:GLU:OE1	2.30	0.63
2:B:17:G:O2'	2:B:56:G:N2	2.28	0.63
3:D:1676:C:O2'	3:D:3914:U:N3	2.31	0.63
3:D:2475:G:O6	28:c:48:ARG:NH2	2.32	0.63
62:AA:96:LYS:HD2	62:AA:132:VAL:HG11	1.80	0.63
61:9:87:ASP:OD1	61:9:129:TYR:OH	2.15	0.63
79:AR:14:HIS:HE1	79:AR:35:SER:HB2	1.62	0.63
2:B:4:U:H3	2:B:68:G:H1	1.46	0.63
3:D:1759:G:H1	3:D:1773:OMU:HN3	1.46	0.63
3:D:1174:G:H1	3:D:1186:U:H3	1.45	0.63
54:2:35:LEU:HD12	54:2:117:ILE:HD13	1.80	0.63
48:w:940:U:H3	48:w:1002:U:H3	1.47	0.63
50:y:71:LEU:HD22	50:y:82:ARG:HB3	1.79	0.63
3:D:4076:G:OP1	12:M:73:ARG:NE	2.24	0.63
75:AN:37:CYS:HB3	75:AN:63:LEU:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:150:U:H3	12:M:162:ASP:HB2	1.62	0.62
8:I:46:LYS:HD2	8:I:113:ARG:HD3	1.80	0.62
48:w:447:A:OP1	57:5:49:ARG:NH1	2.30	0.62
67:AF:27:LYS:H	67:AF:27:LYS:HD3	1.63	0.62
33:h:37:MET:HG3	33:h:97:ILE:HD11	1.80	0.62
51:z:121:ARG:HH12	51:z:123:ARG:HH21	1.44	0.62
3:D:4691:A:H5'	13:N:71:ARG:HH11	1.64	0.62
61:9:130:LYS:NZ	61:9:137:PRO:O	2.32	0.62
64:AC:61:GLU:N	64:AC:61:GLU:OE2	2.28	0.62
3:D:1271:G:H1'	11:L:34:ARG:HH22	1.63	0.62
6:G:27:ALA:O	6:G:128:ARG:NH2	2.32	0.62
48:w:57:U:O2'	48:w:499:G:N3	2.33	0.62
48:w:383:G:H4'	60:8:132:ARG:HD2	1.82	0.62
78:AQ:113:ARG:HB2	78:AQ:113:ARG:NH1	2.14	0.62
48:w:616:A:H4'	78:AQ:81:ARG:CZ	2.29	0.62
79:AR:247:TRP:NE1	79:AR:260:ASP:OD1	2.31	0.62
60:8:35:ARG:NE	60:8:53:GLY:O	2.32	0.62
71:AJ:140:ARG:HD2	71:AJ:141:PRO:HD2	1.81	0.62
3:D:121:A:OP1	12:M:110:LYS:NZ	2.33	0.62
3:D:2472:A:H1'	28:c:48:ARG:HB3	1.82	0.62
9:J:142:PHE:CE1	9:J:171:LEU:HD22	2.35	0.62
48:w:165:G:H1'	55:3:110:ASN:ND2	2.15	0.62
55:3:88:ARG:HB3	55:3:91:GLU:HB2	1.80	0.62
63:AB:25:LEU:HA	63:AB:28:MET:HB2	1.82	0.62
48:w:1139:C:H5	48:w:1149:A:H62	1.48	0.62
56:4:31:GLU:HA	56:4:36:LEU:HD23	1.82	0.62
73:AL:69:THR:HB	73:AL:72:VAL:HG12	1.82	0.62
3:D:194:C:O2	29:d:121:ARG:NH2	2.31	0.62
48:w:1158:G:H5''	70:AI:76:SER:HB2	1.82	0.62
62:AA:39:ASP:OD2	62:AA:40:THR:N	2.33	0.62
72:AK:29:HIS:ND1	72:AK:29:HIS:O	2.32	0.62
3:D:4141:G:H5''	3:D:4142:C:H5'	1.82	0.61
15:P:112:HIS:CE1	15:P:117:ILE:HD13	2.35	0.61
48:w:594:A:H61	48:w:643:A:H5''	1.65	0.61
48:w:1543:U:OP1	64:AC:37:ARG:NH1	2.33	0.61
49:x:8:LEU:HD11	69:AH:39:VAL:HG21	1.81	0.61
58:6:84:ILE:HA	58:6:150:ARG:HA	1.81	0.61
66:AE:142:ARG:HA	73:AL:28:GLY:HA3	1.82	0.61
67:AF:113:VAL:HA	67:AF:123:LEU:HA	1.81	0.61
51:z:199:PRO:HB2	58:6:58:ARG:HH12	1.64	0.61
53:1:107:GLY:HA2	53:1:189:LEU:HG	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:23:A:N3	4:E:118:C:O2'	2.31	0.61
3:D:1172:C:O2'	3:D:1189:G:N2	2.31	0.61
63:AB:108:LYS:HB2	63:AB:111:MET:HG2	1.80	0.61
26:a:45:ILE:HG21	26:a:53:PRO:HB3	1.83	0.61
55:3:214:ALA:HA	55:3:217:MET:HE3	1.82	0.61
59:7:29:MET:SD	59:7:42:ASN:ND2	2.74	0.61
62:AA:85:CYS:HB2	62:AA:124:MET:HE1	1.83	0.61
65:AD:22:THR:O	79:AR:212:LYS:NZ	2.33	0.61
3:D:3641:U:H5	3:D:3646:A:N7	1.99	0.61
55:3:37:ALA:HA	55:3:49:VAL:HG23	1.83	0.61
59:7:64:TRP:CD2	77:AP:23:VAL:HG12	2.35	0.61
68:AG:38:ASP:OD2	68:AG:41:ARG:NH2	2.34	0.61
68:AG:49:LYS:H	68:AG:92:HIS:HE1	1.48	0.61
48:w:568:C:H2'	48:w:569:A:C8	2.36	0.61
48:w:1568:C:OP1	67:AF:96:SER:OG	2.16	0.61
54:2:47:LYS:NZ	64:AC:115:TYR:O	2.33	0.61
14:O:28:ASP:OD2	14:O:32:ARG:NH2	2.34	0.61
16:Q:47:ALA:O	16:Q:49:ARG:N	2.33	0.61
48:w:1434:C:H4'	48:w:1435:C:O5'	2.00	0.61
56:4:25:GLN:HA	56:4:28:LEU:HD22	1.83	0.61
67:AF:29:LYS:HE3	67:AF:29:LYS:HA	1.83	0.61
79:AR:149:GLU:N	79:AR:171:ASP:OD2	2.28	0.61
3:D:741:C:H42	3:D:923:C:H42	1.49	0.60
72:AK:55:ILE:HG22	72:AK:75:ILE:HA	1.83	0.60
3:D:2838:G:H5'	7:H:247:GLY:HA2	1.83	0.60
3:D:5022:U:O2'	3:D:5024:C:OP2	2.18	0.60
43:r:79:GLU:OE2	43:r:81:SER:OG	2.18	0.60
48:w:509:OMG:HM22	48:w:510:G:H5'	1.83	0.60
53:1:121:TYR:HB2	53:1:161:GLN:OE1	2.00	0.60
61:9:3:ARG:HG3	61:9:8:GLY:HA3	1.82	0.60
66:AE:38:ARG:O	66:AE:42:HIS:ND1	2.30	0.60
70:AI:42:MET:HE2	70:AI:49:GLU:HA	1.82	0.60
75:AN:33:MET:HE3	75:AN:79:PHE:CD1	2.36	0.60
3:D:1811:G:H4'	32:g:60:ASN:HD22	1.66	0.60
10:K:120:ASP:OD1	10:K:120:ASP:N	2.34	0.60
16:Q:64:VAL:HA	16:Q:67:HIS:CD2	2.36	0.60
48:w:170:A:O2'	55:3:136:LYS:NZ	2.33	0.60
48:w:1232:PSU:H2'	48:w:1233:G:H8	1.65	0.60
58:6:111:GLN:HE21	58:6:145:PRO:HB3	1.66	0.60
3:D:977:C:OP2	10:K:59:ARG:NH1	2.34	0.60
3:D:1447:C:H2'	3:D:1448:G:H8	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:183:VAL:HG11	53:1:188:ASN:HB2	1.83	0.60
57:5:177:SER:HG	57:5:182:CYS:HG	1.31	0.60
65:AD:41:ILE:HD11	65:AD:47:ARG:HB2	1.82	0.60
68:AG:68:THR:O	77:AP:40:ARG:NH1	2.34	0.60
48:w:11:A:H8	48:w:1357:A:O2'	1.85	0.60
48:w:935:G:O2'	61:9:108:ASP:OD1	2.15	0.60
52:O:67:ARG:NE	59:7:93:THR:O	2.30	0.60
3:D:469:C:N3	10:K:105:ARG:NH1	2.49	0.60
12:M:99:ALA:HB1	12:M:136:LEU:HD11	1.83	0.60
56:4:36:LEU:HG	56:4:39:GLN:HB2	1.82	0.60
64:AC:118:THR:OG1	64:AC:121:VAL:O	2.17	0.60
48:w:1112:U:H2'	48:w:1113:A:C8	2.37	0.60
79:AR:199:THR:HG21	79:AR:240:CYS:HA	1.83	0.60
2:B:52:G:H2'	2:B:53:5MU:H6	1.67	0.60
3:D:5016:A:H2	3:D:5033:G:H21	1.50	0.60
15:P:84:GLU:HG2	15:P:170:TYR:CE1	2.37	0.60
35:j:117:GLN:O	47:v:119:ARG:NH2	2.34	0.60
47:v:97:ILE:HG21	47:v:107:ARG:HB3	1.84	0.60
48:w:913:A:N6	56:4:98:ARG:O	2.32	0.60
30:e:92:ASP:HB3	30:e:95:VAL:HG22	1.82	0.60
49:x:12:GLU:O	49:x:15:VAL:HG22	2.02	0.60
3:D:4092:G:H1'	3:D:4093:G:H21	1.66	0.60
48:w:608:C:H5'	78:AQ:132:SER:HA	1.84	0.60
48:w:1236:G:O2'	63:AB:131:PRO:O	2.14	0.60
56:4:144:ILE:HG13	70:AI:52:ILE:HB	1.84	0.60
79:AR:33:SER:HB3	79:AR:43:TRP:HE1	1.67	0.60
48:w:1373:C:OP1	65:AD:7:LYS:N	2.31	0.59
48:w:1849:G:O2'	48:w:1850:MA6:H8	2.01	0.59
61:9:75:LEU:HD22	61:9:80:LEU:HD11	1.84	0.59
70:AI:28:ARG:HB3	70:AI:29:PRO:HD3	1.83	0.59
35:j:89:LEU:HD13	35:j:118:LEU:HD22	1.83	0.59
48:w:120:U:H2'	48:w:121:OMU:H6	1.84	0.59
63:AB:29:SER:OG	63:AB:31:GLU:OE1	2.20	0.59
72:AK:110:ARG:HE	72:AK:126:GLY:HA3	1.67	0.59
3:D:730:G:OP2	11:L:76:ARG:NE	2.34	0.59
48:w:803:C:O2'	70:AI:80:ASP:OD1	2.15	0.59
48:w:1630:A:OP1	66:AE:40:TYR:HB2	2.03	0.59
58:6:119:LEU:H	58:6:119:LEU:HD23	1.67	0.59
64:AC:118:THR:O	64:AC:120:LEU:N	2.35	0.59
79:AR:199:THR:OG1	79:AR:239:LEU:O	2.17	0.59
3:D:1096:C:O2	3:D:1200:G:N2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:101:VAL:HG22	6:G:165:VAL:HG22	1.85	0.59
14:O:190:LEU:HB3	14:O:197:VAL:HG22	1.85	0.59
3:D:3612:C:H1'	3:D:5016:A:C8	2.37	0.59
48:w:1287:A:C5	48:w:1288:OMU:H1'	2.37	0.59
55:3:223:LYS:O	55:3:227:GLN:N	2.30	0.59
57:5:76:THR:OG1	57:5:105:ASP:OD1	2.21	0.59
62:AA:46:ASP:OD1	62:AA:48:SER:OG	2.19	0.59
79:AR:114:SER:OG	79:AR:116:ASP:OD1	2.19	0.59
58:6:142:VAL:HG12	58:6:144:ILE:H	1.67	0.59
72:AK:16:ARG:H	72:AK:16:ARG:HD3	1.67	0.59
13:N:187:VAL:HG12	13:N:188:GLN:H	1.67	0.59
72:AK:21:LYS:HB2	72:AK:75:ILE:HB	1.85	0.59
48:w:1415:C:H1'	67:AF:128:GLN:HE22	1.68	0.59
49:x:128:ARG:NH2	49:x:151:ASP:O	2.35	0.59
58:6:30:LYS:HA	78:AQ:111:TYR:HE1	1.68	0.59
3:D:2351:OMC:HM22	3:D:2352:U:H5'	1.84	0.59
8:I:204:ARG:NH2	8:I:205:ARG:O	2.36	0.59
20:U:111:SER:HB3	20:U:156:ILE:HD13	1.84	0.59
48:w:1552:G:H8	52:0:3:VAL:HG11	1.66	0.59
49:x:158:ASP:OD2	69:AH:60:ARG:NH1	2.36	0.59
73:AL:56:ASP:N	73:AL:56:ASP:OD1	2.35	0.59
3:D:1351:G:OP1	8:I:33:ARG:NH1	2.36	0.59
19:T:47:PHE:HZ	19:T:144:GLU:HG3	1.68	0.59
53:1:198:ARG:HE	53:1:200:ARG:HE	1.51	0.59
58:6:75:ASN:HA	58:6:78:LEU:HB2	1.85	0.59
3:D:760:G:H4'	3:D:905:C:H1'	1.85	0.58
7:H:293:ILE:HG23	7:H:294:LYS:H	1.66	0.58
20:U:22:LEU:HD13	20:U:90:PHE:HD2	1.68	0.58
48:w:894:G:H3'	48:w:895:G:H5''	1.83	0.58
55:3:76:LEU:HD21	55:3:92:ARG:HD2	1.84	0.58
55:3:135:PRO:HG2	55:3:141:ILE:HD12	1.85	0.58
79:AR:152:SER:H	79:AR:169:GLY:HA2	1.68	0.58
48:w:294:U:OP1	60:8:36:TYR:OH	2.10	0.58
49:x:53:ARG:NH2	69:AH:83:PHE:O	2.36	0.58
3:D:4635:A:O2'	3:D:4637:OMG:OP1	2.20	0.58
6:G:120:PRO:HA	6:G:162:ASN:HB3	1.85	0.58
33:h:105:ILE:HG13	33:h:106:ARG:HD3	1.85	0.58
48:w:560:A:N6	48:w:588:G:O6	2.36	0.58
58:6:70:ARG:HH22	58:6:94:LEU:HD21	1.68	0.58
64:AC:99:TYR:O	79:AR:57:ARG:NH1	2.36	0.58
3:D:217:C:H5	3:D:219:G:H4'	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1701:A:H5''	8:I:304:ALA:HB3	1.85	0.58
3:D:3614:G:O2'	3:D:3615:G:OP1	2.17	0.58
15:P:113:ILE:HG12	15:P:125:ILE:HD11	1.86	0.58
41:p:40:ARG:NH1	41:p:41:TYR:OH	2.35	0.58
45:t:74:GLU:O	45:t:78:ARG:NH2	2.36	0.58
48:w:58:C:H5''	48:w:499:G:H21	1.68	0.58
48:w:525:A:H5''	78:AQ:105:ALA:HB2	1.84	0.58
48:w:1398:G:O2'	79:AR:88:ARG:NH2	2.37	0.58
49:x:104:THR:O	49:x:107:THR:OG1	2.19	0.58
34:i:19:GLU:OE1	34:i:92:ARG:NH1	2.37	0.58
3:D:1574:G:O2'	3:D:1575:A:O5'	2.21	0.58
3:D:1699:A:H3'	3:D:1700:G:H5''	1.85	0.58
3:D:4733:C:H1'	3:D:4734:A:H2'	1.85	0.58
8:I:66:SER:O	8:I:66:SER:OG	2.15	0.58
48:w:371:A:OP2	57:5:10:LYS:HB2	2.04	0.58
48:w:1610:G:P	66:AE:121:ARG:HH21	2.27	0.58
49:x:84:GLN:HG2	49:x:100:ALA:HB1	1.86	0.58
58:6:111:GLN:OE1	58:6:111:GLN:HA	2.03	0.58
72:AK:29:HIS:O	72:AK:29:HIS:CG	2.57	0.58
14:O:54:SER:HB2	14:O:135:ILE:HD11	1.84	0.58
16:Q:128:PRO:HD3	16:Q:143:GLU:OE2	2.04	0.58
61:9:138:ASN:O	61:9:138:ASN:ND2	2.32	0.58
3:D:943:A:N3	8:I:335:MET:HE1	2.19	0.58
7:H:229:LYS:HG3	7:H:272:LYS:HD3	1.86	0.58
21:V:39:THR:HG22	21:V:41:SER:H	1.69	0.58
32:g:110:ALA:C	32:g:112:ILE:H	2.07	0.58
48:w:291:G:H1'	48:w:292:A:H2'	1.84	0.58
48:w:1391:OMC:H4'	77:AP:55:LEU:HD21	1.85	0.58
48:w:1647:A:OP1	64:AC:138:ARG:NH1	2.35	0.58
79:AR:129:ILE:HD13	79:AR:154:VAL:HG11	1.86	0.58
14:O:31:ILE:HD12	14:O:65:LEU:HB3	1.86	0.58
23:X:127:MET:HB3	24:Y:153:PRO:HG2	1.85	0.58
68:AG:85:HIS:HB3	68:AG:87:ARG:HH22	1.69	0.58
3:D:1408:G:H1'	3:D:1411:C:H42	1.68	0.57
3:D:2262:G:OP2	47:v:98:ARG:NH2	2.28	0.57
30:e:50:PRO:HD3	30:e:68:ILE:HG12	1.86	0.57
30:e:89:ILE:HG22	30:e:91:LEU:HG	1.85	0.57
53:1:161:GLN:N	53:1:171:ASP:O	2.35	0.57
70:AI:28:ARG:HB3	70:AI:29:PRO:CD	2.34	0.57
71:AJ:46:HIS:HB3	71:AJ:101:LEU:HD11	1.86	0.57
79:AR:214:GLY:HA2	79:AR:236:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1100:U:O2'	3:D:1167:C:N4	2.37	0.57
20:U:22:LEU:HD13	20:U:90:PHE:CD2	2.39	0.57
48:w:1473:G:N2	48:w:1476:A:OP2	2.30	0.57
79:AR:2:THR:OG1	79:AR:313:THR:O	2.20	0.57
3:D:491:G:H1	3:D:663:G:H1	1.53	0.57
48:w:1550:G:H3'	48:w:1579:A:H61	1.68	0.57
48:w:1616:U:OP2	63:AB:43:ARG:NH2	2.38	0.57
48:w:1673:U:H5''	64:AC:78:VAL:HG12	1.84	0.57
53:1:188:ASN:OD1	53:1:220:THR:OG1	2.22	0.57
58:6:136:ARG:HD2	58:6:139:LYS:HA	1.86	0.57
5:F:14:U:H5''	20:U:123:PRO:HD3	1.87	0.57
48:w:1155:U:OP1	51:z:185:THR:OG1	2.18	0.57
53:1:231:GLY:HA3	53:1:233:LYS:NZ	2.20	0.57
61:9:18:TYR:OH	70:AI:54:ASP:OD1	2.15	0.57
48:w:556:U:O2'	48:w:558:G:OP1	2.21	0.57
2:B:52:G:H2'	2:B:53:5MU:C6	2.40	0.57
6:G:28:ARG:HB2	6:G:123:ARG:HB3	1.86	0.57
29:d:64:GLY:HA3	29:d:66:GLN:HE22	1.69	0.57
48:w:799:OMU:H5''	56:4:111:LYS:HE2	1.85	0.57
48:w:1606:G:O2'	48:w:1607:A:O5'	2.22	0.57
52:0:213:PRO:HD3	65:AD:19:LYS:HD3	1.86	0.57
79:AR:44:LYS:HD2	79:AR:54:ILE:HD11	1.87	0.57
33:h:34:THR:HG23	33:h:95:ALA:HB2	1.87	0.57
36:k:33:VAL:HG23	36:k:38:GLU:HG3	1.87	0.57
62:AA:95:ILE:HD11	62:AA:129:ILE:HG23	1.84	0.57
48:w:122:G:H21	53:1:146:THR:HG21	1.70	0.57
72:AK:106:GLN:NE2	72:AK:109:GLU:OE2	2.37	0.57
73:AL:68:ILE:HB	73:AL:109:TYR:HB2	1.87	0.57
75:AN:11:SER:N	75:AN:14:GLU:OE2	2.37	0.57
79:AR:72:SER:OG	79:AR:74:ASP:O	2.23	0.57
79:AR:199:THR:HG21	79:AR:241:PHE:H	1.70	0.57
3:D:2703:G:OP1	25:Z:113:ARG:NH1	2.38	0.57
12:M:140:VAL:HG21	12:M:166:LEU:O	2.05	0.57
30:e:101:PHE:O	30:e:102:ARG:HD3	2.04	0.57
48:w:3:C:O2	58:6:18:ARG:NH1	2.32	0.57
48:w:527:C:H5'	58:6:125:HIS:HB2	1.87	0.57
53:1:31:PRO:HG2	53:1:38:LEU:HG	1.87	0.57
58:6:114:VAL:HG13	58:6:126:ALA:HB1	1.87	0.57
5:F:16:G:HO2'	5:F:17:A:H8	1.51	0.56
6:G:137:ILE:HD11	6:G:149:LYS:HB2	1.87	0.56
29:d:88:GLU:N	29:d:88:GLU:OE2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:6:159:PHE:HE2	58:6:165:TYR:HB3	1.69	0.56
59:7:24:LYS:HB2	59:7:66:HIS:CE1	2.39	0.56
59:7:47:LYS:HD2	59:7:47:LYS:C	2.30	0.56
3:D:3654:G:O2'	3:D:3693:U:OP1	2.20	0.56
7:H:222:VAL:O	7:H:343:ARG:NH1	2.38	0.56
48:w:379:C:O2	57:5:5:ARG:NE	2.38	0.56
68:AG:19:ARG:HB2	68:AG:117:ALA:HB2	1.85	0.56
71:AJ:49:GLY:N	71:AJ:99:GLU:OE1	2.37	0.56
12:M:50:ASP:OD1	12:M:52:THR:HG23	2.05	0.56
16:Q:65:ARG:HG3	31:f:69:PHE:CG	2.40	0.56
54:2:140:ASP:HB2	76:AO:46:VAL:HG12	1.88	0.56
74:AM:12:LYS:HB2	74:AM:33:ASP:OD2	2.05	0.56
3:D:76:A:N7	16:Q:74:ARG:NH2	2.54	0.56
10:K:162:VAL:HG22	10:K:175:VAL:HG22	1.88	0.56
10:K:245:GLN:NE2	10:K:245:GLN:O	2.38	0.56
16:Q:65:ARG:HD2	16:Q:66:TYR:CZ	2.41	0.56
48:w:1409:A:H61	48:w:1432:U:H3	1.54	0.56
48:w:1861:G:H5''	74:AM:3:LYS:HA	1.88	0.56
49:x:213:GLU:HB2	65:AD:84:TYR:HE1	1.71	0.56
55:3:136:LYS:HG2	55:3:176:ILE:HA	1.86	0.56
72:AK:42:GLU:HB3	72:AK:46:LYS:NZ	2.20	0.56
3:D:1332:C:H5''	35:j:29:VAL:HG23	1.87	0.56
48:w:1144:A:H2'	48:w:1145:A:C8	2.41	0.56
55:3:50:VAL:HG21	55:3:111:LEU:HB3	1.88	0.56
2:C:17:G:O2'	2:C:56:G:N2	2.25	0.56
8:I:38:ASN:O	8:I:42:THR:HG23	2.05	0.56
14:O:33:ILE:HD12	14:O:33:ILE:O	2.05	0.56
20:U:4:TYR:OH	20:U:18:ARG:HG3	2.06	0.56
48:w:1442:OMU:O5'	48:w:1442:OMU:H6	2.06	0.56
57:5:139:LYS:HE3	57:5:146:GLN:HB2	1.88	0.56
59:7:14:LEU:HD12	59:7:17:LYS:HE3	1.87	0.56
64:AC:97:GLN:HG2	64:AC:105:LYS:HD2	1.86	0.56
3:D:1077:C:H4'	3:D:1215:C:N4	2.20	0.56
7:H:107:ALA:HB2	7:H:201:LEU:HD22	1.86	0.56
7:H:219:VAL:HG11	7:H:337:VAL:HG21	1.87	0.56
49:x:16:LEU:HD11	65:AD:114:LEU:HD12	1.86	0.56
53:1:48:LEU:HD22	53:1:61:VAL:HG23	1.88	0.56
70:AI:97:ARG:HG3	70:AI:97:ARG:NH2	2.19	0.56
3:D:491:G:O6	3:D:662:C:N4	2.38	0.56
3:D:3811:G:O2'	3:D:3814:U:OP2	2.22	0.56
48:w:923:G:H5''	61:9:2:GLY:HA2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2:73:THR:HG23	54:2:89:THR:HG22	1.88	0.56
73:AL:50:PHE:HE2	73:AL:55:TYR:HA	1.71	0.56
3:D:4988:U:H1'	3:D:4991:U:O2	2.06	0.56
9:J:3:PHE:HD2	9:J:4:VAL:HG22	1.70	0.56
48:w:290:U:O2'	48:w:292:A:N7	2.29	0.56
48:w:496:C:H5'	53:1:29:PRO:HG3	1.87	0.56
63:AB:29:SER:HB3	63:AB:32:GLN:OE1	2.06	0.56
65:AD:60:ARG:HA	65:AD:63:ARG:NH2	2.20	0.56
79:AR:27:PHE:HB3	79:AR:30:MET:HB3	1.87	0.56
79:AR:68:ASP:HB2	79:AR:110:SER:HA	1.87	0.56
3:D:1962:A:OP2	3:D:2024:G:N1	2.33	0.56
16:Q:126:LEU:N	16:Q:138:ASP:OD2	2.36	0.56
41:p:5:ILE:HD11	41:p:11:PHE:HD1	1.70	0.56
48:w:26:U:H2'	48:w:27:A2M:H8	1.86	0.56
48:w:600:G:H2'	48:w:601:OMG:H8	1.70	0.56
53:1:56:LEU:N	53:1:60:GLU:OE2	2.36	0.56
55:3:39:ASP:OD1	55:3:47:GLY:N	2.39	0.56
57:5:81:VAL:HG12	57:5:102:VAL:HG12	1.88	0.56
3:D:1177:U:HO2'	9:J:286:SER:HG	1.54	0.55
3:D:1518:A:OP1	31:f:27:LYS:NZ	2.29	0.55
3:D:1700:G:OP1	3:D:1704:C:N4	2.39	0.55
5:F:127:U:O2'	5:F:128:C:H6	1.89	0.55
29:d:91:ASN:OD1	29:d:93:THR:HG23	2.05	0.55
45:t:33:LEU:HA	45:t:38:LYS:HG2	1.88	0.55
48:w:332:G:OP1	55:3:196:LYS:NZ	2.38	0.55
60:8:121:GLN:OE1	60:8:121:GLN:N	2.39	0.55
64:AC:23:ALA:HA	64:AC:70:VAL:HG12	1.89	0.55
66:AE:60:THR:OG1	66:AE:62:ASP:OD1	2.24	0.55
48:w:354:U:OP1	60:8:90:ARG:NH1	2.34	0.55
48:w:1434:C:H5'	48:w:1437:C:H42	1.70	0.55
72:AK:41:ARG:HH22	72:AK:53:ASP:HA	1.71	0.55
3:D:4731:G:N3	3:D:4732:G:H1'	2.22	0.55
4:E:117:G:OP1	9:J:253:TYR:OH	2.25	0.55
8:I:7:LEU:HG	8:I:21:ASN:HB3	1.88	0.55
19:T:202:LEU:O	19:T:202:LEU:HD23	2.05	0.55
52:0:135:GLU:HG2	52:0:153:VAL:HG12	1.88	0.55
55:3:53:SER:OG	55:3:110:ASN:OD1	2.24	0.55
55:3:186:GLN:OE1	55:3:187:HIS:ND1	2.39	0.55
65:AD:23:ARG:HB2	79:AR:170:TRP:HZ3	1.70	0.55
79:AR:58:ALA:HB3	79:AR:60:ARG:NE	2.22	0.55
3:D:181:C:N3	3:D:255:C:N4	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1821:G:N3	3:D:1821:G:H2'	2.22	0.55
48:w:1693:G:H21	48:w:1834:A:H8	1.55	0.55
3:D:1498:G:OP1	21:V:150:ARG:NH1	2.39	0.55
3:D:4474:A:H5''	43:r:125:LYS:HD2	1.88	0.55
5:F:110:U:H5''	42:q:8:ARG:HH12	1.72	0.55
42:q:28:ARG:HH21	42:q:28:ARG:HG3	1.71	0.55
45:t:74:GLU:OE1	45:t:77:CYS:N	2.27	0.55
48:w:921:G:C6	70:AI:28:ARG:HD2	2.41	0.55
49:x:57:LYS:NZ	69:AH:66:ASP:OD1	2.38	0.55
55:3:70:HIS:HA	55:3:98:ARG:HH12	1.71	0.55
79:AR:191:HIS:NE2	79:AR:209:SER:OG	2.40	0.55
9:J:62:CYS:HB3	9:J:105:LEU:HD22	1.89	0.55
25:Z:60:VAL:HG11	25:Z:76:VAL:HG13	1.87	0.55
48:w:464:A:H5'	48:w:465:A:C8	2.42	0.55
57:5:64:ASN:HB3	57:5:186:ASP:HB3	1.88	0.55
67:AF:114:GLU:OE1	67:AF:114:GLU:N	2.40	0.55
19:T:61:ARG:HA	19:T:70:PRO:HD2	1.89	0.55
47:v:47:LYS:HB2	47:v:102:TYR:CZ	2.42	0.55
49:x:189:ILE:HG22	49:x:191:ARG:H	1.72	0.55
65:AD:78:ARG:HG2	65:AD:81:ARG:HE	1.72	0.55
72:AK:23:MET:N	72:AK:23:MET:HE3	2.22	0.55
3:D:2096:G:H4'	3:D:2099:G:H4'	1.89	0.55
48:w:525:A:H2'	48:w:526:A:C8	2.37	0.55
51:z:263:LYS:HD3	51:z:264:SER:H	1.71	0.55
53:1:176:ASP:OD1	53:1:179:ASN:ND2	2.40	0.55
56:4:39:GLN:O	56:4:43:LEU:HD13	2.07	0.55
56:4:60:ILE:HD11	56:4:92:VAL:HG12	1.88	0.55
63:AB:130:ARG:HA	63:AB:130:ARG:NE	2.19	0.55
14:O:19:LYS:HA	14:O:23:CYS:SG	2.46	0.55
25:Z:66:SER:OG	25:Z:67:LYS:N	2.39	0.55
52:0:58:VAL:HG23	52:0:59:LEU:HD12	1.87	0.55
8:I:106:LYS:HD3	8:I:108:TRP:CZ2	2.42	0.55
48:w:124:U:OP1	53:1:148:ARG:NH2	2.39	0.55
48:w:681:PSU:H4'	71:AJ:9:THR:HG22	1.89	0.55
78:AQ:94:LYS:NZ	78:AQ:95:GLN:O	2.40	0.55
79:AR:244:ASN:HB3	79:AR:245:ARG:HE	1.71	0.55
3:D:3906:A:H2'	8:I:69:THR:HG23	1.88	0.54
8:I:67:TRP:HB2	8:I:71:ARG:NH1	2.23	0.54
9:J:124:GLU:O	9:J:126:THR:HG23	2.06	0.54
48:w:317:C:OP2	55:3:183:ARG:NH2	2.39	0.54
54:2:124:ASP:HA	54:2:200:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AG:87:ARG:HH21	68:AG:87:ARG:HG2	1.71	0.54
79:AR:104:HIS:CE1	79:AR:124:SER:HB3	2.42	0.54
3:D:1210:C:H41	11:L:66:ARG:CZ	2.20	0.54
3:D:1769:G:H2'	3:D:1770:A:H8	1.72	0.54
6:G:142:GLU:H	6:G:142:GLU:CD	2.15	0.54
48:w:519:A:O2'	58:6:11:LYS:HE2	2.07	0.54
48:w:1834:A:H2	48:w:1837:G:N1	2.03	0.54
63:AB:34:MET:HE1	63:AB:46:ASN:OD1	2.07	0.54
16:Q:121:ARG:HG3	16:Q:121:ARG:HH11	1.73	0.54
25:Z:111:GLU:OE1	25:Z:113:ARG:NH2	2.39	0.54
48:w:149:A:H3'	48:w:150:A:H8	1.73	0.54
48:w:639:C:OP1	78:AQ:114:ARG:NH2	2.36	0.54
48:w:1199:A:OP1	74:AM:2:THR:N	2.40	0.54
52:O:106:ARG:NH1	52:O:174:HIS:O	2.41	0.54
55:3:136:LYS:HA	55:3:176:ILE:HG22	1.88	0.54
55:3:186:GLN:HE22	55:3:187:HIS:CE1	2.25	0.54
61:9:18:TYR:O	70:AI:56:HIS:ND1	2.40	0.54
62:AA:75:MET:HB3	62:AA:114:SER:HB2	1.89	0.54
64:AC:118:THR:C	64:AC:120:LEU:N	2.65	0.54
79:AR:272:GLN:CD	79:AR:272:GLN:H	2.15	0.54
48:w:606:G:O2'	48:w:608:C:OP1	2.23	0.54
48:w:1003:U:H5''	50:y:165:ARG:NH2	2.17	0.54
51:z:229:CYS:O	51:z:232:THR:HG22	2.08	0.54
58:6:137:VAL:HG22	58:6:157:ILE:HG13	1.89	0.54
64:AC:100:VAL:O	79:AR:57:ARG:NH2	2.41	0.54
70:AI:102:ILE:HG13	70:AI:113:HIS:HB3	1.88	0.54
79:AR:11:LEU:HD13	79:AR:307:VAL:HG23	1.88	0.54
53:1:17:HIS:NE2	53:1:107:GLY:O	2.40	0.54
79:AR:285:GLN:HB3	79:AR:303:THR:HB	1.90	0.54
5:F:16:G:O2'	5:F:17:A:H8	1.90	0.54
7:H:47:LEU:HD13	7:H:84:MET:HE1	1.90	0.54
33:h:15:ASN:HA	33:h:18:LEU:HB2	1.89	0.54
34:i:24:GLU:OE1	34:i:87:ARG:NH2	2.36	0.54
38:m:19:LYS:NZ	38:m:23:ASP:OD1	2.30	0.54
48:w:640:A:H2'	48:w:641:A:C8	2.43	0.54
51:z:170:TRP:HA	70:AI:97:ARG:HH11	1.72	0.54
72:AK:112:ASN:HA	72:AK:115:LYS:HE2	1.89	0.54
79:AR:197:THR:HG21	79:AR:238:ALA:HA	1.89	0.54
25:Z:100:LEU:HD12	25:Z:112:LEU:HB3	1.88	0.54
33:h:51:ASN:ND2	46:u:41:PHE:O	2.36	0.54
48:w:837:A:H62	72:AK:8:ARG:HG3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4:158:LEU:HD21	56:4:187:PHE:HD2	1.73	0.54
63:AB:81:ARG:NH1	63:AB:120:SER:OG	2.38	0.54
66:AE:112:GLU:O	66:AE:113:ARG:NH2	2.41	0.54
70:AI:27:ILE:HB	70:AI:61:ILE:CG2	2.38	0.54
3:D:114:G:N2	3:D:158:A:H61	2.06	0.54
3:D:1268:G:N7	32:g:111:ARG:NH2	2.56	0.54
18:S:68:ARG:NH1	18:S:124:ASP:O	2.37	0.54
48:w:420:G:O2'	48:w:660:C:N3	2.38	0.54
48:w:1648:G:N7	64:AC:17:LYS:HD3	2.22	0.54
56:4:21:SER:O	56:4:24:SER:OG	2.17	0.54
60:8:96:ILE:HG13	71:AJ:10:ALA:HB1	1.88	0.54
3:D:407:A:O2'	3:D:410:A:OP1	2.26	0.54
3:D:418:A:N6	5:F:16:G:H1'	2.23	0.54
3:D:1194:G:H2'	3:D:1195:G:C8	2.42	0.54
3:D:1837:A:OP2	24:Y:130:ARG:NH2	2.39	0.54
3:D:2488:C:N4	5:F:126:C:OP1	2.41	0.54
3:D:4092:G:H1'	3:D:4093:G:N2	2.23	0.54
8:I:76:ILE:HD12	8:I:77:PRO:HD2	1.88	0.54
13:N:12:ILE:HG12	13:N:53:LYS:O	2.07	0.54
13:N:141:LYS:HE2	13:N:141:LYS:HA	1.90	0.54
41:p:12:LEU:O	41:p:16:ARG:HG3	2.08	0.54
49:x:85:ARG:NH1	65:AD:81:ARG:O	2.32	0.54
62:AA:31:CYS:HB2	62:AA:44:VAL:HG22	1.89	0.54
66:AE:85:ASN:H	66:AE:97:GLN:HG3	1.73	0.54
3:D:4084:G:O6	6:G:72:ARG:NH2	2.38	0.54
53:1:185:GLY:N	53:1:189:LEU:HD13	2.23	0.54
58:6:109:ARG:HH22	58:6:127:ARG:HH12	1.55	0.54
59:7:80:ARG:NH1	59:7:89:ILE:O	2.25	0.54
66:AE:63:GLU:O	66:AE:67:VAL:HG23	2.08	0.54
78:AQ:81:ARG:NH1	78:AQ:84:LYS:HB3	2.23	0.54
3:D:500:G:O2'	3:D:505:G:OP1	2.24	0.53
3:D:1293:G:OP2	3:D:1293:G:N2	2.29	0.53
3:D:1771:U:H2'	3:D:1772:C:C6	2.43	0.53
52:0:22:ASN:O	52:0:26:THR:HG22	2.08	0.53
79:AR:16:GLY:C	79:AR:305:ASN:HB3	2.34	0.53
79:AR:178:ASN:HB3	79:AR:183:LYS:H	1.73	0.53
3:D:495:C:H2'	3:D:496:G:C8	2.42	0.53
3:D:1646:A:O2'	40:o:49:TRP:O	2.23	0.53
3:D:4378:A:O2'	3:D:4379:A:H2'	2.08	0.53
7:H:378:ARG:HG2	27:b:32:LEU:HD21	1.90	0.53
48:w:1665:G:N2	67:AF:87:VAL:HG22	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AB:31:GLU:O	63:AB:34:MET:HB2	2.08	0.53
3:D:1503:A:H4'	3:D:1504:G:H5'	1.89	0.53
3:D:1761:G:N2	3:D:1771:U:O2	2.33	0.53
48:w:144:U:O4	55:3:178:ARG:NH2	2.41	0.53
48:w:436:OMG:OP2	48:w:471:G:O2'	2.26	0.53
48:w:1617:G:N1	48:w:1620:A:OP2	2.39	0.53
51:z:196:ILE:HB	51:z:223:TYR:HB2	1.89	0.53
3:D:165:A:H61	3:D:270:U:H3	1.56	0.53
3:D:2095:A:H4'	3:D:2096:G:N7	2.23	0.53
12:M:61:ILE:HA	12:M:64:GLN:HG2	1.89	0.53
14:O:169:LYS:NZ	24:Y:157:GLU:OE2	2.34	0.53
48:w:1623:A:N1	66:AE:132:ARG:NH1	2.56	0.53
50:y:34:LYS:O	50:y:98:THR:OG1	2.26	0.53
52:0:210:ILE:HD13	65:AD:16:ILE:HG22	1.91	0.53
55:3:12:CYS:HB3	55:3:124:LEU:HD22	1.91	0.53
66:AE:102:GLY:HA2	66:AE:105:ASN:HD21	1.73	0.53
67:AF:110:LEU:HB3	67:AF:112:MET:HE3	1.90	0.53
79:AR:61:GLY:O	79:AR:88:ARG:NH1	2.39	0.53
48:w:594:A:N6	48:w:643:A:H5''	2.23	0.53
48:w:600:G:H1	48:w:622:C:H5	1.56	0.53
49:x:176:TRP:HE1	49:x:197:VAL:HG23	1.72	0.53
52:0:69:LEU:HA	52:0:72:VAL:HG12	1.90	0.53
53:1:92:ILE:HD11	72:AK:17:LEU:HD11	1.90	0.53
59:7:21:MET:HE3	59:7:22:VAL:N	2.24	0.53
66:AE:141:ARG:O	73:AL:28:GLY:N	2.41	0.53
3:D:1319:U:OP2	31:f:22:ILE:HG22	2.09	0.53
15:P:88:LYS:HB2	15:P:88:LYS:NZ	2.23	0.53
21:V:16:LYS:O	21:V:33:ARG:NH2	2.40	0.53
29:d:50:ARG:HG2	29:d:51:LYS:H	1.71	0.53
33:h:23:LYS:NZ	33:h:23:LYS:HB3	2.23	0.53
48:w:1618:C:H5''	63:AB:47:ARG:HH21	1.72	0.53
57:5:139:LYS:NZ	57:5:140:LYS:O	2.41	0.53
67:AF:82:ARG:NH2	67:AF:90:SER:OG	2.42	0.53
7:H:383:GLU:H	7:H:383:GLU:CD	2.16	0.53
13:N:41:ILE:HG22	13:N:43:VAL:HG13	1.91	0.53
18:S:9:GLU:HB3	39:n:44:ILE:HG13	1.91	0.53
48:w:1606:G:H21	48:w:1607:A:N6	2.07	0.53
61:9:112:LYS:O	61:9:116:ILE:HD12	2.08	0.53
64:AC:50:LYS:HA	64:AC:53:GLU:OE2	2.09	0.53
3:D:320:C:OP1	39:n:84:LYS:NZ	2.39	0.53
3:D:664:G:H2'	3:D:666:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3711:A:H2	3:D:3712:A:H62	1.55	0.53
3:D:4348:A:O3'	3:D:4349:C:H4'	2.08	0.53
48:w:428:OMU:HM22	58:6:7:TRP:HZ3	1.73	0.53
48:w:505:G:O2'	48:w:506:G:O5'	2.26	0.53
48:w:824:C:C2	58:6:144:ILE:HD13	2.44	0.53
52:0:132:LYS:HD3	52:0:156:LEU:HD12	1.91	0.53
53:1:64:ILE:HG23	53:1:69:PHE:HD2	1.72	0.53
59:7:41:PRO:HD2	59:7:44:HIS:CD2	2.44	0.53
66:AE:89:ASP:O	66:AE:91:LYS:N	2.42	0.53
3:D:1194:G:H2'	3:D:1195:G:H8	1.74	0.53
3:D:2848:G:O2'	3:D:3838:U:O4	2.20	0.53
3:D:4093:G:H3'	3:D:4094:G:C8	2.43	0.53
5:F:96:C:H5''	38:m:66:LYS:HD2	1.90	0.53
48:w:303:C:O4'	57:5:64:ASN:ND2	2.42	0.53
48:w:921:G:C5	70:AI:28:ARG:HD2	2.44	0.53
48:w:1527:C:OP1	64:AC:142:GLN:NE2	2.31	0.53
58:6:108:ARG:HH12	58:6:154:GLN:HE22	1.55	0.53
73:AL:50:PHE:CE2	73:AL:55:TYR:HA	2.44	0.53
3:D:175:C:H2'	3:D:176:G:C8	2.44	0.53
3:D:1697:G:H22	3:D:2084:C:P	2.32	0.53
3:D:2464:C:O2'	3:D:2465:C:H6	1.91	0.53
3:D:2527:A:P	22:W:38:ARG:HH22	2.32	0.53
3:D:4093:G:H3'	3:D:4094:G:H8	1.73	0.53
14:O:31:ILE:HG12	14:O:32:ARG:H	1.74	0.53
48:w:186:C:H2'	48:w:187:G:C8	2.43	0.53
48:w:927:C:O2	75:AN:51:GLN:NE2	2.42	0.53
49:x:200:ASP:OD2	49:x:200:ASP:N	2.40	0.53
52:0:25:LEU:HD13	52:0:37:VAL:HG11	1.90	0.53
53:1:63:LYS:NZ	72:AK:84:LYS:O	2.42	0.53
65:AD:16:ILE:HD11	65:AD:54:VAL:HG21	1.91	0.53
77:AP:22:ARG:HG2	77:AP:22:ARG:HH11	1.74	0.53
58:6:111:GLN:OE1	58:6:130:ILE:HD12	2.09	0.52
67:AF:13:GLU:OE2	67:AF:138:VAL:HG21	2.09	0.52
74:AM:57:SER:OG	74:AM:59:PHE:O	2.27	0.52
75:AN:33:MET:HE2	75:AN:73:LEU:HD21	1.92	0.52
3:D:71:C:H1'	16:Q:62:PRO:O	2.09	0.52
3:D:3897:G:H4'	7:H:254:ILE:HD12	1.91	0.52
25:Z:38:ASN:HA	25:Z:41:GLN:HB3	1.91	0.52
48:w:291:G:N2	48:w:293:C:OP2	2.33	0.52
48:w:492:C:H42	48:w:508:A:N6	2.08	0.52
48:w:1597:C:O2'	48:w:1598:G:O4'	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:z:77:SER:O	51:z:79:GLU:N	2.43	0.52
59:7:59:LYS:HG2	59:7:70:TYR:HB2	1.92	0.52
63:AB:41:GLN:NE2	63:AB:113:GLY:O	2.43	0.52
64:AC:53:GLU:OE1	64:AC:53:GLU:N	2.39	0.52
3:D:760:G:H21	3:D:904:C:H42	1.57	0.52
18:S:45:PRO:O	18:S:49:ARG:HG3	2.10	0.52
59:7:46:MET:HE2	59:7:67:PHE:CD1	2.44	0.52
60:8:57:ASP:OD2	60:8:60:CYS:N	2.41	0.52
15:P:160:GLU:O	15:P:164:ARG:HG3	2.09	0.52
24:Y:26:PRO:O	24:Y:29:THR:HG22	2.08	0.52
35:j:109:LYS:NZ	35:j:109:LYS:HB3	2.25	0.52
48:w:1324:G:HO2'	48:w:1510:G:HO2'	1.56	0.52
48:w:1415:C:O2'	67:AF:128:GLN:NE2	2.42	0.52
52:0:27:ARG:HG2	59:7:61:GLN:HE21	1.75	0.52
53:1:106:LYS:HG3	53:1:108:ARG:H	1.74	0.52
67:AF:42:HIS:NE2	67:AF:43:LYS:HE3	2.24	0.52
72:AK:42:GLU:HB3	72:AK:46:LYS:HZ2	1.74	0.52
3:D:119:G:O6	12:M:113:ARG:NH2	2.42	0.52
3:D:1852:U:H5''	31:f:22:ILE:HD11	1.92	0.52
8:I:267:TRP:CE2	8:I:279:LEU:HD11	2.45	0.52
10:K:165:LEU:HD11	10:K:176:THR:HG22	1.91	0.52
12:M:235:ARG:HG2	12:M:235:ARG:HH11	1.74	0.52
17:R:96:GLU:OE2	17:R:100:ARG:NH2	2.42	0.52
38:m:4:ILE:HD12	38:m:9:LEU:HD11	1.91	0.52
48:w:165:G:H2'	48:w:166:A2M:H8	1.91	0.52
48:w:455:A:H2'	48:w:456:C:C6	2.44	0.52
55:3:18:VAL:HG11	55:3:24:LEU:HD21	1.91	0.52
55:3:79:LYS:HD3	55:3:86:PRO:HG3	1.92	0.52
71:AJ:123:VAL:HG12	71:AJ:124:LYS:HG3	1.91	0.52
3:D:967:C:O2'	3:D:969:C:OP2	2.27	0.52
3:D:4415:A:H4'	14:O:74:LYS:HE2	1.91	0.52
15:P:160:GLU:HA	15:P:163:MET:HE2	1.90	0.52
45:t:36:GLN:OE1	45:t:40:ARG:NH1	2.43	0.52
48:w:492:C:H42	48:w:508:A:H62	1.56	0.52
48:w:857:U:H2'	48:w:858:A:C8	2.45	0.52
48:w:1255:G:OP1	48:w:1256:G:O2'	2.22	0.52
57:5:142:SER:O	57:5:146:GLN:HB3	2.10	0.52
57:5:150:ASP:HA	57:5:153:LYS:NZ	2.24	0.52
3:D:4352:U:P	16:Q:190:ARG:HH22	2.32	0.52
3:D:4623:OMG:OP1	7:H:19:ARG:NH2	2.43	0.52
15:P:84:GLU:HG2	15:P:170:TYR:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:106:TYR:O	36:k:108:SER:N	2.43	0.52
48:w:603:C:N4	48:w:620:G:O6	2.42	0.52
48:w:1239:U:H5''	63:AB:124:LYS:HD2	1.92	0.52
53:1:204:SER:OG	53:1:205:PHE:N	2.41	0.52
58:6:82:VAL:HA	58:6:87:LEU:O	2.09	0.52
79:AR:62:HIS:CD2	79:AR:88:ARG:HG3	2.45	0.52
7:H:294:LYS:NZ	7:H:295:ASP:OD1	2.43	0.52
12:M:156:VAL:O	12:M:156:VAL:HG12	2.10	0.52
16:Q:150:LEU:HD23	16:Q:154:VAL:HG12	1.91	0.52
36:k:106:TYR:HB2	36:k:107:PRO:HD3	1.91	0.52
48:w:1300:U:H3'	63:AB:51:ARG:HH12	1.74	0.52
79:AR:234:ASP:HB3	79:AR:252:THR:HB	1.92	0.52
5:F:75:OMG:OP2	29:d:74:TYR:OH	2.25	0.52
7:H:300:LYS:HD2	7:H:301:ASN:N	2.25	0.52
12:M:165:GLU:C	12:M:167:VAL:H	2.18	0.52
18:S:124:ASP:OD1	18:S:125:SER:N	2.42	0.52
40:o:33:THR:HA	40:o:40:PRO:HD3	1.92	0.52
56:4:11:PRO:HD3	56:4:44:ASN:HD22	1.75	0.52
68:AG:22:ILE:HG13	68:AG:89:ILE:HB	1.92	0.52
68:AG:56:MET:HA	68:AG:56:MET:HE2	1.91	0.52
79:AR:126:ASP:OD1	79:AR:128:THR:OG1	2.28	0.52
3:D:175:C:H2'	3:D:176:G:H8	1.74	0.52
3:D:1447:C:H2'	3:D:1448:G:C8	2.44	0.52
7:H:139:ASP:OD2	7:H:140:GLU:N	2.42	0.52
8:I:218:ILE:HA	8:I:229:LEU:HD22	1.91	0.52
14:O:51:HIS:CD2	14:O:168:SER:HB2	2.45	0.52
16:Q:135:LYS:O	16:Q:136:LYS:HG2	2.10	0.52
48:w:494:C:N4	48:w:509:OMG:HN22	2.08	0.52
48:w:1743:G:H21	48:w:1791:A:H62	1.57	0.52
49:x:48:ILE:HD13	65:AD:102:THR:HG22	1.90	0.52
49:x:137:ALA:HB1	49:x:142:LEU:HB3	1.92	0.52
79:AR:143:GLN:NE2	79:AR:145:GLU:OE2	2.43	0.52
3:D:659:G:H2'	3:D:660:A:C8	2.44	0.51
3:D:4472:G:O2'	43:r:100:TYR:O	2.28	0.51
8:I:269:LYS:HB3	8:I:269:LYS:NZ	2.25	0.51
9:J:155:THR:OG1	9:J:179:ARG:NH2	2.41	0.51
16:Q:65:ARG:HD2	16:Q:66:TYR:CE2	2.45	0.51
48:w:557:U:H2'	48:w:558:G:C8	2.45	0.51
3:D:43:U:H5''	18:S:85:VAL:HG23	1.91	0.51
21:V:157:GLY:O	21:V:188:ASN:ND2	2.43	0.51
25:Z:65:ARG:HG2	25:Z:65:ARG:NH1	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:73:HIS:CD2	28:c:115:LYS:HZ3	2.28	0.51
48:w:529:A:H61	48:w:554:A:H61	1.58	0.51
48:w:566:U:H3	48:w:584:G:H1	1.56	0.51
48:w:957:A:OP1	62:AA:57:THR:OG1	2.26	0.51
48:w:1653:U:H3	48:w:1671:G:H1	1.56	0.51
51:z:187:ARG:HD3	51:z:192:LEU:HD12	1.92	0.51
79:AR:44:LYS:HB3	79:AR:54:ILE:HG13	1.91	0.51
3:D:4492:U:OP2	7:H:7:SER:OG	2.25	0.51
3:D:4894:A:H3'	3:D:4895:C:H5'	1.92	0.51
52:0:81:GLU:N	52:0:81:GLU:OE1	2.41	0.51
54:2:168:THR:OG1	54:2:171:GLU:OE2	2.17	0.51
59:7:3:MET:HG2	59:7:47:LYS:HZ3	1.73	0.51
3:D:1777:C:O2'	9:J:2:GLY:HA2	2.11	0.51
48:w:465:A:H4'	48:w:466:G:O5'	2.10	0.51
48:w:1519:U:O2'	48:w:1520:G:H5'	2.09	0.51
52:0:135:GLU:HB2	52:0:157:MET:HE3	1.92	0.51
55:3:118:GLU:OE2	55:3:119:LYS:NZ	2.42	0.51
56:4:100:ILE:HG12	56:4:125:VAL:HG21	1.93	0.51
79:AR:70:VAL:HG11	79:AR:113:PHE:HB2	1.93	0.51
7:H:28:LYS:HG3	7:H:30:LYS:HG3	1.93	0.51
42:q:16:LYS:HD3	42:q:49:LEU:HD22	1.92	0.51
48:w:913:A:OP1	56:4:99:ARG:NH2	2.43	0.51
60:8:151:THR:HA	61:9:133:ARG:HH12	1.75	0.51
61:9:116:ILE:HD12	61:9:116:ILE:H	1.75	0.51
79:AR:143:GLN:HE21	79:AR:145:GLU:HG2	1.76	0.51
3:D:86:U:O2'	31:f:65:ARG:NH1	2.44	0.51
17:R:95:ILE:O	17:R:96:GLU:HB3	2.10	0.51
48:w:332:G:N7	55:3:189:ARG:NH2	2.53	0.51
48:w:656:G:H5'	48:w:662:G:N2	2.26	0.51
60:8:61:PRO:HA	60:8:66:VAL:HG23	1.92	0.51
72:AK:54:VAL:HG13	72:AK:55:ILE:HG23	1.92	0.51
3:D:1301:C:H2'	3:D:1302:U:H4'	1.92	0.51
13:N:76:HIS:O	13:N:80:MET:HG2	2.11	0.51
23:X:161:ARG:HG3	23:X:161:ARG:HH11	1.74	0.51
48:w:507:G:OP2	48:w:508:A:H8	1.94	0.51
48:w:1636:G:H21	54:2:164:ARG:HH22	1.59	0.51
51:z:198:ALA:HB1	51:z:202:THR:HG21	1.91	0.51
53:1:209:HIS:ND1	53:1:219:ALA:HB2	2.26	0.51
54:2:35:LEU:HD21	54:2:146:ARG:HD3	1.92	0.51
58:6:142:VAL:HG21	58:6:147:PHE:CE1	2.45	0.51
62:AA:34:PHE:HB3	62:AA:41:PHE:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AG:20:ILE:HD12	68:AG:20:ILE:O	2.10	0.51
3:D:2621:A:OP1	25:Z:80:LYS:NZ	2.42	0.51
25:Z:107:LYS:O	25:Z:108:GLU:HG3	2.11	0.51
37:l:41:ALA:O	37:l:52:ARG:HD2	2.11	0.51
48:w:70:G:H21	48:w:79:A:H62	1.59	0.51
48:w:985:G:H4'	62:AA:138:ASP:OD1	2.11	0.51
49:x:38:ILE:HG12	49:x:47:TYR:HD1	1.76	0.51
49:x:173:LEU:HD21	49:x:177:MET:HE3	1.92	0.51
54:2:43:GLU:OE1	54:2:44:LYS:HG3	2.10	0.51
33:h:51:ASN:HD21	46:u:41:PHE:C	2.16	0.51
48:w:654:A:OP2	48:w:655:A:O2'	2.24	0.51
48:w:1826:G:OP1	63:AB:145:LYS:NZ	2.35	0.51
53:1:94:LYS:NZ	72:AK:19:GLN:OE1	2.38	0.51
55:3:42:GLY:O	55:3:46:LYS:NZ	2.44	0.51
65:AD:103:LYS:HA	65:AD:106:LEU:HB2	1.93	0.51
69:AH:1:MET:H3	69:AH:9:VAL:HG22	1.76	0.51
70:AI:77:PRO:HG2	70:AI:79:PHE:CE2	2.46	0.51
72:AK:44:LEU:HA	72:AK:47:MET:SD	2.51	0.51
4:E:119:U:H2'	9:J:261:VAL:HG11	1.93	0.51
8:I:267:TRP:CZ2	8:I:279:LEU:HD11	2.46	0.51
10:K:50:LEU:HD23	10:K:50:LEU:H	1.76	0.51
17:R:112:VAL:HG11	19:T:201:LEU:HD21	1.93	0.51
45:t:69:ARG:HG3	45:t:82:MET:HE1	1.93	0.51
52:0:29:LEU:HD22	52:0:58:VAL:HG12	1.93	0.51
53:1:143:ASP:N	53:1:143:ASP:OD1	2.44	0.51
65:AD:98:VAL:HG13	65:AD:103:LYS:NZ	2.26	0.51
66:AE:80:PRO:HG2	67:AF:36:THR:HG21	1.92	0.51
68:AG:25:THR:HG22	68:AG:86:LYS:HE2	1.91	0.51
3:D:1570:G:N7	46:u:3:LYS:NZ	2.60	0.50
25:Z:45:GLU:CD	25:Z:45:GLU:H	2.19	0.50
48:w:203:G:H2'	48:w:204:G:C8	2.45	0.50
55:3:221:LYS:HG2	55:3:225:GLN:HE22	1.76	0.50
56:4:130:LEU:HD21	56:4:156:VAL:HG21	1.93	0.50
60:8:13:GLN:NE2	60:8:36:TYR:HB3	2.26	0.50
3:D:37:U:H4'	31:f:32:ARG:HD2	1.92	0.50
3:D:661:C:H2'	3:D:662:C:C6	2.46	0.50
3:D:1199:G:H2'	3:D:1200:G:C8	2.46	0.50
3:D:3710:G:H4'	3:D:3711:A:C8	2.47	0.50
15:P:15:LEU:HD23	15:P:15:LEU:H	1.77	0.50
26:a:107:ASN:OD1	26:a:108:ASN:N	2.44	0.50
48:w:39:A:H62	48:w:515:G:H21	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:579:C:O2	72:AK:61:ARG:NH1	2.40	0.50
48:w:591:U:H4'	48:w:592:C:O5'	2.11	0.50
48:w:1745:A:O3'	55:3:31:ARG:NH1	2.44	0.50
49:x:12:GLU:HG2	65:AD:111:PHE:HE1	1.75	0.50
49:x:50:ASN:HB3	49:x:53:ARG:HG2	1.92	0.50
2:B:52:G:O2'	2:B:53:5MU:OP1	2.29	0.50
3:D:908:G:H2'	3:D:909:A:H8	1.77	0.50
3:D:2351:OMC:HM23	8:I:95:MET:HG3	1.93	0.50
3:D:3765:G:O2'	3:D:3767:C:N4	2.44	0.50
8:I:201:ARG:HG2	8:I:201:ARG:NH1	2.26	0.50
9:J:217:ASP:HA	9:J:220:LYS:HD3	1.93	0.50
32:g:91:ARG:HB3	32:g:94:ASP:OD1	2.11	0.50
36:k:50:VAL:HG22	36:k:69:VAL:HG12	1.94	0.50
36:k:78:HIS:HB3	36:k:83:MET:O	2.12	0.50
48:w:807:G:H1	48:w:856:C:H5	1.58	0.50
48:w:984:C:O2'	62:AA:138:ASP:HB3	2.11	0.50
48:w:1543:U:H4'	64:AC:43:GLU:CD	2.36	0.50
49:x:147:LEU:O	49:x:165:ASN:ND2	2.37	0.50
58:6:102:ILE:HG23	58:6:103:GLU:OE2	2.10	0.50
63:AB:53:GLN:CD	63:AB:53:GLN:H	2.18	0.50
78:AQ:81:ARG:CZ	78:AQ:84:LYS:HB3	2.41	0.50
3:D:4537:C:H2'	3:D:4538:G:C8	2.46	0.50
7:H:17:LEU:O	7:H:19:ARG:N	2.45	0.50
9:J:262:LYS:H	9:J:262:LYS:HD2	1.77	0.50
15:P:146:ARG:HG2	15:P:147:ARG:HG2	1.92	0.50
16:Q:19:GLN:HA	16:Q:22:VAL:HG13	1.93	0.50
19:T:183:LYS:NZ	19:T:183:LYS:HB3	2.26	0.50
25:Z:40:GLU:HG2	25:Z:44:GLN:HE22	1.77	0.50
25:Z:66:SER:HB3	25:Z:69:LYS:HB2	1.93	0.50
55:3:32:MET:HA	55:3:52:ILE:HG23	1.93	0.50
57:5:89:GLU:O	57:5:93:THR:HG22	2.11	0.50
59:7:49:MET:HA	59:7:52:LEU:HD23	1.93	0.50
61:9:128:TYR:O	61:9:131:THR:OG1	2.26	0.50
63:AB:81:ARG:HH12	63:AB:120:SER:HG	1.59	0.50
3:D:2814:C:H5'	3:D:2815:A2M:OP2	2.12	0.50
26:a:111:GLU:CD	26:a:111:GLU:H	2.19	0.50
48:w:372:U:OP1	60:8:136:LYS:NZ	2.27	0.50
48:w:844:U:H2'	48:w:845:G:C8	2.46	0.50
48:w:1543:U:P	64:AC:37:ARG:HH12	2.34	0.50
53:1:79:ASP:HB3	53:1:82:TYR:HB2	1.92	0.50
73:AL:62:VAL:O	73:AL:65:TYR:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:AM:45:VAL:HG23	74:AM:46:GLU:H	1.76	0.50
3:D:181:C:N4	3:D:254:G:O6	2.44	0.50
3:D:494:U:H2'	3:D:495:C:C6	2.47	0.50
48:w:526:A:O2'	58:6:125:HIS:ND1	2.43	0.50
48:w:606:G:H8	78:AQ:131:ASN:HD21	1.60	0.50
51:z:108:LYS:HE3	51:z:110:MET:HB3	1.94	0.50
57:5:122:GLY:O	57:5:167:GLN:NE2	2.44	0.50
57:5:140:LYS:HD2	57:5:141:ARG:HB2	1.93	0.50
62:AA:61:LYS:HE3	62:AA:80:ASP:OD1	2.11	0.50
71:AJ:52:LEU:HD11	71:AJ:73:GLN:HB2	1.93	0.50
2:C:23:U:H2'	2:C:24:A:C8	2.46	0.50
3:D:963:G:O6	3:D:2095:A:N6	2.45	0.50
3:D:1367:C:O2'	3:D:1369:C:OP2	2.28	0.50
3:D:2705:G:H1	3:D:2710:C:H42	1.58	0.50
3:D:4895:C:H3'	3:D:4895:C:OP2	2.10	0.50
12:M:57:TRP:HB3	12:M:61:ILE:HD11	1.94	0.50
13:N:8:GLN:HG2	13:N:74:CYS:SG	2.52	0.50
48:w:932:G:O2'	48:w:934:G:OP2	2.26	0.50
48:w:1751:C:N4	48:w:1782:G:H1	2.09	0.50
49:x:33:GLN:OE1	49:x:33:GLN:HA	2.12	0.50
53:1:48:LEU:HD23	53:1:48:LEU:O	2.11	0.50
56:4:82:GLU:OE1	56:4:82:GLU:HA	2.10	0.50
64:AC:40:GLU:H	64:AC:40:GLU:CD	2.20	0.50
65:AD:78:ARG:O	65:AD:81:ARG:HG3	2.11	0.50
3:D:2083:C:OP2	21:V:14:ARG:NH1	2.39	0.50
48:w:464:A:H5'	48:w:465:A:N7	2.25	0.50
48:w:1388:A:N6	52:0:161:GLY:HA3	2.27	0.50
50:y:59:SER:HB3	50:y:63:LYS:NZ	2.27	0.50
57:5:81:VAL:HG23	57:5:91:VAL:HG23	1.93	0.50
61:9:4:MET:HE3	61:9:121:ARG:HE	1.76	0.50
65:AD:81:ARG:HD2	65:AD:82:ASP:N	2.27	0.50
69:AH:49:GLN:OE1	69:AH:49:GLN:HA	2.10	0.50
71:AJ:19:ASP:OD1	71:AJ:20:GLN:N	2.44	0.50
79:AR:56:GLN:HG2	79:AR:57:ARG:H	1.77	0.50
10:K:101:ASN:OD1	10:K:105:ARG:NH2	2.44	0.50
37:l:46:CYS:HB3	37:l:82:MET:HE3	1.93	0.50
48:w:198:U:O2'	48:w:202:G:O6	2.29	0.50
51:z:121:ARG:HH12	51:z:123:ARG:NH2	2.09	0.50
61:9:5:HIS:HB3	61:9:117:LEU:HD11	1.94	0.50
3:D:2705:G:H1	3:D:2710:C:N4	2.10	0.49
3:D:4455:G:H5''	7:H:5:LYS:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:5027:C:OP2	57:5:77:ARG:NH1	2.33	0.49
5:F:70:G:N2	5:F:87:G:O2'	2.43	0.49
20:U:54:GLN:HA	20:U:83:TRP:CD1	2.47	0.49
48:w:465:A:H5'	48:w:466:G:C4	2.46	0.49
48:w:951:C:H1'	62:AA:50:LYS:NZ	2.27	0.49
51:z:80:GLU:H	51:z:80:GLU:CD	2.20	0.49
64:AC:76:GLY:O	64:AC:80:GLN:HG3	2.11	0.49
69:AH:41:LYS:H	69:AH:41:LYS:CE	2.24	0.49
3:D:210:C:O2'	3:D:233:U:O2	2.26	0.49
3:D:278:G:H5''	18:S:8:GLN:HE22	1.76	0.49
3:D:387:G:O2'	3:D:412:G:O6	2.16	0.49
3:D:1202:C:N3	3:D:1203:G:O2'	2.44	0.49
9:J:83:LEU:N	9:J:84:PRO:HD2	2.26	0.49
48:w:974:C:O2	62:AA:55:ARG:NH1	2.45	0.49
55:3:197:GLN:H	55:3:197:GLN:CD	2.20	0.49
60:8:4:ILE:HD12	60:8:54:THR:O	2.12	0.49
64:AC:42:ILE:HD11	64:AC:48:GLN:HA	1.95	0.49
65:AD:13:ALA:O	65:AD:17:ILE:HG13	2.12	0.49
72:AK:109:GLU:OE2	72:AK:113:ARG:NH2	2.43	0.49
3:D:3612:C:H1'	3:D:5016:A:H8	1.77	0.49
3:D:4734:A:O2'	3:D:4735:G:OP2	2.29	0.49
13:N:93:ARG:HD2	13:N:143:GLU:HG2	1.93	0.49
20:U:9:GLU:H	20:U:9:GLU:CD	2.15	0.49
37:l:5:LEU:HD11	37:l:32:TYR:CZ	2.47	0.49
48:w:570:C:O2'	72:AK:34:THR:O	2.26	0.49
48:w:1265:A:H2	48:w:1517:G:H22	1.60	0.49
52:0:79:PHE:HE2	52:0:84:VAL:HB	1.77	0.49
55:3:225:GLN:HA	55:3:228:ILE:HG22	1.94	0.49
3:D:1380:G:N2	3:D:1381:U:O4	2.37	0.49
3:D:2480:G:H2'	3:D:2481:G:H8	1.76	0.49
3:D:2743:A:O2'	6:G:21:LYS:NZ	2.45	0.49
3:D:4635:A:H8	3:D:5048:A:N6	2.10	0.49
7:H:285:TYR:CD1	7:H:363:ILE:HD13	2.47	0.49
12:M:187:LYS:HG3	12:M:198:THR:HB	1.94	0.49
19:T:175:MET:HE3	19:T:175:MET:O	2.12	0.49
48:w:493:A:H1'	48:w:574:A:H5'	1.94	0.49
48:w:1743:G:N2	48:w:1791:A:H62	2.09	0.49
53:1:100:ARG:HB2	53:1:114:ILE:HD13	1.94	0.49
61:9:49:GLN:O	61:9:53:ILE:HG22	2.12	0.49
68:AG:32:LEU:HD12	68:AG:87:ARG:HG3	1.94	0.49
74:AM:60:ASP:N	74:AM:60:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:121:GLY:HA3	9:J:168:ASP:O	2.13	0.49
13:N:74:CYS:O	13:N:78:GLN:HG2	2.12	0.49
14:O:34:PHE:HD2	14:O:89:VAL:HG23	1.77	0.49
25:Z:38:ASN:O	25:Z:42:PHE:N	2.43	0.49
60:8:103:GLU:OE1	71:AJ:11:ARG:NH1	2.45	0.49
61:9:87:ASP:HB2	61:9:125:LEU:HD21	1.95	0.49
62:AA:51:GLU:OE1	62:AA:51:GLU:HA	2.10	0.49
64:AC:97:GLN:NE2	64:AC:105:LYS:HE3	2.24	0.49
79:AR:296:GLN:HG2	79:AR:311:GLN:HE22	1.76	0.49
3:D:1431:C:H2'	3:D:1432:G:O4'	2.13	0.49
3:D:4125:C:H5'	12:M:45:ILE:HD12	1.95	0.49
15:P:151:ILE:HG13	15:P:152:GLY:H	1.77	0.49
22:W:140:GLU:O	22:W:144:LYS:HE2	2.13	0.49
38:m:3:LYS:HE2	38:m:3:LYS:N	2.28	0.49
48:w:1617:G:N2	48:w:1619:A:H3'	2.27	0.49
48:w:1693:G:N2	48:w:1834:A:H8	2.10	0.49
51:z:194:ARG:O	51:z:224:THR:HA	2.13	0.49
52:0:64:ARG:O	52:0:68:GLU:HB2	2.13	0.49
65:AD:33:ARG:NH2	65:AD:36:GLU:OE1	2.45	0.49
3:D:963:G:H22	3:D:2093:A:N6	2.06	0.49
3:D:1574:G:O2'	3:D:1575:A:H8	1.94	0.49
15:P:54:ARG:HG3	15:P:55:TYR:CD2	2.47	0.49
20:U:9:GLU:OE2	20:U:9:GLU:N	2.27	0.49
36:k:93:PRO:O	36:k:95:LYS:N	2.46	0.49
48:w:596:U:OP1	71:AJ:137:LYS:NZ	2.43	0.49
48:w:1243:U:OP2	48:w:1518:C:O2'	2.22	0.49
54:2:56:TYR:HA	54:2:62:ARG:HD2	1.95	0.49
57:5:136:ILE:HG22	57:5:137:LEU:HD12	1.95	0.49
60:8:128:VAL:HG12	60:8:142:VAL:HA	1.95	0.49
79:AR:256:ILE:HB	79:AR:270:LEU:HD12	1.93	0.49
3:D:660:A:N6	3:D:661:C:N3	2.60	0.49
3:D:2096:G:N3	3:D:2096:G:H2'	2.28	0.49
15:P:112:HIS:HE1	15:P:117:ILE:HD13	1.76	0.49
29:d:53:ASP:O	29:d:70:VAL:HG12	2.13	0.49
34:i:19:GLU:OE2	34:i:101:LYS:NZ	2.46	0.49
48:w:166:A2M:H8	48:w:166:A2M:H5''	1.95	0.49
48:w:1432:U:H2'	48:w:1438:A:C8	2.48	0.49
53:1:247:THR:OG1	53:1:250:GLU:OE2	2.30	0.49
56:4:10:LYS:HE3	56:4:20:GLU:HG3	1.94	0.49
72:AK:80:ASP:OD1	72:AK:81:TYR:N	2.45	0.49
72:AK:92:ALA:HB2	72:AK:97:TYR:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:699:C:O2'	3:D:968:C:O2	2.30	0.49
3:D:1095:A:H2	3:D:1200:G:H22	1.61	0.49
20:U:46:LYS:NZ	20:U:46:LYS:HB2	2.28	0.49
21:V:148:VAL:HG12	21:V:152:PHE:CZ	2.48	0.49
48:w:166:A2M:HM'2	55:3:11:GLY:HA2	1.95	0.49
48:w:1204:A:O2'	48:w:1700:C:OP2	2.24	0.49
48:w:1230:C:OP1	66:AE:130:ARG:NH2	2.46	0.49
49:x:30:LEU:HD13	49:x:47:TYR:CE1	2.48	0.49
50:y:52:THR:HA	50:y:57:ILE:HA	1.94	0.49
57:5:177:SER:OG	57:5:182:CYS:SG	2.50	0.49
58:6:55:LYS:HA	58:6:58:ARG:HG3	1.93	0.49
3:D:151:G:OP2	18:S:4:TYR:OH	2.27	0.49
3:D:1296:G:H2'	3:D:1297:U:O4'	2.13	0.49
3:D:1601:A:O2'	40:o:2:THR:HG21	2.13	0.49
7:H:153:MET:HB3	7:H:194:LEU:HD11	1.94	0.49
29:d:52:ASP:OD1	29:d:110:LYS:HG2	2.13	0.49
41:p:7:GLU:OE1	41:p:7:GLU:HA	2.12	0.49
48:w:191:A:H5''	57:5:140:LYS:HE2	1.95	0.49
48:w:522:A:N6	48:w:644:OMG:OP1	2.46	0.49
48:w:1230:C:H5'	48:w:1607:A:O2'	2.12	0.49
48:w:1482:C:OP1	77:AP:54:LYS:NZ	2.40	0.49
53:1:21:ASP:OD2	53:1:24:THR:HG23	2.13	0.49
53:1:163:ASP:HB3	53:1:166:THR:HG22	1.95	0.49
55:3:183:ARG:HA	55:3:186:GLN:NE2	2.28	0.49
79:AR:16:GLY:H	79:AR:305:ASN:CB	2.26	0.49
3:D:1279:A:O2'	3:D:1281:G:N7	2.39	0.48
3:D:3599:A:H2'	3:D:3600:G:H8	1.78	0.48
3:D:4913:G:H4'	3:D:4914:C:O5'	2.12	0.48
6:G:82:ILE:HD11	6:G:99:GLY:HA3	1.95	0.48
13:N:92:MET:HE2	13:N:179:ILE:HG22	1.95	0.48
17:R:99:GLU:O	17:R:103:LYS:HG2	2.13	0.48
23:X:84:TYR:CE1	23:X:93:MET:HE3	2.47	0.48
33:h:11:LEU:O	33:h:14:ILE:HG22	2.13	0.48
48:w:442:C:O4'	55:3:92:ARG:NH2	2.46	0.48
56:4:10:LYS:NZ	56:4:17:ASP:OD1	2.45	0.48
57:5:141:ARG:HG3	57:5:144:LYS:HB3	1.94	0.48
60:8:47:PRO:O	60:8:51:ILE:HD12	2.13	0.48
71:AJ:24:ASP:OD1	71:AJ:26:GLN:N	2.46	0.48
74:AM:36:ILE:HB	74:AM:73:TYR:HB2	1.94	0.48
3:D:184:U:N3	3:D:189:G:N7	2.60	0.48
3:D:1633:G:H5'	3:D:1634:A:OP1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2611:A:H5'	3:D:2688:G:H4'	1.95	0.48
19:T:118:MET:HE3	23:X:167:PHE:O	2.12	0.48
45:t:73:VAL:C	45:t:78:ARG:HH22	2.21	0.48
48:w:77:A:OP1	48:w:78:C:N4	2.46	0.48
48:w:1747:C:H2'	48:w:1748:G:O4'	2.13	0.48
51:z:166:ARG:HD3	51:z:181:PRO:HG3	1.95	0.48
51:z:193:VAL:HG11	51:z:240:THR:HA	1.96	0.48
53:1:19:MET:SD	53:1:51:ARG:NH1	2.80	0.48
57:5:101:ILE:HD12	57:5:190:LEU:HD11	1.95	0.48
3:D:739:G:O2'	3:D:740:G:H8	1.95	0.48
11:L:220:MET:O	11:L:221:LYS:HG2	2.14	0.48
17:R:132:LYS:HE2	17:R:132:LYS:HB3	1.60	0.48
24:Y:115:LYS:HB2	24:Y:115:LYS:NZ	2.27	0.48
48:w:595:U:O2'	48:w:596:U:OP2	2.28	0.48
48:w:818:A:OP1	58:6:80:ARG:NH2	2.43	0.48
48:w:1311:C:N4	48:w:1312:G:O6	2.46	0.48
62:AA:82:ALA:HA	62:AA:124:MET:HE3	1.95	0.48
64:AC:58:LEU:HB3	64:AC:62:ARG:HD2	1.96	0.48
68:AG:24:LEU:O	68:AG:32:LEU:HD11	2.12	0.48
79:AR:35:SER:OG	79:AR:36:ARG:N	2.46	0.48
3:D:1071:C:N4	10:K:65:ARG:O	2.46	0.48
3:D:1175:A:H2	3:D:1185:G:H22	1.61	0.48
3:D:1179:U:H3'	3:D:1180:C:H5''	1.94	0.48
3:D:1214:C:N4	32:g:90:SER:OG	2.45	0.48
3:D:5016:A:N6	3:D:5033:G:O2'	2.38	0.48
7:H:370:THR:O	7:H:370:THR:HG22	2.14	0.48
10:K:190:HIS:HB3	10:K:193:PHE:HD2	1.77	0.48
17:R:33:GLN:HG2	17:R:33:GLN:O	2.14	0.48
26:a:30:ASP:OD1	26:a:30:ASP:N	2.46	0.48
28:c:73:HIS:CD2	28:c:115:LYS:NZ	2.82	0.48
34:i:64:ILE:HG23	34:i:68:LEU:HD23	1.95	0.48
48:w:655:A:H4'	48:w:656:G:H3'	1.95	0.48
48:w:1378:A:OP2	49:x:102:ARG:NH2	2.46	0.48
48:w:1839:U:H1'	48:w:1863:A:H2	1.79	0.48
52:0:142:LEU:HG	52:0:150:MET:HE1	1.95	0.48
53:1:63:LYS:O	53:1:67:GLN:HG2	2.13	0.48
76:AO:13:ARG:N	76:AO:33:GLU:O	2.45	0.48
4:E:24:C:H2'	4:E:25:G:O4'	2.13	0.48
7:H:290:GLY:O	7:H:301:ASN:ND2	2.45	0.48
9:J:118:ILE:HG23	9:J:135:ILE:HD11	1.95	0.48
13:N:97:ALA:HB1	43:r:77:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:113:ILE:HG21	15:P:119:TYR:HD1	1.79	0.48
48:w:504:G:N1	48:w:505:G:C6	2.82	0.48
48:w:600:G:H2'	48:w:601:OMG:C8	2.48	0.48
49:x:156:TYR:HD1	69:AH:60:ARG:HB3	1.78	0.48
52:0:162:ASP:O	52:0:164:VAL:N	2.44	0.48
52:0:196:GLY:H	52:0:201:LYS:HE3	1.79	0.48
53:1:42:LEU:HD11	53:1:46:ILE:HD11	1.96	0.48
53:1:44:LEU:HD21	53:1:72:ILE:HD11	1.95	0.48
59:7:26:ASP:N	59:7:26:ASP:OD1	2.47	0.48
75:AN:38:PRO:O	75:AN:40:CYS:N	2.47	0.48
79:AR:132:TRP:HA	79:AR:138:CYS:HA	1.96	0.48
3:D:418:A:H62	5:F:16:G:H1'	1.77	0.48
3:D:1699:A:H1'	11:L:177:ARG:HD3	1.94	0.48
3:D:4942:C:H4'	10:K:154:THR:HG23	1.94	0.48
24:Y:64:VAL:HG13	24:Y:72:VAL:HG13	1.95	0.48
36:k:54:LYS:O	36:k:66:LYS:NZ	2.41	0.48
48:w:149:A:H3'	48:w:150:A:C8	2.49	0.48
48:w:869:A:C5	56:4:114:GLN:HG3	2.47	0.48
50:y:222:LYS:HE2	50:y:222:LYS:HB3	1.57	0.48
56:4:143:ARG:HB3	70:AI:51:GLU:OE1	2.14	0.48
76:AO:13:ARG:NH1	76:AO:55:VAL:HG22	2.28	0.48
3:D:385:A:N3	3:D:387:G:H5''	2.29	0.48
3:D:987:C:O2'	3:D:988:C:OP1	2.25	0.48
3:D:1553:A:N6	3:D:1574:G:H1'	2.29	0.48
43:r:79:GLU:CD	43:r:81:SER:HG	2.18	0.48
52:0:157:MET:HE1	52:0:187:LYS:HB3	1.95	0.48
53:1:127:ARG:N	53:1:140:VAL:O	2.47	0.48
58:6:77:LEU:HA	58:6:80:ARG:HE	1.79	0.48
66:AE:10:GLN:HB2	66:AE:57:GLY:HA2	1.95	0.48
67:AF:111:LYS:HE2	67:AF:124:THR:HG21	1.95	0.48
3:D:1176:C:H42	3:D:1184:A:H61	1.62	0.48
3:D:2266:C:O2'	47:v:39:ARG:NH1	2.47	0.48
16:Q:48:PRO:HA	16:Q:149:GLN:HG2	1.96	0.48
24:Y:80:VAL:HG22	24:Y:81:LYS:H	1.79	0.48
48:w:561:A:H5''	58:6:164:PRO:HG2	1.96	0.48
48:w:616:A:N1	48:w:632:C:H1'	2.28	0.48
48:w:955:A:N1	48:w:968:U:O2'	2.43	0.48
55:3:5:ILE:HG21	55:3:45:TRP:HH2	1.78	0.48
55:3:91:GLU:OE2	55:3:93:LYS:HE3	2.14	0.48
56:4:66:VAL:N	56:4:67:PRO:HD2	2.28	0.48
77:AP:30:LEU:HA	77:AP:39:CYS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1167:C:H2'	3:D:1168:G:H5''	1.96	0.48
7:H:29:VAL:HG12	7:H:31:SER:H	1.78	0.48
20:U:111:SER:HB2	20:U:153:LYS:O	2.13	0.48
45:t:22:LYS:NZ	45:t:22:LYS:HB3	2.28	0.48
48:w:818:A:H5'	58:6:73:GLU:OE1	2.13	0.48
49:x:63:ARG:HG3	49:x:185:MET:HE1	1.96	0.48
49:x:205:ARG:NH2	49:x:210:ILE:HD13	2.28	0.48
53:1:254:LYS:HD2	53:1:254:LYS:H	1.78	0.48
58:6:60:LEU:HA	58:6:63:LEU:HD12	1.94	0.48
73:AL:60:LYS:HA	73:AL:60:LYS:HD2	1.65	0.48
79:AR:178:ASN:HB3	79:AR:183:LYS:N	2.28	0.48
3:D:3641:U:OP2	3:D:3646:A:N6	2.43	0.48
3:D:4742:G:H2'	3:D:4743:G:H8	1.79	0.48
9:J:112:ARG:C	9:J:114:GLY:H	2.22	0.48
10:K:162:VAL:HG23	10:K:177:GLY:H	1.79	0.48
13:N:173:ARG:HB3	43:r:127:VAL:HB	1.94	0.48
15:P:18:ARG:H	15:P:134:LEU:HA	1.78	0.48
31:f:37:GLY:H	31:f:41:HIS:HB2	1.79	0.48
32:g:35:VAL:HG23	32:g:40:LEU:HG	1.96	0.48
48:w:1114:U:O2'	48:w:1115:U:H2'	2.14	0.48
50:y:223:PHE:O	50:y:224:GLU:HG3	2.14	0.48
52:0:34:TYR:CE1	52:0:37:VAL:HG13	2.49	0.48
55:3:58:LYS:HA	55:3:107:SER:OG	2.14	0.48
58:6:75:ASN:O	58:6:79:ARG:N	2.32	0.48
60:8:136:LYS:O	60:8:139:ARG:NH1	2.39	0.48
67:AF:139:ALA:O	67:AF:143:LYS:HG2	2.14	0.48
68:AG:88:LEU:O	68:AG:89:ILE:HD13	2.14	0.48
68:AG:107:GLU:HG2	68:AG:108:PRO:HD3	1.95	0.48
3:D:389:A:H1'	29:d:91:ASN:HA	1.96	0.47
3:D:1590:C:H5''	3:D:1591:U:O5'	2.14	0.47
10:K:112:MET:HG3	10:K:113:PRO:HD2	1.95	0.47
35:j:21:ILE:HD12	35:j:33:ARG:HG3	1.96	0.47
45:t:71:GLU:HB3	45:t:80:LYS:HG2	1.95	0.47
48:w:830:A:H61	48:w:844:U:H3	1.62	0.47
64:AC:123:ASP:OD2	64:AC:125:ARG:HG2	2.14	0.47
79:AR:206:LEU:HD23	79:AR:218:LEU:HD23	1.95	0.47
2:B:9:1MA:O4'	2:B:46:A:H1'	2.15	0.47
3:D:1961:G:H21	3:D:2025:A:H62	1.61	0.47
3:D:4291:G:H5''	3:D:4293:PSU:C6	2.49	0.47
3:D:5016:A:N3	3:D:5016:A:H2'	2.28	0.47
7:H:56:ILE:HD12	7:H:365:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:564:A:H2'	48:w:565:G:O4'	2.14	0.47
48:w:1016:U:H5'	61:9:15:ALA:O	2.14	0.47
50:y:140:VAL:HG13	50:y:213:ARG:HB2	1.96	0.47
52:0:186:VAL:O	52:0:188:ILE:HG13	2.14	0.47
53:1:231:GLY:HA3	53:1:233:LYS:HZ2	1.79	0.47
56:4:70:LYS:HA	56:4:73:GLN:HG3	1.95	0.47
58:6:79:ARG:HA	58:6:82:VAL:HG12	1.95	0.47
3:D:736:C:OP1	17:R:74:ARG:NH1	2.47	0.47
10:K:157:HIS:HB3	10:K:160:LYS:HD2	1.95	0.47
23:X:15:ARG:HB3	23:X:27:LEU:HD23	1.96	0.47
26:a:111:GLU:N	26:a:111:GLU:OE2	2.48	0.47
38:m:4:ILE:O	38:m:4:ILE:HG13	2.15	0.47
48:w:511:U:H2'	48:w:512:A2M:C8	2.44	0.47
48:w:588:G:H5''	48:w:590:A2M:H4'	1.95	0.47
50:y:227:LYS:HA	50:y:230:GLU:OE2	2.15	0.47
58:6:40:LYS:O	58:6:43:VAL:HG22	2.14	0.47
61:9:132:LYS:HA	61:9:132:LYS:HD3	1.64	0.47
79:AR:11:LEU:HD23	79:AR:43:TRP:CE3	2.49	0.47
3:D:737:C:C5	3:D:739:G:H5''	2.49	0.47
6:G:117:GLU:OE2	6:G:163:ARG:NH1	2.47	0.47
12:M:159:HIS:ND1	12:M:185:LYS:HA	2.29	0.47
16:Q:51:ALA:HB2	16:Q:149:GLN:HE22	1.79	0.47
29:d:83:GLU:OE2	29:d:84:ARG:NH2	2.47	0.47
48:w:1606:G:N2	48:w:1632:G:H2'	2.29	0.47
53:1:168:LYS:HE3	53:1:169:ILE:N	2.29	0.47
55:3:147:LEU:HD11	55:3:156:TYR:CG	2.49	0.47
55:3:159:ARG:HB2	55:3:171:THR:HG22	1.96	0.47
64:AC:27:ARG:HB2	64:AC:95:TYR:OH	2.14	0.47
70:AI:55:ASP:HB3	75:AN:25:VAL:HG13	1.97	0.47
70:AI:114:GLU:OE1	70:AI:114:GLU:HA	2.15	0.47
70:AI:114:GLU:OE1	70:AI:118:ARG:NH2	2.41	0.47
71:AJ:48:LYS:HB3	71:AJ:99:GLU:OE1	2.15	0.47
3:D:433:A:C2	3:D:3867:A:H4'	2.49	0.47
3:D:1574:G:HO2'	3:D:1575:A:P	2.38	0.47
5:F:96:C:OP1	38:m:70:ARG:NH1	2.48	0.47
11:L:25:PHE:HD2	11:L:29:LYS:HZ3	1.61	0.47
48:w:334:C:OP2	55:3:190:ARG:NH2	2.28	0.47
49:x:198:MET:HG3	49:x:199:PRO:HD2	1.96	0.47
52:0:151:LYS:O	52:0:153:VAL:HG13	2.15	0.47
79:AR:178:ASN:O	79:AR:182:CYS:HA	2.13	0.47
3:D:280:G:H5''	18:S:14:LYS:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:965:G:N2	3:D:2092:G:H1'	2.30	0.47
12:M:105:GLU:HB2	12:M:109:GLU:HB2	1.96	0.47
25:Z:34:MET:HE3	25:Z:34:MET:HB2	1.77	0.47
29:d:51:LYS:O	29:d:70:VAL:HG13	2.15	0.47
41:p:34:PHE:HE1	41:p:47:ILE:HD11	1.79	0.47
48:w:1621:U:OP1	63:AB:40:ARG:HG2	2.14	0.47
53:1:139:LEU:HG	53:1:150:PRO:HG3	1.97	0.47
53:1:141:THR:OG1	53:1:143:ASP:OD1	2.25	0.47
70:AI:69:LEU:HG	70:AI:70:ASN:O	2.15	0.47
3:D:173:C:H5'	16:Q:129:ARG:HH12	1.79	0.47
9:J:33:ARG:O	9:J:37:VAL:HG12	2.14	0.47
10:K:46:ARG:HB2	10:K:65:ARG:HH21	1.80	0.47
12:M:57:TRP:CE3	12:M:61:ILE:HD11	2.50	0.47
20:U:125:MET:HE3	20:U:141:SER:OG	2.14	0.47
30:e:41:ALA:HB2	30:e:77:TYR:HE1	1.79	0.47
36:k:78:HIS:HB2	36:k:85:ARG:HG3	1.96	0.47
45:t:105:GLN:HG3	45:t:106:PHE:H	1.79	0.47
48:w:146:G:P	55:3:140:ARG:HH22	2.38	0.47
48:w:902:G:C6	48:w:903:A:H8	2.32	0.47
48:w:1736:G:H2'	48:w:1737:G:H8	1.74	0.47
49:x:22:GLY:C	49:x:24:HIS:H	2.23	0.47
49:x:213:GLU:HA	49:x:216:ALA:HB3	1.97	0.47
50:y:174:ARG:HB3	50:y:175:GLU:OE1	2.14	0.47
55:3:22:ARG:HA	55:3:25:ARG:HD3	1.95	0.47
58:6:94:LEU:HD23	58:6:94:LEU:H	1.79	0.47
60:8:4:ILE:HD11	60:8:56:ILE:HD11	1.96	0.47
64:AC:15:ARG:HA	64:AC:19:ALA:O	2.14	0.47
64:AC:51:LEU:O	64:AC:54:PRO:HD2	2.15	0.47
64:AC:96:TYR:HA	64:AC:100:VAL:HG22	1.95	0.47
70:AI:24:GLN:HE22	75:AN:8:LEU:HD11	1.79	0.47
70:AI:86:LEU:HD21	70:AI:113:HIS:HB2	1.96	0.47
3:D:93:G:H2'	3:D:94:A:C8	2.50	0.47
3:D:2485:U:H2'	3:D:2486:G:H8	1.80	0.47
3:D:4739:C:H2'	3:D:4740:G:H5'	1.96	0.47
9:J:256:LYS:CD	9:J:256:LYS:H	2.28	0.47
14:O:182:GLU:HA	14:O:182:GLU:OE1	2.15	0.47
21:V:71:LYS:HD2	21:V:71:LYS:O	2.15	0.47
48:w:868:G:N2	56:4:111:LYS:HD2	2.27	0.47
48:w:1082:A:H2'	48:w:1084:A:H5''	1.96	0.47
48:w:1370:A:N3	48:w:1372:U:H5'	2.30	0.47
65:AD:37:GLU:CD	65:AD:37:GLU:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:188:G:N1	3:D:191:G:O6	2.28	0.47
3:D:958:G:H21	10:K:125:LEU:H	1.63	0.47
3:D:1475:G:H2'	3:D:1476:C:C6	2.50	0.47
5:F:92:U:H2'	5:F:93:C:O4'	2.14	0.47
12:M:158:ALA:HB2	12:M:190:LEU:HD12	1.96	0.47
26:a:99:GLU:HG3	27:b:21:TYR:OH	2.15	0.47
48:w:382:C:H2'	48:w:383:G:C8	2.46	0.47
48:w:1030:A:H2'	48:w:1031:A2M:H8	1.97	0.47
48:w:1128:C:OP1	75:AN:17:ARG:NE	2.48	0.47
48:w:1240:A:C2	63:AB:100:LYS:HB2	2.50	0.47
48:w:1515:G:N2	63:AB:99:GLY:O	2.41	0.47
48:w:1535:U:O2'	48:w:1536:G:OP2	2.33	0.47
49:x:184:ARG:HG2	49:x:191:ARG:HG2	1.96	0.47
64:AC:58:LEU:HD22	64:AC:108:ILE:HG12	1.97	0.47
79:AR:16:GLY:H	79:AR:305:ASN:HB3	1.79	0.47
79:AR:162:ASN:O	79:AR:164:ILE:N	2.47	0.47
3:D:1820:C:O2'	3:D:1821:G:N7	2.47	0.47
3:D:4694:G:O2'	13:N:71:ARG:NH2	2.48	0.47
7:H:308:ASP:O	7:H:309:LEU:HD23	2.15	0.47
10:K:111:LYS:HE3	47:v:87:ARG:HH12	1.79	0.47
11:L:95:ILE:O	11:L:223:LYS:HD2	2.14	0.47
13:N:63:ASN:O	13:N:67:LEU:HB2	2.15	0.47
17:R:32:ASP:HA	23:X:145:PHE:CZ	2.49	0.47
20:U:154:GLU:H	20:U:154:GLU:CD	2.23	0.47
30:e:89:ILE:HD13	30:e:121:ARG:HE	1.80	0.47
37:l:69:LYS:HG3	37:l:73:HIS:CD2	2.50	0.47
51:z:170:TRP:CD1	70:AI:97:ARG:NH1	2.82	0.47
53:1:183:VAL:HG13	53:1:224:ASN:HB3	1.96	0.47
53:1:230:LYS:H	53:1:235:TRP:HE1	1.63	0.47
55:3:216:ARG:HA	55:3:216:ARG:NE	2.30	0.47
72:AK:47:MET:HE1	72:AK:48:TYR:CD2	2.50	0.47
3:D:1339:U:H2'	3:D:1340:OMC:C6	2.49	0.46
3:D:1780:A:N3	14:O:198:LYS:NZ	2.63	0.46
3:D:4405:G:H5'	14:O:8:CYS:SG	2.55	0.46
3:D:4600:G:O2'	3:D:4601:U:P	2.73	0.46
5:F:16:G:O2'	5:F:17:A:O5'	2.34	0.46
23:X:7:LEU:O	23:X:103:ALA:HB1	2.15	0.46
48:w:126:G:N1	55:3:192:ILE:HD11	2.30	0.46
55:3:46:LYS:O	55:3:118:GLU:HG2	2.15	0.46
55:3:193:ALA:HA	55:3:196:LYS:HE3	1.96	0.46
60:8:117:PHE:C	60:8:119:ASP:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:9:83:ASP:N	61:9:83:ASP:OD1	2.46	0.46
66:AE:81:ASP:OD1	66:AE:95:TYR:HD2	1.98	0.46
66:AE:86:ARG:HG2	66:AE:106:LYS:HE3	1.96	0.46
68:AG:26:SER:OG	68:AG:27:ARG:N	2.47	0.46
74:AM:43:ASN:HA	74:AM:66:LYS:HA	1.97	0.46
3:D:302:C:OP1	18:S:68:ARG:HB2	2.15	0.46
3:D:4281:A:O2'	3:D:4282:A:H2'	2.15	0.46
9:J:263:LYS:HA	9:J:263:LYS:CE	2.44	0.46
12:M:144:THR:O	12:M:148:GLU:HG3	2.15	0.46
17:R:128:LYS:HB2	17:R:128:LYS:NZ	2.29	0.46
19:T:10:ASP:OD1	19:T:37:ARG:HD3	2.16	0.46
22:W:105:LEU:HD23	22:W:138:LEU:HD23	1.97	0.46
38:m:82:ASP:OD2	38:m:82:ASP:N	2.48	0.46
47:v:97:ILE:CG2	47:v:107:ARG:HB3	2.44	0.46
48:w:165:G:H1'	55:3:110:ASN:HD21	1.80	0.46
48:w:834:C:N4	48:w:835:C:N3	2.63	0.46
48:w:877:C:O2	48:w:910:G:N2	2.48	0.46
48:w:886:A:N1	48:w:901:G:H1'	2.30	0.46
48:w:1351:G:O2'	48:w:1378:A:N1	2.43	0.46
52:0:55:THR:HA	52:0:58:VAL:HG22	1.98	0.46
52:0:80:PRO:O	52:0:83:SER:OG	2.32	0.46
58:6:35:TYR:HA	58:6:123:ILE:HD13	1.97	0.46
58:6:111:GLN:HE21	58:6:145:PRO:CB	2.27	0.46
58:6:147:PHE:HD2	58:6:148:ILE:N	2.13	0.46
64:AC:107:GLU:H	64:AC:107:GLU:CD	2.18	0.46
65:AD:76:GLU:O	65:AD:79:GLU:HB3	2.15	0.46
69:AH:1:MET:N	69:AH:9:VAL:HG22	2.30	0.46
79:AR:73:SER:HB2	79:AR:117:ASN:HD21	1.80	0.46
3:D:1773:OMU:H2'	3:D:1774:C:C6	2.49	0.46
23:X:84:TYR:HE1	23:X:93:MET:HE3	1.79	0.46
31:f:72:THR:HG22	31:f:110:LYS:HB3	1.98	0.46
47:v:108:MET:O	47:v:112:ARG:HG2	2.15	0.46
48:w:172:OMU:N3	48:w:337:C:O2'	2.47	0.46
48:w:1289:U:H2'	48:w:1290:G:C8	2.50	0.46
48:w:1600:G:H4'	73:AL:43:LYS:HE3	1.97	0.46
50:y:146:ARG:HB2	50:y:149:GLN:HB2	1.96	0.46
52:0:79:PHE:HB2	52:0:80:PRO:HD2	1.98	0.46
54:2:37:ASP:OD1	54:2:37:ASP:N	2.48	0.46
58:6:30:LYS:HA	78:AQ:111:TYR:CE1	2.50	0.46
61:9:11:LEU:HD12	61:9:11:LEU:O	2.16	0.46
3:D:1397:A:H5''	31:f:113:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3668:C:H5'	6:G:8:GLN:O	2.15	0.46
4:E:39:C:N3	15:P:73:THR:HG22	2.31	0.46
11:L:171:ASP:OD1	11:L:172:ASN:N	2.49	0.46
40:o:34:CYS:HB3	40:o:39:TYR:H	1.80	0.46
48:w:1415:C:H2'	48:w:1416:C:C6	2.50	0.46
51:z:170:TRP:CA	70:AI:97:ARG:HH11	2.27	0.46
51:z:211:LYS:O	51:z:215:MET:HG3	2.15	0.46
72:AK:76:TYR:OH	72:AK:86:GLU:OE1	2.19	0.46
74:AM:22:ARG:NH1	74:AM:27:ALA:O	2.47	0.46
3:D:2431:A:OP1	42:q:41:ARG:NH1	2.37	0.46
3:D:2705:G:H2'	3:D:2706:G:O4'	2.15	0.46
22:W:90:PRO:HB2	22:W:93:VAL:HG12	1.97	0.46
48:w:32:U:H4'	48:w:643:A:N6	2.30	0.46
48:w:917:U:O4'	56:4:118:ARG:HD2	2.15	0.46
48:w:1033:G:N1	48:w:1080:A:O2'	2.39	0.46
56:4:134:VAL:HG12	56:4:173:PHE:CE2	2.50	0.46
63:AB:28:MET:HG3	63:AB:32:GLN:HE21	1.80	0.46
76:AO:16:LYS:HB2	76:AO:16:LYS:HE3	1.48	0.46
3:D:1574:G:O2'	3:D:1575:A:P	2.74	0.46
3:D:3718:A2M:O5'	3:D:3718:A2M:H8	2.16	0.46
3:D:4939:C:OP1	10:K:187:ARG:NH1	2.48	0.46
8:I:228:THR:HG23	8:I:248:ARG:HH22	1.81	0.46
13:N:12:ILE:HG22	13:N:81:ILE:HD11	1.97	0.46
24:Y:159:MET:HA	24:Y:159:MET:HE3	1.98	0.46
50:y:139:CYS:SG	50:y:172:MET:HE2	2.56	0.46
54:2:35:LEU:O	54:2:39:ILE:HG12	2.15	0.46
56:4:63:PHE:CE1	56:4:95:ILE:HD11	2.51	0.46
65:AD:72:LYS:HE2	65:AD:73:LEU:HD23	1.97	0.46
66:AE:69:THR:O	66:AE:73:ASN:ND2	2.48	0.46
71:AJ:66:ILE:O	71:AJ:68:LYS:NZ	2.47	0.46
79:AR:87:LEU:HD21	79:AR:111:VAL:HG11	1.98	0.46
3:D:182:G:H1	3:D:254:G:H22	1.63	0.46
3:D:1083:U:H3	3:D:1216:C:N4	2.13	0.46
3:D:4699:U:H1'	3:D:4700:A:H5''	1.97	0.46
23:X:9:GLU:HG2	23:X:67:VAL:HB	1.97	0.46
48:w:527:C:OP1	58:6:122:SER:OG	2.23	0.46
70:AI:114:GLU:OE1	70:AI:117:ARG:NH1	2.48	0.46
76:AO:46:VAL:HG11	76:AO:56:LEU:HD21	1.98	0.46
3:D:2333:G:N7	8:I:189:MET:HE3	2.30	0.46
3:D:4717:A:OP2	7:H:30:LYS:NZ	2.42	0.46
7:H:185:VAL:HG13	7:H:193:LYS:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:128:PRO:HB3	16:Q:134:PRO:HD2	1.98	0.46
17:R:122:ILE:HB	19:T:189:ILE:HD11	1.97	0.46
17:R:124:LYS:HB2	17:R:124:LYS:NZ	2.30	0.46
23:X:45:TRP:HZ3	23:X:54:MET:HE2	1.80	0.46
28:c:72:ASP:O	28:c:76:ILE:HG12	2.15	0.46
28:c:115:LYS:NZ	28:c:115:LYS:HB3	2.31	0.46
48:w:633:C:O3'	78:AQ:86:ARG:NE	2.41	0.46
48:w:952:G:O2'	62:AA:51:GLU:OE1	2.25	0.46
64:AC:113:ILE:HD12	64:AC:114:GLN:N	2.30	0.46
3:D:3717:A:H2'	3:D:3718:A2M:C8	2.46	0.46
22:W:99:MET:HE1	22:W:127:VAL:O	2.16	0.46
25:Z:28:PRO:HB3	25:Z:100:LEU:HD11	1.98	0.46
36:k:88:PHE:CD1	36:k:92:LEU:HD21	2.51	0.46
43:r:92:ASP:O	43:r:105:PRO:HG3	2.15	0.46
48:w:39:A:H62	48:w:515:G:N2	2.13	0.46
48:w:197:U:C5	48:w:198:U:H1'	2.51	0.46
48:w:563:G:N2	48:w:592:C:O2	2.28	0.46
48:w:960:U:H1'	48:w:963:A:N7	2.30	0.46
51:z:178:HIS:CG	51:z:200:ARG:HE	2.34	0.46
55:3:221:LYS:HG3	55:3:224:ARG:NH1	2.31	0.46
59:7:52:LEU:HD22	59:7:55:ARG:HH21	1.81	0.46
64:AC:42:ILE:O	64:AC:45:ARG:HG3	2.16	0.46
66:AE:82:TRP:CD1	66:AE:82:TRP:H	2.34	0.46
79:AR:274:VAL:HG13	79:AR:276:SER:H	1.80	0.46
3:D:44:A:OP2	18:S:85:VAL:HG21	2.16	0.46
3:D:1705:G:H2'	3:D:1706:A:O4'	2.16	0.46
3:D:4546:A:N7	6:G:215:ASN:ND2	2.62	0.46
5:F:83:C:O2'	5:F:84:A:H5''	2.16	0.46
6:G:178:PRO:HG2	46:u:26:VAL:HG13	1.98	0.46
7:H:295:ASP:HA	7:H:296:GLY:HA2	1.76	0.46
48:w:60:A:N3	48:w:316:G:O2'	2.41	0.46
53:1:185:GLY:HA2	53:1:189:LEU:HD22	1.97	0.46
55:3:52:ILE:HD11	55:3:109:LEU:CD1	2.46	0.46
58:6:115:PHE:HA	58:6:120:ALA:HB3	1.98	0.46
60:8:77:VAL:HA	60:8:88:ILE:HG22	1.98	0.46
63:AB:19:GLY:N	66:AE:92:ASP:HA	2.30	0.46
68:AG:26:SER:HB2	68:AG:110:VAL:HA	1.98	0.46
75:AN:36:LYS:HD2	75:AN:80:ARG:HH12	1.81	0.46
79:AR:152:SER:HB2	79:AR:168:CYS:SG	2.56	0.46
79:AR:215:GLN:HA	79:AR:231:ASP:HA	1.98	0.46
3:D:908:G:H2'	3:D:909:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:981:C:H2'	10:K:73:TYR:CE1	2.51	0.45
8:I:74:ALA:O	8:I:76:ILE:N	2.49	0.45
38:m:22:ASP:OD2	38:m:23:ASP:N	2.50	0.45
48:w:112:U:H5'	48:w:113:G:H5'	1.98	0.45
48:w:1278:A:N6	48:w:1318:G:O6	2.49	0.45
48:w:1330:G:H4'	48:w:1331:C:H3'	1.97	0.45
48:w:1332:A:H2'	52:0:141:LYS:HE2	1.97	0.45
56:4:38:ALA:H	56:4:41:ARG:NH2	2.14	0.45
62:AA:28:PHE:HA	62:AA:92:ALA:O	2.16	0.45
65:AD:77:GLU:HG2	65:AD:80:ARG:HE	1.81	0.45
77:AP:22:ARG:HG2	77:AP:22:ARG:NH1	2.31	0.45
3:D:1613:A:H5''	6:G:183:GLY:HA2	1.97	0.45
3:D:4479:A:OP1	13:N:170:LYS:NZ	2.50	0.45
3:D:4518:A:H8	3:D:4518:A:OP2	1.99	0.45
48:w:428:OMU:H4'	58:6:2:PRO:HG3	1.98	0.45
52:0:39:VAL:HG13	52:0:48:ILE:HG22	1.97	0.45
53:1:11:ARG:HH21	53:1:20:LEU:HB3	1.82	0.45
57:5:105:ASP:HA	57:5:169:GLY:O	2.16	0.45
59:7:46:MET:HE2	59:7:67:PHE:HD1	1.80	0.45
70:AI:102:ILE:HG22	70:AI:128:PHE:HB3	1.98	0.45
79:AR:247:TRP:CE3	79:AR:258:ILE:HD11	2.52	0.45
23:X:15:ARG:HG3	23:X:16:CYS:O	2.17	0.45
25:Z:45:GLU:O	25:Z:53:ALA:HB1	2.16	0.45
48:w:570:C:O2	72:AK:34:THR:OG1	2.26	0.45
48:w:594:A:N1	48:w:642:U:O2'	2.46	0.45
55:3:230:LYS:HA	55:3:233:ARG:HG2	1.99	0.45
57:5:69:SER:HB3	60:8:19:ASN:O	2.17	0.45
59:7:49:MET:HE1	59:7:69:TRP:CZ2	2.51	0.45
63:AB:37:TYR:CE1	63:AB:41:GLN:HB3	2.51	0.45
65:AD:26:ASN:OD1	65:AD:26:ASN:N	2.45	0.45
67:AF:126:GLN:HG3	67:AF:129:ARG:HH11	1.82	0.45
69:AH:16:LYS:HD2	69:AH:21:ASN:OD1	2.16	0.45
72:AK:39:GLU:HA	72:AK:42:GLU:CD	2.41	0.45
2:C:52:G:H2'	2:C:53:5MU:C6	2.52	0.45
3:D:1702:C:H5'	8:I:308:LYS:HD2	1.97	0.45
3:D:4620:OMU:O5'	3:D:4620:OMU:H6	2.16	0.45
5:F:122:G:H1	5:F:128:C:H42	1.65	0.45
12:M:224:THR:HA	12:M:228:ASP:HB2	1.98	0.45
14:O:32:ARG:HD3	14:O:32:ARG:HA	1.88	0.45
19:T:54:TYR:OH	19:T:73:PHE:O	2.34	0.45
30:e:101:PHE:C	30:e:102:ARG:HD3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:502:C:N4	53:1:67:GLN:OE1	2.49	0.45
48:w:533:A:H2'	48:w:534:G:C8	2.51	0.45
48:w:1112:U:H2'	48:w:1113:A:H8	1.81	0.45
48:w:1228:A:H2'	48:w:1229:G:C8	2.51	0.45
48:w:1395:C:O2'	48:w:1396:A:OP1	2.32	0.45
51:z:183:LYS:HA	51:z:195:LEU:O	2.16	0.45
53:1:73:ASP:HB3	53:1:164:LEU:HD22	1.97	0.45
53:1:160:ILE:HD12	53:1:169:ILE:HG22	1.99	0.45
54:2:158:ALA:N	54:2:176:GLU:OE2	2.50	0.45
56:4:148:LEU:HA	70:AI:42:MET:SD	2.57	0.45
57:5:65:PHE:CE1	57:5:78:ILE:HD11	2.52	0.45
57:5:129:LEU:HG	57:5:132:GLU:HB2	1.98	0.45
63:AB:85:ILE:HG12	63:AB:114:HIS:O	2.17	0.45
69:AH:20:SER:OG	69:AH:22:ARG:HG2	2.16	0.45
70:AI:15:ASN:ND2	70:AI:18:GLU:OE2	2.50	0.45
79:AR:239:LEU:HB3	79:AR:250:ALA:HA	1.98	0.45
79:AR:299:PHE:HD1	79:AR:309:VAL:HG12	1.82	0.45
2:B:33:U:OP2	64:AC:146:ARG:NH1	2.49	0.45
3:D:406:C:O2'	3:D:407:A:OP1	2.31	0.45
3:D:690:C:OP2	10:K:111:LYS:NZ	2.49	0.45
3:D:987:C:H2'	3:D:988:C:C6	2.52	0.45
3:D:1354:A:OP2	21:V:106:THR:HG21	2.15	0.45
3:D:1418:C:H2'	3:D:1419:G:O4'	2.17	0.45
3:D:2529:A:O2'	3:D:2531:C:OP2	2.35	0.45
3:D:2560:C:H2'	3:D:2561:C:C6	2.51	0.45
15:P:39:VAL:HG22	15:P:123:ILE:HD12	1.98	0.45
46:u:45:THR:HG22	46:u:45:THR:O	2.16	0.45
48:w:1415:C:H2'	48:w:1416:C:H6	1.82	0.45
53:1:254:LYS:HD2	53:1:254:LYS:N	2.31	0.45
57:5:113:TYR:O	57:5:117:TYR:HB2	2.16	0.45
57:5:139:LYS:CE	57:5:146:GLN:HB2	2.46	0.45
66:AE:6:PRO:HD3	73:AL:49:LEU:HD23	1.98	0.45
70:AI:106:THR:HG23	70:AI:122:GLY:O	2.17	0.45
79:AR:104:HIS:HD2	79:AR:108:VAL:HB	1.81	0.45
3:D:1082:C:O2'	3:D:1083:U:O5'	2.28	0.45
3:D:3599:A:H2'	3:D:3600:G:C8	2.52	0.45
3:D:3773:U:H1'	3:D:3775:A:H2	1.82	0.45
3:D:3792:OMG:HM23	3:D:3792:OMG:H1'	1.81	0.45
6:G:116:LEU:HD23	6:G:164:ALA:HB2	1.97	0.45
13:N:6:SER:HB2	13:N:67:LEU:HD11	1.99	0.45
38:m:60:VAL:O	38:m:64:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1415:C:C1'	67:AF:128:GLN:HE22	2.28	0.45
51:z:69:LEU:HD11	51:z:266:TYR:HB3	1.98	0.45
51:z:137:VAL:C	51:z:162:ILE:HG13	2.42	0.45
51:z:170:TRP:CE2	51:z:199:PRO:HG3	2.52	0.45
58:6:11:LYS:HA	58:6:11:LYS:HD3	1.59	0.45
2:C:52:G:HO2'	2:C:53:5MU:P	2.39	0.45
3:D:2631:U:OP2	25:Z:48:LYS:NZ	2.49	0.45
9:J:215:ASP:C	9:J:215:ASP:OD1	2.60	0.45
47:v:68:SER:OG	47:v:69:GLY:N	2.50	0.45
62:AA:47:LEU:HD23	62:AA:47:LEU:HA	1.79	0.45
6:G:117:GLU:HA	6:G:124:GLY:HA2	1.98	0.45
9:J:79:TYR:O	9:J:82:GLU:HG2	2.17	0.45
45:t:101:GLY:HA2	45:t:102:GLN:HB3	1.98	0.45
45:t:104:ILE:HA	45:t:105:GLN:HA	1.71	0.45
48:w:670:A:O2'	48:w:1163:C:O2'	2.32	0.45
48:w:1864:U:H5'	74:AM:79:ILE:HD11	1.99	0.45
53:1:189:LEU:O	53:1:245:ARG:NH2	2.49	0.45
56:4:82:GLU:OE1	56:4:85:LYS:NZ	2.49	0.45
56:4:127:ASP:O	56:4:131:GLU:HG2	2.16	0.45
57:5:79:ILE:HG13	57:5:80:ASP:OD1	2.17	0.45
72:AK:114:MET:HA	72:AK:125:VAL:HG11	1.99	0.45
75:AN:11:SER:HB3	75:AN:14:GLU:OE1	2.17	0.45
3:D:1660:U:H2'	31:f:12:ARG:O	2.16	0.45
3:D:2480:G:H2'	3:D:2481:G:C8	2.51	0.45
10:K:118:THR:HG21	35:j:92:ASN:OD1	2.16	0.45
11:L:107:LYS:O	11:L:110:GLN:HG2	2.17	0.45
13:N:37:ASP:C	13:N:37:ASP:OD1	2.60	0.45
15:P:151:ILE:HG13	15:P:152:GLY:N	2.32	0.45
22:W:114:LYS:O	22:W:146:LYS:NZ	2.40	0.45
29:d:47:MET:HE3	29:d:47:MET:HB3	1.87	0.45
48:w:608:C:H2'	48:w:609:PSU:H6	1.81	0.45
48:w:1136:U:H2'	48:w:1137:U:C6	2.52	0.45
48:w:1265:A:H5'	48:w:1326:OMU:HM21	1.99	0.45
56:4:122:LEU:HA	56:4:125:VAL:HG22	1.99	0.45
65:AD:31:ASN:OD1	65:AD:31:ASN:N	2.50	0.45
68:AG:62:ARG:NH2	77:AP:56:ASP:OD2	2.50	0.45
76:AO:13:ARG:HH11	76:AO:55:VAL:HG22	1.81	0.45
79:AR:72:SER:HA	79:AR:113:PHE:CE2	2.52	0.45
3:D:4741:C:H4'	3:D:4742:G:H5'	1.98	0.45
12:M:210:GLU:N	12:M:210:GLU:OE2	2.49	0.45
24:Y:79:GLN:HE21	24:Y:79:GLN:C	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:103:ASP:OD1	24:Y:103:ASP:N	2.50	0.45
48:w:1639:G7M:H2'	48:w:1640:A:C8	2.52	0.45
49:x:117:ARG:HG3	49:x:119:PRO:HD3	1.99	0.45
51:z:163:VAL:HG23	69:AH:27:LYS:HZ3	1.82	0.45
54:2:152:TRP:O	54:2:156:THR:HG22	2.17	0.45
55:3:167:LYS:HB3	55:3:167:LYS:HE3	1.73	0.45
55:3:221:LYS:HG2	55:3:225:GLN:NE2	2.32	0.45
57:5:150:ASP:HA	57:5:153:LYS:HZ2	1.81	0.45
72:AK:21:LYS:HE2	72:AK:75:ILE:HG21	1.99	0.45
79:AR:244:ASN:HB3	79:AR:245:ARG:NE	2.32	0.45
3:D:1448:G:H2'	3:D:1449:C:C6	2.53	0.44
3:D:1769:G:H2'	3:D:1770:A:C8	2.50	0.44
3:D:2474:G:H2'	3:D:2502:G:N2	2.31	0.44
3:D:2527:A:OP2	22:W:38:ARG:NH2	2.49	0.44
9:J:191:ASN:OD1	9:J:194:VAL:HG23	2.16	0.44
24:Y:64:VAL:HG22	24:Y:72:VAL:HG11	1.99	0.44
34:i:92:ARG:HA	34:i:102:LEU:HD23	1.98	0.44
48:w:678:U:H2'	48:w:679:A:C8	2.52	0.44
48:w:1299:A:OP1	63:AB:59:ARG:NH2	2.48	0.44
48:w:1454:A:H5''	65:AD:3:ARG:HD2	1.97	0.44
50:y:60:ASP:OD1	50:y:60:ASP:N	2.49	0.44
50:y:167:LYS:O	50:y:171:ILE:HG12	2.16	0.44
51:z:168:GLY:HA2	69:AH:1:MET:HE1	1.98	0.44
53:1:18:TRP:N	53:1:18:TRP:CD1	2.84	0.44
53:1:210:VAL:HB	53:1:218:PHE:CE1	2.52	0.44
55:3:226:GLU:O	55:3:230:LYS:HG3	2.17	0.44
61:9:26:LEU:HD11	61:9:60:VAL:HG12	1.98	0.44
63:AB:136:THR:HG22	63:AB:138:SER:H	1.81	0.44
64:AC:101:ASP:OD1	64:AC:102:GLU:N	2.50	0.44
68:AG:22:ILE:HA	68:AG:113:GLU:O	2.17	0.44
72:AK:16:ARG:H	72:AK:16:ARG:CD	2.30	0.44
3:D:2094:G:C8	3:D:2095:A:C6	3.05	0.44
3:D:4397:A:H2'	3:D:4452:U:O4	2.18	0.44
6:G:31:ALA:HB2	6:G:123:ARG:HH21	1.82	0.44
10:K:114:ARG:HG2	47:v:87:ARG:HG3	1.99	0.44
15:P:96:LYS:O	15:P:159:LYS:NZ	2.50	0.44
16:Q:121:ARG:HG3	16:Q:121:ARG:NH1	2.32	0.44
25:Z:25:CYS:HB3	25:Z:112:LEU:HD13	1.99	0.44
48:w:494:C:H41	48:w:509:OMG:HN22	1.63	0.44
48:w:554:A:H2'	48:w:555:A:C8	2.51	0.44
48:w:874:G:H1	48:w:912:C:H42	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1752:C:H2'	48:w:1753:C:C5	2.52	0.44
49:x:34:MET:HG2	49:x:154:LEU:HD11	1.98	0.44
50:y:28:LYS:HB3	50:y:28:LYS:HE2	1.74	0.44
79:AR:49:GLU:C	79:AR:51:ASN:H	2.26	0.44
79:AR:149:GLU:HG3	79:AR:171:ASP:OD1	2.18	0.44
3:D:6:C:H2'	3:D:7:C:C6	2.53	0.44
3:D:1604:G:H2'	3:D:1605:G:C8	2.52	0.44
3:D:2872:C:H5''	44:s:25:LYS:HE2	1.99	0.44
7:H:71:GLU:OE2	27:b:1:MET:N	2.44	0.44
12:M:134:PRO:HB3	12:M:206:GLN:NE2	2.32	0.44
15:P:168:GLN:N	15:P:168:GLN:OE1	2.50	0.44
30:e:83:THR:CG2	30:e:85:TYR:HD2	2.31	0.44
34:i:40:LYS:HE2	34:i:40:LYS:HB3	1.63	0.44
48:w:379:C:OP1	57:5:56:ARG:NH1	2.50	0.44
48:w:676:C:H5''	61:9:5:HIS:HD2	1.82	0.44
48:w:927:C:H1'	75:AN:51:GLN:HE21	1.82	0.44
48:w:1233:G:C6	48:w:1526:G:C6	3.05	0.44
56:4:11:PRO:HD2	56:4:45:ILE:O	2.18	0.44
57:5:41:ARG:HD3	57:5:43:ILE:HD12	1.98	0.44
2:C:21:A:N6	2:C:47:5MC:OP2	2.49	0.44
3:D:278:G:OP2	39:n:30:ARG:NH2	2.43	0.44
3:D:1773:OMU:HM23	3:D:1773:OMU:H1'	1.56	0.44
3:D:3925:OMU:HM23	3:D:3925:OMU:H1'	1.73	0.44
3:D:4196:OMG:HM23	3:D:4196:OMG:H1'	1.65	0.44
3:D:4749:C:H2'	3:D:4750:G:O4'	2.17	0.44
43:r:99:CYS:HB2	43:r:115:CYS:HB3	2.00	0.44
49:x:40:LYS:HE3	65:AD:101:ASP:CG	2.43	0.44
55:3:217:MET:O	55:3:221:LYS:N	2.39	0.44
56:4:8:ILE:HG22	56:4:9:VAL:HG23	1.99	0.44
56:4:42:GLU:N	56:4:42:GLU:OE1	2.51	0.44
56:4:79:LEU:HD23	56:4:94:PHE:HE2	1.82	0.44
67:AF:74:SER:O	67:AF:78:ILE:HD12	2.18	0.44
69:AH:1:MET:N	69:AH:9:VAL:H	2.15	0.44
72:AK:54:VAL:HG22	72:AK:76:TYR:HB2	1.99	0.44
79:AR:5:MET:HG2	79:AR:312:VAL:HA	1.99	0.44
79:AR:7:LEU:HD12	79:AR:8:ARG:N	2.32	0.44
3:D:516:C:OP2	3:D:516:C:H6	1.99	0.44
3:D:4138:C:H2'	3:D:4139:G:C8	2.53	0.44
11:L:137:GLU:N	11:L:138:PRO:HD2	2.32	0.44
12:M:231:ASP:O	12:M:235:ARG:NH1	2.50	0.44
26:a:20:LEU:HD22	26:a:26:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:954:U:H2'	48:w:955:A:C8	2.53	0.44
48:w:1217:A:H2'	48:w:1218:C:C6	2.52	0.44
53:1:230:LYS:O	53:1:233:LYS:HD2	2.18	0.44
54:2:185:SER:H	54:2:190:ILE:HD12	1.82	0.44
56:4:83:LEU:HD21	56:4:92:VAL:HG21	1.98	0.44
57:5:110:ARG:HA	57:5:121:LEU:HD23	2.00	0.44
58:6:32:ILE:HG13	58:6:37:LEU:HB2	1.99	0.44
61:9:38:TYR:CZ	61:9:78:LYS:HG3	2.52	0.44
63:AB:98:ASN:OD1	63:AB:122:THR:HA	2.18	0.44
64:AC:109:LYS:O	64:AC:113:ILE:HG13	2.18	0.44
66:AE:62:ASP:OD1	66:AE:62:ASP:N	2.50	0.44
69:AH:62:MET:HE2	69:AH:64:GLU:HG3	1.99	0.44
3:D:124:C:OP1	18:S:144:ARG:HD2	2.18	0.44
3:D:1372:A:OP1	18:S:202:ARG:NH2	2.40	0.44
3:D:2485:U:H2'	3:D:2486:G:C8	2.53	0.44
6:G:108:PRO:HB2	46:u:86:LEU:HD22	2.00	0.44
6:G:205:ASN:HB2	6:G:206:PRO:HD2	2.00	0.44
15:P:63:ARG:HE	15:P:63:ARG:HB2	1.57	0.44
17:R:25:VAL:HG12	17:R:45:VAL:HG21	1.98	0.44
29:d:53:ASP:OD1	29:d:110:LYS:HB3	2.17	0.44
37:l:10:ARG:HD3	37:l:10:ARG:HA	1.72	0.44
42:q:28:ARG:HG3	42:q:28:ARG:NH2	2.33	0.44
45:t:64:LYS:HE2	45:t:64:LYS:HB3	1.85	0.44
48:w:444:G:N1	48:w:447:A:OP2	2.51	0.44
48:w:1634:A:C6	48:w:1635:C:C2	3.05	0.44
48:w:1636:G:H21	54:2:164:ARG:NH2	2.15	0.44
49:x:145:ILE:HG13	49:x:159:ILE:HB	1.98	0.44
51:z:105:GLU:OE1	51:z:106:VAL:N	2.46	0.44
57:5:10:LYS:HE2	60:8:136:LYS:HE3	1.99	0.44
60:8:101:ARG:HG2	71:AJ:7:LEU:HA	2.00	0.44
61:9:19:ARG:NH1	75:AN:83:GLN:HE21	2.15	0.44
63:AB:96:VAL:HG11	63:AB:116:LEU:HG	1.99	0.44
68:AG:21:ARG:HB3	68:AG:115:THR:HG23	2.00	0.44
2:C:5:C:H2'	2:C:6:2MG:O4'	2.18	0.44
3:D:1720:C:H2'	3:D:1721:G:O4'	2.17	0.44
3:D:4475:G:H5''	3:D:4476:C:H5''	1.99	0.44
3:D:4743:G:H2'	3:D:4744:A:C8	2.51	0.44
3:D:4859:C:H5''	3:D:4860:G:C8	2.53	0.44
7:H:293:ILE:HG23	7:H:294:LYS:N	2.30	0.44
10:K:150:LEU:HD11	10:K:164:PHE:HB2	1.99	0.44
23:X:69:GLU:OE2	23:X:101:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:115:LYS:HG2	24:Y:126:VAL:HG11	1.98	0.44
34:i:106:VAL:O	34:i:106:VAL:HG12	2.17	0.44
48:w:523:A:H4'	58:6:131:ARG:NE	2.33	0.44
48:w:927:C:H1'	75:AN:51:GLN:NE2	2.33	0.44
48:w:1139:C:H2'	48:w:1140:G:O4'	2.18	0.44
48:w:1556:A:H3'	77:AP:13:LYS:HZ3	1.83	0.44
48:w:1808:U:H2'	48:w:1809:A:C8	2.53	0.44
49:x:11:LYS:HB3	49:x:13:GLU:OE1	2.17	0.44
60:8:119:ASP:O	60:8:147:LYS:NZ	2.49	0.44
65:AD:7:LYS:O	65:AD:11:LYS:HG2	2.18	0.44
65:AD:92:ASP:N	65:AD:92:ASP:OD1	2.50	0.44
65:AD:119:VAL:HG12	65:AD:120:THR:C	2.43	0.44
3:D:1271:G:O2'	11:L:34:ARG:NH2	2.51	0.44
3:D:1411:C:O2'	3:D:1412:G:O5'	2.33	0.44
7:H:189:THR:O	7:H:193:LYS:HB2	2.17	0.44
36:k:93:PRO:C	36:k:95:LYS:H	2.25	0.44
48:w:57:U:H4'	48:w:504:G:H21	1.83	0.44
48:w:618:C:H2'	48:w:619:A:O4'	2.18	0.44
48:w:981:A:H2'	48:w:982:G:C8	2.53	0.44
48:w:1622:U:O2'	48:w:1623:A:OP1	2.31	0.44
50:y:108:ASP:N	50:y:108:ASP:OD1	2.48	0.44
55:3:144:LEU:HD23	55:3:145:PHE:CE1	2.53	0.44
60:8:127:THR:HG22	60:8:144:LYS:HB3	2.00	0.44
61:9:91:LEU:HG	61:9:122:ILE:HG13	1.99	0.44
63:AB:30:TYR:O	63:AB:34:MET:N	2.51	0.44
66:AE:98:VAL:HG11	66:AE:106:LYS:HE2	2.00	0.44
79:AR:289:LEU:HD22	79:AR:298:LEU:HD21	2.00	0.44
3:D:278:G:H5''	18:S:8:GLN:NE2	2.33	0.44
3:D:4146:G:H2'	3:D:4147:G:C8	2.53	0.44
13:N:23:ARG:NH2	13:N:41:ILE:O	2.51	0.44
15:P:35:ARG:O	15:P:39:VAL:HG23	2.18	0.44
20:U:29:THR:HA	20:U:32:THR:HG22	2.00	0.44
30:e:9:LYS:NZ	30:e:83:THR:O	2.38	0.44
33:h:47:ILE:HD12	33:h:94:LEU:HD11	1.99	0.44
48:w:571:U:H5''	72:AK:37:LYS:HG3	1.99	0.44
48:w:1454:A:C2	48:w:1476:A:H2'	2.53	0.44
48:w:1521:C:O2'	66:AE:136:THR:O	2.29	0.44
51:z:183:LYS:HD3	51:z:194:ARG:NH2	2.33	0.44
58:6:147:PHE:C	58:6:147:PHE:CD2	2.96	0.44
60:8:72:ILE:HD12	60:8:72:ILE:N	2.33	0.44
67:AF:128:GLN:NE2	67:AF:132:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3681:G:OP2	6:G:128:ARG:NH1	2.50	0.43
3:D:4744:A:H2'	3:D:4745:G:O4'	2.18	0.43
4:E:47:G:C2	4:E:48:G:H1'	2.53	0.43
16:Q:65:ARG:HG3	31:f:69:PHE:CD1	2.53	0.43
19:T:80:PHE:HA	19:T:83:THR:HG22	2.00	0.43
23:X:158:VAL:HG11	23:X:160:ARG:HH11	1.82	0.43
23:X:160:ARG:HD3	23:X:160:ARG:HA	1.61	0.43
30:e:83:THR:HG22	30:e:85:TYR:H	1.83	0.43
47:v:107:ARG:O	47:v:111:ILE:HG12	2.17	0.43
48:w:90:G:H2'	48:w:91:A:O4'	2.18	0.43
48:w:951:C:H1'	62:AA:50:LYS:HZ2	1.82	0.43
48:w:1446:A:O2'	48:w:1447:G:H5''	2.18	0.43
50:y:217:MET:HG2	50:y:220:LYS:NZ	2.32	0.43
54:2:194:ASP:N	54:2:194:ASP:OD1	2.50	0.43
55:3:126:ASP:N	55:3:126:ASP:OD1	2.49	0.43
74:AM:41:ILE:O	74:AM:41:ILE:HG22	2.18	0.43
79:AR:231:ASP:OD1	79:AR:232:GLY:N	2.51	0.43
3:D:760:G:N2	3:D:904:C:H42	2.15	0.43
3:D:2637:U:OP1	37:l:28:ASN:ND2	2.51	0.43
3:D:2653:C:OP2	37:l:51:GLY:HA2	2.18	0.43
3:D:3868:G:H22	3:D:3900:G:H1'	1.83	0.43
3:D:4910:G:N2	19:T:106:ASP:O	2.51	0.43
4:E:75:G:N2	4:E:100:A:OP2	2.43	0.43
41:p:19:ASP:O	41:p:38:CYS:HA	2.18	0.43
48:w:149:A:C8	48:w:150:A:C8	3.06	0.43
48:w:155:G:OP1	55:3:15:LEU:HD12	2.18	0.43
48:w:380:G:N1	48:w:383:G:OP2	2.44	0.43
48:w:619:A:O2'	48:w:621:C:N4	2.35	0.43
48:w:811:A:O2'	48:w:812:A:OP1	2.34	0.43
50:y:27:LYS:HA	50:y:51:ARG:NH2	2.33	0.43
57:5:62:VAL:HA	57:5:77:ARG:HA	2.00	0.43
58:6:111:GLN:CD	58:6:127:ARG:HA	2.42	0.43
67:AF:37:VAL:C	67:AF:39:LEU:H	2.26	0.43
75:AN:19:HIS:HB3	75:AN:21:LYS:O	2.17	0.43
79:AR:282:GLU:O	79:AR:284:PRO:HD3	2.17	0.43
3:D:1834:U:H2'	24:Y:116:LYS:HE2	2.01	0.43
3:D:2382:A:N1	3:D:2829:U:O2'	2.47	0.43
3:D:4625:C:O2'	3:D:4626:A:H5'	2.19	0.43
3:D:4992:G:H2'	3:D:4993:G:C8	2.53	0.43
7:H:297:LYS:HE3	7:H:297:LYS:HB3	1.73	0.43
16:Q:7:GLY:O	31:f:49:HIS:NE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:145:LYS:C	16:Q:146:LEU:HD12	2.44	0.43
23:X:99:ASP:OD1	23:X:100:LEU:N	2.46	0.43
48:w:433:A:H2'	48:w:434:G:C8	2.53	0.43
48:w:560:A:H5'	58:6:174:LYS:HB3	2.00	0.43
48:w:869:A:C4	48:w:915:G:H1'	2.53	0.43
48:w:1259:A:H1'	48:w:1264:C:N4	2.33	0.43
48:w:1678:A2M:HM'3	48:w:1678:A2M:H1'	1.60	0.43
51:z:76:LYS:HD2	51:z:76:LYS:HA	1.77	0.43
51:z:109:ILE:HD13	51:z:126:ALA:HA	2.00	0.43
53:1:118:GLU:HA	53:1:121:TYR:CE2	2.52	0.43
53:1:198:ARG:NE	53:1:200:ARG:HE	2.13	0.43
55:3:215:LYS:HB3	55:3:216:ARG:NH1	2.33	0.43
57:5:76:THR:HG21	57:5:104:ILE:HD12	2.01	0.43
58:6:42:GLU:H	58:6:42:GLU:HG2	1.64	0.43
58:6:164:PRO:HB3	58:6:170:PRO:HA	1.99	0.43
79:AR:40:ILE:HB	79:AR:59:LEU:HD12	2.00	0.43
79:AR:282:GLU:N	79:AR:283:PRO:HD3	2.33	0.43
2:C:17:G:HO2'	2:C:56:G:H22	1.55	0.43
6:G:14:SER:H	6:G:17:ARG:HE	1.65	0.43
8:I:347:HIS:O	8:I:351:VAL:HG22	2.18	0.43
9:J:262:LYS:HD2	9:J:262:LYS:N	2.33	0.43
10:K:50:LEU:HD22	10:K:56:ARG:HA	2.00	0.43
11:L:164:LYS:HD3	11:L:164:LYS:HA	1.83	0.43
18:S:136:ASP:OD1	18:S:139:HIS:HB2	2.19	0.43
26:a:13:LYS:HD2	26:a:128:LEU:HD11	2.00	0.43
32:g:16:TRP:CD1	32:g:21:ILE:HD11	2.53	0.43
48:w:97:U:O2	48:w:434:G:N2	2.51	0.43
48:w:113:G:N2	48:w:292:A:H1'	2.33	0.43
48:w:453:C:O2'	55:3:92:ARG:O	2.35	0.43
48:w:678:U:H2'	48:w:679:A:H8	1.82	0.43
48:w:1103:C:OP1	50:y:157:GLN:NE2	2.46	0.43
49:x:110:ASN:C	49:x:111:GLN:HG3	2.44	0.43
51:z:165:VAL:HG11	51:z:217:ALA:HB1	2.01	0.43
52:0:102:ALA:HB2	52:0:186:VAL:HG21	1.99	0.43
54:2:43:GLU:C	54:2:45:TYR:H	2.25	0.43
54:2:171:GLU:OE2	54:2:171:GLU:N	2.39	0.43
57:5:206:LYS:HD3	57:5:206:LYS:HA	1.87	0.43
58:6:136:ARG:HB3	58:6:141:VAL:HG12	1.99	0.43
59:7:5:LYS:HE3	59:7:5:LYS:HB3	1.57	0.43
59:7:53:LYS:HE3	59:7:53:LYS:HB3	1.85	0.43
66:AE:33:ILE:HG23	66:AE:100:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:AL:77:LEU:HB3	73:AL:79:ILE:HG12	2.00	0.43
75:AN:21:LYS:C	75:AN:23:ARG:H	2.27	0.43
1:A:28:G:H1	48:w:1331:C:N4	2.07	0.43
3:D:208:A:H2	3:D:233:U:H5''	1.83	0.43
3:D:508:G:H21	31:f:85:GLN:HE22	1.66	0.43
3:D:1083:U:H3	3:D:1216:C:H41	1.67	0.43
3:D:4591:U:H2'	3:D:4592:C:C6	2.53	0.43
3:D:4691:A:H5'	13:N:71:ARG:NH1	2.33	0.43
15:P:144:LYS:HE2	15:P:146:ARG:O	2.18	0.43
53:1:145:ARG:NH1	53:1:162:ILE:HD12	2.33	0.43
58:6:107:GLU:O	58:6:112:THR:OG1	2.36	0.43
65:AD:102:THR:O	65:AD:105:MET:HG3	2.17	0.43
68:AG:19:ARG:NH1	68:AG:92:HIS:HB3	2.33	0.43
79:AR:17:TRP:HE3	79:AR:303:THR:HA	1.83	0.43
3:D:490:C:H2'	3:D:491:G:C8	2.54	0.43
3:D:4393:G:O4'	3:D:4447:5MC:HM53	2.18	0.43
3:D:4637:OMG:H1'	3:D:4637:OMG:HM23	1.75	0.43
12:M:206:GLN:O	12:M:206:GLN:CD	2.61	0.43
17:R:36:ALA:HB2	17:R:52:PHE:CZ	2.54	0.43
45:t:77:CYS:C	45:t:78:ARG:HD2	2.44	0.43
48:w:21:U:O2'	48:w:22:A:H5'	2.18	0.43
48:w:212:C:H2'	48:w:213:G:C8	2.54	0.43
48:w:799:OMU:HM23	48:w:799:OMU:H1'	1.56	0.43
48:w:1158:G:O3'	70:AI:76:SER:OG	2.23	0.43
49:x:9:GLN:H	49:x:11:LYS:NZ	2.16	0.43
55:3:46:LYS:HD3	55:3:46:LYS:HA	1.86	0.43
58:6:93:LYS:HG2	58:6:96:TYR:HD2	1.82	0.43
67:AF:126:GLN:HG3	67:AF:129:ARG:NH1	2.33	0.43
3:D:923:C:O2'	3:D:924:C:O4'	2.37	0.43
3:D:3943:A:H5'	3:D:3944:OMG:OP2	2.19	0.43
3:D:4870:G:O6	23:X:157:ARG:NH1	2.51	0.43
3:D:5021:C:H3'	3:D:5022:U:H5''	2.00	0.43
9:J:212:MET:HE3	9:J:219:TYR:CZ	2.54	0.43
37:l:105:LYS:HB2	37:l:105:LYS:NZ	2.33	0.43
47:v:32:LEU:O	47:v:33:LYS:HB2	2.19	0.43
48:w:70:G:N2	48:w:79:A:H62	2.17	0.43
48:w:142:C:H41	48:w:330:G:P	2.41	0.43
48:w:1597:C:H4'	48:w:1603:G:O6	2.17	0.43
52:0:115:VAL:HG11	52:0:142:LEU:HD11	2.01	0.43
52:0:129:SER:O	52:0:129:SER:OG	2.32	0.43
54:2:187:SER:HB3	54:2:190:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4:75:ILE:HG22	56:4:79:LEU:HB2	2.01	0.43
57:5:40:PRO:HG2	57:5:59:ARG:NH2	2.34	0.43
78:AQ:86:ARG:HH12	78:AQ:91:LYS:NZ	2.17	0.43
79:AR:33:SER:CB	79:AR:43:TRP:HE1	2.31	0.43
79:AR:40:ILE:HB	79:AR:59:LEU:HB2	2.01	0.43
3:D:462:G:H2'	3:D:463:A:C8	2.54	0.43
3:D:505:G:H22	3:D:653:U:H3	1.65	0.43
3:D:2029:A:H2'	3:D:2030:A:C8	2.54	0.43
3:D:2669:C:H2'	3:D:2670:C:O4'	2.19	0.43
3:D:2693:G:OP1	41:p:35:LYS:NZ	2.42	0.43
3:D:3923:A:H2'	3:D:3924:C:C6	2.54	0.43
3:D:4260:U:H2'	3:D:4261:C:C6	2.53	0.43
3:D:4773:C:O2'	3:D:4774:C:H5'	2.19	0.43
7:H:92:TYR:HB2	7:H:159:VAL:HB	2.01	0.43
8:I:154:VAL:HG11	8:I:174:LEU:HD11	2.00	0.43
11:L:240:ILE:HD12	11:L:240:ILE:HA	1.92	0.43
16:Q:135:LYS:HD3	16:Q:136:LYS:HB3	2.00	0.43
33:h:20:LEU:HG	33:h:101:ASP:OD1	2.18	0.43
33:h:51:ASN:HB2	33:h:77:ASN:HB2	2.01	0.43
48:w:179:C:H3'	48:w:180:G:C8	2.54	0.43
48:w:222:U:H5''	60:8:17:PHE:CD2	2.54	0.43
53:1:104:ASP:N	53:1:108:ARG:O	2.49	0.43
59:7:4:PRO:HD2	59:7:7:ASN:OD1	2.19	0.43
67:AF:1:MET:HE3	67:AF:1:MET:HB3	1.76	0.43
67:AF:23:LYS:HA	67:AF:23:LYS:HD2	1.63	0.43
3:D:165:A:N6	3:D:270:U:H3	2.16	0.43
3:D:3710:G:H5'	3:D:3711:A:OP1	2.19	0.43
9:J:135:ILE:HG13	9:J:138:GLN:HB2	2.00	0.43
28:c:127:LEU:O	28:c:134:LYS:HA	2.19	0.43
31:f:125:LYS:HA	31:f:145:VAL:O	2.19	0.43
48:w:17:C:H2'	48:w:18:C:C6	2.53	0.43
48:w:445:A:H4'	57:5:50:GLY:O	2.19	0.43
48:w:527:C:H42	48:w:558:G:H1	1.66	0.43
48:w:831:G:H2'	48:w:832:G:H8	1.84	0.43
48:w:918:U:P	61:9:64:ARG:HH12	2.36	0.43
48:w:1401:A:N6	48:w:1441:U:O2'	2.52	0.43
48:w:1746:U:H4'	55:3:65:GLN:NE2	2.33	0.43
49:x:33:GLN:HB3	49:x:154:LEU:HD12	1.99	0.43
52:0:79:PHE:CE2	52:0:84:VAL:HB	2.52	0.43
53:1:104:ASP:CG	53:1:110:ALA:HB2	2.44	0.43
56:4:12:ASN:OD1	56:4:12:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AE:53:THR:HG23	66:AE:54:LYS:HE3	2.01	0.43
75:AN:83:GLN:NE2	75:AN:84:HIS:OXT	2.52	0.43
76:AO:34:PHE:C	76:AO:36:ASP:H	2.27	0.43
11:L:87:PRO:HG2	11:L:144:TYR:CE2	2.54	0.43
12:M:180:PRO:HG2	12:M:219:VAL:HG13	2.00	0.43
15:P:154:LYS:H	15:P:154:LYS:HG2	1.62	0.43
17:R:63:LYS:HE2	17:R:63:LYS:HB2	1.88	0.43
36:k:63:LYS:HB2	36:k:63:LYS:NZ	2.34	0.43
48:w:475:C:H1'	48:w:507:G:H2'	2.00	0.43
48:w:1472:C:H2'	48:w:1473:G:O4'	2.18	0.43
48:w:1737:G:H2'	48:w:1738:C:C6	2.53	0.43
49:x:111:GLN:HA	49:x:116:PHE:CG	2.53	0.43
51:z:104:ASP:OD1	51:z:104:ASP:C	2.61	0.43
53:1:103:TYR:CD1	53:1:189:LEU:HD11	2.54	0.43
54:2:144:LEU:HD23	76:AO:49:PRO:HG2	2.01	0.43
54:2:191:LYS:HB2	54:2:191:LYS:HE3	1.71	0.43
55:3:4:ASN:HB3	55:3:110:ASN:HA	2.00	0.43
63:AB:23:ASP:OD1	63:AB:24:GLN:N	2.52	0.43
63:AB:49:LEU:HD12	63:AB:53:GLN:HB2	2.00	0.43
68:AG:23:THR:OG1	68:AG:113:GLU:HB2	2.19	0.43
69:AH:80:SER:O	69:AH:83:PHE:N	2.49	0.43
74:AM:22:ARG:NH1	74:AM:27:ALA:HB1	2.34	0.43
3:D:4457:PSU:H1'	7:H:252:ALA:HB3	2.01	0.42
3:D:4938:A:P	10:K:183:ARG:HH21	2.42	0.42
6:G:200:ARG:NH2	6:G:217:GLN:OE1	2.52	0.42
8:I:25:PRO:HG2	8:I:28:PHE:CE2	2.54	0.42
8:I:315:LYS:HD2	11:L:168:ALA:HB1	2.00	0.42
13:N:44:GLU:HB3	13:N:58:ASP:HB2	2.01	0.42
16:Q:185:ALA:HB2	39:n:7:MET:HE1	2.01	0.42
26:a:65:VAL:HG23	26:a:73:ARG:HA	2.01	0.42
32:g:99:ILE:O	32:g:109:ARG:NH1	2.52	0.42
48:w:36:PSU:HN3	48:w:519:A:H61	1.66	0.42
48:w:440:G:O2'	48:w:1737:G:H1'	2.19	0.42
48:w:678:U:OP2	48:w:1026:C:N4	2.43	0.42
48:w:1481:G:O3'	77:AP:54:LYS:NZ	2.52	0.42
49:x:51:LEU:HA	49:x:54:THR:HB	2.00	0.42
53:1:188:ASN:N	53:1:188:ASN:HD22	2.17	0.42
53:1:230:LYS:H	53:1:235:TRP:NE1	2.17	0.42
53:1:235:TRP:N	53:1:235:TRP:CD1	2.86	0.42
55:3:188:LYS:O	55:3:192:ILE:HG22	2.18	0.42
57:5:113:TYR:CG	57:5:121:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:7:16:PHE:CZ	59:7:89:ILE:HG12	2.54	0.42
59:7:62:PHE:HD2	59:7:67:PHE:CE2	2.37	0.42
60:8:93:LEU:HD23	60:8:104:LYS:HA	2.01	0.42
65:AD:24:LEU:CD2	65:AD:34:VAL:HG21	2.49	0.42
79:AR:17:TRP:CD1	79:AR:36:ARG:HG2	2.54	0.42
79:AR:89:LEU:HB2	79:AR:99:ARG:HB3	2.01	0.42
3:D:75:G:H3'	16:Q:74:ARG:HD2	2.01	0.42
17:R:104:MET:SD	19:T:199:HIS:HB3	2.59	0.42
48:w:2:A:H8	48:w:2:A:OP1	2.02	0.42
48:w:1144:A:H5'	48:w:1355:C:H41	1.84	0.42
48:w:1232:PSU:H2'	48:w:1233:G:C8	2.51	0.42
52:0:5:ILE:HG22	52:0:10:LYS:HE3	2.01	0.42
52:0:40:ARG:HH12	68:AG:108:PRO:C	2.26	0.42
54:2:48:TYR:CZ	64:AC:56:LEU:HD23	2.54	0.42
55:3:32:MET:SD	55:3:100:CYS:HB2	2.60	0.42
58:6:121:LYS:HB3	58:6:121:LYS:HE3	1.72	0.42
65:AD:25:GLY:H	65:AD:31:ASN:HD21	1.66	0.42
69:AH:80:SER:O	69:AH:82:ASN:N	2.52	0.42
3:D:2563:C:H3'	3:D:2564:G:C8	2.54	0.42
22:W:181:LYS:HA	22:W:181:LYS:HD3	1.84	0.42
27:b:54:LEU:HD23	27:b:54:LEU:HA	1.84	0.42
40:o:67:LEU:HD23	40:o:67:LEU:HA	1.93	0.42
48:w:85:A:H2'	48:w:86:C:C6	2.54	0.42
48:w:384:U:H5'	60:8:133:PRO:O	2.20	0.42
52:0:27:ARG:O	59:7:61:GLN:NE2	2.50	0.42
54:2:73:THR:O	54:2:89:THR:HG21	2.18	0.42
59:7:49:MET:O	59:7:52:LEU:HB2	2.20	0.42
61:9:15:ALA:HB2	75:AN:20:LYS:HD3	2.01	0.42
68:AG:28:ASN:OD1	68:AG:28:ASN:C	2.63	0.42
72:AK:86:GLU:OE2	72:AK:90:ARG:NH1	2.52	0.42
73:AL:69:THR:HG22	73:AL:71:ALA:H	1.84	0.42
79:AR:38:LYS:HA	79:AR:66:VAL:HG23	2.02	0.42
79:AR:153:CYS:SG	79:AR:197:THR:HA	2.59	0.42
3:D:2092:G:O2'	3:D:2093:A:OP2	2.36	0.42
3:D:2787:A2M:HM'1	3:D:2789:A:H3'	1.99	0.42
3:D:3910:C:H2'	3:D:3911:C:C6	2.55	0.42
9:J:125:VAL:HG23	9:J:126:THR:H	1.83	0.42
12:M:157:ILE:H	12:M:157:ILE:HG13	1.57	0.42
17:R:24:LEU:H	17:R:43:THR:HG21	1.85	0.42
32:g:20:GLY:O	32:g:22:LYS:HG2	2.20	0.42
45:t:14:LYS:HD2	45:t:77:CYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:130:G:H2'	48:w:130:G:N3	2.34	0.42
48:w:1204:A:H2'	48:w:1205:C:O4'	2.20	0.42
48:w:1679:A:H2'	54:2:60:ARG:HD2	2.01	0.42
51:z:85:SER:O	51:z:85:SER:OG	2.35	0.42
52:0:98:ALA:HB1	52:0:186:VAL:HG23	2.01	0.42
54:2:106:GLU:OE2	54:2:106:GLU:HA	2.19	0.42
55:3:84:TYR:CE1	55:3:93:LYS:HB2	2.54	0.42
58:6:142:VAL:HG21	58:6:147:PHE:CD1	2.54	0.42
67:AF:39:LEU:HD23	67:AF:39:LEU:HA	1.83	0.42
73:AL:66:LYS:HD3	73:AL:111:ARG:HH22	1.85	0.42
79:AR:127:LYS:HD2	79:AR:149:GLU:HA	2.00	0.42
3:D:184:U:O2'	3:D:189:G:O4'	2.37	0.42
3:D:2084:C:C4	21:V:14:ARG:HD2	2.55	0.42
3:D:2478:C:N4	3:D:2479:G:O6	2.53	0.42
3:D:4138:C:H2'	3:D:4139:G:H8	1.83	0.42
3:D:5060:A:O2'	3:D:5061:A:OP1	2.34	0.42
9:J:125:VAL:HG23	9:J:126:THR:N	2.34	0.42
12:M:261:LEU:HD23	12:M:261:LEU:HA	1.89	0.42
13:N:91:LYS:HG2	13:N:145:ILE:HG12	2.01	0.42
17:R:90:ARG:O	17:R:94:LYS:HG3	2.20	0.42
29:d:55:VAL:HG22	29:d:104:VAL:HB	2.00	0.42
37:l:19:LYS:HD3	37:l:19:LYS:HA	1.77	0.42
42:q:24:PRO:HG2	42:q:27:ILE:HG12	2.01	0.42
48:w:900:C:H3'	48:w:901:G:H8	1.84	0.42
48:w:989:C:OP2	50:y:155:TYR:OH	2.31	0.42
50:y:103:MET:HE3	50:y:188:LEU:HD22	2.00	0.42
50:y:122:GLU:OE2	50:y:140:VAL:HG12	2.20	0.42
53:1:56:LEU:H	53:1:60:GLU:CD	2.25	0.42
58:6:33:GLY:HA3	78:AQ:111:TYR:CD1	2.55	0.42
58:6:65:GLU:O	58:6:66:LYS:HG2	2.18	0.42
63:AB:13:ARG:HH21	63:AB:14:LYS:HB3	1.84	0.42
63:AB:108:LYS:HB3	63:AB:110:GLU:OE1	2.20	0.42
66:AE:78:LYS:HE2	66:AE:78:LYS:HB2	1.88	0.42
67:AF:42:HIS:HA	67:AF:83:GLN:HG3	2.02	0.42
79:AR:26:GLN:HE21	79:AR:75:GLY:N	2.17	0.42
3:D:2487:G:N2	3:D:2492:C:H1'	2.27	0.42
3:D:3844:U:OP2	7:H:239:LYS:HG2	2.20	0.42
7:H:14:LEU:O	7:H:17:LEU:HB2	2.19	0.42
37:l:69:LYS:HG3	37:l:73:HIS:HD2	1.85	0.42
48:w:614:C:H2'	48:w:626:G:C4	2.54	0.42
48:w:1018:U:H5''	61:9:71:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:1604:G:C6	48:w:1605:G:C4	3.08	0.42
48:w:1623:A:H5'	66:AE:133:GLY:HA3	2.01	0.42
51:z:128:VAL:HG13	51:z:158:ALA:HB2	2.01	0.42
52:0:34:TYR:HE1	52:0:37:VAL:HG13	1.84	0.42
54:2:162:ALA:HB2	54:2:172:CYS:SG	2.59	0.42
63:AB:15:PHE:CZ	63:AB:22:LEU:HB2	2.54	0.42
63:AB:30:TYR:O	63:AB:34:MET:HG2	2.20	0.42
65:AD:106:LEU:HA	65:AD:109:LEU:HB2	2.02	0.42
79:AR:3:GLU:HB3	79:AR:267:VAL:HG13	2.01	0.42
79:AR:31:ILE:HG23	79:AR:43:TRP:HB2	2.01	0.42
79:AR:113:PHE:HE2	79:AR:117:ASN:HD22	1.66	0.42
2:B:61:C:H2'	2:B:62:C:C6	2.54	0.42
3:D:667:A:N6	8:I:291:ARG:HH22	2.18	0.42
3:D:987:C:H1'	3:D:1067:G:N2	2.34	0.42
3:D:1412:G:H2'	3:D:1413:C:C6	2.55	0.42
3:D:1846:G:H2'	3:D:1847:C:C6	2.54	0.42
3:D:1855:G:OP1	32:g:4:SER:HB2	2.20	0.42
3:D:2666:U:O4	22:W:128:LYS:HE2	2.20	0.42
3:D:3880:G:H2'	3:D:3881:G:C8	2.54	0.42
8:I:334:THR:HG21	11:L:51:TYR:OH	2.20	0.42
9:J:179:ARG:HA	9:J:179:ARG:HD3	1.89	0.42
10:K:176:THR:HG23	10:K:176:THR:O	2.19	0.42
11:L:31:LYS:HA	11:L:31:LYS:HD3	1.82	0.42
14:O:206:LEU:HD12	14:O:206:LEU:HA	1.88	0.42
17:R:40:GLY:H	17:R:45:VAL:HG23	1.85	0.42
29:d:31:SER:HA	29:d:48:PRO:HA	2.02	0.42
29:d:120:GLU:OE2	29:d:120:GLU:N	2.48	0.42
48:w:107:A:H2'	48:w:108:G:C8	2.55	0.42
48:w:456:C:H1'	48:w:1800:A:C8	2.55	0.42
48:w:492:C:OP2	72:AK:107:ARG:NH2	2.53	0.42
48:w:623:G:O6	48:w:624:C:N4	2.53	0.42
48:w:1636:G:OP1	48:w:1636:G:H3'	2.20	0.42
49:x:63:ARG:NH1	69:AH:38:GLU:HA	2.33	0.42
50:y:224:GLU:HB2	50:y:227:LYS:HG2	2.00	0.42
57:5:129:LEU:O	57:5:133:GLU:HG2	2.20	0.42
57:5:153:LYS:HA	57:5:156:ALA:HB3	2.00	0.42
64:AC:28:GLY:HA3	64:AC:67:ASP:OD2	2.20	0.42
64:AC:128:GLU:OE2	64:AC:138:ARG:NH2	2.53	0.42
71:AJ:47:ALA:O	71:AJ:101:LEU:HD12	2.20	0.42
72:AK:46:LYS:O	72:AK:49:LYS:HD2	2.20	0.42
76:AO:62:GLU:N	76:AO:62:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:498:C:H42	3:D:656:C:H42	1.67	0.42
3:D:667:A:N6	8:I:291:ARG:NH2	2.67	0.42
3:D:1340:OMC:OP1	31:f:6:ARG:NH2	2.52	0.42
6:G:205:ASN:O	6:G:208:GLU:HG2	2.19	0.42
7:H:53:MET:HE2	7:H:53:MET:HB3	1.96	0.42
13:N:26:ILE:HD12	13:N:35:ARG:HG2	2.01	0.42
14:O:32:ARG:O	14:O:33:ILE:C	2.63	0.42
19:T:34:VAL:HG22	19:T:103:LYS:HB2	2.02	0.42
21:V:103:LEU:HD23	21:V:103:LEU:H	1.85	0.42
37:l:15:THR:O	37:l:19:LYS:HE3	2.20	0.42
48:w:651:PSU:H2'	48:w:652:U:C6	2.55	0.42
48:w:808:A:N6	48:w:809:A:N1	2.68	0.42
48:w:831:G:N7	72:AK:11:LYS:NZ	2.42	0.42
48:w:838:G:N2	48:w:840:C:O2'	2.53	0.42
48:w:1301:A:OP1	63:AB:51:ARG:NH1	2.51	0.42
48:w:1633:A:C5	48:w:1634:A:N7	2.87	0.42
49:x:6:ASP:HA	49:x:9:GLN:HG2	2.01	0.42
53:1:48:LEU:O	53:1:55:ALA:N	2.46	0.42
53:1:232:ASN:OD1	53:1:233:LYS:HE3	2.19	0.42
55:3:91:GLU:HG2	55:3:92:ARG:N	2.35	0.42
58:6:35:TYR:N	58:6:35:TYR:CD1	2.88	0.42
58:6:113:GLN:HA	58:6:116:LYS:HG2	2.01	0.42
58:6:142:VAL:HG11	58:6:147:PHE:HD1	1.85	0.42
66:AE:91:LYS:HG3	66:AE:92:ASP:N	2.35	0.42
70:AI:42:MET:HE3	70:AI:50:PHE:CD2	2.54	0.42
75:AN:56:CYS:SG	75:AN:59:CYS:HB2	2.60	0.42
3:D:959:G:N7	10:K:123:ARG:HG3	2.35	0.42
3:D:2459:G:H2'	3:D:2461:G:OP2	2.19	0.42
3:D:2544:G:O2'	3:D:2547:G:H5'	2.19	0.42
3:D:2561:C:H2'	3:D:2562:G:O4'	2.20	0.42
3:D:3688:U:OP2	6:G:198:ARG:NH1	2.53	0.42
9:J:51:MET:HB2	9:J:144:CYS:SG	2.59	0.42
13:N:105:ILE:HD12	13:N:112:VAL:HG22	2.02	0.42
17:R:95:ILE:C	17:R:97:ALA:H	2.28	0.42
30:e:58:GLY:O	30:e:62:ILE:HG13	2.20	0.42
48:w:835:C:C5	72:AK:8:ARG:HD3	2.54	0.42
53:1:160:ILE:HA	53:1:172:PHE:HA	2.02	0.42
54:2:50:PRO:HG2	54:2:90:VAL:HG23	2.02	0.42
59:7:49:MET:HE1	59:7:69:TRP:CH2	2.55	0.42
68:AG:66:ARG:HD2	68:AG:66:ARG:HA	1.82	0.42
71:AJ:125:VAL:O	71:AJ:128:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:677:G:H2'	3:D:678:C:C6	2.55	0.42
3:D:1442:C:O2'	3:D:1443:A:H5'	2.20	0.42
3:D:4745:G:H22	3:D:4955:A:H2	1.68	0.42
8:I:293:LEU:O	8:I:298:ILE:HD11	2.19	0.42
18:S:159:ARG:HB2	18:S:164:LEU:HB2	2.02	0.42
37:l:82:MET:HE2	37:l:86:CYS:HB3	2.02	0.42
48:w:1593:C:O2'	67:AF:12:GLN:NE2	2.53	0.42
50:y:71:LEU:HA	50:y:74:LEU:HB2	2.02	0.42
53:1:206:ASP:O	53:1:222:LEU:HB2	2.19	0.42
55:3:55:GLY:HA3	55:3:108:VAL:O	2.20	0.42
56:4:103:LYS:HA	56:4:104:PRO:HD3	1.91	0.42
58:6:12:THR:HA	58:6:48:PHE:CD2	2.55	0.42
60:8:55:TYR:CD1	60:8:55:TYR:C	2.98	0.42
3:D:1834:U:OP1	24:Y:116:LYS:NZ	2.35	0.41
3:D:4870:G:H5''	17:R:91:TRP:CD2	2.55	0.41
5:F:77:A:H2'	5:F:78:G:O4'	2.20	0.41
6:G:192:LYS:HE2	6:G:192:LYS:HB3	1.89	0.41
7:H:359:ALA:C	7:H:360:LEU:HD23	2.45	0.41
12:M:50:ASP:HB2	28:c:40:ILE:HD12	2.01	0.41
16:Q:18:TRP:CD1	16:Q:18:TRP:H	2.37	0.41
20:U:125:MET:HE2	20:U:143:PRO:HG3	2.02	0.41
29:d:2:LYS:HB3	29:d:2:LYS:HE3	1.83	0.41
31:f:137:ILE:O	31:f:140:VAL:HG12	2.21	0.41
34:i:40:LYS:HA	34:i:43:PRO:HG2	2.01	0.41
48:w:120:U:H2'	48:w:121:OMU:C6	2.50	0.41
48:w:1208:A:OP2	48:w:1835:A:O2'	2.34	0.41
48:w:1398:G:H1'	79:AR:63:SER:OG	2.20	0.41
48:w:1804:OMU:HM23	48:w:1804:OMU:H1'	1.70	0.41
51:z:72:ASP:OD2	51:z:74:LYS:NZ	2.39	0.41
58:6:29:LEU:HD11	78:AQ:110:GLN:HE22	1.84	0.41
59:7:3:MET:HE3	59:7:47:LYS:HZ1	1.84	0.41
59:7:64:TRP:CE2	77:AP:23:VAL:HG12	2.55	0.41
61:9:29:THR:OG1	61:9:30:SER:N	2.51	0.41
63:AB:26:LEU:HD12	63:AB:26:LEU:HA	1.87	0.41
79:AR:165:ILE:HD11	79:AR:177:TRP:HB2	2.02	0.41
79:AR:200:VAL:HG22	79:AR:207:CYS:SG	2.60	0.41
2:B:9:1MA:N3	2:B:45:G:H2'	2.35	0.41
3:D:1294:A:H1'	3:D:1296:G:N1	2.34	0.41
3:D:1443:A:H2'	3:D:1444:G:O4'	2.20	0.41
3:D:1617:G:H1'	3:D:2513:A:N6	2.35	0.41
3:D:2864:A:H2'	3:D:2865:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4734:A:H1'	3:D:4735:G:C8	2.54	0.41
3:D:4896:G:N2	3:D:4926:C:H41	2.18	0.41
5:F:125:C:O3'	5:F:126:C:H2'	2.20	0.41
13:N:27:VAL:HG23	13:N:80:MET:HE2	2.02	0.41
15:P:101:ASP:OD2	15:P:101:ASP:N	2.46	0.41
15:P:112:HIS:HE1	15:P:117:ILE:HG21	1.85	0.41
17:R:104:MET:HE3	17:R:109:ARG:HG2	2.01	0.41
19:T:190:ASP:OD2	19:T:190:ASP:N	2.51	0.41
21:V:161:SER:O	21:V:161:SER:OG	2.32	0.41
32:g:114:LYS:O	32:g:117:ARG:NH1	2.53	0.41
33:h:77:ASN:OD1	33:h:80:GLU:HG2	2.20	0.41
48:w:492:C:N4	48:w:508:A:H62	2.17	0.41
53:1:150:PRO:O	55:3:209:TYR:HE1	2.02	0.41
53:1:175:PHE:HE2	53:1:198:ARG:HD2	1.84	0.41
57:5:140:LYS:HE3	57:5:140:LYS:HB3	1.96	0.41
66:AE:73:ASN:HB3	66:AE:76:GLN:NE2	2.35	0.41
67:AF:65:TYR:HD1	67:AF:66:LEU:HD22	1.85	0.41
73:AL:72:VAL:O	73:AL:75:GLU:HG3	2.20	0.41
74:AM:41:ILE:HD13	74:AM:41:ILE:HA	1.86	0.41
79:AR:301:GLY:HA2	79:AR:307:VAL:HG12	2.02	0.41
3:D:398:A2M:HM'3	3:D:398:A2M:H1'	1.89	0.41
3:D:2097:U:O3'	3:D:2098:G:H4'	2.19	0.41
7:H:28:LYS:HB2	7:H:28:LYS:HE3	1.70	0.41
19:T:140:ARG:O	19:T:144:GLU:HG2	2.20	0.41
42:q:38:ASN:C	42:q:40:LYS:H	2.29	0.41
47:v:105:ASP:OD1	47:v:105:ASP:N	2.51	0.41
48:w:343:A:H2'	48:w:344:U:O4'	2.20	0.41
48:w:395:G:N2	57:5:14:THR:O	2.53	0.41
48:w:1093:A:H1'	70:AI:9:ASP:OD1	2.20	0.41
48:w:1585:U:O2'	48:w:1587:G:OP2	2.26	0.41
64:AC:47:LEU:HD11	64:AC:78:VAL:HG23	2.02	0.41
64:AC:111:ILE:HD13	64:AC:111:ILE:HA	1.84	0.41
72:AK:47:MET:HE1	72:AK:48:TYR:CE2	2.55	0.41
76:AO:11:LEU:HD23	76:AO:57:THR:HA	2.02	0.41
3:D:75:G:N7	16:Q:102:ARG:HG2	2.35	0.41
3:D:2415:OMU:HM23	3:D:2415:OMU:H1'	1.56	0.41
3:D:2730:U:H2'	3:D:2731:C:C6	2.56	0.41
3:D:4620:OMU:HM23	3:D:4620:OMU:H1'	1.77	0.41
7:H:76:VAL:HA	7:H:334:LYS:O	2.19	0.41
8:I:218:ILE:O	8:I:222:ARG:HB2	2.20	0.41
16:Q:58:ILE:HD13	16:Q:157:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:18:LEU:HD23	33:h:18:LEU:HA	1.88	0.41
48:w:2:A:H5''	51:z:205:VAL:HG11	2.02	0.41
48:w:1035:A:H2'	48:w:1036:A:O4'	2.21	0.41
50:y:106:THR:HB	62:AA:130:GLU:OE2	2.20	0.41
54:2:102:LEU:HD11	73:AL:67:LEU:HD13	2.01	0.41
56:4:38:ALA:N	56:4:41:ARG:NH2	2.67	0.41
57:5:84:ASN:ND2	57:5:100:CYS:SG	2.86	0.41
58:6:114:VAL:CG1	58:6:126:ALA:HB1	2.50	0.41
63:AB:85:ILE:O	63:AB:112:ILE:HG13	2.21	0.41
65:AD:81:ARG:HD2	65:AD:81:ARG:C	2.45	0.41
65:AD:100:PRO:HD3	65:AD:119:VAL:HB	2.03	0.41
72:AK:12:PHE:HZ	72:AK:21:LYS:HD2	1.85	0.41
78:AQ:81:ARG:HG2	78:AQ:81:ARG:NH2	2.36	0.41
3:D:172:C:H2'	3:D:173:C:O4'	2.20	0.41
3:D:1081:C:O2'	3:D:1082:C:H2'	2.20	0.41
3:D:1202:C:H3'	3:D:1203:G:C5'	2.50	0.41
9:J:123:VAL:HG12	9:J:248:ARG:CZ	2.51	0.41
10:K:251:LYS:HB2	10:K:251:LYS:HE2	1.89	0.41
14:O:38:ARG:NH2	14:O:45:GLU:OE1	2.36	0.41
21:V:64:SER:HB3	21:V:92:VAL:HG11	2.02	0.41
37:l:60:ARG:HA	37:l:60:ARG:HD2	1.88	0.41
41:p:54:GLU:HA	41:p:54:GLU:OE2	2.20	0.41
48:w:50:A:N6	48:w:477:G:H1'	2.35	0.41
50:y:70:SER:HA	50:y:83:LYS:HA	2.02	0.41
50:y:71:LEU:H	50:y:71:LEU:HD23	1.86	0.41
50:y:174:ARG:NH2	50:y:175:GLU:OE2	2.39	0.41
53:1:180:LEU:HD12	53:1:229:GLY:HA3	2.02	0.41
55:3:231:ARG:HH11	55:3:234:LEU:HD13	1.85	0.41
65:AD:103:LYS:HD2	65:AD:118:GLN:OE1	2.20	0.41
66:AE:13:LEU:O	66:AE:15:VAL:HG23	2.20	0.41
67:AF:37:VAL:HG21	67:AF:52:TRP:CZ2	2.54	0.41
71:AJ:46:HIS:CD2	71:AJ:103:ALA:HB2	2.55	0.41
71:AJ:52:LEU:HD21	71:AJ:73:GLN:OE1	2.20	0.41
72:AK:117:VAL:HG23	72:AK:122:LYS:HG2	2.02	0.41
3:D:208:A:C2	3:D:233:U:H5''	2.55	0.41
3:D:1326:A2M:OP2	3:D:4445:U:O2'	2.33	0.41
3:D:1553:A:H62	3:D:1574:G:H1'	1.85	0.41
3:D:1863:U:OP1	14:O:15:LYS:HE3	2.21	0.41
3:D:4325:A:N3	9:J:36:LEU:HB3	2.36	0.41
3:D:4458:C:H2'	3:D:4459:U:C6	2.56	0.41
3:D:4648:A:OP1	22:W:62:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:47:LEU:HD11	7:H:181:MET:SD	2.60	0.41
12:M:164:ILE:O	12:M:164:ILE:HG23	2.21	0.41
13:N:27:VAL:CG2	13:N:80:MET:HE2	2.51	0.41
17:R:100:ARG:HD3	19:T:198:THR:O	2.21	0.41
48:w:383:G:O2'	60:8:132:ARG:HG2	2.20	0.41
48:w:556:U:H1'	48:w:558:G:OP2	2.21	0.41
48:w:1619:A:OP2	63:AB:47:ARG:NH2	2.53	0.41
49:x:53:ARG:HG2	49:x:53:ARG:H	1.67	0.41
49:x:57:LYS:HE2	49:x:160:ALA:O	2.20	0.41
52:0:211:VAL:HG22	65:AD:38:ILE:O	2.20	0.41
55:3:52:ILE:HD12	55:3:52:ILE:HA	1.79	0.41
56:4:49:LYS:HD3	56:4:49:LYS:HA	1.75	0.41
58:6:64:ASP:OD1	58:6:65:GLU:N	2.54	0.41
59:7:13:GLU:O	59:7:17:LYS:HD3	2.20	0.41
59:7:47:LYS:HA	59:7:50:GLN:HG2	2.02	0.41
72:AK:32:LYS:HB3	72:AK:32:LYS:HE2	1.84	0.41
78:AQ:81:ARG:HG2	78:AQ:81:ARG:HH21	1.86	0.41
79:AR:132:TRP:CE3	79:AR:138:CYS:HB3	2.56	0.41
79:AR:170:TRP:HA	79:AR:194:TYR:HB2	2.02	0.41
79:AR:217:MET:HE2	79:AR:217:MET:HB3	1.88	0.41
3:D:659:G:C6	3:D:660:A:C6	3.08	0.41
3:D:1406:G:H2'	3:D:1407:C:C5	2.56	0.41
3:D:4581:G:P	7:H:26:ARG:HH22	2.43	0.41
10:K:178:PRO:HG3	10:K:257:ILE:HD11	2.01	0.41
12:M:148:GLU:OE2	18:S:6:TYR:OH	2.23	0.41
21:V:3:VAL:HG23	21:V:5:ILE:HG12	2.02	0.41
22:W:172:ARG:HH21	48:w:909:G:P	2.41	0.41
28:c:87:MET:O	28:c:91:GLU:HG3	2.20	0.41
31:f:92:LYS:HE2	31:f:92:LYS:HB2	1.72	0.41
48:w:641:A:H2'	48:w:642:U:O4'	2.20	0.41
48:w:827:A:OP1	58:6:10:ARG:HB3	2.21	0.41
52:0:173:ARG:HA	52:0:173:ARG:HD3	1.95	0.41
53:1:139:LEU:O	53:1:146:THR:HA	2.21	0.41
55:3:84:TYR:HD1	55:3:95:LYS:HE2	1.86	0.41
59:7:60:GLU:HG3	59:7:69:TRP:NE1	2.36	0.41
64:AC:40:GLU:N	64:AC:40:GLU:OE2	2.53	0.41
65:AD:24:LEU:HD21	65:AD:34:VAL:HG21	2.03	0.41
66:AE:63:GLU:HB3	66:AE:66:ARG:HH21	1.85	0.41
67:AF:13:GLU:OE2	67:AF:13:GLU:C	2.64	0.41
68:AG:64:THR:HG22	68:AG:77:TRP:HE3	1.86	0.41
79:AR:203:ASP:OD1	79:AR:204:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:758:G:C2	3:D:759:G:H1'	2.56	0.41
3:D:1214:C:N3	32:g:90:SER:OG	2.54	0.41
3:D:1556:C:O2'	3:D:2669:C:OP1	2.31	0.41
3:D:4274:A:H2'	3:D:4275:G:C8	2.56	0.41
3:D:4966:A:H2'	3:D:4967:A:O4'	2.21	0.41
5:F:122:G:H1	5:F:128:C:N4	2.18	0.41
8:I:67:TRP:HB2	8:I:71:ARG:HH12	1.85	0.41
8:I:150:LEU:HD12	8:I:150:LEU:HA	1.71	0.41
40:o:25:LYS:HD2	42:q:51:LEU:HA	2.02	0.41
44:s:19:LYS:HE2	44:s:19:LYS:HB3	1.78	0.41
48:w:89:C:O2'	48:w:499:G:H5''	2.21	0.41
48:w:115:U:H2'	48:w:116:OMU:C6	2.50	0.41
48:w:878:G:C2	48:w:909:G:C2	3.09	0.41
48:w:1113:A:C2'	48:w:1114:U:H5'	2.51	0.41
48:w:1471:C:H42	48:w:1476:A:H62	1.67	0.41
48:w:1849:G:O2'	48:w:1850:MA6:C8	2.66	0.41
49:x:12:GLU:HG2	65:AD:111:PHE:CE1	2.55	0.41
49:x:122:LEU:HB2	49:x:142:LEU:HD21	2.02	0.41
50:y:112:SER:O	50:y:115:LYS:NZ	2.45	0.41
53:1:10:LYS:HD3	53:1:10:LYS:HA	1.93	0.41
57:5:23:LYS:HB3	57:5:23:LYS:HE2	1.79	0.41
57:5:81:VAL:HA	57:5:102:VAL:HA	2.03	0.41
58:6:136:ARG:HA	58:6:141:VAL:HA	2.02	0.41
59:7:63:ALA:O	59:7:64:TRP:C	2.64	0.41
60:8:130:GLU:HB3	60:8:140:PHE:CZ	2.56	0.41
64:AC:34:VAL:N	64:AC:37:ARG:O	2.45	0.41
66:AE:65:GLU:HA	66:AE:68:ILE:HG22	2.03	0.41
68:AG:20:ILE:HD11	68:AG:91:LEU:HB2	2.02	0.41
68:AG:47:ASN:HB3	68:AG:91:LEU:HD22	2.02	0.41
79:AR:230:LEU:HD23	79:AR:259:TRP:CD2	2.55	0.41
2:C:23:U:H2'	2:C:24:A:H8	1.86	0.41
3:D:2313:A:O2'	3:D:2314:G:H5'	2.21	0.41
3:D:2461:G:H2'	3:D:2462:C:C6	2.56	0.41
3:D:4467:A:O2'	3:D:4510:A:N3	2.50	0.41
3:D:4910:G:H4'	7:H:95:THR:HG22	2.02	0.41
3:D:5006:U:H4'	3:D:5007:A:H5'	2.03	0.41
5:F:52:A:O5'	42:q:21:ARG:HD3	2.21	0.41
7:H:397:ILE:HG13	7:H:398:ALA:N	2.35	0.41
8:I:111:TRP:O	8:I:112:HIS:HB2	2.19	0.41
10:K:69:TYR:O	10:K:70:LYS:HB3	2.21	0.41
11:L:105:VAL:HG13	11:L:136:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:106:THR:N	12:M:109:GLU:OE2	2.49	0.41
13:N:4:ILE:HG12	13:N:61:TRP:CH2	2.56	0.41
14:O:31:ILE:HG12	14:O:32:ARG:N	2.34	0.41
14:O:183:ASP:O	14:O:187:LYS:HG2	2.21	0.41
15:P:160:GLU:OE1	15:P:160:GLU:N	2.50	0.41
21:V:128:LEU:HD12	21:V:128:LEU:HA	1.89	0.41
26:a:26:ILE:HD12	26:a:101:ASN:CB	2.51	0.41
28:c:50:LYS:HE3	28:c:50:LYS:HB2	1.88	0.41
46:u:26:VAL:O	46:u:30:GLU:HG2	2.20	0.41
48:w:85:A:OP1	72:AK:118:ARG:HG2	2.21	0.41
48:w:186:C:H2'	48:w:187:G:H8	1.84	0.41
48:w:583:C:OP1	58:6:162:ARG:NH1	2.54	0.41
48:w:839:C:N4	72:AK:10:ARG:HA	2.35	0.41
48:w:889:U:O5'	48:w:890:U:H5'	2.21	0.41
48:w:1057:C:H5	48:w:1060:A:OP2	2.03	0.41
48:w:1098:C:H2'	48:w:1099:G:C8	2.56	0.41
48:w:1388:A:H61	52:0:161:GLY:HA3	1.86	0.41
48:w:1442:OMU:HM23	48:w:1442:OMU:H1'	1.78	0.41
48:w:1619:A:O2'	63:AB:82:ASP:OD2	2.32	0.41
48:w:1842:4AC:O7	48:w:1842:4AC:H5	2.21	0.41
49:x:198:MET:HE1	65:AD:86:PRO:O	2.20	0.41
50:y:78:GLU:HG2	50:y:79:VAL:H	1.85	0.41
51:z:254:ASP:OD2	51:z:254:ASP:N	2.54	0.41
52:0:162:ASP:C	52:0:164:VAL:H	2.27	0.41
53:1:102:ILE:HG21	53:1:239:PRO:HG3	2.03	0.41
53:1:116:PRO:O	53:1:120:LYS:HG2	2.21	0.41
53:1:198:ARG:HH22	53:1:222:LEU:HD12	1.85	0.41
55:3:5:ILE:HG22	55:3:113:ILE:HD11	2.02	0.41
55:3:136:LYS:O	55:3:136:LYS:HD2	2.20	0.41
55:3:159:ARG:HB3	55:3:173:ALA:HB2	2.03	0.41
55:3:177:GLN:HG3	55:3:178:ARG:N	2.36	0.41
57:5:162:LEU:HD12	57:5:162:LEU:HA	1.93	0.41
57:5:172:LEU:O	57:5:172:LEU:HD12	2.21	0.41
59:7:31:LYS:NZ	59:7:36:ALA:O	2.42	0.41
60:8:2:ALA:O	60:8:4:ILE:HG22	2.21	0.41
64:AC:119:LEU:HD23	64:AC:119:LEU:HA	1.86	0.41
66:AE:89:ASP:O	66:AE:92:ASP:N	2.47	0.41
68:AG:36:CYS:SG	68:AG:37:ALA:N	2.94	0.41
69:AH:79:VAL:HG12	69:AH:79:VAL:O	2.20	0.41
70:AI:105:THR:HG22	70:AI:124:LYS:HB2	2.03	0.41
79:AR:35:SER:O	79:AR:66:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AR:73:SER:H	79:AR:117:ASN:ND2	2.18	0.41
3:D:1399:G:N2	3:D:1419:G:H1'	2.36	0.41
3:D:1919:G:H1'	23:X:164:LYS:NZ	2.35	0.41
3:D:2465:C:H2'	3:D:2466:G:O4'	2.21	0.41
6:G:144:LYS:HE2	6:G:144:LYS:HB2	1.79	0.41
7:H:47:LEU:H	7:H:84:MET:CE	2.34	0.41
10:K:101:ASN:OD1	10:K:102:GLY:N	2.54	0.41
25:Z:21:PHE:CE1	25:Z:80:LYS:HB2	2.57	0.41
48:w:617:G:H4'	71:AJ:88:ASP:HB2	2.03	0.41
49:x:126:ASP:OD1	49:x:126:ASP:C	2.64	0.41
58:6:21:GLU:HG3	58:6:24:ARG:HB3	2.03	0.41
58:6:87:LEU:HD11	58:6:91:LYS:HG3	2.03	0.41
59:7:1:MET:SD	59:7:47:LYS:HE2	2.61	0.41
62:AA:113:GLN:OE1	74:AM:45:VAL:HA	2.21	0.41
79:AR:87:LEU:HB2	79:AR:101:PHE:CG	2.55	0.41
3:D:43:U:H5''	18:S:85:VAL:CG2	2.52	0.40
3:D:684:G:OP1	10:K:100:LYS:NZ	2.36	0.40
3:D:4146:G:H2'	3:D:4147:G:H8	1.86	0.40
3:D:4414:A:H5''	14:O:154:ARG:NH1	2.37	0.40
3:D:4524:G:C2	7:H:252:ALA:HB1	2.56	0.40
7:H:92:TYR:HB3	7:H:99:LEU:HD22	2.03	0.40
8:I:94:ASN:OD1	8:I:94:ASN:N	2.50	0.40
8:I:232:VAL:O	8:I:233:SER:OG	2.32	0.40
19:T:187:LYS:HA	19:T:187:LYS:CE	2.47	0.40
21:V:76:GLU:H	21:V:76:GLU:CD	2.27	0.40
29:d:89:LYS:HB3	29:d:89:LYS:HE3	1.90	0.40
48:w:112:U:H2'	48:w:115:U:C5	2.56	0.40
48:w:159:A2M:HM'3	48:w:159:A2M:H1'	1.75	0.40
48:w:581:U:O2	72:AK:34:THR:HG23	2.21	0.40
48:w:1520:G:H3'	48:w:1521:C:C5	2.56	0.40
50:y:55:THR:O	50:y:57:ILE:HG23	2.20	0.40
51:z:88:ILE:O	51:z:160:LEU:HD12	2.21	0.40
51:z:172:ASN:OD1	51:z:172:ASN:N	2.54	0.40
52:0:48:ILE:HG13	52:0:86:LEU:HG	2.03	0.40
52:0:130:GLY:O	52:0:191:PRO:HG3	2.20	0.40
55:3:147:LEU:HD21	55:3:156:TYR:CZ	2.56	0.40
57:5:74:ARG:HH21	57:5:112:TRP:CD1	2.39	0.40
60:8:104:LYS:HG3	71:AJ:8:ARG:NH1	2.36	0.40
60:8:125:ILE:HD12	60:8:125:ILE:N	2.35	0.40
63:AB:119:PHE:CE2	66:AE:117:ILE:HD12	2.56	0.40
71:AJ:73:GLN:HG3	71:AJ:80:LYS:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:AJ:102:VAL:CG1	71:AJ:120:PHE:HB3	2.51	0.40
76:AO:13:ARG:HA	76:AO:13:ARG:NE	2.36	0.40
76:AO:26:GLN:OE1	76:AO:26:GLN:N	2.51	0.40
79:AR:64:HIS:ND1	79:AR:65:PHE:N	2.69	0.40
79:AR:119:GLN:O	79:AR:120:ILE:HD13	2.21	0.40
3:D:2034:G:OP1	23:X:86:SER:HB2	2.20	0.40
3:D:3877:A:N3	3:D:4401:G:O2'	2.43	0.40
3:D:4145:C:H2'	3:D:4146:G:C8	2.56	0.40
3:D:4229:U:OP1	45:t:63:THR:OG1	2.38	0.40
9:J:112:ARG:O	9:J:113:PHE:HB2	2.22	0.40
16:Q:42:LYS:O	16:Q:46:ILE:HG12	2.21	0.40
17:R:55:MET:HE2	17:R:55:MET:HB3	1.91	0.40
27:b:3:VAL:CG1	27:b:12:LYS:HG2	2.51	0.40
29:d:50:ARG:HD2	29:d:115:ARG:HD3	2.02	0.40
36:k:43:LEU:HA	36:k:43:LEU:HD12	1.78	0.40
48:w:944:A:H5'	62:AA:134:PRO:CB	2.50	0.40
51:z:76:LYS:HA	51:z:97:PHE:HE1	1.86	0.40
52:0:46:THR:O	52:0:84:VAL:HA	2.21	0.40
56:4:154:ILE:HB	56:4:185:VAL:HG23	2.02	0.40
57:5:12:ARG:HG2	57:5:16:GLY:O	2.21	0.40
60:8:37:TYR:CD1	60:8:37:TYR:C	3.00	0.40
68:AG:50:VAL:HG12	68:AG:91:LEU:HD21	2.03	0.40
73:AL:50:PHE:CZ	73:AL:58:LEU:HD13	2.46	0.40
75:AN:20:LYS:HG3	75:AN:21:LYS:N	2.36	0.40
75:AN:24:LEU:HD23	75:AN:24:LEU:HA	1.75	0.40
79:AR:126:ASP:OD1	79:AR:126:ASP:N	2.52	0.40
3:D:158:A:H5''	3:D:159:C:H2'	2.04	0.40
3:D:966:A:H5''	3:D:2092:G:H22	1.87	0.40
3:D:3712:A:H2'	3:D:3713:U:O4'	2.21	0.40
3:D:4508:C:N3	3:D:4512:U:H5	2.19	0.40
8:I:64:ALA:HB3	8:I:92:PHE:CE2	2.56	0.40
8:I:138:MET:HB3	8:I:138:MET:HE3	1.77	0.40
10:K:278:THR:OG1	10:K:279:ASN:N	2.54	0.40
17:R:114:LYS:HD3	17:R:114:LYS:HA	1.91	0.40
19:T:53:LYS:HB2	19:T:53:LYS:HE2	1.92	0.40
30:e:99:ASP:C	30:e:99:ASP:OD1	2.64	0.40
32:g:16:TRP:HD1	32:g:21:ILE:HD11	1.87	0.40
32:g:101:HIS:CE1	32:g:104:LEU:HD13	2.56	0.40
48:w:360:A:N6	48:w:400:C:O2'	2.54	0.40
48:w:436:OMG:H5''	48:w:473:A:N6	2.36	0.40
48:w:1237:C:H5'	63:AB:131:PRO:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:x:82:THR:HG22	49:x:204:TYR:CD2	2.57	0.40
50:y:57:ILE:HG13	50:y:58:ALA:N	2.28	0.40
53:1:11:ARG:NH2	53:1:20:LEU:HB3	2.36	0.40
55:3:18:VAL:HG23	55:3:23:LYS:HD2	2.03	0.40
57:5:71:CYS:SG	57:5:71:CYS:O	2.79	0.40
58:6:138:ARG:HG2	58:6:156:HIS:HB2	2.03	0.40
59:7:4:PRO:O	59:7:8:ARG:HB2	2.21	0.40
66:AE:70:ILE:H	66:AE:70:ILE:HG13	1.69	0.40
67:AF:75:MET:HA	67:AF:78:ILE:HD13	2.02	0.40
72:AK:22:GLN:C	72:AK:23:MET:HE3	2.47	0.40
79:AR:104:HIS:NE2	79:AR:124:SER:HB3	2.36	0.40
79:AR:168:CYS:HB3	79:AR:198:VAL:HG13	2.02	0.40
3:D:959:G:C5	10:K:123:ARG:HG3	2.56	0.40
3:D:2464:C:HO2'	3:D:2465:C:P	2.44	0.40
3:D:3724:A2M:H1'	3:D:3724:A2M:HM'3	1.86	0.40
7:H:238:LYS:HE2	7:H:238:LYS:HB2	1.94	0.40
12:M:165:GLU:C	12:M:167:VAL:N	2.79	0.40
16:Q:48:PRO:HB2	38:m:120:ALA:HB2	2.03	0.40
20:U:20:SER:HB3	20:U:21:ASN:H	1.77	0.40
34:i:117:LEU:HD23	34:i:117:LEU:HA	1.91	0.40
40:o:20:ARG:H	40:o:20:ARG:HG3	1.76	0.40
50:y:52:THR:HG22	50:y:57:ILE:HB	2.03	0.40
53:1:197:ASN:HD21	53:1:209:HIS:CD2	2.39	0.40
56:4:58:LYS:O	56:4:90:LYS:HA	2.21	0.40
56:4:76:GLN:OE1	56:4:94:PHE:HB2	2.22	0.40
56:4:83:LEU:HG	56:4:92:VAL:HG11	2.02	0.40
57:5:116:HIS:HD1	57:5:117:TYR:HD1	1.68	0.40
60:8:55:TYR:OH	60:8:116:CYS:HB3	2.22	0.40
63:AB:83:MET:SD	63:AB:84:ILE:N	2.94	0.40
65:AD:40:ILE:HD12	65:AD:40:ILE:N	2.36	0.40
66:AE:34:LYS:HB3	66:AE:34:LYS:HE2	1.76	0.40
72:AK:118:ARG:HG2	72:AK:119:GLY:H	1.85	0.40
74:AM:45:VAL:HG23	74:AM:46:GLU:N	2.36	0.40
74:AM:55:GLU:HA	74:AM:55:GLU:OE2	2.21	0.40
2:B:14:A:H2'	2:B:15:G:O4'	2.21	0.40
3:D:1082:C:HO2'	3:D:1083:U:P	2.43	0.40
3:D:2493:G:H21	5:F:126:C:H5''	1.86	0.40
3:D:4143:G:H1'	3:D:4145:C:OP1	2.21	0.40
3:D:4578:G:H2'	3:D:4579:PSU:C6	2.56	0.40
4:E:7:G:H4'	9:J:33:ARG:NH1	2.36	0.40
7:H:289:GLN:NE2	7:H:292:LEU:HD11	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:49:ARG:NH1	8:I:111:TRP:HB3	2.33	0.40
13:N:115:ARG:O	13:N:116:ASN:C	2.64	0.40
13:N:187:VAL:HG12	13:N:188:GLN:N	2.34	0.40
16:Q:47:ALA:C	16:Q:49:ARG:N	2.80	0.40
25:Z:55:ASN:OD1	25:Z:55:ASN:C	2.64	0.40
45:t:31:ASP:OD1	45:t:31:ASP:N	2.54	0.40
48:w:22:A:H4'	58:6:17:ARG:HA	2.03	0.40
48:w:416:U:O4	48:w:417:C:N4	2.50	0.40
48:w:456:C:H1'	48:w:1800:A:H8	1.85	0.40
48:w:830:A:C5	48:w:831:G:H1'	2.57	0.40
48:w:1663:A:O2'	48:w:1664:A:H5'	2.22	0.40
53:1:209:HIS:HA	53:1:219:ALA:HA	2.02	0.40
56:4:8:ILE:HD12	56:4:28:LEU:HD12	2.03	0.40
59:7:16:PHE:CE2	59:7:89:ILE:HG12	2.57	0.40
67:AF:18:LEU:HB2	67:AF:134:ILE:HG21	2.04	0.40
72:AK:62:THR:HB	72:AK:69:THR:HG22	2.04	0.40
78:AQ:81:ARG:HH21	78:AQ:82:ALA:HA	1.87	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%)	369 (93%)	27 (7%)	0	100	100
8	I	361/427 (84%)	340 (94%)	21 (6%)	0	100	100
9	J	291/297 (98%)	272 (94%)	19 (6%)	0	100	100
10	K	211/288 (73%)	190 (90%)	21 (10%)	0	100	100
11	L	223/248 (90%)	213 (96%)	10 (4%)	0	100	100
12	M	223/266 (84%)	206 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	N	188/192 (98%)	174 (93%)	14 (7%)	0	100	100
14	O	202/214 (94%)	182 (90%)	19 (9%)	1 (0%)	24	24
15	P	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
16	Q	206/211 (98%)	190 (92%)	13 (6%)	3 (2%)	8	4
17	R	134/215 (62%)	121 (90%)	13 (10%)	0	100	100
18	S	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
19	T	198/203 (98%)	193 (98%)	5 (2%)	0	100	100
20	U	155/184 (84%)	142 (92%)	13 (8%)	0	100	100
21	V	185/188 (98%)	174 (94%)	11 (6%)	0	100	100
22	W	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
23	X	173/176 (98%)	160 (92%)	13 (8%)	0	100	100
24	Y	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
25	Z	99/128 (77%)	91 (92%)	8 (8%)	0	100	100
26	a	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
27	b	61/157 (39%)	60 (98%)	1 (2%)	0	100	100
28	c	118/156 (76%)	111 (94%)	7 (6%)	0	100	100
29	d	132/145 (91%)	126 (96%)	6 (4%)	0	100	100
30	e	133/136 (98%)	123 (92%)	9 (7%)	1 (1%)	16	14
31	f	145/148 (98%)	132 (91%)	13 (9%)	0	100	100
32	g	100/159 (63%)	90 (90%)	8 (8%)	2 (2%)	6	3
33	h	95/115 (83%)	91 (96%)	4 (4%)	0	100	100
34	i	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
35	j	126/135 (93%)	123 (98%)	3 (2%)	0	100	100
36	k	107/110 (97%)	98 (92%)	9 (8%)	0	100	100
37	l	110/117 (94%)	105 (96%)	5 (4%)	0	100	100
38	m	119/123 (97%)	115 (97%)	4 (3%)	0	100	100
39	n	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
40	o	84/97 (87%)	78 (93%)	5 (6%)	1 (1%)	10	7
41	p	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
42	q	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	r	50/128 (39%)	49 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	84 (94%)	5 (6%)	0	100	100
47	v	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
49	x	213/295 (72%)	197 (92%)	16 (8%)	0	100	100
50	y	210/264 (80%)	194 (92%)	16 (8%)	0	100	100
51	z	210/293 (72%)	200 (95%)	9 (4%)	1 (0%)	24	24
52	0	210/243 (86%)	187 (89%)	23 (11%)	0	100	100
53	1	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
54	2	185/204 (91%)	166 (90%)	19 (10%)	0	100	100
55	3	235/249 (94%)	229 (97%)	6 (3%)	0	100	100
56	4	185/194 (95%)	168 (91%)	17 (9%)	0	100	100
57	5	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
58	6	180/194 (93%)	168 (93%)	12 (7%)	0	100	100
59	7	94/165 (57%)	86 (92%)	8 (8%)	0	100	100
60	8	138/158 (87%)	128 (93%)	9 (6%)	1 (1%)	18	17
61	9	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
62	AA	132/151 (87%)	120 (91%)	12 (9%)	0	100	100
63	AB	132/145 (91%)	124 (94%)	8 (6%)	0	100	100
64	AC	140/146 (96%)	125 (89%)	14 (10%)	1 (1%)	18	17
65	AD	129/135 (96%)	108 (84%)	19 (15%)	2 (2%)	7	4
66	AE	142/152 (93%)	128 (90%)	14 (10%)	0	100	100
67	AF	141/145 (97%)	132 (94%)	9 (6%)	0	100	100
68	AG	100/119 (84%)	95 (95%)	5 (5%)	0	100	100
69	AH	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
70	AI	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
71	AJ	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
72	AK	121/133 (91%)	119 (98%)	2 (2%)	0	100	100
73	AL	84/125 (67%)	75 (89%)	9 (11%)	0	100	100
74	AM	97/115 (84%)	91 (94%)	6 (6%)	0	100	100
75	AN	81/84 (96%)	70 (86%)	10 (12%)	1 (1%)	10	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	AO	59/69 (86%)	54 (92%)	5 (8%)	0	100	100
77	AP	43/56 (77%)	41 (95%)	2 (5%)	0	100	100
78	AQ	55/59 (93%)	49 (89%)	6 (11%)	0	100	100
79	AR	311/317 (98%)	267 (86%)	44 (14%)	0	100	100
All	All	10947/12400 (88%)	10194 (93%)	739 (7%)	14 (0%)	49	56

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	48	PRO
32	g	111	ARG
64	AC	119	LEU
65	AD	119	VAL
30	e	33	THR
32	g	110	ALA
65	AD	118	GLN
16	Q	47	ALA
51	z	78	LEU
16	Q	5	ARG
60	8	118	ARG
40	o	40	PRO
75	AN	39	GLY
14	O	16	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%)	345 (100%)	1 (0%)	86	90
8	I	301/348 (86%)	300 (100%)	1 (0%)	86	90
9	J	245/250 (98%)	244 (100%)	1 (0%)	84	89
10	K	193/252 (77%)	192 (100%)	1 (0%)	81	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	194/215 (90%)	194 (100%)	0	100	100
12	M	195/223 (87%)	193 (99%)	2 (1%)	68	77
13	N	169/171 (99%)	167 (99%)	2 (1%)	63	74
14	O	174/181 (96%)	172 (99%)	2 (1%)	65	75
15	P	143/149 (96%)	140 (98%)	3 (2%)	47	58
16	Q	174/177 (98%)	173 (99%)	1 (1%)	78	84
17	R	116/161 (72%)	115 (99%)	1 (1%)	70	79
18	S	171/172 (99%)	171 (100%)	0	100	100
19	T	172/174 (99%)	171 (99%)	1 (1%)	78	84
20	U	138/163 (85%)	136 (99%)	2 (1%)	59	70
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%)	155 (99%)	1 (1%)	78	84
24	Y	139/140 (99%)	137 (99%)	2 (1%)	59	70
25	Z	90/115 (78%)	89 (99%)	1 (1%)	65	75
26	a	101/107 (94%)	100 (99%)	1 (1%)	68	77
27	b	55/126 (44%)	52 (94%)	3 (6%)	19	20
28	c	107/133 (80%)	107 (100%)	0	100	100
29	d	124/135 (92%)	122 (98%)	2 (2%)	55	66
30	e	117/118 (99%)	116 (99%)	1 (1%)	70	79
31	f	120/121 (99%)	119 (99%)	1 (1%)	73	80
32	g	81/126 (64%)	80 (99%)	1 (1%)	63	74
33	h	82/97 (84%)	79 (96%)	3 (4%)	30	37
34	i	98/110 (89%)	96 (98%)	2 (2%)	48	59
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%)	108 (99%)	1 (1%)	70	79
39	n	86/89 (97%)	86 (100%)	0	100	100
40	o	73/80 (91%)	72 (99%)	1 (1%)	59	70
41	p	64/65 (98%)	63 (98%)	1 (2%)	55	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	q	47/48 (98%)	45 (96%)	2 (4%)	26	31
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%)	92 (99%)	1 (1%)	65	75
46	u	74/75 (99%)	72 (97%)	2 (3%)	39	49
47	v	109/121 (90%)	107 (98%)	2 (2%)	51	63
49	x	178/243 (73%)	176 (99%)	2 (1%)	65	75
50	y	194/231 (84%)	192 (99%)	2 (1%)	68	77
51	z	176/225 (78%)	176 (100%)	0	100	100
52	0	175/202 (87%)	172 (98%)	3 (2%)	53	65
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%)	205 (100%)	1 (0%)	81	87
56	4	168/174 (97%)	168 (100%)	0	100	100
57	5	175/180 (97%)	172 (98%)	3 (2%)	53	65
58	6	160/168 (95%)	160 (100%)	0	100	100
59	7	87/136 (64%)	85 (98%)	2 (2%)	44	55
60	8	125/142 (88%)	125 (100%)	0	100	100
61	9	130/131 (99%)	126 (97%)	4 (3%)	35	44
62	AA	104/119 (87%)	101 (97%)	3 (3%)	37	47
63	AB	120/130 (92%)	120 (100%)	0	100	100
64	AC	117/121 (97%)	115 (98%)	2 (2%)	53	65
65	AD	117/122 (96%)	115 (98%)	2 (2%)	53	65
66	AE	119/132 (90%)	118 (99%)	1 (1%)	73	80
67	AF	113/115 (98%)	112 (99%)	1 (1%)	70	79
68	AG	89/107 (83%)	88 (99%)	1 (1%)	65	75
69	AH	67/67 (100%)	67 (100%)	0	100	100
70	AI	112/113 (99%)	112 (100%)	0	100	100
71	AJ	113/115 (98%)	113 (100%)	0	100	100
72	AK	106/115 (92%)	106 (100%)	0	100	100
73	AL	73/103 (71%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	AM	86/98 (88%)	84 (98%)	2 (2%)	44	55
75	AN	73/76 (96%)	71 (97%)	2 (3%)	39	49
76	AO	54/62 (87%)	54 (100%)	0	100	100
77	AP	39/49 (80%)	39 (100%)	0	100	100
78	AQ	46/48 (96%)	46 (100%)	0	100	100
79	AR	272/275 (99%)	272 (100%)	0	100	100
All	All	9509/10553 (90%)	9432 (99%)	77 (1%)	70	80

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	289	GLN
8	I	111	TRP
9	J	135	ILE
10	K	245	GLN
12	M	166	LEU
12	M	224	THR
13	N	66	GLU
13	N	143	GLU
14	O	28	ASP
14	O	60	LEU
15	P	117	ILE
15	P	134	LEU
15	P	148	THR
16	Q	149	GLN
17	R	132	LYS
19	T	189	ILE
20	U	21	ASN
20	U	58	VAL
23	X	7	LEU
24	Y	79	GLN
24	Y	127	GLN
25	Z	22	THR
26	a	48	ARG
27	b	1	MET
27	b	25	ASP
27	b	48	GLN
29	d	111	LEU
29	d	118	ILE
30	e	31	ASP

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Mol	Chain	Res	Type
31	f	140	VAL
32	g	11	ASN
33	h	15	ASN
33	h	80	GLU
33	h	93	THR
34	i	22	THR
34	i	46	LEU
38	m	116	LEU
40	o	48	ASN
41	p	5	ILE
42	q	16	LYS
42	q	47	THR
45	t	90	HIS
46	u	5	THR
46	u	88	GLU
47	v	43	LEU
47	v	108	MET
49	x	113	GLN
49	x	170	SER
50	y	77	ASP
50	y	193	ILE
52	0	157	MET
52	0	162	ASP
52	0	189	MET
55	3	114	VAL
57	5	46	VAL
57	5	153	LYS
57	5	186	ASP
59	7	49	MET
59	7	50	GLN
61	9	69	ASN
61	9	87	ASP
61	9	134	VAL
61	9	138	ASN
62	AA	61	LYS
62	AA	79	GLN
62	AA	90	ILE
64	AC	46	THR
64	AC	109	LYS
65	AD	9	VAL
65	AD	105	MET
66	AE	85	ASN

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Mol	Chain	Res	Type
67	AF	33	TRP
68	AG	101	ILE
74	AM	2	THR
74	AM	74	CYS
75	AN	8	LEU
75	AN	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
6	G	22	HIS
7	H	145	GLN
7	H	245	HIS
7	H	302	ASN
8	I	21	ASN
8	I	43	ASN
8	I	61	GLN
8	I	329	ASN
8	I	347	HIS
9	J	229	ASN
10	K	191	GLN
11	L	206	ASN
11	L	239	GLN
12	M	94	GLN
12	M	153	GLN
12	M	206	GLN
13	N	98	HIS
13	N	102	ASN
14	O	73	ASN
15	P	46	GLN
15	P	112	HIS
16	Q	205	GLN
17	R	34	ASN
17	R	66	HIS
18	S	29	GLN
19	T	26	GLN
19	T	180	GLN
20	U	145	HIS
21	V	7	HIS
21	V	45	GLN
24	Y	127	GLN
24	Y	144	ASN

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Mol	Chain	Res	Type
28	c	73	HIS
28	c	151	ASN
29	d	14	ASN
29	d	96	HIS
31	f	60	HIS
32	g	6	ASN
34	i	116	ASN
35	j	52	GLN
36	k	21	GLN
36	k	24	HIS
37	l	73	HIS
38	m	65	GLN
38	m	107	GLN
39	n	15	HIS
40	o	66	HIS
43	r	117	HIS
47	v	4	HIS
49	x	50	ASN
49	x	111	GLN
50	y	92	GLN
50	y	158	HIS
53	1	161	GLN
53	1	209	HIS
55	3	110	ASN
57	5	167	GLN
57	5	181	GLN
58	6	111	GLN
58	6	154	GLN
58	6	156	HIS
59	7	44	HIS
59	7	77	GLN
60	8	11	GLN
63	AB	79	HIS
64	AC	8	GLN
64	AC	97	GLN
66	AE	11	HIS
66	AE	97	GLN
66	AE	105	ASN
66	AE	120	HIS
67	AF	85	ASN
67	AF	128	GLN
68	AG	18	HIS

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Mol	Chain	Res	Type
68	AG	92	HIS
72	AK	124	ASN
73	AL	64	ASN
75	AN	83	GLN
79	AR	117	ASN
79	AR	143	GLN
79	AR	196	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	13/14 (92%)	2 (15%)	0
2	B	74/75 (98%)	13 (17%)	0
2	C	74/75 (98%)	14 (18%)	1 (1%)
3	D	3496/5070 (68%)	618 (17%)	29 (0%)
4	E	119/120 (99%)	16 (13%)	0
48	w	1624/1869 (86%)	392 (24%)	0
5	F	155/156 (99%)	27 (17%)	3 (1%)
All	All	5555/7379 (75%)	1082 (19%)	33 (0%)

All (1082) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	28	G
1	A	29	A
2	B	3	C
2	B	9	1MA
2	B	13	PSU
2	B	17	G
2	B	18	G
2	B	21	A
2	B	46	A
2	B	47	5MC
2	B	48	5MC
2	B	53	5MU
2	B	73	C
2	B	74	C
2	B	75	A
2	C	4	U
2	C	6	2MG
2	C	9	1MA

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Mol	Chain	Res	Type
2	C	17	G
2	C	21	A
2	C	26	C
2	C	33	U
2	C	34	56B
2	C	46	A
2	C	47	5MC
2	C	48	5MC
2	C	53	5MU
2	C	66	C
2	C	73	C
3	D	2	G
3	D	39	A
3	D	42	A
3	D	48	G
3	D	56	A
3	D	59	A
3	D	64	A
3	D	65	A
3	D	69	A
3	D	91	G
3	D	98	A
3	D	108	A
3	D	109	G
3	D	110	C
3	D	119	G
3	D	120	A
3	D	143	C
3	D	144	G
3	D	152	U
3	D	159	C
3	D	170	C
3	D	171	U
3	D	172	C
3	D	180	C
3	D	181	C
3	D	183	C
3	D	185	C
3	D	186	G
3	D	188	G
3	D	189	G
3	D	200	U

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Mol	Chain	Res	Type
3	D	209	U
3	D	218	A
3	D	220	C
3	D	234	G
3	D	256	G
3	D	257	C
3	D	259	C
3	D	261	G
3	D	265	C
3	D	266	C
3	D	267	G
3	D	275	C
3	D	276	C
3	D	280	G
3	D	306	A
3	D	315	G
3	D	316	U
3	D	340	C
3	D	344	A
3	D	345	C
3	D	350	C
3	D	386	A
3	D	387	G
3	D	399	G
3	D	407	A
3	D	410	A
3	D	412	G
3	D	413	G
3	D	432	U
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	487	G
3	D	491	G
3	D	494	U

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Mol	Chain	Res	Type
3	D	495	C
3	D	496	G
3	D	498	C
3	D	499	G
3	D	500	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	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	703	G
3	D	704	C
3	D	731	G
3	D	738	C
3	D	739	G
3	D	740	G
3	D	746	A
3	D	754	U
3	D	760	G
3	D	904	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	926	G

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Mol	Chain	Res	Type
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	972	C
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	1078	A
3	D	1082	C
3	D	1083	U
3	D	1094	G
3	D	1168	G
3	D	1171	G
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	1196	G
3	D	1202	C
3	D	1203	G
3	D	1210	C
3	D	1211	G
3	D	1214	C

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Mol	Chain	Res	Type
3	D	1215	C
3	D	1217	G
3	D	1219	G
3	D	1241	C
3	D	1262	G
3	D	1266	G
3	D	1269	G
3	D	1270	A
3	D	1271	G
3	D	1272	C
3	D	1273	G
3	D	1275	G
3	D	1277	G
3	D	1280	C
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	1312	A
3	D	1313	C
3	D	1326	A2M
3	D	1337	A
3	D	1354	A
3	D	1358	G
3	D	1359	G
3	D	1365	C
3	D	1366	G
3	D	1377	G
3	D	1379	C
3	D	1387	A
3	D	1394	G
3	D	1397	A
3	D	1398	A
3	D	1403	G
3	D	1404	G
3	D	1407	C

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Mol	Chain	Res	Type
3	D	1408	G
3	D	1409	C
3	D	1410	U
3	D	1411	C
3	D	1412	G
3	D	1414	C
3	D	1415	G
3	D	1417	C
3	D	1420	A
3	D	1439	C
3	D	1441	C
3	D	1442	C
3	D	1443	A
3	D	1482	G
3	D	1483	C
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	1591	U
3	D	1596	U
3	D	1624	G
3	D	1625	OMG
3	D	1631	A
3	D	1633	G
3	D	1634	A
3	D	1640	C
3	D	1642	A
3	D	1654	G
3	D	1661	C
3	D	1676	C
3	D	1677	PSU
3	D	1678	C
3	D	1698	C
3	D	1699	A

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Mol	Chain	Res	Type
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	1734	G
3	D	1735	U
3	D	1741	G
3	D	1742	A
3	D	1756	U
3	D	1757	U
3	D	1758	G
3	D	1760	OMG
3	D	1763	C
3	D	1787	A
3	D	1797	G
3	D	1804	A
3	D	1810	G
3	D	1821	G
3	D	1822	U
3	D	1836	G
3	D	1837	A
3	D	1842	G
3	D	1843	A
3	D	1855	G
3	D	1869	G
3	D	1882	U
3	D	1892	A
3	D	1897	A
3	D	1918	U
3	D	1919	G
3	D	1920	C
3	D	1921	C
3	D	1922	G
3	D	1925	G
3	D	1931	C
3	D	1932	A
3	D	1940	G
3	D	1948	G
3	D	1951	G
3	D	1960	A

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Mol	Chain	Res	Type
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	2099	G
3	D	2102	G
3	D	2103	G
3	D	2104	G
3	D	2105	A
3	D	2257	C
3	D	2258	C
3	D	2259	G
3	D	2289	C
3	D	2300	A
3	D	2301	G
3	D	2313	A
3	D	2316	G
3	D	2333	G
3	D	2348	G
3	D	2351	OMC
3	D	2395	A
3	D	2397	G
3	D	2416	G
3	D	2421	G
3	D	2422	OMC
3	D	2424	OMG
3	D	2425	U
3	D	2447	U

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Mol	Chain	Res	Type
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	2490	U
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	2506	G
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
3	D	2547	G
3	D	2554	U
3	D	2583	C
3	D	2587	A
3	D	2601	A
3	D	2618	G
3	D	2627	C
3	D	2653	C
3	D	2662	G
3	D	2669	C
3	D	2676	A
3	D	2687	U
3	D	2694	G
3	D	2695	A
3	D	2696	A

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Mol	Chain	Res	Type
3	D	2703	G
3	D	2706	G
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	2729	C
3	D	2739	C
3	D	2742	G
3	D	2743	A
3	D	2746	A
3	D	2754	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	2829	U
3	D	2838	G
3	D	2848	G
3	D	2855	G
3	D	2856	C
3	D	2867	C
3	D	2874	U
3	D	2877	G
3	D	2892	C
3	D	2900	U
3	D	3604	A
3	D	3605	C
3	D	3606	U
3	D	3615	G
3	D	3618	C
3	D	3626	G

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Mol	Chain	Res	Type
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	3735	G
3	D	3736	A
3	D	3748	A
3	D	3750	G
3	D	3753	G
3	D	3757	G
3	D	3758	PSU
3	D	3760	A2M
3	D	3763	A
3	D	3771	C
3	D	3776	G
3	D	3777	G
3	D	3783	A
3	D	3784	A
3	D	3786	U
3	D	3802	U
3	D	3811	G
3	D	3812	C
3	D	3814	U
3	D	3817	A
3	D	3818	UY1
3	D	3819	G
3	D	3823	G
3	D	3838	U
3	D	3839	G
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

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Mol	Chain	Res	Type
3	D	3906	A
3	D	3907	G
3	D	3908	A
3	D	3915	U
3	D	3938	G
3	D	3939	G
3	D	3943	A
3	D	3944	OMG
3	D	3946	G
3	D	4076	G
3	D	4086	G
3	D	4093	G
3	D	4094	G
3	D	4097	G
3	D	4098	A
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
3	D	4170	A
3	D	4183	G
3	D	4184	G
3	D	4191	G
3	D	4201	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

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Mol	Chain	Res	Type
3	D	4258	C
3	D	4268	A
3	D	4273	A
3	D	4281	A
3	D	4290	U
3	D	4291	G
3	D	4297	G
3	D	4305	G
3	D	4329	G
3	D	4330	G
3	D	4332	C
3	D	4339	A
3	D	4349	C
3	D	4364	G
3	D	4373	G
3	D	4376	A
3	D	4377	G
3	D	4378	A
3	D	4379	A
3	D	4380	A
3	D	4387	C
3	D	4391	G
3	D	4394	A
3	D	4405	G
3	D	4421	C
3	D	4422	A
3	D	4444	C
3	D	4448	G
3	D	4449	A
3	D	4452	U
3	D	4453	C
3	D	4464	A
3	D	4475	G
3	D	4500	PSU
3	D	4512	U
3	D	4513	A
3	D	4519	C
3	D	4524	G
3	D	4545	G
3	D	4548	A
3	D	4554	G
3	D	4560	C

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Mol	Chain	Res	Type
3	D	4567	G
3	D	4570	G
3	D	4573	G
3	D	4575	G
3	D	4590	A
3	D	4600	G
3	D	4601	U
3	D	4617	G
3	D	4636	U
3	D	4637	OMG
3	D	4647	G
3	D	4656	A
3	D	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	4720	C
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	4862	G
3	D	4870	G
3	D	4871	C
3	D	4875	G
3	D	4882	U
3	D	4883	C

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Mol	Chain	Res	Type
3	D	4889	G
3	D	4895	C
3	D	4896	G
3	D	4900	C
3	D	4901	G
3	D	4902	C
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	4960	G
3	D	4963	G
3	D	4966	A
3	D	4976	U
3	D	4989	U
3	D	4990	C
3	D	4991	U
3	D	5007	A
3	D	5014	A
3	D	5016	A
3	D	5017	G
3	D	5022	U
3	D	5024	C
3	D	5025	C
3	D	5026	U
3	D	5028	G
3	D	5030	U
3	D	5034	A
3	D	5041	G
3	D	5050	C
3	D	5054	C
3	D	5058	A
3	D	5060	A
3	D	5061	A
3	D	5062	G
3	D	5069	U
4	E	7	G

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Mol	Chain	Res	Type
4	E	20	U
4	E	22	A
4	E	24	C
4	E	31	G
4	E	42	A
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	103	A
4	E	110	G
4	E	120	U
5	F	2	G
5	F	17	A
5	F	23	C
5	F	34	U
5	F	35	C
5	F	48	A
5	F	59	A
5	F	63	U
5	F	81	C
5	F	82	A
5	F	83	C
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	124	U
5	F	125	C
5	F	126	C
5	F	127	U
5	F	128	C
5	F	150	C
5	F	151	G
5	F	153	C

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Mol	Chain	Res	Type
48	w	2	A
48	w	17	C
48	w	21	U
48	w	22	A
48	w	33	G
48	w	34	PSU
48	w	35	C
48	w	41	G
48	w	42	A
48	w	43	U
48	w	44	U
48	w	45	A
48	w	46	A
48	w	49	C
48	w	59	U
48	w	60	A
48	w	61	A
48	w	62	G
48	w	66	G
48	w	67	C
48	w	68	A
48	w	69	C
48	w	78	C
48	w	79	A
48	w	80	G
48	w	81	U
48	w	83	A
48	w	89	C
48	w	98	C
48	w	99	A2M
48	w	103	A
48	w	113	G
48	w	115	U
48	w	116	OMU
48	w	117	C
48	w	120	U
48	w	121	OMU
48	w	126	G
48	w	129	C
48	w	130	G
48	w	143	U
48	w	149	A

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Mol	Chain	Res	Type
48	w	150	A
48	w	154	U
48	w	155	G
48	w	159	A2M
48	w	161	U
48	w	162	C
48	w	163	U
48	w	166	A2M
48	w	173	A
48	w	182	C
48	w	190	G
48	w	191	A
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	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	295	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	370	G
48	w	380	G
48	w	381	C
48	w	385	G
48	w	386	C

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Mol	Chain	Res	Type
48	w	398	A
48	w	400	C
48	w	407	G
48	w	408	A
48	w	409	C
48	w	413	G
48	w	418	A
48	w	421	G
48	w	428	OMU
48	w	438	G
48	w	441	C
48	w	447	A
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	467	G
48	w	468	A2M
48	w	471	G
48	w	472	C
48	w	473	A
48	w	474	G
48	w	482	G
48	w	485	A
48	w	487	U
48	w	488	U
48	w	489	A
48	w	491	C
48	w	493	A
48	w	496	C
48	w	497	C
48	w	498	C
48	w	500	A
48	w	506	G
48	w	507	G
48	w	512	A2M
48	w	516	A
48	w	519	A
48	w	523	A

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Mol	Chain	Res	Type
48	w	528	A
48	w	531	A
48	w	532	C
48	w	533	A
48	w	534	G
48	w	551	U
48	w	552	G
48	w	554	A
48	w	556	U
48	w	557	U
48	w	558	G
48	w	560	A
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	598	G
48	w	604	A
48	w	605	A
48	w	606	G
48	w	608	C
48	w	613	G
48	w	614	C
48	w	616	A
48	w	622	C
48	w	627	OMU
48	w	629	A
48	w	632	C
48	w	634	A
48	w	643	A
48	w	655	A
48	w	660	C
48	w	664	A
48	w	668	A2M

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Mol	Chain	Res	Type
48	w	669	A
48	w	671	A
48	w	672	A
48	w	688	U
48	w	808	A
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	835	C
48	w	836	G
48	w	837	A
48	w	838	G
48	w	839	C
48	w	840	C
48	w	841	G
48	w	842	C
48	w	847	A
48	w	853	C
48	w	869	A
48	w	870	A
48	w	872	A
48	w	874	G
48	w	878	G
48	w	880	G
48	w	881	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

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Mol	Chain	Res	Type
48	w	901	G
48	w	904	A
48	w	909	G
48	w	912	C
48	w	913	A
48	w	917	U
48	w	920	A
48	w	930	C
48	w	933	G
48	w	934	G
48	w	943	U
48	w	944	A
48	w	958	G
48	w	963	A
48	w	970	G
48	w	972	A
48	w	990	A
48	w	992	A
48	w	999	G
48	w	1001	A
48	w	1017	U
48	w	1023	A
48	w	1027	A
48	w	1032	C
48	w	1060	A
48	w	1061	U
48	w	1062	A
48	w	1083	A
48	w	1085	C
48	w	1109	C
48	w	1114	U
48	w	1115	U
48	w	1116	C
48	w	1119	A
48	w	1126	G
48	w	1133	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

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Mol	Chain	Res	Type
48	w	1207	G
48	w	1208	A
48	w	1215	C
48	w	1217	A
48	w	1221	G
48	w	1224	G
48	w	1242	U
48	w	1243	U
48	w	1251	A
48	w	1253	A
48	w	1256	G
48	w	1257	G
48	w	1259	A
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	1288	OMU
48	w	1293	A
48	w	1295	A
48	w	1298	G
48	w	1301	A
48	w	1302	G
48	w	1308	U
48	w	1309	C
48	w	1331	C
48	w	1332	A
48	w	1342	U
48	w	1371	U
48	w	1372	U
48	w	1373	C
48	w	1378	A
48	w	1396	A
48	w	1397	U
48	w	1401	A
48	w	1402	A
48	w	1404	U
48	w	1406	G
48	w	1408	U
48	w	1417	C

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Mol	Chain	Res	Type
48	w	1428	G
48	w	1429	G
48	w	1433	C
48	w	1434	C
48	w	1435	C
48	w	1436	C
48	w	1438	A
48	w	1449	G
48	w	1450	G
48	w	1452	A
48	w	1454	A
48	w	1462	U
48	w	1463	U
48	w	1464	C
48	w	1476	A
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	1523	C
48	w	1528	G
48	w	1533	A
48	w	1536	G
48	w	1543	U
48	w	1545	A
48	w	1546	G
48	w	1548	G
48	w	1552	G
48	w	1553	C
48	w	1555	U
48	w	1569	A
48	w	1570	G
48	w	1574	C
48	w	1575	G
48	w	1580	A

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Mol	Chain	Res	Type
48	w	1585	U
48	w	1586	U
48	w	1588	A
48	w	1599	U
48	w	1601	A
48	w	1602	U
48	w	1607	A
48	w	1610	G
48	w	1621	U
48	w	1623	A
48	w	1624	U
48	w	1630	A
48	w	1632	G
48	w	1633	A
48	w	1635	C
48	w	1637	A
48	w	1638	G
48	w	1639	G7M
48	w	1640	A
48	w	1648	G
48	w	1654	G
48	w	1661	A
48	w	1663	A
48	w	1665	G
48	w	1671	G
48	w	1698	C
48	w	1721	U
48	w	1722	G
48	w	1742	C
48	w	1744	G
48	w	1745	A
48	w	1748	G
48	w	1751	C
48	w	1753	C
48	w	1754	G
48	w	1778	C
48	w	1779	G
48	w	1782	G
48	w	1783	C
48	w	1784	G
48	w	1786	U
48	w	1801	A

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Mol	Chain	Res	Type
48	w	1813	A
48	w	1824	A
48	w	1829	G
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 (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	5	C
3	D	1	C
3	D	406	C
3	D	515	C
3	D	914	U
3	D	922	C
3	D	987	C
3	D	1081	C
3	D	1574	G
3	D	1590	C
3	D	1625	OMG
3	D	1633	G
3	D	1677	PSU
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	3876	A
3	D	4092	G
3	D	4113	U
3	D	4115	G
3	D	4348	A

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Mol	Chain	Res	Type
3	D	4378	A
3	D	4600	G
3	D	4678	G
3	D	4699	U
3	D	4913	G
3	D	5016	A
5	F	16	G
5	F	86	U
5	F	126	C

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

216 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
3	PSU	D	1744	80,3	18,21,22	0.99	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	4312	3	18,21,22	1.05	1 (5%)	22,30,33	1.89	5 (22%)
5	OMG	F	75	5	23,26,27	2.55	9 (39%)	33,38,41	1.93	9 (27%)
3	PSU	D	3851	3	18,21,22	1.04	1 (5%)	22,30,33	1.79	4 (18%)
3	UR3	D	4530	3	19,22,23	2.59	6 (31%)	26,32,35	1.29	3 (11%)
48	PSU	w	866	48	18,21,22	1.06	1 (5%)	22,30,33	1.83	5 (22%)
3	A2M	D	3760	3	22,25,26	1.41	1 (4%)	31,36,39	1.13	2 (6%)
3	OMU	D	1773	3	19,22,23	2.92	8 (42%)	26,31,34	1.61	4 (15%)
48	PSU	w	34	48	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
48	PSU	w	815	48	18,21,22	1.09	1 (5%)	22,30,33	1.86	5 (22%)
48	PSU	w	1692	48	18,21,22	1.02	1 (5%)	22,30,33	1.84	4 (18%)
3	PSU	D	1683	80,3	18,21,22	1.07	2 (11%)	22,30,33	1.89	4 (18%)
3	OMC	D	2422	80,3	19,22,23	2.83	8 (42%)	26,31,34	0.71	0
2	H2U	C	19	2	18,21,22	1.06	2 (11%)	21,30,33	0.79	0
3	A2M	D	3825	3	22,25,26	1.40	1 (4%)	31,36,39	1.04	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	w	1347	48	18,21,22	0.99	1 (5%)	22,30,33	1.80	4 (18%)
48	6MZ	w	1832	48,80	22,25,26	2.81	4 (18%)	30,36,39	2.20	10 (33%)
48	OMU	w	1442	48,80	19,22,23	2.85	6 (31%)	26,31,34	1.73	5 (19%)
3	PSU	D	4403	80,3	18,21,22	1.08	1 (5%)	22,30,33	1.89	4 (18%)
48	PSU	w	1244	48	18,21,22	1.01	1 (5%)	22,30,33	1.82	5 (22%)
3	PSU	D	3764	3	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	OMC	D	4536	3	19,22,23	2.80	8 (42%)	26,31,34	0.73	0
3	PSU	D	1677	3	18,21,22	1.14	2 (11%)	22,30,33	1.83	4 (18%)
2	2MG	B	6	2	23,26,27	2.63	7 (30%)	32,38,41	2.15	10 (31%)
3	OMG	D	4623	3	23,26,27	2.50	9 (39%)	33,38,41	1.99	10 (30%)
2	5MC	B	48	2	18,22,23	3.78	8 (44%)	26,32,35	1.03	2 (7%)
3	A2M	D	1534	80,3	22,25,26	1.36	2 (9%)	31,36,39	1.35	7 (22%)
48	PSU	w	1056	48	18,21,22	1.04	1 (5%)	22,30,33	1.82	4 (18%)
48	OMG	w	1490	48,80	23,26,27	2.58	8 (34%)	33,38,41	1.95	9 (27%)
48	OMC	w	174	48	19,22,23	3.02	8 (42%)	26,31,34	0.73	0
2	5MU	C	53	2	19,22,23	4.67	6 (31%)	28,32,35	3.60	9 (32%)
3	A2M	D	398	3	22,25,26	1.35	1 (4%)	31,36,39	1.01	3 (9%)
3	1MA	D	1322	3	21,25,26	0.74	0	31,37,40	0.82	1 (3%)
48	PSU	w	1232	48	18,21,22	1.08	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	3695	3	18,21,22	1.01	1 (5%)	22,30,33	1.91	4 (18%)
3	PSU	D	1782	3	18,21,22	1.02	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	D	4576	3	18,21,22	1.00	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	D	1862	3	18,21,22	1.01	1 (5%)	22,30,33	1.95	5 (22%)
3	A2M	D	2787	80,3	22,25,26	1.38	1 (4%)	31,36,39	1.01	2 (6%)
48	PSU	w	966	48	18,21,22	1.03	1 (5%)	22,30,33	1.90	5 (22%)
3	A2M	D	3718	3	22,25,26	1.35	1 (4%)	31,36,39	0.98	2 (6%)
48	OMC	w	462	48	19,22,23	3.02	8 (42%)	26,31,34	0.77	0
2	2MG	C	6	2	23,26,27	2.65	7 (30%)	32,38,41	2.16	9 (28%)
3	PSU	D	4423	3	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
48	MA6	w	1850	48	23,26,27	1.45	4 (17%)	34,38,41	2.18	11 (32%)
3	OMC	D	3808	3	19,22,23	2.76	8 (42%)	26,31,34	0.74	0
3	OMG	D	3744	3	23,26,27	2.56	9 (39%)	33,38,41	1.92	9 (27%)
48	OMU	w	428	48	19,22,23	2.97	8 (42%)	26,31,34	1.73	4 (15%)
48	PSU	w	1045	48	18,21,22	1.04	1 (5%)	22,30,33	1.95	5 (22%)
3	OMG	D	4494	3	23,26,27	2.56	10 (43%)	33,38,41	1.96	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	D	4431	3	18,21,22	1.04	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	4689	3	18,21,22	1.07	1 (5%)	22,30,33	1.80	4 (18%)
48	A2M	w	1031	48	22,25,26	1.43	1 (4%)	31,36,39	1.04	1 (3%)
2	5MC	B	38	2	18,22,23	3.68	8 (44%)	26,32,35	1.09	2 (7%)
48	OMU	w	1288	48	19,22,23	2.95	8 (42%)	26,31,34	1.68	4 (15%)
3	PSU	D	3758	3	18,21,22	0.97	1 (5%)	22,30,33	1.82	4 (18%)
48	PSU	w	1625	48	18,21,22	1.05	1 (5%)	22,30,33	1.83	5 (22%)
48	OMU	w	1804	48	19,22,23	2.84	6 (31%)	26,31,34	1.76	5 (19%)
3	PSU	D	3920	80,3	18,21,22	1.08	1 (5%)	22,30,33	1.83	4 (18%)
3	PSU	D	4296	3	18,21,22	1.05	1 (5%)	22,30,33	1.84	4 (18%)
48	PSU	w	109	48	18,21,22	1.07	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	1792	3	18,21,22	0.96	1 (5%)	22,30,33	1.80	3 (13%)
48	PSU	w	210	48	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
3	PSU	D	4500	3	18,21,22	1.00	1 (5%)	22,30,33	1.91	5 (22%)
3	PSU	D	3768	3	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
2	PSU	B	54	2	18,21,22	1.04	1 (5%)	22,30,33	1.75	4 (18%)
48	A2M	w	668	48,80	22,25,26	1.61	2 (9%)	31,36,39	1.05	4 (12%)
3	PSU	D	3734	3	18,21,22	1.02	1 (5%)	22,30,33	1.87	5 (22%)
48	PSU	w	1081	48	18,21,22	1.03	1 (5%)	22,30,33	1.83	4 (18%)
3	A2M	D	2815	3	22,25,26	1.52	1 (4%)	31,36,39	1.00	3 (9%)
48	PSU	w	1177	48	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
48	A2M	w	512	48	22,25,26	1.52	3 (13%)	31,36,39	1.07	2 (6%)
3	OMG	D	3792	3	23,26,27	2.54	10 (43%)	33,38,41	1.87	8 (24%)
2	5MC	C	48	2	18,22,23	3.78	8 (44%)	26,32,35	1.00	1 (3%)
48	A2M	w	1383	48	22,25,26	1.44	1 (4%)	31,36,39	1.17	5 (16%)
3	PSU	D	3715	3	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
2	PSU	C	54	2	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
2	56B	C	34	2,81	29,35,36	3.02	11 (37%)	36,52,55	2.36	8 (22%)
3	PSU	D	1781	3	18,21,22	1.03	1 (5%)	22,30,33	1.84	4 (18%)
2	1MA	B	9	2	21,25,26	0.82	1 (4%)	31,37,40	0.75	0
48	PSU	w	822	48	18,21,22	1.11	1 (5%)	22,30,33	1.76	5 (22%)
2	PSU	B	13	2	18,21,22	1.01	1 (5%)	22,30,33	1.84	5 (22%)
48	4AC	w	1842	48	21,24,25	0.59	0	29,34,37	1.12	4 (13%)
48	OMU	w	1326	48	19,22,23	2.88	7 (36%)	26,31,34	1.84	6 (23%)
3	OMU	D	4306	3	19,22,23	2.73	6 (31%)	26,31,34	1.83	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	D	1326	3	22,25,26	1.41	1 (4%)	31,36,39	1.00	1 (3%)
3	A2M	D	1871	80,3	22,25,26	1.44	2 (9%)	31,36,39	1.15	4 (12%)
48	A2M	w	484	48	22,25,26	1.59	3 (13%)	31,36,39	0.99	2 (6%)
3	A2M	D	400	3	22,25,26	1.45	2 (9%)	31,36,39	1.01	2 (6%)
3	OMC	D	1340	3	19,22,23	2.77	8 (42%)	26,31,34	0.73	0
48	OMG	w	601	48	23,26,27	2.62	8 (34%)	33,38,41	1.93	9 (27%)
48	OMU	w	121	48	19,22,23	2.95	7 (36%)	26,31,34	1.67	4 (15%)
48	OMG	w	683	48	23,26,27	2.59	8 (34%)	33,38,41	1.96	9 (27%)
48	OMC	w	1703	48,80	19,22,23	2.85	8 (42%)	26,31,34	0.73	0
3	UY1	D	3818	80,3	19,22,23	1.11	2 (10%)	22,31,34	0.93	1 (4%)
48	PSU	w	93	48	18,21,22	1.06	1 (5%)	22,30,33	1.79	3 (13%)
3	PSU	D	4532	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
3	5MC	D	3782	80,3	18,22,23	3.55	7 (38%)	26,32,35	1.15	2 (7%)
3	PSU	D	4420	3	18,21,22	1.02	1 (5%)	22,30,33	1.81	6 (27%)
2	1MA	B	57	2	21,25,26	0.87	1 (4%)	31,37,40	0.77	1 (3%)
48	A2M	w	99	48,80	22,25,26	1.41	2 (9%)	31,36,39	1.08	3 (9%)
48	PSU	w	119	48	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
2	5MU	B	53	2	19,22,23	4.65	6 (31%)	28,32,35	3.60	9 (32%)
48	OMG	w	644	48	23,26,27	2.63	9 (39%)	33,38,41	1.97	10 (30%)
48	PSU	w	572	48	18,21,22	1.09	1 (5%)	22,30,33	1.76	3 (13%)
48	B8N	w	1248	48	24,29,30	0.80	0	29,42,45	1.00	2 (6%)
48	OMG	w	1328	48	23,26,27	2.61	8 (34%)	33,38,41	1.96	9 (27%)
48	OMU	w	116	48	19,22,23	2.89	6 (31%)	26,31,34	1.67	5 (19%)
2	H2U	B	19	2	18,21,22	1.08	2 (11%)	21,30,33	0.85	0
3	A2M	D	3785	80,3	22,25,26	1.50	2 (9%)	31,36,39	1.34	3 (9%)
48	PSU	w	1004	48	18,21,22	1.06	1 (5%)	22,30,33	1.85	4 (18%)
48	OMU	w	627	48	19,22,23	2.88	7 (36%)	26,31,34	1.69	5 (19%)
3	OMU	D	4498	3	19,22,23	2.73	6 (31%)	26,31,34	1.79	5 (19%)
3	PSU	D	4972	80,3	18,21,22	1.01	1 (5%)	22,30,33	1.91	5 (22%)
48	PSU	w	105	48	18,21,22	1.03	1 (5%)	22,30,33	1.79	5 (22%)
3	OMG	D	1625	80,3	23,26,27	2.57	9 (39%)	33,38,41	1.95	8 (24%)
3	OMC	D	2861	3	19,22,23	2.80	8 (42%)	26,31,34	0.66	0
3	OMU	D	3925	3	19,22,23	2.71	6 (31%)	26,31,34	1.81	4 (15%)
3	OMC	D	4456	3	19,22,23	2.79	8 (42%)	26,31,34	0.65	0
3	OMG	D	3627	3	23,26,27	2.54	10 (43%)	33,38,41	2.00	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	A2M	w	468	48	22,25,26	1.57	2 (9%)	31,36,39	1.05	1 (3%)
3	OMG	D	4637	3	23,26,27	2.55	9 (39%)	33,38,41	1.94	9 (27%)
48	A2M	w	576	48	22,25,26	1.44	2 (9%)	31,36,39	1.01	2 (6%)
48	OMC	w	1391	48	19,22,23	2.91	8 (42%)	26,31,34	0.74	0
48	PSU	w	406	48	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4457	3	18,21,22	1.04	1 (5%)	22,30,33	1.85	4 (18%)
48	A2M	w	590	48	22,25,26	1.48	2 (9%)	31,36,39	0.98	1 (3%)
48	PSU	w	1643	48,80	18,21,22	1.03	1 (5%)	22,30,33	1.80	4 (18%)
3	A2M	D	2401	3	22,25,26	1.40	1 (4%)	31,36,39	1.01	2 (6%)
48	PSU	w	1367	48	18,21,22	1.03	1 (5%)	22,30,33	1.86	5 (22%)
3	OMC	D	2804	3	19,22,23	2.78	7 (36%)	26,31,34	0.67	0
2	1MA	C	57	2	21,25,26	0.86	1 (4%)	31,37,40	0.77	1 (3%)
3	OMC	D	2365	80,3	19,22,23	2.75	8 (42%)	26,31,34	0.65	0
3	PSU	D	4471	3	18,21,22	1.07	1 (5%)	22,30,33	1.85	4 (18%)
3	PSU	D	4299	3	18,21,22	1.02	2 (11%)	22,30,33	1.82	4 (18%)
3	PSU	D	4579	3	18,21,22	1.06	2 (11%)	22,30,33	1.85	4 (18%)
2	PSU	C	13	2	18,21,22	1.05	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	4628	3	18,21,22	1.04	1 (5%)	22,30,33	1.85	4 (18%)
48	PSU	w	1174	48,80	18,21,22	1.02	1 (5%)	22,30,33	1.76	4 (18%)
48	OMC	w	517	48,80	19,22,23	3.00	8 (42%)	26,31,34	0.71	0
3	A2M	D	3830	3	22,25,26	1.39	1 (4%)	31,36,39	1.08	2 (6%)
3	OMG	D	4370	3	23,26,27	2.54	10 (43%)	33,38,41	1.96	10 (30%)
3	OMG	D	2364	3	23,26,27	2.51	10 (43%)	33,38,41	1.92	9 (27%)
3	OMU	D	2837	3	19,22,23	2.73	6 (31%)	26,31,34	1.93	5 (19%)
48	G7M	w	1639	48,2	23,26,27	2.81	8 (34%)	35,39,42	1.86	9 (25%)
3	6MZ	D	4220	3	22,25,26	2.79	4 (18%)	30,36,39	2.26	10 (33%)
3	OMC	D	2824	3	19,22,23	2.80	8 (42%)	26,31,34	0.73	0
3	OMC	D	3841	3	19,22,23	2.77	8 (42%)	26,31,34	0.74	0
48	PSU	w	1046	48	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
3	OMG	D	4618	3	23,26,27	2.55	9 (39%)	33,38,41	1.95	10 (30%)
3	PSU	D	3762	3	18,21,22	1.07	1 (5%)	22,30,33	1.83	5 (22%)
48	OMG	w	509	48	23,26,27	2.67	8 (34%)	33,38,41	1.92	9 (27%)
3	OMC	D	2351	80,3	19,22,23	2.73	7 (36%)	26,31,34	0.82	1 (3%)
48	PSU	w	814	48	18,21,22	1.06	1 (5%)	22,30,33	1.83	4 (18%)
3	PSU	D	4521	80,3	18,21,22	1.06	1 (5%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	w	681	48,80	18,21,22	1.08	1 (5%)	22,30,33	1.89	5 (22%)
48	A2M	w	159	48	22,25,26	1.52	2 (9%)	31,36,39	1.07	3 (9%)
48	PSU	w	1445	48	18,21,22	1.05	1 (5%)	22,30,33	1.85	5 (22%)
3	OMG	D	3944	3	23,26,27	2.60	8 (34%)	33,38,41	1.95	9 (27%)
2	56B	B	34	2,81	29,35,36	3.01	12 (41%)	36,52,55	2.37	9 (25%)
3	OMU	D	4620	3	19,22,23	2.74	6 (31%)	26,31,34	1.84	5 (19%)
3	PSU	D	4552	3	18,21,22	1.10	2 (11%)	22,30,33	1.85	4 (18%)
3	OMU	D	2415	3	19,22,23	2.77	6 (31%)	26,31,34	1.94	5 (19%)
3	OMG	D	1316	3	23,26,27	2.52	9 (39%)	33,38,41	1.98	10 (30%)
48	OMU	w	799	48	19,22,23	2.94	8 (42%)	26,31,34	1.66	4 (15%)
3	OMU	D	4227	3	19,22,23	2.81	6 (31%)	26,31,34	1.90	4 (15%)
3	OMG	D	4196	2,80,3	23,26,27	2.52	10 (43%)	33,38,41	1.90	9 (27%)
2	1MA	C	9	2	21,25,26	0.89	1 (4%)	31,37,40	0.77	1 (3%)
3	PSU	D	2632	3	18,21,22	1.01	1 (5%)	22,30,33	1.83	4 (18%)
3	PSU	D	4353	3	18,21,22	1.05	1 (5%)	22,30,33	1.84	4 (18%)
48	PSU	w	1238	48	18,21,22	1.04	1 (5%)	22,30,33	1.78	5 (22%)
3	A2M	D	4523	80,3	22,25,26	1.48	2 (9%)	31,36,39	1.12	4 (12%)
48	PSU	w	36	48	18,21,22	1.07	1 (5%)	22,30,33	1.80	5 (22%)
48	4AC	w	1337	48	21,24,25	0.57	0	29,34,37	1.20	5 (17%)
48	A2M	w	1678	48	22,25,26	1.43	1 (4%)	31,36,39	0.95	1 (3%)
3	PSU	D	3730	3	18,21,22	1.02	1 (5%)	22,30,33	1.90	5 (22%)
3	PSU	D	1536	3	18,21,22	1.07	2 (11%)	22,30,33	1.81	3 (13%)
2	5MC	C	47	2	18,22,23	3.76	8 (44%)	26,32,35	1.03	2 (7%)
3	OMG	D	1522	3	23,26,27	2.49	8 (34%)	33,38,41	1.92	10 (30%)
3	PSU	D	5001	80,3	18,21,22	1.07	1 (5%)	22,30,33	1.81	3 (13%)
48	PSU	w	651	48	18,21,22	1.05	1 (5%)	22,30,33	1.83	5 (22%)
48	PSU	w	649	48	18,21,22	1.03	1 (5%)	22,30,33	1.80	4 (18%)
3	A2M	D	3724	3	22,25,26	1.39	1 (4%)	31,36,39	1.03	2 (6%)
3	OMG	D	4228	3	23,26,27	2.54	9 (39%)	33,38,41	2.04	10 (30%)
48	PSU	w	686	48	18,21,22	1.05	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	2508	3	18,21,22	1.03	2 (11%)	22,30,33	1.86	5 (22%)
48	PSU	w	609	48	18,21,22	1.09	1 (5%)	22,30,33	1.79	4 (18%)
48	MA6	w	1851	48	23,26,27	1.34	4 (17%)	34,38,41	2.28	10 (29%)
3	OMG	D	2424	3	23,26,27	2.57	9 (39%)	33,38,41	1.92	8 (24%)
3	PSU	D	1860	3	18,21,22	1.02	1 (5%)	22,30,33	1.85	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	D	4361	3	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
3	A2M	D	1524	3	22,25,26	1.53	2 (9%)	31,36,39	1.15	4 (12%)
3	PSU	D	3639	3	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
3	PSU	D	3853	80,3	18,21,22	1.01	1 (5%)	22,30,33	1.75	4 (18%)
48	OMG	w	436	48	23,26,27	2.58	8 (34%)	33,38,41	1.99	10 (30%)
48	PSU	w	863	48	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)
3	OMC	D	3887	3	19,22,23	2.80	8 (42%)	26,31,34	0.77	1 (3%)
2	5MC	C	38	2	18,22,23	3.75	8 (44%)	26,32,35	1.02	2 (7%)
3	OMG	D	3899	3	23,26,27	2.51	10 (43%)	33,38,41	2.01	10 (30%)
48	PSU	w	801	48	18,21,22	1.07	1 (5%)	22,30,33	1.83	5 (22%)
3	OMG	D	1760	3	23,26,27	2.63	8 (34%)	33,38,41	1.93	11 (33%)
3	5MC	D	4447	80,3	18,22,23	3.55	7 (38%)	26,32,35	1.19	2 (7%)
3	PSU	D	3637	80,3	18,21,22	1.06	1 (5%)	22,30,33	1.96	5 (22%)
3	PSU	D	3770	3	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)
2	5MC	B	47	2	18,22,23	3.73	8 (44%)	26,32,35	1.07	2 (7%)
3	PSU	D	5010	3	18,21,22	1.04	1 (5%)	22,30,33	1.87	4 (18%)
48	A2M	w	27	48	22,25,26	1.44	1 (4%)	31,36,39	1.03	2 (6%)
48	PSU	w	218	48	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
48	A2M	w	166	48	22,25,26	1.54	3 (13%)	31,36,39	1.06	3 (9%)
3	A2M	D	2363	80,3	22,25,26	1.41	2 (9%)	31,36,39	0.98	1 (3%)
3	PSU	D	4442	3	18,21,22	1.04	2 (11%)	22,30,33	1.88	5 (22%)
3	PSU	D	4293	3	18,21,22	1.05	2 (11%)	22,30,33	1.84	4 (18%)
48	OMU	w	172	48	19,22,23	2.96	8 (42%)	26,31,34	1.72	4 (15%)
3	OMG	D	4499	2,3	23,26,27	2.55	10 (43%)	33,38,41	1.97	10 (30%)
3	OMC	D	3701	80,3	19,22,23	2.80	8 (42%)	26,31,34	0.77	0
3	OMG	D	4392	3	23,26,27	2.51	9 (39%)	33,38,41	2.03	10 (30%)

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
3	PSU	D	1744	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	4312	3	-	0/7/25/26	0/2/2/2
5	OMG	F	75	5	-	0/9/27/28	0/3/3/3
3	PSU	D	3851	3	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UR3	D	4530	3	-	0/7/25/26	0/2/2/2
48	PSU	w	866	48	-	0/7/25/26	0/2/2/2
3	A2M	D	3760	3	-	2/9/27/28	0/3/3/3
3	OMU	D	1773	3	-	1/9/27/28	0/2/2/2
48	PSU	w	34	48	-	3/7/25/26	0/2/2/2
48	PSU	w	815	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1692	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1683	80,3	-	0/7/25/26	0/2/2/2
3	OMC	D	2422	80,3	-	1/9/27/28	0/2/2/2
2	H2U	C	19	2	-	0/7/38/39	0/2/2/2
3	A2M	D	3825	3	-	0/9/27/28	0/3/3/3
48	PSU	w	1347	48	-	0/7/25/26	0/2/2/2
48	6MZ	w	1832	48,80	-	0/9/27/28	0/3/3/3
48	OMU	w	1442	48,80	-	1/9/27/28	0/2/2/2
3	PSU	D	4403	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	1244	48	-	0/7/25/26	0/2/2/2
3	PSU	D	3764	3	-	0/7/25/26	0/2/2/2
3	OMC	D	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	D	1677	3	-	5/7/25/26	0/2/2/2
2	2MG	B	6	2	-	0/9/27/28	0/3/3/3
3	OMG	D	4623	3	-	0/9/27/28	0/3/3/3
2	5MC	B	48	2	-	2/7/25/26	0/2/2/2
3	A2M	D	1534	80,3	-	3/9/27/28	0/3/3/3
48	PSU	w	1056	48	-	0/7/25/26	0/2/2/2
48	OMG	w	1490	48,80	-	3/9/27/28	0/3/3/3
48	OMC	w	174	48	-	0/9/27/28	0/2/2/2
2	5MU	C	53	2	-	2/7/25/26	0/2/2/2
3	A2M	D	398	3	-	0/9/27/28	0/3/3/3
3	1MA	D	1322	3	-	2/7/25/26	0/3/3/3
48	PSU	w	1232	48	-	0/7/25/26	0/2/2/2
3	PSU	D	3695	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1782	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1862	3	-	0/7/25/26	0/2/2/2
3	A2M	D	2787	80,3	-	3/9/27/28	0/3/3/3
48	PSU	w	966	48	-	0/7/25/26	0/2/2/2
3	A2M	D	3718	3	-	0/9/27/28	0/3/3/3
48	OMC	w	462	48	-	0/9/27/28	0/2/2/2
2	2MG	C	6	2	-	0/9/27/28	0/3/3/3
3	PSU	D	4423	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	OMG	D	3744	3	-	0/9/27/28	0/3/3/3
48	OMU	w	428	48	-	7/9/27/28	0/2/2/2
48	PSU	w	1045	48	-	0/7/25/26	0/2/2/2
3	OMG	D	4494	3	-	1/9/27/28	0/3/3/3
3	PSU	D	4431	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4689	3	-	0/7/25/26	0/2/2/2
48	A2M	w	1031	48	-	0/9/27/28	0/3/3/3
2	5MC	B	38	2	-	0/7/25/26	0/2/2/2
48	OMU	w	1288	48	-	4/9/27/28	0/2/2/2
3	PSU	D	3758	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1625	48	-	0/7/25/26	0/2/2/2
48	OMU	w	1804	48	-	1/9/27/28	0/2/2/2
3	PSU	D	3920	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	4296	3	-	0/7/25/26	0/2/2/2
48	PSU	w	109	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1792	3	-	0/7/25/26	0/2/2/2
48	PSU	w	210	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4500	3	-	3/7/25/26	0/2/2/2
3	PSU	D	3768	3	-	0/7/25/26	0/2/2/2
2	PSU	B	54	2	-	0/7/25/26	0/2/2/2
48	A2M	w	668	48,80	-	3/9/27/28	0/3/3/3
3	PSU	D	3734	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1081	48	-	0/7/25/26	0/2/2/2
3	A2M	D	2815	3	-	2/9/27/28	0/3/3/3
48	PSU	w	1177	48	-	0/7/25/26	0/2/2/2
48	A2M	w	512	48	-	2/9/27/28	0/3/3/3
3	OMG	D	3792	3	-	0/9/27/28	0/3/3/3
2	5MC	C	48	2	-	2/7/25/26	0/2/2/2
48	A2M	w	1383	48	-	0/9/27/28	0/3/3/3
3	PSU	D	3715	3	-	1/7/25/26	0/2/2/2
2	PSU	C	54	2	-	0/7/25/26	0/2/2/2
2	56B	C	34	2,81	-	2/12/43/44	0/4/4/4
3	PSU	D	1781	3	-	0/7/25/26	0/2/2/2
2	1MA	B	9	2	-	0/7/25/26	0/3/3/3
48	PSU	w	822	48	-	2/7/25/26	0/2/2/2
2	PSU	B	13	2	-	1/7/25/26	0/2/2/2
48	4AC	w	1842	48	-	0/11/29/30	0/2/2/2
48	OMU	w	1326	48	-	5/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	D	4306	3	-	0/9/27/28	0/2/2/2
3	A2M	D	1326	3	-	0/9/27/28	0/3/3/3
3	A2M	D	1871	80,3	-	0/9/27/28	0/3/3/3
48	A2M	w	484	48	-	1/9/27/28	0/3/3/3
3	A2M	D	400	3	-	0/9/27/28	0/3/3/3
3	OMC	D	1340	3	-	0/9/27/28	0/2/2/2
48	OMG	w	601	48	-	0/9/27/28	0/3/3/3
48	OMU	w	121	48	-	0/9/27/28	0/2/2/2
48	OMG	w	683	48	-	1/9/27/28	0/3/3/3
48	OMC	w	1703	48,80	-	2/9/27/28	0/2/2/2
3	UY1	D	3818	80,3	-	5/9/27/28	0/2/2/2
48	PSU	w	93	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4532	3	-	0/7/25/26	0/2/2/2
3	5MC	D	3782	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	4420	3	-	0/7/25/26	0/2/2/2
2	1MA	B	57	2	-	0/7/25/26	0/3/3/3
48	A2M	w	99	48,80	-	2/9/27/28	0/3/3/3
48	PSU	w	119	48	-	0/7/25/26	0/2/2/2
2	5MU	B	53	2	-	2/7/25/26	0/2/2/2
48	OMG	w	644	48	-	3/9/27/28	0/3/3/3
48	PSU	w	572	48	-	0/7/25/26	0/2/2/2
48	B8N	w	1248	48	-	2/16/34/35	0/2/2/2
48	OMG	w	1328	48	-	0/9/27/28	0/3/3/3
48	OMU	w	116	48	-	2/9/27/28	0/2/2/2
2	H2U	B	19	2	-	0/7/38/39	0/2/2/2
3	A2M	D	3785	80,3	-	3/9/27/28	0/3/3/3
48	PSU	w	1004	48	-	0/7/25/26	0/2/2/2
48	OMU	w	627	48	-	7/9/27/28	0/2/2/2
3	OMU	D	4498	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4972	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	105	48	-	0/7/25/26	0/2/2/2
3	OMG	D	1625	80,3	-	1/9/27/28	0/3/3/3
3	OMC	D	2861	3	-	0/9/27/28	0/2/2/2
3	OMU	D	3925	3	-	1/9/27/28	0/2/2/2
3	OMC	D	4456	3	-	0/9/27/28	0/2/2/2
3	OMG	D	3627	3	-	0/9/27/28	0/3/3/3
48	A2M	w	468	48	-	2/9/27/28	0/3/3/3
3	OMG	D	4637	3	-	1/9/27/28	0/3/3/3
48	A2M	w	576	48	-	3/9/27/28	0/3/3/3
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
48	PSU	w	406	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4457	3	-	0/7/25/26	0/2/2/2
48	A2M	w	590	48	-	2/9/27/28	0/3/3/3
48	PSU	w	1643	48,80	-	0/7/25/26	0/2/2/2
3	A2M	D	2401	3	-	1/9/27/28	0/3/3/3
48	PSU	w	1367	48	-	0/7/25/26	0/2/2/2
3	OMC	D	2804	3	-	0/9/27/28	0/2/2/2
2	1MA	C	57	2	-	0/7/25/26	0/3/3/3
3	OMC	D	2365	80,3	-	0/9/27/28	0/2/2/2
3	PSU	D	4471	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4579	3	-	0/7/25/26	0/2/2/2
2	PSU	C	13	2	-	0/7/25/26	0/2/2/2
3	PSU	D	4628	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1174	48,80	-	0/7/25/26	0/2/2/2
48	OMC	w	517	48,80	-	0/9/27/28	0/2/2/2
3	A2M	D	3830	3	-	0/9/27/28	0/3/3/3
3	OMG	D	4370	3	-	0/9/27/28	0/3/3/3
3	OMG	D	2364	3	-	2/9/27/28	0/3/3/3
3	OMU	D	2837	3	-	0/9/27/28	0/2/2/2
48	G7M	w	1639	48,2	-	2/7/25/26	0/3/3/3
3	6MZ	D	4220	3	-	0/9/27/28	0/3/3/3
3	OMC	D	2824	3	-	0/9/27/28	0/2/2/2
3	OMC	D	3841	3	-	0/9/27/28	0/2/2/2
48	PSU	w	1046	48	-	0/7/25/26	0/2/2/2
3	OMG	D	4618	3	-	0/9/27/28	0/3/3/3
3	PSU	D	3762	3	-	0/7/25/26	0/2/2/2
48	OMG	w	509	48	-	0/9/27/28	0/3/3/3
3	OMC	D	2351	80,3	-	2/9/27/28	0/2/2/2
48	PSU	w	814	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4521	80,3	-	2/7/25/26	0/2/2/2
48	PSU	w	681	48,80	-	0/7/25/26	0/2/2/2
48	A2M	w	159	48	-	3/9/27/28	0/3/3/3
48	PSU	w	1445	48	-	0/7/25/26	0/2/2/2
3	OMG	D	3944	3	-	4/9/27/28	0/3/3/3
2	56B	B	34	2,81	-	2/12/43/44	0/4/4/4
3	OMU	D	4620	3	-	1/9/27/28	0/2/2/2
3	PSU	D	4552	3	-	0/7/25/26	0/2/2/2
3	OMU	D	2415	3	-	1/9/27/28	0/2/2/2
3	OMG	D	1316	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMU	w	799	48	-	3/9/27/28	0/2/2/2
3	OMU	D	4227	3	-	0/9/27/28	0/2/2/2
3	OMG	D	4196	2,80,3	-	1/9/27/28	0/3/3/3
2	1MA	C	9	2	-	2/7/25/26	0/3/3/3
3	PSU	D	2632	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4353	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1238	48	-	2/7/25/26	0/2/2/2
3	A2M	D	4523	80,3	-	0/9/27/28	0/3/3/3
48	PSU	w	36	48	-	0/7/25/26	0/2/2/2
48	4AC	w	1337	48	-	2/11/29/30	0/2/2/2
48	A2M	w	1678	48	-	1/9/27/28	0/3/3/3
3	PSU	D	3730	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1536	3	-	0/7/25/26	0/2/2/2
2	5MC	C	47	2	-	3/7/25/26	0/2/2/2
3	OMG	D	1522	3	-	0/9/27/28	0/3/3/3
3	PSU	D	5001	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	651	48	-	0/7/25/26	0/2/2/2
48	PSU	w	649	48	-	0/7/25/26	0/2/2/2
3	A2M	D	3724	3	-	0/9/27/28	0/3/3/3
3	OMG	D	4228	3	-	0/9/27/28	0/3/3/3
48	PSU	w	686	48	-	0/7/25/26	0/2/2/2
3	PSU	D	2508	3	-	0/7/25/26	0/2/2/2
48	PSU	w	609	48	-	0/7/25/26	0/2/2/2
48	MA6	w	1851	48	-	3/11/29/30	0/3/3/3
3	OMG	D	2424	3	-	2/9/27/28	0/3/3/3
3	PSU	D	1860	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4361	3	-	0/7/25/26	0/2/2/2
3	A2M	D	1524	3	-	2/9/27/28	0/3/3/3
3	PSU	D	3639	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3853	80,3	-	0/7/25/26	0/2/2/2
48	OMG	w	436	48	-	0/9/27/28	0/3/3/3
48	PSU	w	863	48	-	0/7/25/26	0/2/2/2
3	OMC	D	3887	3	-	1/9/27/28	0/2/2/2
2	5MC	C	38	2	-	0/7/25/26	0/2/2/2
3	OMG	D	3899	3	-	0/9/27/28	0/3/3/3
48	PSU	w	801	48	-	0/7/25/26	0/2/2/2
3	OMG	D	1760	3	-	2/9/27/28	0/3/3/3
3	5MC	D	4447	80,3	-	4/7/25/26	0/2/2/2
3	PSU	D	3637	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	3770	3	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	B	47	2	-	3/7/25/26	0/2/2/2
3	PSU	D	5010	3	-	0/7/25/26	0/2/2/2
48	A2M	w	27	48	-	1/9/27/28	0/3/3/3
48	PSU	w	218	48	-	0/7/25/26	0/2/2/2
48	A2M	w	166	48	-	2/9/27/28	0/3/3/3
3	A2M	D	2363	80,3	-	0/9/27/28	0/3/3/3
3	PSU	D	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4293	3	-	0/7/25/26	0/2/2/2
48	OMU	w	172	48	-	0/9/27/28	0/2/2/2
3	OMG	D	4499	2,3	-	1/9/27/28	0/3/3/3
3	OMC	D	3701	80,3	-	4/9/27/28	0/2/2/2
3	OMG	D	4392	3	-	0/9/27/28	0/3/3/3

All (814) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	1832	6MZ	C6-N6	11.94	1.47	1.34
3	D	4220	6MZ	C6-N6	11.91	1.47	1.34
2	B	53	5MU	C2-N1	10.71	1.55	1.38
2	C	53	5MU	C6-N1	10.64	1.56	1.38
2	B	53	5MU	C6-N1	10.53	1.56	1.38
2	C	53	5MU	C2-N1	10.51	1.55	1.38
2	C	48	5MC	C6-C5	9.51	1.50	1.34
2	B	48	5MC	C6-C5	9.45	1.50	1.34
2	C	38	5MC	C6-C5	9.40	1.50	1.34
2	B	47	5MC	C6-C5	9.36	1.50	1.34
2	C	47	5MC	C6-C5	9.35	1.50	1.34
3	D	4447	5MC	C6-C5	9.31	1.49	1.34
2	B	38	5MC	C6-C5	9.23	1.49	1.34
2	C	53	5MU	C4-C5	9.10	1.59	1.44
3	D	3782	5MC	C6-C5	9.02	1.49	1.34
2	B	53	5MU	C4-C5	8.99	1.59	1.44
2	B	6	2MG	C2-N3	7.69	1.46	1.31
2	C	6	2MG	C2-N3	7.69	1.46	1.31
48	w	509	OMG	C4-N3	7.46	1.52	1.34
2	C	47	5MC	C4-N3	7.37	1.46	1.34
2	B	53	5MU	C4-N3	-7.37	1.25	1.38
2	C	53	5MU	C4-N3	-7.36	1.25	1.38
3	D	1760	OMG	C4-N3	7.33	1.51	1.34
48	w	436	OMG	C4-N3	7.33	1.51	1.34
2	B	48	5MC	C4-N3	7.31	1.46	1.34
3	D	3944	OMG	C4-N3	7.30	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	38	5MC	C4-N3	7.29	1.46	1.34
48	w	601	OMG	C4-N3	7.27	1.51	1.34
48	w	683	OMG	C4-N3	7.25	1.51	1.34
2	C	48	5MC	C4-N3	7.24	1.46	1.34
2	B	47	5MC	C4-N3	7.23	1.46	1.34
48	w	644	OMG	C4-N3	7.23	1.51	1.34
48	w	172	OMU	C2-N1	7.22	1.50	1.38
48	w	1490	OMG	C4-N3	7.22	1.51	1.34
48	w	428	OMU	C2-N1	7.22	1.50	1.38
48	w	1328	OMG	C4-N3	7.22	1.51	1.34
48	w	121	OMU	C2-N1	7.18	1.50	1.38
48	w	1288	OMU	C2-N1	7.13	1.49	1.38
48	w	799	OMU	C2-N1	7.13	1.49	1.38
3	D	1625	OMG	C4-N3	7.09	1.51	1.34
3	D	3744	OMG	C4-N3	7.08	1.51	1.34
3	D	4494	OMG	C4-N3	7.06	1.51	1.34
5	F	75	OMG	C4-N3	7.04	1.51	1.34
2	C	34	56B	C14-C13	7.02	1.53	1.32
3	D	4637	OMG	C4-N3	7.02	1.50	1.34
2	B	34	56B	C14-C13	7.02	1.53	1.32
2	B	38	5MC	C4-N3	7.01	1.46	1.34
3	D	4228	OMG	C4-N3	7.01	1.50	1.34
3	D	3792	OMG	C4-N3	7.01	1.50	1.34
3	D	4618	OMG	C4-N3	7.00	1.50	1.34
3	D	3627	OMG	C4-N3	6.97	1.50	1.34
3	D	1773	OMU	C2-N1	6.96	1.49	1.38
3	D	2424	OMG	C4-N3	6.96	1.50	1.34
48	w	116	OMU	C2-N1	6.95	1.49	1.38
3	D	4370	OMG	C4-N3	6.94	1.50	1.34
3	D	4196	OMG	C4-N3	6.92	1.50	1.34
3	D	4499	OMG	C4-N3	6.89	1.50	1.34
3	D	4227	OMU	C2-N1	6.88	1.49	1.38
48	w	1326	OMU	C2-N1	6.87	1.49	1.38
3	D	1522	OMG	C4-N3	6.85	1.50	1.34
48	w	627	OMU	C2-N1	6.82	1.49	1.38
48	w	1442	OMU	C2-N1	6.82	1.49	1.38
3	D	4392	OMG	C4-N3	6.82	1.50	1.34
3	D	2364	OMG	C4-N3	6.80	1.50	1.34
48	w	1804	OMU	C2-N1	6.80	1.49	1.38
3	D	4623	OMG	C4-N3	6.78	1.50	1.34
3	D	3782	5MC	C4-N3	6.78	1.45	1.34
3	D	1316	OMG	C4-N3	6.72	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3899	OMG	C4-N3	6.72	1.50	1.34
48	w	1288	OMU	C2-N3	6.67	1.49	1.38
48	w	121	OMU	C2-N3	6.66	1.49	1.38
3	D	2415	OMU	C2-N1	6.66	1.49	1.38
48	w	172	OMU	C2-N3	6.65	1.49	1.38
3	D	1773	OMU	C2-N3	6.63	1.49	1.38
48	w	428	OMU	C2-N3	6.60	1.49	1.38
48	w	799	OMU	C2-N3	6.59	1.49	1.38
2	C	6	2MG	C4-N3	6.55	1.49	1.34
48	w	116	OMU	C2-N3	6.54	1.49	1.38
48	w	627	OMU	C2-N3	6.53	1.49	1.38
2	C	53	5MU	C6-C5	6.53	1.45	1.34
48	w	1326	OMU	C2-N3	6.52	1.49	1.38
2	C	47	5MC	C2-N3	6.51	1.49	1.36
3	D	3925	OMU	C2-N1	6.51	1.48	1.38
2	B	6	2MG	C4-N3	6.51	1.49	1.34
2	C	48	5MC	C2-N3	6.50	1.49	1.36
48	w	1639	G7M	C2-N2	6.49	1.49	1.34
3	D	4530	UR3	C2-N1	6.46	1.47	1.38
48	w	1442	OMU	C2-N3	6.44	1.49	1.38
2	B	48	5MC	C2-N3	6.43	1.49	1.36
2	B	47	5MC	C2-N3	6.42	1.49	1.36
2	C	38	5MC	C2-N3	6.42	1.49	1.36
48	w	1639	G7M	C4-N3	6.40	1.49	1.34
48	w	1804	OMU	C2-N3	6.37	1.49	1.38
3	D	4306	OMU	C2-N1	6.36	1.48	1.38
3	D	4447	5MC	C4-N3	6.36	1.44	1.34
48	w	174	OMC	C2-N3	6.34	1.49	1.36
2	B	53	5MU	C6-C5	6.33	1.45	1.34
48	w	462	OMC	C2-N3	6.32	1.49	1.36
3	D	4620	OMU	C2-N1	6.31	1.48	1.38
2	B	38	5MC	C2-N3	6.28	1.49	1.36
3	D	4498	OMU	C2-N1	6.26	1.48	1.38
48	w	517	OMC	C2-N3	6.25	1.49	1.36
3	D	2837	OMU	C2-N3	6.20	1.49	1.38
3	D	2837	OMU	C2-N1	6.19	1.48	1.38
2	C	34	56B	C4-N3	6.13	1.48	1.34
2	B	34	56B	C4-N3	6.12	1.48	1.34
3	D	2415	OMU	C2-N3	6.11	1.48	1.38
48	w	462	OMC	C6-C5	6.11	1.49	1.35
48	w	1391	OMC	C2-N3	6.11	1.48	1.36
48	w	174	OMC	C6-C5	6.09	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3782	5MC	C2-N3	6.09	1.48	1.36
48	w	517	OMC	C6-C5	6.04	1.49	1.35
3	D	4306	OMU	C2-N3	6.01	1.48	1.38
3	D	4227	OMU	C2-N3	6.00	1.48	1.38
3	D	4620	OMU	C2-N3	5.98	1.48	1.38
2	C	34	56B	O11-C11	-5.98	1.28	1.43
2	B	34	56B	O11-C11	-5.96	1.28	1.43
3	D	4498	OMU	C2-N3	5.96	1.48	1.38
48	w	428	OMU	C6-C5	5.95	1.48	1.35
3	D	4536	OMC	C2-N3	5.89	1.48	1.36
48	w	172	OMU	C6-C5	5.89	1.48	1.35
3	D	2804	OMC	C2-N3	5.89	1.48	1.36
48	w	1703	OMC	C6-C5	5.88	1.48	1.35
3	D	2422	OMC	C2-N3	5.88	1.48	1.36
3	D	3701	OMC	C6-C5	5.87	1.48	1.35
48	w	1391	OMC	C6-C5	5.86	1.48	1.35
48	w	1703	OMC	C2-N3	5.85	1.48	1.36
48	w	799	OMU	C6-C5	5.84	1.48	1.35
48	w	627	OMU	C6-C5	5.84	1.48	1.35
48	w	121	OMU	C6-C5	5.83	1.48	1.35
3	D	4530	UR3	C6-C5	5.83	1.48	1.35
3	D	1773	OMU	C6-C5	5.83	1.48	1.35
3	D	2422	OMC	C6-C5	5.82	1.48	1.35
48	w	509	OMG	C2-N3	5.79	1.47	1.33
48	w	1288	OMU	C6-C5	5.78	1.48	1.35
3	D	2861	OMC	C2-N3	5.78	1.48	1.36
3	D	2861	OMC	C6-C5	5.77	1.48	1.35
3	D	3887	OMC	C2-N3	5.76	1.48	1.36
3	D	1340	OMC	C2-N3	5.75	1.48	1.36
48	w	1639	G7M	C2-N3	5.75	1.47	1.33
3	D	3925	OMU	C2-N3	5.74	1.48	1.38
3	D	3841	OMC	C2-N3	5.74	1.48	1.36
3	D	2824	OMC	C2-N3	5.73	1.48	1.36
3	D	4536	OMC	C6-C5	5.72	1.48	1.35
48	w	116	OMU	C6-C5	5.71	1.48	1.35
3	D	2824	OMC	C6-C5	5.71	1.48	1.35
3	D	3701	OMC	C2-N3	5.70	1.47	1.36
48	w	1442	OMU	C6-C5	5.70	1.48	1.35
3	D	4456	OMC	C2-N3	5.70	1.47	1.36
3	D	2365	OMC	C2-N3	5.69	1.47	1.36
3	D	3785	A2M	O5'-C5'	-5.69	1.30	1.44
3	D	3887	OMC	C6-C5	5.68	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4456	OMC	C6-C5	5.67	1.48	1.35
3	D	2365	OMC	C6-C5	5.67	1.48	1.35
3	D	2351	OMC	C2-N3	5.66	1.47	1.36
3	D	3808	OMC	C2-N3	5.65	1.47	1.36
48	w	1326	OMU	C6-C5	5.65	1.48	1.35
3	D	3841	OMC	C6-C5	5.65	1.48	1.35
3	D	4447	5MC	C2-N3	5.65	1.47	1.36
3	D	3808	OMC	C6-C5	5.64	1.48	1.35
48	w	1804	OMU	C6-C5	5.63	1.48	1.35
3	D	2804	OMC	C6-C5	5.63	1.48	1.35
3	D	1340	OMC	C6-C5	5.61	1.48	1.35
3	D	2815	A2M	O5'-C5'	-5.60	1.31	1.44
3	D	2351	OMC	C6-C5	5.60	1.48	1.35
3	D	4620	OMU	C6-C5	5.57	1.48	1.35
3	D	4227	OMU	C6-C5	5.57	1.48	1.35
3	D	1760	OMG	C2-N3	5.54	1.46	1.33
3	D	4498	OMU	C6-C5	5.54	1.47	1.35
3	D	4306	OMU	C6-C5	5.54	1.47	1.35
48	w	644	OMG	C2-N3	5.53	1.46	1.33
2	B	34	56B	C11-C10	5.52	1.62	1.54
2	C	34	56B	C2-N3	5.52	1.46	1.33
2	C	34	56B	C11-C10	5.51	1.62	1.54
48	w	1328	OMG	C2-N3	5.50	1.46	1.33
3	D	2415	OMU	C6-C5	5.49	1.47	1.35
3	D	1524	A2M	O5'-C5'	-5.47	1.31	1.44
2	B	34	56B	C2-N3	5.47	1.46	1.33
3	D	2837	OMU	C6-C5	5.46	1.47	1.35
3	D	3925	OMU	C6-C5	5.43	1.47	1.35
48	w	601	OMG	C2-N3	5.40	1.46	1.33
48	w	1490	OMG	C2-N3	5.39	1.46	1.33
3	D	3944	OMG	C2-N3	5.37	1.46	1.33
3	D	1625	OMG	C2-N3	5.36	1.46	1.33
48	w	683	OMG	C2-N3	5.34	1.46	1.33
48	w	668	A2M	O5'-C5'	-5.32	1.31	1.44
48	w	436	OMG	C2-N3	5.26	1.45	1.33
48	w	509	OMG	C2-N2	5.24	1.46	1.34
3	D	2424	OMG	C2-N3	5.24	1.45	1.33
3	D	3792	OMG	C2-N3	5.24	1.45	1.33
3	D	4494	OMG	C2-N3	5.22	1.45	1.33
3	D	1760	OMG	C2-N2	5.21	1.46	1.34
48	w	644	OMG	C2-N2	5.19	1.46	1.34
3	D	400	A2M	O5'-C5'	-5.18	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2401	A2M	O5'-C5'	-5.17	1.32	1.44
48	w	484	A2M	O5'-C5'	-5.17	1.32	1.44
5	F	75	OMG	C2-N3	5.16	1.45	1.33
2	B	48	5MC	C6-N1	5.15	1.46	1.38
3	D	4523	A2M	O5'-C5'	-5.15	1.32	1.44
48	w	468	A2M	O5'-C5'	-5.15	1.32	1.44
3	D	4637	OMG	C2-N3	5.15	1.45	1.33
3	D	3830	A2M	O5'-C5'	-5.14	1.32	1.44
3	D	4196	OMG	C2-N3	5.14	1.45	1.33
48	w	601	OMG	C2-N2	5.14	1.46	1.34
3	D	1871	A2M	O5'-C5'	-5.13	1.32	1.44
3	D	3744	OMG	C2-N3	5.13	1.45	1.33
48	w	174	OMC	C4-N3	5.12	1.44	1.34
2	C	48	5MC	C6-N1	5.11	1.46	1.38
48	w	1328	OMG	C2-N2	5.11	1.46	1.34
3	D	1326	A2M	O5'-C5'	-5.11	1.32	1.44
48	w	517	OMC	C4-N3	5.11	1.44	1.34
3	D	4370	OMG	C2-N3	5.10	1.45	1.33
3	D	3944	OMG	C2-N2	5.10	1.46	1.34
3	D	4618	OMG	C2-N3	5.10	1.45	1.33
48	w	683	OMG	C2-N2	5.09	1.46	1.34
2	C	47	5MC	C6-N1	5.08	1.46	1.38
48	w	462	OMC	C4-N3	5.08	1.44	1.34
3	D	3825	A2M	O5'-C5'	-5.08	1.32	1.44
3	D	3627	OMG	C2-N3	5.08	1.45	1.33
48	w	1031	A2M	O5'-C5'	-5.07	1.32	1.44
3	D	4499	OMG	C2-N3	5.07	1.45	1.33
48	w	27	A2M	O5'-C5'	-5.06	1.32	1.44
2	C	6	2MG	C2-N1	5.06	1.44	1.36
3	D	4228	OMG	C2-N3	5.05	1.45	1.33
48	w	1383	A2M	O5'-C5'	-5.04	1.32	1.44
48	w	1490	OMG	C2-N2	5.04	1.46	1.34
2	C	38	5MC	C6-N1	5.04	1.46	1.38
3	D	2424	OMG	C2-N2	5.03	1.46	1.34
3	D	2364	OMG	C2-N3	5.02	1.45	1.33
48	w	436	OMG	C2-N2	5.01	1.46	1.34
3	D	3760	A2M	O5'-C5'	-4.96	1.32	1.44
2	B	38	5MC	C6-N1	4.95	1.46	1.38
3	D	2787	A2M	O5'-C5'	-4.95	1.32	1.44
48	w	1391	OMC	C4-N3	4.94	1.44	1.34
2	B	47	5MC	C6-N1	4.94	1.46	1.38
3	D	3744	OMG	C2-N2	4.94	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4392	OMG	C2-N3	4.94	1.45	1.33
3	D	4447	5MC	C6-N1	4.93	1.46	1.38
3	D	1625	OMG	C2-N2	4.93	1.45	1.34
48	w	174	OMC	C4-N4	4.92	1.45	1.33
3	D	4623	OMG	C2-N3	4.92	1.45	1.33
3	D	4499	OMG	C2-N2	4.90	1.45	1.34
48	w	462	OMC	C4-N4	4.90	1.45	1.33
3	D	4618	OMG	C2-N2	4.89	1.45	1.34
2	B	6	2MG	C2-N1	4.88	1.44	1.36
5	F	75	OMG	C2-N2	4.88	1.45	1.34
3	D	1522	OMG	C2-N3	4.87	1.44	1.33
3	D	3899	OMG	C2-N3	4.87	1.44	1.33
3	D	4228	OMG	C2-N2	4.86	1.45	1.34
48	w	517	OMC	C4-N4	4.84	1.45	1.33
48	w	166	A2M	O5'-C5'	-4.84	1.32	1.44
3	D	3718	A2M	O5'-C5'	-4.83	1.32	1.44
48	w	159	A2M	O5'-C5'	-4.83	1.32	1.44
3	D	3724	A2M	O5'-C5'	-4.83	1.33	1.44
3	D	2363	A2M	O5'-C5'	-4.82	1.33	1.44
3	D	3627	OMG	C2-N2	4.82	1.45	1.34
3	D	4494	OMG	C2-N2	4.82	1.45	1.34
3	D	1316	OMG	C2-N3	4.82	1.44	1.33
3	D	2364	OMG	C2-N2	4.80	1.45	1.34
48	w	1391	OMC	C4-N4	4.79	1.45	1.33
3	D	4637	OMG	C2-N2	4.78	1.45	1.34
3	D	3899	OMG	C2-N2	4.78	1.45	1.34
3	D	4370	OMG	C2-N2	4.78	1.45	1.34
3	D	398	A2M	O5'-C5'	-4.75	1.33	1.44
48	w	512	A2M	O5'-C5'	-4.75	1.33	1.44
3	D	4623	OMG	C2-N2	4.75	1.45	1.34
3	D	3792	OMG	C2-N2	4.75	1.45	1.34
3	D	4392	OMG	C2-N2	4.73	1.45	1.34
48	w	576	A2M	O5'-C5'	-4.72	1.33	1.44
48	w	1639	G7M	C5-N7	-4.71	1.33	1.39
3	D	1316	OMG	C2-N2	4.71	1.45	1.34
48	w	1703	OMC	C4-N4	4.70	1.45	1.33
2	C	34	56B	C2-N2	4.69	1.45	1.34
3	D	4196	OMG	C2-N2	4.68	1.45	1.34
48	w	1703	OMC	C4-N3	4.68	1.43	1.34
3	D	3887	OMC	C4-N3	4.66	1.43	1.34
3	D	2804	OMC	C4-N3	4.65	1.43	1.34
3	D	4536	OMC	C4-N4	4.64	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2824	OMC	C4-N3	4.64	1.43	1.34
3	D	2861	OMC	C4-N4	4.63	1.44	1.33
2	B	34	56B	C2-N2	4.62	1.45	1.34
3	D	1522	OMG	C2-N2	4.62	1.45	1.34
48	w	590	A2M	O5'-C5'	-4.62	1.33	1.44
3	D	3701	OMC	C4-N4	4.62	1.44	1.33
48	w	1678	A2M	O5'-C5'	-4.62	1.33	1.44
3	D	2422	OMC	C4-N4	4.62	1.44	1.33
3	D	1534	A2M	O5'-C5'	-4.61	1.33	1.44
3	D	4530	UR3	C2-N3	4.59	1.47	1.39
3	D	4456	OMC	C4-N3	4.59	1.43	1.34
3	D	3887	OMC	C4-N4	4.59	1.44	1.33
48	w	99	A2M	O5'-C5'	-4.58	1.33	1.44
3	D	3701	OMC	C4-N3	4.58	1.43	1.34
3	D	4456	OMC	C4-N4	4.58	1.44	1.33
3	D	3808	OMC	C4-N4	4.57	1.44	1.33
3	D	2365	OMC	C4-N4	4.55	1.44	1.33
3	D	3782	5MC	C6-N1	4.55	1.45	1.38
3	D	1340	OMC	C4-N3	4.54	1.43	1.34
3	D	2804	OMC	C4-N4	4.53	1.44	1.33
3	D	3841	OMC	C4-N4	4.53	1.44	1.33
3	D	2422	OMC	C4-N3	4.52	1.43	1.34
3	D	2824	OMC	C4-N4	4.52	1.44	1.33
3	D	4536	OMC	C4-N3	4.52	1.43	1.34
48	w	462	OMC	C2-N1	4.52	1.49	1.40
48	w	174	OMC	C2-N1	4.51	1.49	1.40
3	D	3808	OMC	C4-N3	4.49	1.43	1.34
3	D	1340	OMC	C4-N4	4.49	1.44	1.33
3	D	2861	OMC	C4-N3	4.48	1.43	1.34
3	D	2365	OMC	C4-N3	4.46	1.43	1.34
3	D	2351	OMC	C4-N4	4.44	1.44	1.33
48	w	517	OMC	C2-N1	4.43	1.49	1.40
3	D	3841	OMC	C4-N3	4.40	1.43	1.34
3	D	2351	OMC	C4-N3	4.36	1.43	1.34
2	B	48	5MC	C2-N1	4.28	1.49	1.40
48	w	1391	OMC	C2-N1	4.25	1.49	1.40
2	C	48	5MC	C2-N1	4.22	1.49	1.40
2	B	47	5MC	C2-N1	4.15	1.49	1.40
2	B	47	5MC	C4-N4	4.13	1.44	1.34
2	B	48	5MC	C4-N4	4.13	1.44	1.34
2	C	38	5MC	C2-N1	4.11	1.48	1.40
2	B	38	5MC	C2-N1	4.11	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	47	5MC	C2-N1	4.10	1.48	1.40
2	C	48	5MC	C4-N4	4.09	1.44	1.34
2	C	47	5MC	C4-N4	4.06	1.44	1.34
2	C	38	5MC	C4-N4	4.06	1.44	1.34
2	C	34	56B	C5-C6	4.05	1.53	1.44
3	D	2824	OMC	C2-N1	4.04	1.48	1.40
48	w	1703	OMC	C2-N1	4.03	1.48	1.40
3	D	2422	OMC	C2-N1	3.98	1.48	1.40
2	B	38	5MC	C4-N4	3.96	1.44	1.34
2	B	34	56B	C5-C6	3.93	1.53	1.44
3	D	3841	OMC	C2-N1	3.92	1.48	1.40
3	D	1340	OMC	C2-N1	3.91	1.48	1.40
3	D	2861	OMC	C2-N1	3.88	1.48	1.40
3	D	3808	OMC	C2-N1	3.87	1.48	1.40
3	D	3887	OMC	C2-N1	3.87	1.48	1.40
3	D	2351	OMC	C2-N1	3.85	1.48	1.40
3	D	4456	OMC	C2-N1	3.83	1.48	1.40
3	D	3782	5MC	C4-N4	3.83	1.44	1.34
3	D	2804	OMC	C2-N1	3.83	1.48	1.40
3	D	3782	5MC	C2-N1	3.82	1.48	1.40
3	D	3701	OMC	C2-N1	3.80	1.48	1.40
3	D	4447	5MC	C4-N4	3.76	1.43	1.34
3	D	2365	OMC	C2-N1	3.74	1.48	1.40
48	w	1639	G7M	C5-C6	3.73	1.53	1.43
3	D	4536	OMC	C2-N1	3.72	1.48	1.40
3	D	4447	5MC	C2-N1	3.71	1.48	1.40
48	w	1288	OMU	C4-N3	3.58	1.45	1.38
48	w	822	PSU	C6-C5	3.57	1.39	1.35
48	w	815	PSU	C6-C5	3.55	1.39	1.35
48	w	609	PSU	C6-C5	3.54	1.39	1.35
48	w	210	PSU	C6-C5	3.50	1.39	1.35
48	w	119	PSU	C6-C5	3.49	1.39	1.35
48	w	172	OMU	C4-N3	3.48	1.44	1.38
48	w	116	OMU	C4-N3	3.47	1.44	1.38
48	w	572	PSU	C6-C5	3.45	1.39	1.35
48	w	1850	MA6	C8-N9	-3.45	1.31	1.37
48	w	799	OMU	C4-N3	3.44	1.44	1.38
3	D	1773	OMU	C4-N3	3.41	1.44	1.38
48	w	109	PSU	C6-C5	3.41	1.39	1.35
3	D	4392	OMG	C5-N7	-3.40	1.32	1.39
2	C	54	PSU	C6-C5	3.40	1.39	1.35
48	w	428	OMU	C4-N3	3.39	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1625	OMG	C5-N7	-3.39	1.32	1.39
3	D	3899	OMG	C5-N7	-3.39	1.32	1.39
48	w	121	OMU	C4-N3	3.38	1.44	1.38
48	w	866	PSU	C6-C5	3.38	1.39	1.35
3	D	4196	OMG	C5-N7	-3.38	1.32	1.39
3	D	4392	OMG	O6-C6	-3.38	1.17	1.23
48	w	627	OMU	C4-N3	3.38	1.44	1.38
3	D	1316	OMG	C5-N7	-3.37	1.32	1.39
48	w	801	PSU	C6-C5	3.36	1.39	1.35
48	w	1232	PSU	C6-C5	3.36	1.39	1.35
48	w	93	PSU	C6-C5	3.35	1.39	1.35
3	D	3792	OMG	C5-N7	-3.35	1.32	1.39
48	w	218	PSU	C6-C5	3.35	1.39	1.35
3	D	4370	OMG	C5-N7	-3.35	1.32	1.39
3	D	3841	OMC	O2-C2	-3.35	1.17	1.23
48	w	863	PSU	C6-C5	3.34	1.39	1.35
48	w	36	PSU	C6-C5	3.34	1.39	1.35
48	w	686	PSU	C6-C5	3.34	1.39	1.35
2	C	13	PSU	C6-C5	3.33	1.39	1.35
3	D	2364	OMG	C5-N7	-3.33	1.32	1.39
3	D	3899	OMG	O6-C6	-3.33	1.17	1.23
3	D	4637	OMG	C5-N7	-3.31	1.32	1.39
48	w	34	PSU	C6-C5	3.31	1.39	1.35
48	w	1004	PSU	C6-C5	3.29	1.39	1.35
48	w	517	OMC	C6-N1	3.28	1.45	1.38
3	D	4536	OMC	O2-C2	-3.28	1.17	1.23
3	D	4306	OMU	O2-C2	-3.27	1.17	1.23
3	D	3762	PSU	C6-C5	3.27	1.39	1.35
3	D	3925	OMU	O2-C2	-3.27	1.17	1.23
48	w	462	OMC	C6-N1	3.26	1.45	1.38
48	w	1326	OMU	C4-N3	3.25	1.44	1.38
48	w	1442	OMU	C4-N3	3.25	1.44	1.38
48	w	174	OMC	C6-N1	3.25	1.45	1.38
2	B	54	PSU	C6-C5	3.25	1.39	1.35
3	D	4494	OMG	C5-N7	-3.24	1.32	1.39
3	D	4456	OMC	O2-C2	-3.24	1.17	1.23
3	D	2351	OMC	O2-C2	-3.24	1.17	1.23
48	w	1804	OMU	C4-N3	3.23	1.44	1.38
48	w	105	PSU	C6-C5	3.23	1.39	1.35
3	D	1522	OMG	O6-C6	-3.23	1.17	1.23
3	D	1522	OMG	C5-N7	-3.23	1.32	1.39
3	D	2424	OMG	C5-N7	-3.23	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2837	OMU	O4-C4	-3.22	1.18	1.24
3	D	4637	OMG	O6-C6	-3.22	1.17	1.23
3	D	4623	OMG	C5-N7	-3.22	1.32	1.39
48	w	1851	MA6	C5-C4	-3.21	1.33	1.39
3	D	3744	OMG	C5-N7	-3.21	1.32	1.39
3	D	3770	PSU	C6-C5	3.21	1.39	1.35
2	B	13	PSU	C6-C5	3.21	1.39	1.35
3	D	3768	PSU	C6-C5	3.20	1.39	1.35
3	D	3925	OMU	O4-C4	-3.20	1.18	1.24
3	D	4618	OMG	C5-N7	-3.20	1.32	1.39
3	D	3627	OMG	O6-C6	-3.20	1.17	1.23
48	w	1625	PSU	C6-C5	3.20	1.39	1.35
3	D	4228	OMG	O6-C6	-3.19	1.17	1.23
3	D	2365	OMC	O2-C2	-3.19	1.17	1.23
3	D	2824	OMC	O2-C2	-3.19	1.17	1.23
3	D	4499	OMG	C5-N7	-3.18	1.32	1.39
48	w	1046	PSU	C6-C5	3.18	1.39	1.35
3	D	3627	OMG	C5-N7	-3.18	1.32	1.39
3	D	3808	OMC	O2-C2	-3.18	1.17	1.23
48	w	814	PSU	C6-C5	3.18	1.39	1.35
3	D	4620	OMU	O2-C2	-3.17	1.17	1.23
5	F	75	OMG	C5-N7	-3.17	1.32	1.39
3	D	1340	OMC	O2-C2	-3.17	1.17	1.23
3	D	2422	OMC	O2-C2	-3.16	1.17	1.23
3	D	2861	OMC	O2-C2	-3.15	1.17	1.23
3	D	3715	PSU	C6-C5	3.15	1.39	1.35
48	w	406	PSU	C6-C5	3.15	1.39	1.35
48	w	649	PSU	C6-C5	3.15	1.39	1.35
3	D	4494	OMG	O6-C6	-3.15	1.17	1.23
3	D	3792	OMG	O6-C6	-3.14	1.17	1.23
48	w	1445	PSU	C6-C5	3.14	1.39	1.35
3	D	4196	OMG	O6-C6	-3.14	1.17	1.23
3	D	1316	OMG	O6-C6	-3.14	1.17	1.23
48	w	1367	PSU	C6-C5	3.13	1.39	1.35
3	D	4370	OMG	O6-C6	-3.12	1.17	1.23
3	D	3887	OMC	O2-C2	-3.12	1.17	1.23
48	w	1703	OMC	O2-C2	-3.12	1.17	1.23
3	D	4498	OMU	O2-C2	-3.12	1.17	1.23
3	D	4623	OMG	O6-C6	-3.11	1.17	1.23
3	D	2364	OMG	O6-C6	-3.11	1.17	1.23
3	D	2804	OMC	O2-C2	-3.11	1.18	1.23
48	w	651	PSU	C6-C5	3.10	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	966	PSU	C6-C5	3.10	1.38	1.35
48	w	1238	PSU	C6-C5	3.09	1.38	1.35
3	D	4228	OMG	C5-N7	-3.09	1.33	1.39
3	D	4620	OMU	O4-C4	-3.08	1.18	1.24
48	w	681	PSU	C6-C5	3.08	1.38	1.35
3	D	4618	OMG	O6-C6	-3.08	1.17	1.23
3	D	4420	PSU	C6-C5	3.07	1.38	1.35
3	D	4423	PSU	C6-C5	3.07	1.38	1.35
3	D	4498	OMU	O4-C4	-3.07	1.18	1.24
48	w	1045	PSU	C6-C5	3.06	1.38	1.35
3	D	4499	OMG	O6-C6	-3.06	1.17	1.23
48	w	1643	PSU	C6-C5	3.05	1.38	1.35
3	D	2837	OMU	O2-C2	-3.04	1.17	1.23
48	w	1490	OMG	C5-N7	-3.04	1.33	1.39
3	D	4227	OMU	O2-C2	-3.04	1.17	1.23
3	D	3764	PSU	C6-C5	3.03	1.38	1.35
3	D	4306	OMU	O4-C4	-3.03	1.18	1.24
48	w	509	OMG	C5-N7	-3.03	1.33	1.39
3	D	3734	PSU	C6-C5	3.02	1.38	1.35
3	D	3744	OMG	O6-C6	-3.01	1.17	1.23
48	w	1391	OMC	C6-N1	3.01	1.45	1.38
3	D	3818	UY1	C2-N1	3.01	1.40	1.36
3	D	4227	OMU	O4-C4	-3.01	1.18	1.24
48	w	1177	PSU	C6-C5	3.01	1.38	1.35
2	C	34	56B	C11-C12	3.01	1.58	1.53
3	D	2415	OMU	C4-N3	3.01	1.43	1.38
48	w	668	A2M	O4'-C4'	-3.00	1.38	1.45
2	B	34	56B	C11-C12	3.00	1.58	1.53
3	D	4431	PSU	C6-C5	2.99	1.38	1.35
3	D	3701	OMC	O2-C2	-2.99	1.18	1.23
48	w	1244	PSU	C6-C5	2.99	1.38	1.35
3	D	1625	OMG	O6-C6	-2.99	1.17	1.23
48	w	1850	MA6	C5-C4	-2.99	1.33	1.39
48	w	1056	PSU	C6-C5	2.99	1.38	1.35
3	D	5010	PSU	C6-C5	2.99	1.38	1.35
3	D	3887	OMC	C6-N1	2.98	1.45	1.38
48	w	1692	PSU	C6-C5	2.98	1.38	1.35
48	w	1347	PSU	C6-C5	2.97	1.38	1.35
3	D	2415	OMU	O4-C4	-2.97	1.18	1.24
3	D	4500	PSU	C6-C5	2.96	1.38	1.35
2	B	6	2MG	C5-N7	-2.96	1.33	1.39
48	w	1703	OMC	C6-N1	2.96	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3944	OMG	C5-N7	-2.96	1.33	1.39
48	w	644	OMG	C5-C6	2.95	1.55	1.44
3	D	2424	OMG	O6-C6	-2.94	1.18	1.23
3	D	4532	PSU	C6-C5	2.94	1.38	1.35
5	F	75	OMG	O6-C6	-2.94	1.18	1.23
3	D	2861	OMC	C6-N1	2.94	1.45	1.38
48	w	1850	MA6	C5-N7	-2.94	1.33	1.39
48	w	601	OMG	C5-N7	-2.93	1.33	1.39
48	w	683	OMG	C5-N7	-2.93	1.33	1.39
48	w	1328	OMG	C5-N7	-2.92	1.33	1.39
3	D	4689	PSU	C6-C5	2.92	1.38	1.35
3	D	5001	PSU	C6-C5	2.92	1.38	1.35
3	D	4498	OMU	C4-N3	2.92	1.43	1.38
48	w	1328	OMG	C5-C6	2.91	1.55	1.44
3	D	4447	5MC	O2-C2	-2.91	1.18	1.23
3	D	3730	PSU	C6-C5	2.91	1.38	1.35
3	D	2415	OMU	O2-C2	-2.91	1.17	1.23
2	C	6	2MG	C5-N7	-2.90	1.33	1.39
3	D	4361	PSU	C6-C5	2.90	1.38	1.35
3	D	3701	OMC	C6-N1	2.90	1.45	1.38
3	D	4456	OMC	C6-N1	2.90	1.45	1.38
48	w	1081	PSU	C6-C5	2.90	1.38	1.35
48	w	1174	PSU	C6-C5	2.89	1.38	1.35
48	w	1326	OMU	O2-C2	-2.89	1.17	1.23
3	D	4471	PSU	C6-C5	2.89	1.38	1.35
3	D	2422	OMC	C6-N1	2.88	1.44	1.38
3	D	4227	OMU	C4-N3	2.88	1.43	1.38
48	w	1804	OMU	O4-C4	-2.87	1.18	1.24
48	w	1490	OMG	O6-C6	-2.87	1.18	1.23
3	D	1340	OMC	C6-N1	2.87	1.44	1.38
3	D	2632	PSU	C6-C5	2.87	1.38	1.35
48	w	683	OMG	C5-C6	2.86	1.55	1.44
3	D	4403	PSU	C6-C5	2.86	1.38	1.35
3	D	4552	PSU	C6-C5	2.86	1.38	1.35
48	w	1850	MA6	C6-N6	2.86	1.45	1.36
3	D	1860	PSU	C6-C5	2.85	1.38	1.35
3	D	1781	PSU	C6-C5	2.84	1.38	1.35
3	D	2824	OMC	C6-N1	2.84	1.44	1.38
48	w	1639	G7M	C2-N1	2.84	1.44	1.37
48	w	436	OMG	C5-C6	2.84	1.54	1.44
3	D	1760	OMG	C5-C6	2.84	1.54	1.44
2	C	9	1MA	C2-N1	2.83	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3841	OMC	C6-N1	2.82	1.44	1.38
48	w	436	OMG	O6-C6	-2.82	1.18	1.23
3	D	4312	PSU	C6-C5	2.82	1.38	1.35
48	w	601	OMG	C5-C6	2.82	1.54	1.44
2	B	57	1MA	C2-N1	2.81	1.41	1.35
3	D	2837	OMU	C4-N3	2.81	1.43	1.38
48	w	644	OMG	C5-N7	-2.81	1.33	1.39
2	C	57	1MA	C2-N1	2.81	1.41	1.35
3	D	4536	OMC	C6-N1	2.81	1.44	1.38
3	D	4353	PSU	C6-C5	2.80	1.38	1.35
48	w	436	OMG	C5-N7	-2.80	1.33	1.39
3	D	2365	OMC	C6-N1	2.80	1.44	1.38
48	w	1326	OMU	O4-C4	-2.80	1.19	1.24
3	D	1782	PSU	C6-C5	2.79	1.38	1.35
3	D	2351	OMC	C6-N1	2.79	1.44	1.38
3	D	3944	OMG	C5-C6	2.79	1.54	1.44
48	w	509	OMG	C5-C6	2.79	1.54	1.44
48	w	1391	OMC	O2-C2	-2.78	1.18	1.23
48	w	1490	OMG	C5-C6	2.78	1.54	1.44
48	w	601	OMG	O6-C6	-2.78	1.18	1.23
48	w	1639	G7M	C6-N1	2.77	1.44	1.38
3	D	1760	OMG	C5-N7	-2.77	1.33	1.39
48	w	1328	OMG	O6-C6	-2.77	1.18	1.23
3	D	1760	OMG	C6-N1	2.76	1.44	1.38
3	D	4220	6MZ	C5-C4	-2.76	1.33	1.39
3	D	4521	PSU	C6-C5	2.76	1.38	1.35
3	D	3637	PSU	C6-C5	2.76	1.38	1.35
48	w	683	OMG	O6-C6	-2.76	1.18	1.23
3	D	4628	PSU	C6-C5	2.76	1.38	1.35
3	D	4620	OMU	C4-N3	2.75	1.43	1.38
3	D	4972	PSU	C6-C5	2.75	1.38	1.35
48	w	1851	MA6	C6-N6	2.75	1.45	1.36
3	D	3944	OMG	O6-C6	-2.75	1.18	1.23
48	w	644	OMG	C6-N1	2.75	1.43	1.38
3	D	2804	OMC	C6-N1	2.75	1.44	1.38
48	w	1442	OMU	O2-C2	-2.74	1.18	1.23
48	w	1442	OMU	O4-C4	-2.74	1.19	1.24
48	w	428	OMU	O4-C4	-2.73	1.19	1.24
3	D	3808	OMC	C6-N1	2.73	1.44	1.38
48	w	428	OMU	O2-C2	-2.73	1.18	1.23
3	D	4579	PSU	C6-C5	2.73	1.38	1.35
48	w	1832	6MZ	C5-C4	-2.73	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3758	PSU	C6-C5	2.72	1.38	1.35
3	D	4296	PSU	C6-C5	2.72	1.38	1.35
48	w	517	OMC	O2-C2	-2.72	1.18	1.23
5	F	75	OMG	C5-C6	2.72	1.54	1.44
3	D	4530	UR3	C6-N1	2.71	1.44	1.38
2	B	34	56B	O6-C6	-2.71	1.18	1.23
3	D	3920	PSU	C6-C5	2.71	1.38	1.35
3	D	1744	PSU	C6-C5	2.71	1.38	1.35
48	w	116	OMU	O4-C4	-2.70	1.19	1.24
3	D	1760	OMG	O6-C6	-2.70	1.18	1.23
2	C	34	56B	O6-C6	-2.70	1.18	1.23
48	w	509	OMG	C6-N1	2.69	1.43	1.38
3	D	1862	PSU	C6-C5	2.69	1.38	1.35
3	D	4442	PSU	C6-C5	2.69	1.38	1.35
3	D	3744	OMG	C5-C6	2.69	1.54	1.44
48	w	601	OMG	C6-N1	2.69	1.43	1.38
48	w	121	OMU	O4-C4	-2.69	1.19	1.24
3	D	4499	OMG	C5-C6	2.68	1.54	1.44
3	D	4618	OMG	C5-C6	2.68	1.54	1.44
2	B	19	H2U	C2-N3	-2.68	1.33	1.38
48	w	509	OMG	O6-C6	-2.68	1.18	1.23
3	D	3792	OMG	C5-C6	2.67	1.54	1.44
3	D	4457	PSU	C6-C5	2.67	1.38	1.35
3	D	4228	OMG	C5-C6	2.67	1.54	1.44
3	D	4576	PSU	C6-C5	2.67	1.38	1.35
2	C	34	56B	C2-N1	2.67	1.44	1.37
48	w	121	OMU	O2-C2	-2.67	1.18	1.23
3	D	1522	OMG	C5-C6	2.67	1.54	1.44
48	w	436	OMG	C6-N1	2.67	1.43	1.38
48	w	644	OMG	O6-C6	-2.67	1.18	1.23
3	D	4392	OMG	C5-C6	2.67	1.54	1.44
3	D	4293	PSU	C6-C5	2.66	1.38	1.35
3	D	1625	OMG	C5-C6	2.66	1.54	1.44
3	D	4623	OMG	C5-C6	2.66	1.54	1.44
2	C	19	H2U	C2-N3	-2.66	1.33	1.38
48	w	1804	OMU	O2-C2	-2.66	1.18	1.23
2	B	9	1MA	C2-N1	2.66	1.40	1.35
3	D	4494	OMG	C5-C6	2.66	1.54	1.44
48	w	627	OMU	O4-C4	-2.65	1.19	1.24
3	D	1316	OMG	C4-N9	-2.65	1.31	1.38
48	w	1851	MA6	C5-N7	-2.64	1.34	1.39
3	D	4370	OMG	C5-C6	2.64	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3695	PSU	C6-C5	2.63	1.38	1.35
48	w	462	OMC	O2-C2	-2.63	1.18	1.23
3	D	3851	PSU	C6-C5	2.63	1.38	1.35
48	w	1288	OMU	O4-C4	-2.63	1.19	1.24
3	D	2424	OMG	C5-C6	2.63	1.54	1.44
2	C	6	2MG	C5-C6	2.63	1.54	1.44
3	D	4306	OMU	C4-N3	2.63	1.43	1.38
3	D	4637	OMG	C5-C6	2.63	1.54	1.44
3	D	2508	PSU	C6-C5	2.63	1.38	1.35
48	w	509	OMG	C2-N1	2.63	1.44	1.37
48	w	172	OMU	O4-C4	-2.62	1.19	1.24
48	w	799	OMU	O4-C4	-2.62	1.19	1.24
3	D	1773	OMU	O4-C4	-2.62	1.19	1.24
48	w	1639	G7M	O6-C6	-2.62	1.18	1.23
3	D	1760	OMG	C2-N1	2.62	1.44	1.37
3	D	2364	OMG	C5-C6	2.61	1.54	1.44
48	w	644	OMG	C2-N1	2.61	1.44	1.37
3	D	1773	OMU	O2-C2	-2.60	1.18	1.23
48	w	116	OMU	O2-C2	-2.60	1.18	1.23
3	D	3944	OMG	C6-N1	2.60	1.43	1.38
3	D	1536	PSU	C6-C5	2.59	1.38	1.35
2	B	34	56B	C2-N1	2.59	1.44	1.37
3	D	3627	OMG	C5-C6	2.59	1.54	1.44
48	w	683	OMG	C6-N1	2.59	1.43	1.38
3	D	3639	PSU	C6-C5	2.58	1.38	1.35
48	w	1328	OMG	C6-N1	2.58	1.43	1.38
3	D	3853	PSU	C6-C5	2.58	1.38	1.35
3	D	1683	PSU	C6-C5	2.58	1.38	1.35
3	D	3899	OMG	C5-C6	2.57	1.53	1.44
3	D	4196	OMG	C5-C6	2.56	1.53	1.44
3	D	3782	5MC	O2-C2	-2.55	1.19	1.23
3	D	4530	UR3	O2-C2	-2.55	1.17	1.22
2	B	19	H2U	C4-N3	-2.55	1.33	1.37
3	D	4299	PSU	C6-C5	2.55	1.38	1.35
48	w	627	OMU	O2-C2	-2.55	1.18	1.23
48	w	799	OMU	O2-C2	-2.55	1.18	1.23
48	w	174	OMC	C5-C4	2.54	1.48	1.42
3	D	1792	PSU	C6-C5	2.54	1.38	1.35
48	w	462	OMC	C5-C4	2.54	1.48	1.42
48	w	601	OMG	C2-N1	2.54	1.43	1.37
2	C	19	H2U	C4-N3	-2.53	1.33	1.37
3	D	3925	OMU	C4-N3	2.53	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	172	OMU	O2-C2	-2.53	1.18	1.23
48	w	1288	OMU	O2-C2	-2.52	1.18	1.23
48	w	174	OMC	O2-C2	-2.52	1.19	1.23
3	D	1316	OMG	C5-C6	2.52	1.53	1.44
48	w	517	OMC	C5-C4	2.51	1.48	1.42
3	D	1677	PSU	O4'-C1'	-2.50	1.40	1.43
48	w	1328	OMG	C2-N1	2.49	1.43	1.37
2	B	6	2MG	C5-C6	2.48	1.53	1.44
3	D	4530	UR3	O4-C4	-2.47	1.18	1.23
3	D	2363	A2M	O4'-C4'	-2.47	1.39	1.45
3	D	3899	OMG	C4-N9	-2.45	1.31	1.38
48	w	1851	MA6	C8-N9	-2.45	1.33	1.37
3	D	1522	OMG	C4-N9	-2.44	1.31	1.38
48	w	1832	6MZ	C8-N9	-2.44	1.33	1.37
48	w	683	OMG	C2-N1	2.43	1.43	1.37
3	D	3944	OMG	C2-N1	2.43	1.43	1.37
3	D	1524	A2M	O4'-C4'	-2.43	1.39	1.45
48	w	436	OMG	C2-N1	2.39	1.43	1.37
3	D	4220	6MZ	C8-N9	-2.37	1.33	1.37
5	F	75	OMG	C6-N1	2.37	1.43	1.38
2	C	6	2MG	C6-N1	2.37	1.43	1.38
48	w	99	A2M	C5'-C4'	2.37	1.59	1.51
2	C	38	5MC	O2-C2	-2.37	1.19	1.23
3	D	4623	OMG	C4-N9	-2.36	1.31	1.38
3	D	1677	PSU	C6-C5	2.36	1.38	1.35
3	D	3744	OMG	C6-N1	2.36	1.43	1.38
48	w	1490	OMG	C6-N1	2.35	1.43	1.38
2	B	38	5MC	O2-C2	-2.35	1.19	1.23
3	D	3627	OMG	C4-N9	-2.34	1.32	1.38
3	D	2364	OMG	C4-N9	-2.34	1.32	1.38
3	D	2424	OMG	C6-N1	2.34	1.43	1.38
2	B	6	2MG	O6-C6	-2.34	1.19	1.23
3	D	4499	OMG	C6-N1	2.33	1.43	1.38
3	D	4499	OMG	C4-N9	-2.33	1.32	1.38
3	D	2424	OMG	C4-N9	-2.32	1.32	1.38
48	w	1391	OMC	C5-C4	2.32	1.48	1.42
3	D	4370	OMG	C6-N1	2.30	1.43	1.38
48	w	1832	6MZ	C5-N7	-2.30	1.34	1.39
5	F	75	OMG	C2-N1	2.29	1.43	1.37
48	w	1703	OMC	C5-C4	2.29	1.48	1.42
2	C	47	5MC	O2-C2	-2.29	1.19	1.23
3	D	4228	OMG	C6-N1	2.28	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3744	OMG	C2-N1	2.28	1.43	1.37
3	D	4392	OMG	C4-N9	-2.28	1.32	1.38
3	D	4499	OMG	C2-N1	2.27	1.43	1.37
2	B	6	2MG	C6-N1	2.26	1.43	1.38
3	D	4618	OMG	C6-N1	2.26	1.43	1.38
3	D	3701	OMC	C5-C4	2.26	1.48	1.42
48	w	512	A2M	C5-C4	2.26	1.43	1.39
3	D	4618	OMG	C4-N9	-2.26	1.32	1.38
3	D	4523	A2M	O4'-C4'	-2.26	1.40	1.45
3	D	2424	OMG	C2-N1	2.26	1.43	1.37
48	w	1490	OMG	C2-N1	2.25	1.43	1.37
3	D	1316	OMG	C8-N9	-2.25	1.32	1.37
2	C	48	5MC	CM5-C5	2.25	1.56	1.50
3	D	3785	A2M	O4'-C1'	-2.25	1.36	1.42
2	B	48	5MC	O2-C2	-2.25	1.19	1.23
48	w	166	A2M	C5-C4	2.24	1.43	1.39
3	D	3818	UY1	O4'-C1'	-2.24	1.40	1.43
3	D	4370	OMG	C4-N9	-2.24	1.32	1.38
2	C	34	56B	C6-N1	2.24	1.43	1.38
2	C	48	5MC	O2-C2	-2.24	1.19	1.23
3	D	4228	OMG	C4-N9	-2.23	1.32	1.38
2	C	6	2MG	O6-C6	-2.22	1.19	1.23
2	C	38	5MC	CM5-C5	2.22	1.56	1.50
2	B	48	5MC	CM5-C5	2.22	1.56	1.50
2	B	47	5MC	O2-C2	-2.22	1.19	1.23
2	B	47	5MC	CM5-C5	2.22	1.56	1.50
48	w	576	A2M	C5-C4	2.21	1.43	1.39
48	w	512	A2M	C8-N9	2.21	1.41	1.37
3	D	4228	OMG	C2-N1	2.21	1.43	1.37
3	D	1625	OMG	C6-N1	2.20	1.42	1.38
3	D	2861	OMC	C5-C4	2.20	1.48	1.42
3	D	4196	OMG	C4-N9	-2.20	1.32	1.38
3	D	2422	OMC	C5-C4	2.19	1.47	1.42
3	D	4494	OMG	C2-N1	2.19	1.43	1.37
2	C	47	5MC	CM5-C5	2.19	1.56	1.50
3	D	4637	OMG	C4-N9	-2.18	1.32	1.38
3	D	4220	6MZ	C5-N7	-2.18	1.34	1.39
2	B	38	5MC	CM5-C5	2.18	1.56	1.50
3	D	4456	OMC	C5-C4	2.17	1.47	1.42
3	D	4618	OMG	C2-N1	2.17	1.43	1.37
3	D	3887	OMC	C5-C4	2.16	1.47	1.42
3	D	3744	OMG	C4-N9	-2.16	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	172	OMU	C5-C4	2.16	1.48	1.43
48	w	1326	OMU	C6-N1	2.16	1.43	1.38
3	D	4494	OMG	C6-N1	2.16	1.42	1.38
5	F	75	OMG	C4-N9	-2.16	1.32	1.38
2	B	34	56B	C6-N1	2.15	1.42	1.38
3	D	4494	OMG	C4-N9	-2.15	1.32	1.38
3	D	1625	OMG	C2-N1	2.15	1.43	1.37
48	w	428	OMU	C5-C4	2.14	1.48	1.43
3	D	4196	OMG	C8-N9	-2.14	1.32	1.37
3	D	3899	OMG	C8-N9	-2.14	1.32	1.37
3	D	1534	A2M	C3'-C4'	-2.14	1.47	1.53
48	w	166	A2M	C8-N9	2.14	1.41	1.37
48	w	172	OMU	C6-N1	2.13	1.43	1.38
48	w	121	OMU	C6-N1	2.13	1.43	1.38
3	D	1316	OMG	C6-N1	2.12	1.42	1.38
3	D	3808	OMC	C5-C4	2.12	1.47	1.42
48	w	590	A2M	C5-C4	2.11	1.43	1.39
3	D	2364	OMG	C8-N9	-2.11	1.32	1.37
3	D	2824	OMC	C5-C4	2.11	1.47	1.42
3	D	3627	OMG	C6-N1	2.11	1.42	1.38
48	w	799	OMU	C5-C4	2.10	1.48	1.43
3	D	1871	A2M	O3'-C3'	-2.10	1.38	1.43
3	D	4623	OMG	C6-N1	2.10	1.42	1.38
48	w	428	OMU	C6-N1	2.09	1.43	1.38
48	w	1288	OMU	C6-N1	2.09	1.43	1.38
3	D	4637	OMG	C8-N9	-2.09	1.32	1.37
3	D	3899	OMG	C2-N1	2.09	1.42	1.37
3	D	2365	OMC	C5-C4	2.09	1.47	1.42
3	D	1683	PSU	C4-C5	-2.09	1.38	1.44
3	D	3792	OMG	C4-N9	-2.09	1.32	1.38
3	D	4442	PSU	O4'-C1'	-2.09	1.40	1.43
3	D	3841	OMC	C5-C4	2.09	1.47	1.42
3	D	1522	OMG	C8-N9	-2.08	1.32	1.37
3	D	4623	OMG	C2-N1	2.08	1.42	1.37
3	D	4370	OMG	C2-N1	2.08	1.42	1.37
3	D	1773	OMU	C6-N1	2.08	1.43	1.38
48	w	484	A2M	C8-N9	2.08	1.41	1.37
3	D	4196	OMG	C2-N1	2.07	1.42	1.37
3	D	3792	OMG	C8-N9	-2.07	1.32	1.37
48	w	799	OMU	C6-N1	2.07	1.43	1.38
2	C	53	5MU	O2-C2	-2.07	1.19	1.23
3	D	4299	PSU	C4-C5	-2.07	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4536	OMC	C5-C4	2.07	1.47	1.42
3	D	3627	OMG	C2-N1	2.07	1.42	1.37
3	D	4494	OMG	C8-N9	-2.06	1.33	1.37
3	D	400	A2M	O4'-C4'	-2.06	1.40	1.45
3	D	4392	OMG	C6-N1	2.06	1.42	1.38
3	D	3792	OMG	C2-N1	2.05	1.42	1.37
3	D	4293	PSU	C4-C5	-2.05	1.38	1.44
3	D	4579	PSU	C4-C5	-2.05	1.38	1.44
48	w	468	A2M	C5-C4	2.05	1.42	1.39
48	w	627	OMU	C5-C4	2.05	1.48	1.43
48	w	644	OMG	C4-N9	-2.05	1.32	1.38
3	D	3899	OMG	C6-N1	2.05	1.42	1.38
3	D	4392	OMG	C8-N9	-2.04	1.33	1.37
3	D	4637	OMG	C2-N1	2.04	1.42	1.37
3	D	1773	OMU	C5-C4	2.04	1.48	1.43
3	D	2364	OMG	C2-N1	2.04	1.42	1.37
3	D	2508	PSU	C4-C5	-2.03	1.38	1.44
3	D	4370	OMG	C8-N9	-2.03	1.33	1.37
3	D	4499	OMG	C8-N9	-2.03	1.33	1.37
48	w	159	A2M	C2'-C1'	2.03	1.58	1.53
2	B	34	56B	C5-C4	-2.03	1.37	1.44
2	B	53	5MU	O2-C2	-2.03	1.19	1.23
3	D	3627	OMG	C8-N9	-2.03	1.33	1.37
3	D	1340	OMC	C5-C4	2.02	1.47	1.42
3	D	1536	PSU	C4-C5	-2.02	1.38	1.44
48	w	484	A2M	C5-C4	2.02	1.42	1.39
3	D	3792	OMG	C6-N1	2.02	1.42	1.38
48	w	1288	OMU	C5-C4	2.02	1.48	1.43
3	D	2364	OMG	C6-N1	2.02	1.42	1.38
3	D	4552	PSU	C4-C5	-2.01	1.38	1.44
3	D	4196	OMG	C6-N1	2.01	1.42	1.38
3	D	1625	OMG	C8-N9	-2.01	1.33	1.37

All (949) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	53	5MU	C5-C4-N3	12.32	125.82	115.31
2	C	53	5MU	C5-C4-N3	12.04	125.59	115.31
2	C	53	5MU	C5-C6-N1	-9.90	113.15	123.34
2	B	53	5MU	C5-C6-N1	-9.51	113.56	123.34
2	C	34	56B	C1'-N9-C4	-7.80	103.34	126.50
2	B	34	56B	C1'-N9-C4	-7.29	104.85	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	34	56B	C5-C4-N3	-6.60	119.80	127.52
2	C	6	2MG	C2-N3-C4	6.49	120.09	112.04
2	B	6	2MG	C2-N3-C4	6.40	119.97	112.04
2	C	34	56B	C5-C4-N3	-6.15	120.32	127.52
3	D	4227	OMU	C4-N3-C2	-6.04	118.62	126.58
48	w	1851	MA6	N1-C2-N3	-6.01	119.19	128.60
3	D	2837	OMU	C4-N3-C2	-5.96	118.72	126.58
3	D	4220	6MZ	N1-C2-N3	-5.92	119.33	128.60
48	w	1832	6MZ	N1-C2-N3	-5.83	119.48	128.60
3	D	2415	OMU	C4-N3-C2	-5.75	118.99	126.58
3	D	1625	OMG	C5-C4-N3	-5.71	119.19	128.46
48	w	1850	MA6	N1-C2-N3	-5.63	119.79	128.60
3	D	4498	OMU	C4-N3-C2	-5.63	119.15	126.58
48	w	1490	OMG	C5-C4-N3	-5.56	119.44	128.46
3	D	3925	OMU	C4-N3-C2	-5.53	119.29	126.58
3	D	4620	OMU	C4-N3-C2	-5.47	119.36	126.58
3	D	4306	OMU	C4-N3-C2	-5.47	119.36	126.58
3	D	4392	OMG	C5-C4-N3	-5.46	119.61	128.46
48	w	1804	OMU	C4-N3-C2	-5.44	119.41	126.58
48	w	509	OMG	C5-C4-N3	-5.41	119.68	128.46
3	D	3792	OMG	C5-C4-N3	-5.38	119.74	128.46
3	D	4637	OMG	C5-C4-N3	-5.35	119.78	128.46
48	w	428	OMU	C4-N3-C2	-5.33	119.56	126.58
48	w	683	OMG	C5-C4-N3	-5.29	119.88	128.46
3	D	3637	PSU	N1-C2-N3	5.29	121.12	115.13
2	B	53	5MU	O4-C4-C5	-5.28	118.78	124.90
48	w	172	OMU	C4-N3-C2	-5.28	119.62	126.58
3	D	4494	OMG	C5-C4-N3	-5.27	119.92	128.46
48	w	627	OMU	C4-N3-C2	-5.25	119.66	126.58
48	w	1442	OMU	C4-N3-C2	-5.23	119.68	126.58
3	D	4196	OMG	C5-C4-N3	-5.23	119.98	128.46
2	C	6	2MG	C5-C4-N3	-5.22	120.00	128.46
3	D	3944	OMG	C5-C4-N3	-5.19	120.03	128.46
48	w	799	OMU	C4-N3-C2	-5.18	119.75	126.58
48	w	1328	OMG	C5-C4-N3	-5.18	120.06	128.46
5	F	75	OMG	C5-C4-N3	-5.16	120.09	128.46
48	w	1326	OMU	C4-N3-C2	-5.12	119.82	126.58
48	w	436	OMG	C5-C4-N3	-5.11	120.17	128.46
3	D	4618	OMG	C5-C4-N3	-5.10	120.19	128.46
2	B	6	2MG	C5-C4-N3	-5.09	120.20	128.46
3	D	2364	OMG	C5-C4-N3	-5.08	120.22	128.46
48	w	1288	OMU	C4-N3-C2	-5.08	119.88	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	601	OMG	C5-C4-N3	-5.06	120.25	128.46
3	D	1862	PSU	N1-C2-N3	5.05	120.85	115.13
3	D	3744	OMG	C5-C4-N3	-5.05	120.27	128.46
3	D	4370	OMG	C5-C4-N3	-5.04	120.29	128.46
3	D	3637	PSU	C4-N3-C2	-5.03	119.09	126.34
3	D	4972	PSU	C4-N3-C2	-5.03	119.09	126.34
3	D	4499	OMG	C5-C4-N3	-5.03	120.31	128.46
3	D	3695	PSU	C4-N3-C2	-5.02	119.11	126.34
3	D	4228	OMG	C5-C4-N3	-5.00	120.36	128.46
3	D	4403	PSU	N1-C2-N3	4.99	120.79	115.13
48	w	116	OMU	C4-N3-C2	-4.99	120.00	126.58
3	D	4623	OMG	C5-C4-N3	-4.98	120.38	128.46
3	D	1862	PSU	C4-N3-C2	-4.98	119.17	126.34
2	C	53	5MU	O4-C4-C5	-4.97	119.14	124.90
3	D	4521	PSU	C4-N3-C2	-4.96	119.19	126.34
3	D	2424	OMG	C5-C4-N3	-4.96	120.42	128.46
3	D	3627	OMG	C5-C4-N3	-4.96	120.42	128.46
3	D	1683	PSU	N1-C2-N3	4.95	120.74	115.13
3	D	3695	PSU	N1-C2-N3	4.94	120.73	115.13
48	w	121	OMU	C4-N3-C2	-4.93	120.07	126.58
48	w	644	OMG	C5-C4-N3	-4.93	120.47	128.46
3	D	4312	PSU	N1-C2-N3	4.92	120.71	115.13
3	D	4403	PSU	C4-N3-C2	-4.92	119.25	126.34
3	D	1677	PSU	C4-N3-C2	-4.92	119.26	126.34
48	w	1045	PSU	C4-N3-C2	-4.91	119.26	126.34
3	D	1792	PSU	C4-N3-C2	-4.91	119.27	126.34
3	D	4457	PSU	N1-C2-N3	4.90	120.69	115.13
48	w	681	PSU	N1-C2-N3	4.90	120.69	115.13
3	D	3899	OMG	C5-C4-N3	-4.90	120.51	128.46
48	w	1692	PSU	C4-N3-C2	-4.90	119.28	126.34
3	D	4972	PSU	N1-C2-N3	4.89	120.67	115.13
48	w	681	PSU	C4-N3-C2	-4.89	119.30	126.34
3	D	1316	OMG	C5-C4-N3	-4.88	120.54	128.46
3	D	1773	OMU	C4-N3-C2	-4.88	120.14	126.58
48	w	814	PSU	C4-N3-C2	-4.88	119.31	126.34
3	D	4293	PSU	C4-N3-C2	-4.88	119.31	126.34
3	D	4353	PSU	C4-N3-C2	-4.87	119.32	126.34
3	D	1536	PSU	C4-N3-C2	-4.87	119.33	126.34
3	D	1683	PSU	C4-N3-C2	-4.87	119.33	126.34
3	D	4457	PSU	C4-N3-C2	-4.87	119.33	126.34
3	D	3730	PSU	C4-N3-C2	-4.86	119.33	126.34
3	D	4312	PSU	C4-N3-C2	-4.86	119.34	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4471	PSU	C4-N3-C2	-4.86	119.34	126.34
3	D	4442	PSU	C4-N3-C2	-4.86	119.34	126.34
48	w	1367	PSU	C4-N3-C2	-4.86	119.34	126.34
3	D	1781	PSU	C4-N3-C2	-4.85	119.35	126.34
3	D	4552	PSU	N1-C2-N3	4.84	120.62	115.13
48	w	93	PSU	C4-N3-C2	-4.84	119.36	126.34
3	D	5010	PSU	N1-C2-N3	4.83	120.60	115.13
48	w	966	PSU	N1-C2-N3	4.83	120.60	115.13
3	D	4500	PSU	N1-C2-N3	4.83	120.60	115.13
3	D	2508	PSU	C4-N3-C2	-4.83	119.38	126.34
3	D	4471	PSU	N1-C2-N3	4.83	120.60	115.13
3	D	1782	PSU	C4-N3-C2	-4.82	119.39	126.34
48	w	1045	PSU	N1-C2-N3	4.82	120.59	115.13
3	D	4628	PSU	N1-C2-N3	4.82	120.59	115.13
3	D	4579	PSU	N1-C2-N3	4.82	120.59	115.13
3	D	4442	PSU	N1-C2-N3	4.81	120.58	115.13
3	D	4576	PSU	C4-N3-C2	-4.81	119.41	126.34
2	B	13	PSU	N1-C2-N3	4.80	120.57	115.13
3	D	1860	PSU	N1-C2-N3	4.80	120.57	115.13
3	D	3730	PSU	N1-C2-N3	4.80	120.57	115.13
3	D	4299	PSU	C4-N3-C2	-4.80	119.42	126.34
3	D	3920	PSU	C4-N3-C2	-4.80	119.43	126.34
3	D	4552	PSU	C4-N3-C2	-4.80	119.43	126.34
48	w	966	PSU	C4-N3-C2	-4.79	119.43	126.34
48	w	815	PSU	C4-N3-C2	-4.79	119.44	126.34
3	D	4296	PSU	C4-N3-C2	-4.78	119.45	126.34
48	w	1445	PSU	C4-N3-C2	-4.78	119.45	126.34
3	D	4521	PSU	N1-C2-N3	4.78	120.54	115.13
3	D	5010	PSU	C4-N3-C2	-4.77	119.46	126.34
48	w	1832	6MZ	C5-C4-N3	-4.77	120.53	126.75
3	D	2508	PSU	N1-C2-N3	4.77	120.53	115.13
3	D	3758	PSU	C4-N3-C2	-4.76	119.48	126.34
3	D	3734	PSU	C4-N3-C2	-4.76	119.48	126.34
48	w	1244	PSU	C4-N3-C2	-4.76	119.48	126.34
3	D	4296	PSU	N1-C2-N3	4.75	120.52	115.13
48	w	1056	PSU	C4-N3-C2	-4.75	119.49	126.34
48	w	1081	PSU	C4-N3-C2	-4.75	119.50	126.34
3	D	4500	PSU	C4-N3-C2	-4.75	119.50	126.34
48	w	1177	PSU	C4-N3-C2	-4.75	119.50	126.34
3	D	4361	PSU	C4-N3-C2	-4.75	119.50	126.34
3	D	3734	PSU	N1-C2-N3	4.74	120.50	115.13
3	D	1760	OMG	C5-C4-N3	-4.74	120.77	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2632	PSU	C4-N3-C2	-4.74	119.52	126.34
3	D	4392	OMG	C2-N3-C4	4.73	120.73	112.30
48	w	572	PSU	C4-N3-C2	-4.73	119.52	126.34
48	w	1692	PSU	N1-C2-N3	4.73	120.49	115.13
3	D	1522	OMG	C5-C4-N3	-4.73	120.79	128.46
48	w	1347	PSU	C4-N3-C2	-4.73	119.53	126.34
48	w	1004	PSU	C4-N3-C2	-4.73	119.53	126.34
3	D	1860	PSU	C4-N3-C2	-4.72	119.54	126.34
3	D	4220	6MZ	N9-C8-N7	-4.72	107.46	113.91
48	w	866	PSU	C4-N3-C2	-4.71	119.55	126.34
48	w	1004	PSU	N1-C2-N3	4.71	120.47	115.13
48	w	406	PSU	C4-N3-C2	-4.71	119.56	126.34
3	D	4689	PSU	N1-C2-N3	4.71	120.46	115.13
3	D	5001	PSU	C4-N3-C2	-4.71	119.56	126.34
3	D	3764	PSU	C4-N3-C2	-4.70	119.56	126.34
3	D	4628	PSU	C4-N3-C2	-4.70	119.56	126.34
48	w	801	PSU	N1-C2-N3	4.70	120.45	115.13
3	D	3851	PSU	C4-N3-C2	-4.69	119.58	126.34
3	D	4353	PSU	N1-C2-N3	4.69	120.45	115.13
3	D	4579	PSU	C4-N3-C2	-4.69	119.58	126.34
48	w	609	PSU	N1-C2-N3	4.69	120.44	115.13
48	w	1625	PSU	N1-C2-N3	4.69	120.44	115.13
48	w	649	PSU	C4-N3-C2	-4.69	119.58	126.34
3	D	5001	PSU	N1-C2-N3	4.69	120.44	115.13
3	D	1781	PSU	N1-C2-N3	4.69	120.44	115.13
3	D	1677	PSU	N1-C2-N3	4.68	120.44	115.13
3	D	4689	PSU	C4-N3-C2	-4.68	119.59	126.34
3	D	3764	PSU	N1-C2-N3	4.68	120.43	115.13
48	w	801	PSU	C4-N3-C2	-4.68	119.60	126.34
3	D	3762	PSU	N1-C2-N3	4.68	120.43	115.13
48	w	651	PSU	C4-N3-C2	-4.68	119.60	126.34
48	w	1625	PSU	C4-N3-C2	-4.67	119.61	126.34
48	w	1643	PSU	N1-C2-N3	4.67	120.42	115.13
2	C	53	5MU	C4-N3-C2	-4.67	121.31	127.35
3	D	4299	PSU	N1-C2-N3	4.67	120.42	115.13
2	B	13	PSU	C4-N3-C2	-4.66	119.62	126.34
48	w	1367	PSU	N1-C2-N3	4.66	120.41	115.13
3	D	4431	PSU	N1-C2-N3	4.66	120.41	115.13
3	D	2632	PSU	N1-C2-N3	4.65	120.40	115.13
3	D	3853	PSU	C4-N3-C2	-4.65	119.64	126.34
3	D	4532	PSU	C4-N3-C2	-4.65	119.64	126.34
48	w	1643	PSU	C4-N3-C2	-4.65	119.64	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3920	PSU	N1-C2-N3	4.64	120.39	115.13
3	D	3762	PSU	C4-N3-C2	-4.64	119.66	126.34
2	C	54	PSU	C4-N3-C2	-4.63	119.66	126.34
3	D	4293	PSU	N1-C2-N3	4.63	120.38	115.13
48	w	218	PSU	C4-N3-C2	-4.63	119.67	126.34
3	D	4532	PSU	N1-C2-N3	4.63	120.37	115.13
3	D	4576	PSU	N1-C2-N3	4.63	120.37	115.13
48	w	1081	PSU	N1-C2-N3	4.63	120.37	115.13
48	w	1177	PSU	N1-C2-N3	4.63	120.37	115.13
3	D	3851	PSU	N1-C2-N3	4.63	120.37	115.13
48	w	815	PSU	N1-C2-N3	4.62	120.37	115.13
48	w	1232	PSU	N1-C2-N3	4.62	120.36	115.13
3	D	4220	6MZ	C5-C4-N3	-4.61	120.73	126.75
48	w	210	PSU	C4-N3-C2	-4.61	119.69	126.34
3	D	1782	PSU	N1-C2-N3	4.60	120.34	115.13
48	w	1056	PSU	N1-C2-N3	4.60	120.34	115.13
3	D	3639	PSU	N1-C2-N3	4.60	120.34	115.13
3	D	1744	PSU	C4-N3-C2	-4.60	119.71	126.34
3	D	4530	UR3	C4-N3-C2	-4.60	120.23	124.56
48	w	866	PSU	N1-C2-N3	4.60	120.34	115.13
48	w	683	OMG	C2-N3-C4	4.59	120.48	112.30
48	w	1244	PSU	N1-C2-N3	4.59	120.33	115.13
48	w	1445	PSU	N1-C2-N3	4.59	120.33	115.13
3	D	3639	PSU	C4-N3-C2	-4.59	119.73	126.34
2	C	13	PSU	N1-C2-N3	4.59	120.33	115.13
3	D	4420	PSU	C4-N3-C2	-4.59	119.73	126.34
48	w	651	PSU	N1-C2-N3	4.58	120.32	115.13
48	w	109	PSU	N1-C2-N3	4.58	120.32	115.13
48	w	863	PSU	C4-N3-C2	-4.58	119.74	126.34
48	w	686	PSU	N1-C2-N3	4.58	120.32	115.13
48	w	1174	PSU	C4-N3-C2	-4.58	119.74	126.34
48	w	1238	PSU	C4-N3-C2	-4.58	119.74	126.34
48	w	1850	MA6	C2-N1-C6	4.57	122.56	111.75
3	D	3715	PSU	C4-N3-C2	-4.57	119.76	126.34
3	D	4423	PSU	C4-N3-C2	-4.56	119.76	126.34
48	w	34	PSU	N1-C2-N3	4.56	120.30	115.13
48	w	1850	MA6	C5-C4-N3	-4.56	120.80	126.75
2	C	54	PSU	N1-C2-N3	4.56	120.30	115.13
48	w	863	PSU	N1-C2-N3	4.56	120.29	115.13
48	w	36	PSU	N1-C2-N3	4.56	120.29	115.13
2	B	54	PSU	C4-N3-C2	-4.56	119.78	126.34
48	w	1046	PSU	N1-C2-N3	4.55	120.29	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	13	PSU	C4-N3-C2	-4.55	119.78	126.34
3	D	3768	PSU	C4-N3-C2	-4.55	119.78	126.34
48	w	649	PSU	N1-C2-N3	4.55	120.28	115.13
48	w	119	PSU	C4-N3-C2	-4.54	119.79	126.34
3	D	1536	PSU	N1-C2-N3	4.54	120.27	115.13
48	w	1851	MA6	C5-C4-N3	-4.54	120.83	126.75
48	w	1232	PSU	C4-N3-C2	-4.54	119.80	126.34
48	w	1490	OMG	C2-N3-C4	4.53	120.38	112.30
48	w	1046	PSU	C4-N3-C2	-4.53	119.81	126.34
3	D	3768	PSU	N1-C2-N3	4.53	120.27	115.13
48	w	119	PSU	N1-C2-N3	4.53	120.26	115.13
3	D	4431	PSU	C4-N3-C2	-4.53	119.81	126.34
3	D	3770	PSU	N1-C2-N3	4.53	120.26	115.13
48	w	1639	G7M	C2-N3-C4	4.52	120.36	112.30
3	D	3758	PSU	N1-C2-N3	4.52	120.25	115.13
3	D	3853	PSU	N1-C2-N3	4.51	120.24	115.13
3	D	4420	PSU	N1-C2-N3	4.51	120.24	115.13
2	B	34	56B	C2-N3-C4	4.51	120.34	112.30
48	w	436	OMG	C2-N3-C4	4.50	120.31	112.30
3	D	4361	PSU	N1-C2-N3	4.49	120.22	115.13
48	w	686	PSU	C4-N3-C2	-4.49	119.87	126.34
48	w	406	PSU	N1-C2-N3	4.49	120.22	115.13
48	w	1851	MA6	C2-N1-C6	4.49	122.35	111.75
48	w	1832	6MZ	N9-C8-N7	-4.49	107.78	113.91
3	D	1792	PSU	N1-C2-N3	4.49	120.21	115.13
2	B	53	5MU	C4-N3-C2	-4.48	121.55	127.35
48	w	109	PSU	C4-N3-C2	-4.48	119.88	126.34
48	w	814	PSU	N1-C2-N3	4.48	120.21	115.13
48	w	105	PSU	C4-N3-C2	-4.48	119.88	126.34
3	D	4423	PSU	N1-C2-N3	4.48	120.20	115.13
48	w	105	PSU	N1-C2-N3	4.47	120.19	115.13
3	D	4306	OMU	N3-C2-N1	4.47	120.82	114.89
48	w	1347	PSU	N1-C2-N3	4.47	120.19	115.13
3	D	3715	PSU	N1-C2-N3	4.46	120.19	115.13
48	w	1174	PSU	N1-C2-N3	4.46	120.18	115.13
3	D	4228	OMG	C2-N3-C4	4.46	120.25	112.30
3	D	1625	OMG	C2-N3-C4	4.45	120.23	112.30
3	D	1744	PSU	N1-C2-N3	4.45	120.17	115.13
3	D	3627	OMG	C2-N3-C4	4.45	120.22	112.30
48	w	36	PSU	C4-N3-C2	-4.45	119.93	126.34
48	w	822	PSU	C4-N3-C2	-4.44	119.94	126.34
48	w	609	PSU	C4-N3-C2	-4.44	119.94	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	93	PSU	N1-C2-N3	4.43	120.15	115.13
48	w	218	PSU	N1-C2-N3	4.43	120.15	115.13
48	w	1238	PSU	N1-C2-N3	4.43	120.14	115.13
48	w	210	PSU	N1-C2-N3	4.41	120.13	115.13
3	D	4499	OMG	C2-N3-C4	4.41	120.15	112.30
3	D	4618	OMG	C2-N3-C4	4.41	120.15	112.30
3	D	4227	OMU	N3-C2-N1	4.40	120.73	114.89
3	D	3770	PSU	C4-N3-C2	-4.40	120.00	126.34
3	D	3744	OMG	C2-N3-C4	4.39	120.13	112.30
3	D	3899	OMG	C2-N3-C4	4.39	120.12	112.30
2	B	54	PSU	N1-C2-N3	4.39	120.10	115.13
3	D	4620	OMU	N3-C2-N1	4.38	120.71	114.89
2	C	34	56B	C2-N3-C4	4.38	120.10	112.30
3	D	3944	OMG	C2-N3-C4	4.37	120.09	112.30
48	w	1851	MA6	N9-C8-N7	-4.37	107.93	113.91
48	w	601	OMG	C2-N3-C4	4.37	120.09	112.30
3	D	4494	OMG	C2-N3-C4	4.37	120.08	112.30
48	w	1850	MA6	C4-C5-C6	4.36	120.76	115.88
3	D	4370	OMG	C2-N3-C4	4.36	120.07	112.30
2	C	53	5MU	N3-C2-N1	4.35	120.66	114.89
3	D	2364	OMG	C2-N3-C4	4.34	120.03	112.30
48	w	572	PSU	N1-C2-N3	4.34	120.05	115.13
5	F	75	OMG	C2-N3-C4	4.33	120.02	112.30
48	w	1328	OMG	C2-N3-C4	4.31	119.98	112.30
3	D	1316	OMG	C2-N3-C4	4.30	119.96	112.30
48	w	822	PSU	N1-C2-N3	4.30	120.00	115.13
3	D	4637	OMG	C2-N3-C4	4.29	119.95	112.30
3	D	4623	OMG	C2-N3-C4	4.28	119.93	112.30
2	C	6	2MG	C2-N1-C6	-4.28	119.55	124.48
3	D	2424	OMG	C2-N3-C4	4.27	119.91	112.30
3	D	2837	OMU	N3-C2-N1	4.25	120.53	114.89
48	w	34	PSU	C4-N3-C2	-4.25	120.22	126.34
48	w	509	OMG	C2-N3-C4	4.24	119.86	112.30
48	w	644	OMG	C2-N3-C4	4.24	119.86	112.30
2	B	6	2MG	C2-N1-C6	-4.24	119.60	124.48
48	w	1639	G7M	C5-C4-N3	-4.24	120.02	128.15
2	B	53	5MU	C5M-C5-C4	4.22	123.41	118.77
3	D	4196	OMG	C2-N3-C4	4.20	119.79	112.30
3	D	3792	OMG	C2-N3-C4	4.17	119.74	112.30
3	D	4447	5MC	C5-C6-N1	-4.16	119.06	123.34
3	D	1760	OMG	C2-N3-C4	4.13	119.66	112.30
3	D	1625	OMG	N9-C4-N3	4.13	134.23	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3925	OMU	N3-C2-N1	4.11	120.35	114.89
3	D	1522	OMG	C2-N3-C4	4.09	119.59	112.30
3	D	4498	OMU	N3-C2-N1	4.06	120.28	114.89
48	w	1639	G7M	C5-C6-N1	4.06	120.26	111.79
48	w	428	OMU	N3-C2-N1	4.05	120.26	114.89
2	C	34	56B	C7-C5-C4	-4.03	107.99	112.66
2	C	53	5MU	C5M-C5-C6	-4.00	117.50	122.85
2	B	53	5MU	N3-C2-N1	3.99	120.19	114.89
2	B	34	56B	C7-C5-C4	-3.99	108.04	112.66
2	C	53	5MU	C5M-C5-C4	3.99	123.16	118.77
3	D	2415	OMU	N3-C2-N1	3.94	120.12	114.89
48	w	1326	OMU	N3-C2-N1	3.93	120.11	114.89
48	w	509	OMG	N9-C4-N3	3.93	133.83	125.94
48	w	1442	OMU	N3-C2-N1	3.93	120.10	114.89
48	w	1490	OMG	N9-C4-N3	3.88	133.74	125.94
3	D	3792	OMG	N9-C4-N3	3.88	133.73	125.94
2	B	53	5MU	C5M-C5-C6	-3.87	117.68	122.85
48	w	121	OMU	N3-C2-N1	3.83	119.98	114.89
48	w	172	OMU	N3-C2-N1	3.83	119.97	114.89
3	D	4637	OMG	N9-C4-N3	3.80	133.57	125.94
3	D	2415	OMU	C5-C4-N3	3.80	120.52	114.84
3	D	4220	6MZ	C5-N7-C8	3.78	108.88	103.51
2	B	34	56B	C7-C8-N9	-3.77	107.36	111.06
48	w	627	OMU	N3-C2-N1	3.75	119.87	114.89
3	D	4227	OMU	C5-C4-N3	3.73	120.43	114.84
48	w	799	OMU	N3-C2-N1	3.73	119.84	114.89
48	w	1850	MA6	N9-C8-N7	-3.72	108.83	113.91
2	C	34	56B	C7-C8-N9	-3.70	107.43	111.06
3	D	4498	OMU	C5-C4-N3	3.69	120.37	114.84
3	D	3944	OMG	N9-C4-N3	3.68	133.33	125.94
48	w	1337	4AC	O7-C7-N4	3.68	127.77	121.82
3	D	4220	6MZ	C2-N3-C4	3.68	120.44	111.75
3	D	2837	OMU	C5-C4-N3	3.67	120.34	114.84
48	w	1851	MA6	C4-C5-C6	3.67	119.98	115.88
48	w	683	OMG	N9-C4-N3	3.66	133.28	125.94
2	B	38	5MC	C5-C6-N1	-3.65	119.58	123.34
48	w	1804	OMU	N3-C2-N1	3.64	119.72	114.89
48	w	1804	OMU	C5-C4-N3	3.64	120.28	114.84
3	D	4196	OMG	N9-C4-N3	3.64	133.24	125.94
3	D	4494	OMG	N9-C4-N3	3.61	133.19	125.94
2	B	34	56B	N9-C4-N3	3.61	133.19	125.94
48	w	1832	6MZ	C2-N3-C4	3.59	120.22	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3899	OMG	N9-C8-N7	-3.57	106.66	113.39
3	D	4370	OMG	N9-C8-N7	-3.57	106.67	113.39
3	D	4228	OMG	N9-C8-N7	-3.55	106.70	113.39
3	D	3925	OMU	C5-C4-N3	3.55	120.16	114.84
3	D	1760	OMG	N9-C8-N7	-3.53	106.74	113.39
3	D	1773	OMU	N3-C2-N1	3.53	119.58	114.89
48	w	1288	OMU	N3-C2-N1	3.53	119.58	114.89
3	D	4392	OMG	C2-N1-C6	-3.52	118.68	125.10
48	w	1832	6MZ	C5-N7-C8	3.51	108.50	103.51
3	D	4623	OMG	N9-C8-N7	-3.51	106.79	113.39
48	w	644	OMG	N9-C8-N7	-3.50	106.79	113.39
48	w	1842	4AC	O7-C7-N4	3.49	127.46	121.82
48	w	1328	OMG	N9-C8-N7	-3.48	106.83	113.39
3	D	4392	OMG	N9-C4-N3	3.48	132.94	125.94
3	D	1316	OMG	N9-C8-N7	-3.48	106.83	113.39
3	D	3782	5MC	C5-C6-N1	-3.48	119.75	123.34
3	D	4499	OMG	N9-C8-N7	-3.47	106.85	113.39
3	D	3627	OMG	N9-C8-N7	-3.47	106.86	113.39
48	w	1639	G7M	O6-C6-C5	-3.46	120.25	128.06
48	w	1851	MA6	C5-N7-C8	3.46	108.42	103.51
48	w	436	OMG	N9-C8-N7	-3.45	106.89	113.39
48	w	1328	OMG	N9-C4-N3	3.45	132.87	125.94
2	C	6	2MG	N9-C4-N3	3.45	132.86	125.94
3	D	2364	OMG	N9-C4-N3	3.45	132.86	125.94
3	D	1522	OMG	N9-C8-N7	-3.44	106.91	113.39
2	B	47	5MC	C5-C6-N1	-3.44	119.80	123.34
48	w	601	OMG	N9-C4-N3	3.44	132.84	125.94
5	F	75	OMG	N9-C4-N3	3.44	132.84	125.94
48	w	436	OMG	N9-C4-N3	3.43	132.83	125.94
2	B	6	2MG	N9-C4-N3	3.42	132.80	125.94
48	w	116	OMU	C5-C4-N3	3.42	119.95	114.84
48	w	1851	MA6	C2-N3-C4	3.41	119.81	111.75
2	B	48	5MC	C5-C6-N1	-3.41	119.83	123.34
3	D	4228	OMG	C1'-N9-C4	-3.41	116.38	126.50
3	D	4618	OMG	N9-C4-N3	3.39	132.74	125.94
3	D	4370	OMG	N9-C4-N3	3.37	132.70	125.94
48	w	1326	OMU	C5-C4-N3	3.37	119.88	114.84
3	D	3944	OMG	N9-C8-N7	-3.36	107.06	113.39
3	D	2364	OMG	N9-C8-N7	-3.35	107.07	113.39
3	D	4494	OMG	N9-C8-N7	-3.35	107.07	113.39
48	w	601	OMG	N9-C8-N7	-3.35	107.08	113.39
3	D	3744	OMG	N9-C4-N3	3.35	132.66	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	47	5MC	C5-C6-N1	-3.34	119.90	123.34
3	D	4220	6MZ	C4-C5-N7	-3.34	106.55	110.62
3	D	2424	OMG	N9-C4-N3	3.34	132.65	125.94
48	w	172	OMU	C5-C4-N3	3.34	119.84	114.84
48	w	1288	OMU	C5-C4-N3	3.34	119.84	114.84
48	w	683	OMG	N9-C8-N7	-3.34	107.11	113.39
3	D	4620	OMU	C5-C4-N3	3.33	119.82	114.84
48	w	627	OMU	C5-C4-N3	3.32	119.81	114.84
48	w	116	OMU	N3-C2-N1	3.32	119.29	114.89
3	D	4499	OMG	N9-C4-N3	3.32	132.60	125.94
5	F	75	OMG	N9-C8-N7	-3.31	107.15	113.39
3	D	1760	OMG	N9-C4-N3	3.29	132.55	125.94
48	w	799	OMU	C5-C4-N3	3.29	119.77	114.84
3	D	1625	OMG	C2-N1-C6	-3.29	119.10	125.10
3	D	4196	OMG	N9-C8-N7	-3.28	107.20	113.39
3	D	4637	OMG	N9-C8-N7	-3.28	107.20	113.39
3	D	2424	OMG	N9-C8-N7	-3.28	107.21	113.39
3	D	4618	OMG	N9-C8-N7	-3.28	107.21	113.39
3	D	4637	OMG	C2-N1-C6	-3.28	119.12	125.10
2	C	38	5MC	C5-C6-N1	-3.28	119.97	123.34
3	D	4500	PSU	O2-C2-N1	-3.27	119.19	122.79
3	D	4196	OMG	C2-N1-C6	-3.27	119.13	125.10
2	B	6	2MG	N9-C8-N7	-3.27	107.23	113.39
3	D	3627	OMG	N9-C4-N3	3.27	132.50	125.94
48	w	1442	OMU	C5-C4-N3	3.27	119.72	114.84
48	w	428	OMU	C5-C4-N3	3.26	119.72	114.84
48	w	1639	G7M	N9-C4-N3	3.26	132.48	125.94
2	C	6	2MG	N9-C8-N7	-3.25	107.26	113.39
3	D	2424	OMG	C2-N1-C6	-3.25	119.17	125.10
48	w	644	OMG	N9-C4-N3	3.25	132.47	125.94
2	C	34	56B	N9-C4-N3	3.24	132.45	125.94
3	D	3785	A2M	C2'-C1'-N9	-3.24	108.07	113.53
3	D	4392	OMG	N9-C8-N7	-3.23	107.30	113.39
3	D	4623	OMG	C1'-N9-C4	-3.23	116.91	126.50
3	D	3899	OMG	N9-C4-N3	3.22	132.41	125.94
3	D	1773	OMU	C5-C4-N3	3.22	119.65	114.84
3	D	3744	OMG	N9-C8-N7	-3.20	107.36	113.39
48	w	1328	OMG	C2-N1-C6	-3.19	119.27	125.10
3	D	1522	OMG	C1'-N9-C4	-3.18	117.06	126.50
48	w	1832	6MZ	C4-C5-C6	3.18	119.27	116.81
3	D	3899	OMG	C1'-N9-C4	-3.18	117.07	126.50
3	D	4499	OMG	C2-N1-C6	-3.17	119.31	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4228	OMG	N9-C4-N3	3.17	132.31	125.94
48	w	1639	G7M	C2-N1-C6	-3.16	119.33	125.10
48	w	683	OMG	C2-N1-C6	-3.16	119.34	125.10
3	D	3627	OMG	C1'-N9-C4	-3.16	117.13	126.50
48	w	1490	OMG	N9-C8-N7	-3.15	107.45	113.39
48	w	121	OMU	C5-C4-N3	3.15	119.56	114.84
3	D	2364	OMG	C2-N1-C6	-3.15	119.36	125.10
3	D	4623	OMG	N9-C4-N3	3.15	132.26	125.94
3	D	3792	OMG	N9-C8-N7	-3.13	107.49	113.39
48	w	644	OMG	C1'-N9-C4	-3.13	117.19	126.50
3	D	1534	A2M	O2'-C2'-C1'	3.13	115.18	109.08
3	D	4228	OMG	C2-N1-C6	-3.12	119.40	125.10
3	D	1316	OMG	C2-N1-C6	-3.12	119.41	125.10
3	D	4306	OMU	C5-C4-N3	3.12	119.50	114.84
48	w	1850	MA6	C5-N7-C8	3.12	107.94	103.51
2	C	48	5MC	C5-C6-N1	-3.11	120.14	123.34
3	D	4618	OMG	C2-N1-C6	-3.10	119.44	125.10
3	D	1760	OMG	C1'-N9-C4	-3.10	117.29	126.50
5	F	75	OMG	C2-N1-C6	-3.10	119.45	125.10
48	w	509	OMG	N9-C8-N7	-3.09	107.56	113.39
48	w	1490	OMG	C2-N1-C6	-3.09	119.47	125.10
3	D	4392	OMG	C5-C6-N1	3.09	121.03	113.19
3	D	1625	OMG	N9-C8-N7	-3.09	107.58	113.39
48	w	109	PSU	O2-C2-N1	-3.08	119.39	122.79
48	w	1850	MA6	C2-N3-C4	3.08	119.03	111.75
3	D	1522	OMG	N9-C4-N3	3.08	132.13	125.94
3	D	1316	OMG	N9-C4-N3	3.08	132.12	125.94
2	B	34	56B	C2-N1-C6	-3.07	119.50	125.10
3	D	4494	OMG	C2-N1-C6	-3.07	119.50	125.10
48	w	644	OMG	C2-N1-C6	-3.06	119.51	125.10
3	D	3627	OMG	C2-N1-C6	-3.06	119.52	125.10
3	D	1316	OMG	C1'-N9-C4	-3.06	117.41	126.50
3	D	3944	OMG	C2-N1-C6	-3.06	119.52	125.10
3	D	3792	OMG	C2-N1-C6	-3.05	119.53	125.10
48	w	436	OMG	C2-N1-C6	-3.05	119.53	125.10
3	D	2837	OMU	O4-C4-C5	-3.05	119.80	125.16
48	w	116	OMU	O4-C4-C5	-3.05	119.80	125.16
3	D	4370	OMG	C2-N1-C6	-3.04	119.56	125.10
48	w	509	OMG	C2-N1-C6	-3.04	119.56	125.10
3	D	4623	OMG	C2-N1-C6	-3.03	119.57	125.10
2	C	34	56B	C2-N1-C6	-3.02	119.59	125.10
3	D	3899	OMG	C2-N1-C6	-3.02	119.59	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1288	OMU	O4-C4-C5	-3.02	119.86	125.16
3	D	1744	PSU	O2-C2-N1	-3.00	119.49	122.79
48	w	601	OMG	C2-N1-C6	-3.00	119.63	125.10
48	w	1804	OMU	O4-C4-C5	-2.99	119.90	125.16
3	D	4296	PSU	O2-C2-N1	-2.98	119.51	122.79
3	D	1522	OMG	C2-N1-C6	-2.97	119.69	125.10
48	w	686	PSU	O2-C2-N1	-2.96	119.54	122.79
3	D	4499	OMG	C1'-N9-C4	-2.95	117.72	126.50
3	D	3627	OMG	C5-C6-N1	2.95	120.69	113.19
3	D	4370	OMG	C1'-N9-C4	-2.94	117.76	126.50
48	w	436	OMG	C1'-N9-C4	-2.94	117.77	126.50
48	w	966	PSU	O2-C2-N1	-2.92	119.58	122.79
48	w	1851	MA6	C4-C5-N7	-2.91	107.07	110.62
48	w	1326	OMU	O4-C4-C5	-2.91	120.04	125.16
3	D	3734	PSU	O2-C2-N1	-2.91	119.59	122.79
48	w	1832	6MZ	C4-C5-N7	-2.91	107.08	110.62
3	D	2424	OMG	C5-C6-N1	2.90	120.54	113.19
3	D	3744	OMG	C2-N1-C6	-2.89	119.82	125.10
3	D	4228	OMG	C5-C6-N1	2.89	120.53	113.19
3	D	3730	PSU	O2-C2-N1	-2.89	119.61	122.79
48	w	1851	MA6	N1-C6-N6	-2.89	113.93	117.08
48	w	1442	OMU	O4-C4-C5	-2.89	120.08	125.16
3	D	1760	OMG	C2-N1-C6	-2.88	119.84	125.10
3	D	2415	OMU	O4-C4-C5	-2.88	120.09	125.16
3	D	4637	OMG	C5-C6-N1	2.88	120.49	113.19
3	D	4628	PSU	O2-C2-N1	-2.88	119.62	122.79
48	w	683	OMG	C5-C6-N1	2.87	120.48	113.19
48	w	36	PSU	O2-C2-N1	-2.87	119.63	122.79
3	D	1683	PSU	O2-C2-N1	-2.87	119.64	122.79
3	D	4498	OMU	O4-C4-C5	-2.86	120.13	125.16
48	w	436	OMG	C5-C6-N1	2.85	120.43	113.19
3	D	1862	PSU	O2-C2-N1	-2.85	119.65	122.79
48	w	1328	OMG	C1'-N9-C4	-2.85	118.04	126.50
3	D	2364	OMG	C5-C6-N1	2.84	120.39	113.19
3	D	4196	OMG	C5-C6-N1	2.84	120.39	113.19
3	D	4618	OMG	C5-C6-N1	2.83	120.39	113.19
3	D	4618	OMG	C1'-N9-C4	-2.83	118.09	126.50
48	w	1347	PSU	O2-C2-N1	-2.83	119.67	122.79
48	w	1004	PSU	O2-C2-N1	-2.83	119.68	122.79
48	w	627	OMU	O4-C4-C5	-2.83	120.19	125.16
48	w	1045	PSU	O2-C2-N1	-2.82	119.68	122.79
48	w	1639	G7M	CN7-N7-C5	2.82	130.27	126.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4220	6MZ	C5-C4-N9	2.82	109.06	105.78
3	D	3899	OMG	C5-C6-N1	2.82	120.35	113.19
48	w	1445	PSU	O2-C2-N1	-2.82	119.69	122.79
48	w	1367	PSU	O2-C2-N1	-2.81	119.69	122.79
3	D	4532	PSU	O2-C2-N1	-2.81	119.69	122.79
48	w	1850	MA6	C4-C5-N7	-2.81	107.19	110.62
3	D	4499	OMG	C5-C6-N1	2.81	120.33	113.19
48	w	1238	PSU	O2-C2-N1	-2.81	119.69	122.79
3	D	3768	PSU	O2-C2-N1	-2.81	119.70	122.79
3	D	2424	OMG	C1'-N9-C4	-2.80	118.18	126.50
48	w	172	OMU	O4-C4-C5	-2.80	120.23	125.16
2	C	34	56B	C9-N10-C10	-2.80	107.25	113.35
3	D	4972	PSU	O2-C2-N1	-2.80	119.71	122.79
48	w	801	PSU	O2-C2-N1	-2.80	119.71	122.79
3	D	4442	PSU	O2-C2-N1	-2.79	119.72	122.79
3	D	2424	OMG	O6-C6-C5	-2.79	119.20	126.60
3	D	1860	PSU	O2-C2-N1	-2.79	119.72	122.79
3	D	1625	OMG	C5-C6-N1	2.79	120.27	113.19
3	D	5010	PSU	O2-C2-N1	-2.79	119.72	122.79
3	D	4494	OMG	C5-C6-N1	2.79	120.26	113.19
48	w	1046	PSU	O2-C2-N1	-2.78	119.73	122.79
3	D	1522	OMG	C5-C6-N1	2.78	120.25	113.19
3	D	4293	PSU	O2-C2-N1	-2.78	119.73	122.79
48	w	1490	OMG	C5-C6-N1	2.78	120.24	113.19
3	D	1316	OMG	C5-C6-N1	2.77	120.24	113.19
3	D	3944	OMG	C5-C6-N1	2.77	120.24	113.19
3	D	3782	5MC	CM5-C5-C6	-2.77	119.14	122.85
48	w	1328	OMG	C5-C6-N1	2.77	120.23	113.19
3	D	4228	OMG	O6-C6-C5	-2.77	119.24	126.60
48	w	1045	PSU	C6-C5-C4	2.77	120.14	118.20
3	D	2837	OMU	O2-C2-N1	-2.77	119.10	122.79
3	D	3925	OMU	O4-C4-C5	-2.77	120.29	125.16
2	B	6	2MG	C5-C6-N1	2.77	120.22	113.19
3	D	4370	OMG	C5-C6-N1	2.76	120.21	113.19
48	w	121	OMU	O4-C4-C5	-2.76	120.31	125.16
48	w	866	PSU	O2-C2-N1	-2.75	119.76	122.79
3	D	1773	OMU	O4-C4-C5	-2.75	120.33	125.16
3	D	2632	PSU	O2-C2-N1	-2.74	119.77	122.79
48	w	601	OMG	C5-C6-N1	2.74	120.15	113.19
2	C	13	PSU	O2-C2-N1	-2.74	119.78	122.79
48	w	119	PSU	O2-C2-N1	-2.73	119.79	122.79
48	w	609	PSU	O2-C2-N1	-2.73	119.79	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	799	OMU	O4-C4-C5	-2.72	120.37	125.16
5	F	75	OMG	C5-C6-N1	2.72	120.09	113.19
48	w	644	OMG	C5-C6-N1	2.72	120.09	113.19
3	D	4392	OMG	C1'-N9-C4	-2.72	118.44	126.50
3	D	1677	PSU	O2-C2-N1	-2.71	119.81	122.79
3	D	1760	OMG	C5-C6-N1	2.71	120.08	113.19
3	D	3744	OMG	C5-C6-N1	2.71	120.06	113.19
3	D	3762	PSU	O2-C2-N1	-2.71	119.81	122.79
3	D	1534	A2M	C3'-C2'-C1'	-2.71	97.80	102.89
48	w	1625	PSU	O2-C2-N1	-2.70	119.81	122.79
48	w	428	OMU	O4-C4-C5	-2.70	120.41	125.16
3	D	4623	OMG	C5-C6-N1	2.70	120.05	113.19
3	D	4227	OMU	O4-C4-C5	-2.70	120.41	125.16
3	D	4431	PSU	O2-C2-N1	-2.70	119.82	122.79
2	C	6	2MG	C5-C6-N1	2.69	120.03	113.19
48	w	815	PSU	O2-C2-N1	-2.69	119.83	122.79
48	w	1232	PSU	O2-C2-N1	-2.69	119.83	122.79
5	F	75	OMG	C1'-N9-C4	-2.69	118.52	126.50
48	w	601	OMG	C1'-N9-C4	-2.68	118.53	126.50
3	D	3744	OMG	C1'-N9-C4	-2.68	118.53	126.50
3	D	4579	PSU	O2-C2-N1	-2.68	119.84	122.79
48	w	105	PSU	O2-C2-N1	-2.68	119.84	122.79
48	w	509	OMG	C5-C6-N1	2.67	119.97	113.19
48	w	822	PSU	O2-C2-N1	-2.67	119.85	122.79
3	D	4306	OMU	O4-C4-C5	-2.66	120.48	125.16
3	D	4576	PSU	O2-C2-N1	-2.66	119.86	122.79
3	D	3760	A2M	C3'-C2'-C1'	-2.65	97.90	102.89
3	D	2364	OMG	C1'-N9-C4	-2.65	118.63	126.50
3	D	1781	PSU	O2-C2-N1	-2.65	119.87	122.79
3	D	1625	OMG	O6-C6-C5	-2.65	119.58	126.60
48	w	1174	PSU	O2-C2-N1	-2.64	119.88	122.79
3	D	4420	PSU	O2-C2-N1	-2.64	119.88	122.79
3	D	3792	OMG	C5-C6-N1	2.64	119.89	113.19
48	w	863	PSU	O2-C2-N1	-2.64	119.89	122.79
48	w	1851	MA6	C5-C4-N9	2.64	108.85	105.78
48	w	509	OMG	O6-C6-C5	-2.63	119.61	126.60
48	w	601	OMG	O6-C6-C5	-2.63	119.63	126.60
3	D	4392	OMG	O6-C6-C5	-2.62	119.64	126.60
3	D	3764	PSU	O2-C2-N1	-2.62	119.91	122.79
3	D	4620	OMU	O4-C4-C5	-2.61	120.57	125.16
3	D	4499	OMG	O6-C6-C5	-2.60	119.70	126.60
3	D	4228	OMG	C1'-N9-C8	2.60	134.09	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3944	OMG	O6-C6-C5	-2.59	119.72	126.60
5	F	75	OMG	O6-C6-C5	-2.59	119.72	126.60
48	w	1244	PSU	O2-C2-N1	-2.59	119.94	122.79
2	B	6	2MG	O6-C6-C5	-2.59	119.74	126.60
3	D	3639	PSU	O2-C2-N1	-2.58	119.95	122.79
3	D	3770	PSU	O2-C2-N1	-2.58	119.95	122.79
48	w	436	OMG	O6-C6-C5	-2.57	119.77	126.60
3	D	2364	OMG	O6-C6-C5	-2.57	119.78	126.60
3	D	4637	OMG	O6-C6-C5	-2.57	119.79	126.60
3	D	4299	PSU	O2-C2-N1	-2.57	119.96	122.79
3	D	1860	PSU	C6-N1-C2	-2.57	120.06	122.68
48	w	218	PSU	O2-C2-N1	-2.56	119.97	122.79
48	w	36	PSU	C6-N1-C2	-2.56	120.07	122.68
3	D	4220	6MZ	C4-C5-C6	2.55	118.79	116.81
3	D	4618	OMG	O6-C6-C5	-2.55	119.82	126.60
48	w	1692	PSU	O2-C2-N1	-2.55	119.98	122.79
3	D	3695	PSU	O2-C2-N1	-2.55	119.98	122.79
3	D	4494	OMG	C1'-N9-C4	-2.55	118.93	126.50
3	D	1760	OMG	O6-C6-C5	-2.55	119.84	126.60
3	D	3627	OMG	O6-C6-C5	-2.55	119.84	126.60
2	B	13	PSU	O2-C2-N1	-2.55	119.99	122.79
48	w	683	OMG	O6-C6-C5	-2.55	119.85	126.60
48	w	1490	OMG	O6-C6-C5	-2.54	119.85	126.60
48	w	1643	PSU	O2-C2-N1	-2.54	120.00	122.79
48	w	109	PSU	C6-N1-C2	-2.54	120.09	122.68
48	w	1337	4AC	CM7-C7-N4	-2.53	110.91	115.29
48	w	651	PSU	C6-C5-C4	2.53	119.97	118.20
2	C	53	5MU	O4-C4-N3	-2.53	115.27	120.12
3	D	4196	OMG	O6-C6-C5	-2.53	119.90	126.60
2	B	6	2MG	N1-C2-N3	-2.52	120.05	123.95
3	D	4306	OMU	O2-C2-N1	-2.52	119.44	122.79
2	C	53	5MU	O2-C2-N1	-2.52	119.44	122.79
48	w	406	PSU	O2-C2-N1	-2.52	120.02	122.79
48	w	644	OMG	O6-C6-C5	-2.52	119.92	126.60
48	w	99	A2M	C2'-C1'-N9	-2.52	109.30	113.53
3	D	1534	A2M	O4'-C1'-N9	-2.51	103.11	108.06
3	D	3758	PSU	O2-C2-N1	-2.51	120.03	122.79
3	D	4312	PSU	O2-C2-N1	-2.51	120.03	122.79
3	D	1683	PSU	C6-N1-C2	-2.51	120.12	122.68
48	w	649	PSU	O2-C2-N1	-2.50	120.04	122.79
3	D	3920	PSU	O2-C2-N1	-2.50	120.04	122.79
3	D	4552	PSU	O2-C2-N1	-2.50	120.04	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3944	OMG	C1'-N9-C4	-2.50	119.08	126.50
3	D	3899	OMG	O6-C6-C5	-2.50	119.97	126.60
48	w	1232	PSU	C6-N1-C2	-2.50	120.13	122.68
48	w	34	PSU	O2-C2-N1	-2.50	120.04	122.79
3	D	4628	PSU	C6-N1-C2	-2.49	120.13	122.68
48	w	609	PSU	C6-N1-C2	-2.49	120.13	122.68
3	D	3851	PSU	O2-C2-N1	-2.49	120.05	122.79
48	w	683	OMG	C1'-N9-C4	-2.49	119.10	126.50
2	C	54	PSU	O2-C2-N1	-2.49	120.05	122.79
3	D	3792	OMG	O6-C6-C5	-2.49	120.00	126.60
3	D	4423	PSU	O2-C2-N1	-2.48	120.06	122.79
3	D	4457	PSU	C6-N1-C2	-2.48	120.15	122.68
3	D	4494	OMG	O6-C6-C5	-2.48	120.03	126.60
3	D	4579	PSU	C6-N1-C2	-2.48	120.15	122.68
48	w	1081	PSU	O2-C2-N1	-2.47	120.08	122.79
3	D	3744	OMG	O6-C6-C5	-2.47	120.06	126.60
3	D	4620	OMU	O2-C2-N1	-2.46	119.52	122.79
2	B	53	5MU	O4-C4-N3	-2.46	115.40	120.12
3	D	1316	OMG	O6-C6-C5	-2.46	120.08	126.60
48	w	1383	A2M	C2'-C1'-N9	-2.46	109.39	113.53
3	D	1536	PSU	O2-C2-N1	-2.45	120.09	122.79
48	w	210	PSU	O2-C2-N1	-2.45	120.09	122.79
48	w	686	PSU	C6-N1-C2	-2.45	120.18	122.68
48	w	34	PSU	C6-N1-C2	-2.44	120.18	122.68
48	w	966	PSU	C6-C5-C4	2.44	119.90	118.20
3	D	2508	PSU	O2-C2-N1	-2.44	120.11	122.79
3	D	1524	A2M	N3-C4-N9	2.44	131.10	127.08
2	C	6	2MG	O6-C6-C5	-2.44	120.14	126.60
48	w	1832	6MZ	C5-C4-N9	2.43	108.61	105.78
2	C	6	2MG	N1-C2-N3	-2.43	120.19	123.95
2	B	54	PSU	O2-C2-N1	-2.43	120.12	122.79
3	D	4623	OMG	C1'-N9-C8	2.43	133.61	126.70
48	w	1056	PSU	O2-C2-N1	-2.43	120.12	122.79
48	w	1383	A2M	C3'-C2'-C1'	-2.42	98.33	102.89
48	w	572	PSU	O2-C2-N1	-2.42	120.13	122.79
3	D	4353	PSU	O2-C2-N1	-2.42	120.13	122.79
3	D	4689	PSU	C6-N1-C2	-2.41	120.22	122.68
48	w	1326	OMU	C1'-N1-C2	2.41	121.93	117.57
3	D	4500	PSU	C6-N1-C2	-2.41	120.22	122.68
3	D	3715	PSU	O2-C2-N1	-2.41	120.14	122.79
3	D	4521	PSU	O2-C2-N1	-2.40	120.14	122.79
48	w	822	PSU	O4'-C1'-C2'	2.40	108.53	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4403	PSU	O2-C2-N1	-2.40	120.14	122.79
48	w	1004	PSU	C6-N1-C2	-2.40	120.23	122.68
3	D	4370	OMG	C8-N7-C5	2.40	108.59	104.24
3	D	4457	PSU	O2-C2-N1	-2.40	120.15	122.79
48	w	1328	OMG	O6-C6-C5	-2.40	120.24	126.60
3	D	4431	PSU	C6-N1-C2	-2.40	120.23	122.68
3	D	4370	OMG	O6-C6-C5	-2.39	120.25	126.60
3	D	1792	PSU	O2-C2-N1	-2.39	120.16	122.79
3	D	3639	PSU	C6-N1-C2	-2.39	120.24	122.68
48	w	1177	PSU	O2-C2-N1	-2.39	120.16	122.79
3	D	1782	PSU	O2-C2-N1	-2.38	120.17	122.79
3	D	4623	OMG	O6-C6-C5	-2.38	120.29	126.60
3	D	4637	OMG	C1'-N9-C4	-2.38	119.44	126.50
3	D	3770	PSU	C6-N1-C2	-2.37	120.26	122.68
3	D	5010	PSU	C6-N1-C2	-2.37	120.26	122.68
3	D	2815	A2M	N3-C4-N9	2.37	130.99	127.08
3	D	3637	PSU	C6-N1-C2	-2.37	120.26	122.68
3	D	4523	A2M	C2'-C1'-N9	-2.37	109.55	113.53
3	D	4296	PSU	C6-N1-C2	-2.36	120.27	122.68
48	w	1046	PSU	C6-N1-C2	-2.36	120.27	122.68
3	D	4423	PSU	C6-N1-C2	-2.35	120.28	122.68
3	D	4530	UR3	C6-N1-C2	-2.35	119.69	121.79
48	w	1643	PSU	C6-N1-C2	-2.35	120.28	122.68
3	D	4471	PSU	O2-C2-N1	-2.35	120.21	122.79
3	D	3899	OMG	C8-N7-C5	2.34	108.48	104.24
3	D	4196	OMG	C1'-N9-C4	-2.34	119.55	126.50
3	D	3762	PSU	C6-N1-C2	-2.34	120.29	122.68
3	D	4403	PSU	C6-N1-C2	-2.34	120.29	122.68
48	w	1328	OMG	C8-N7-C5	2.34	108.47	104.24
3	D	4532	PSU	C6-N1-C2	-2.34	120.29	122.68
3	D	3853	PSU	O2-C2-N1	-2.34	120.22	122.79
48	w	1326	OMU	O2'-C2'-C1'	2.33	113.62	109.08
3	D	3830	A2M	N3-C4-N9	2.33	130.92	127.08
48	w	166	A2M	N3-C4-N9	2.33	130.92	127.08
3	D	1871	A2M	C2'-C1'-N9	-2.33	109.61	113.53
48	w	681	PSU	O2-C2-N1	-2.32	120.23	122.79
3	D	1871	A2M	C3'-C2'-C1'	-2.32	98.54	102.89
48	w	1850	MA6	N3-C4-N9	2.31	130.90	127.08
2	B	13	PSU	C6-N1-C2	-2.31	120.32	122.68
3	D	2415	OMU	O3'-C3'-C2'	2.31	117.72	111.17
48	w	1031	A2M	N3-C4-N9	2.31	130.89	127.08
3	D	4498	OMU	O2-C2-N1	-2.31	119.72	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3627	OMG	C1'-N9-C8	2.31	133.26	126.70
48	w	484	A2M	N3-C4-N9	2.30	130.88	127.08
3	D	1522	OMG	C1'-N9-C8	2.30	133.25	126.70
3	D	3768	PSU	C6-N1-C2	-2.30	120.33	122.68
48	w	1832	6MZ	N3-C4-N9	2.29	130.86	127.08
48	w	436	OMG	C8-N7-C5	2.29	108.39	104.24
3	D	4228	OMG	C8-N7-C5	2.29	108.38	104.24
3	D	4623	OMG	C8-N7-C5	2.29	108.38	104.24
3	D	3734	PSU	C6-N1-C2	-2.28	120.35	122.68
48	w	814	PSU	O2-C2-N1	-2.28	120.28	122.79
3	D	4552	PSU	C6-N1-C2	-2.28	120.35	122.68
3	D	3899	OMG	C1'-N9-C8	2.28	133.18	126.70
48	w	644	OMG	C8-N7-C5	2.28	108.36	104.24
3	D	1522	OMG	O6-C6-C5	-2.28	120.56	126.60
3	D	1524	A2M	C2-N1-C6	-2.27	114.87	118.77
2	C	13	PSU	C6-N1-C2	-2.27	120.36	122.68
2	C	6	2MG	C8-N7-C5	2.27	108.35	104.24
48	w	801	PSU	C6-N1-C2	-2.27	120.36	122.68
48	w	1625	PSU	C6-N1-C2	-2.27	120.36	122.68
48	w	815	PSU	C6-C5-C4	2.27	119.78	118.20
3	D	1677	PSU	C6-C5-C4	2.27	119.78	118.20
48	w	966	PSU	C6-N1-C2	-2.27	120.37	122.68
48	w	576	A2M	N3-C4-N9	2.26	130.81	127.08
3	D	3758	PSU	C6-N1-C2	-2.26	120.37	122.68
48	w	105	PSU	C6-N1-C2	-2.26	120.37	122.68
48	w	644	OMG	C1'-N9-C8	2.26	133.13	126.70
3	D	2815	A2M	C5-C4-N3	-2.26	123.80	126.75
48	w	863	PSU	C6-N1-C2	-2.25	120.38	122.68
48	w	27	A2M	N3-C4-N9	2.25	130.80	127.08
48	w	512	A2M	N3-C4-N9	2.25	130.79	127.08
48	w	668	A2M	O4'-C1'-N9	-2.25	103.62	108.06
48	w	681	PSU	C6-C5-C4	2.25	119.77	118.20
48	w	159	A2M	N3-C4-N9	2.25	130.79	127.08
3	D	3695	PSU	C6-N1-C2	-2.25	120.39	122.68
3	D	4420	PSU	C6-N1-C2	-2.24	120.39	122.68
48	w	116	OMU	C1'-N1-C2	2.24	121.63	117.57
48	w	512	A2M	C3'-C2'-C1'	-2.24	98.68	102.89
48	w	1842	4AC	C5-C4-N4	-2.24	119.03	122.92
3	D	3637	PSU	O2-C2-N1	-2.24	120.33	122.79
3	D	3730	PSU	C6-C5-C4	2.23	119.76	118.20
48	w	651	PSU	O2-C2-N1	-2.23	120.33	122.79
3	D	3764	PSU	C6-N1-C2	-2.23	120.40	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	93	PSU	O2-C2-N1	-2.23	120.34	122.79
48	w	468	A2M	N3-C4-N9	2.23	130.75	127.08
2	B	38	5MC	CM5-C5-C6	-2.23	119.88	122.85
3	D	1534	A2M	C2-N1-C6	-2.23	114.95	118.77
2	B	57	1MA	C6-C5-N7	-2.22	128.15	132.20
3	D	1316	OMG	C1'-N9-C8	2.22	133.02	126.70
3	D	5001	PSU	C6-N1-C2	-2.22	120.41	122.68
48	w	1850	MA6	N1-C6-N6	-2.22	114.66	117.08
3	D	2632	PSU	C6-N1-C2	-2.22	120.42	122.68
3	D	1862	PSU	C6-C5-C4	2.22	119.75	118.20
3	D	2787	A2M	N3-C4-N9	2.22	130.73	127.08
48	w	105	PSU	C6-C5-C4	2.21	119.75	118.20
48	w	1056	PSU	C6-N1-C2	-2.21	120.42	122.68
3	D	1862	PSU	C6-N1-C2	-2.21	120.42	122.68
48	w	119	PSU	C6-N1-C2	-2.21	120.42	122.68
2	B	53	5MU	C1'-N1-C2	2.21	121.57	117.57
3	D	4442	PSU	C6-N1-C2	-2.21	120.42	122.68
2	B	34	56B	O12-C12-C11	-2.21	108.52	113.47
3	D	1760	OMG	C8-N7-C5	2.21	108.23	104.24
3	D	398	A2M	N3-C4-N9	2.21	130.72	127.08
48	w	1081	PSU	O4'-C1'-C2'	2.20	108.25	105.14
3	D	4471	PSU	C6-N1-C2	-2.20	120.43	122.68
3	D	4293	PSU	C6-N1-C2	-2.20	120.43	122.68
3	D	1871	A2M	N3-C4-N9	2.20	130.71	127.08
3	D	3785	A2M	N3-C4-N9	2.20	130.71	127.08
3	D	4447	5MC	O2-C2-N3	-2.20	118.75	122.33
3	D	1534	A2M	C5-C4-N3	-2.20	123.88	126.75
3	D	1781	PSU	C6-N1-C2	-2.20	120.44	122.68
3	D	3730	PSU	C6-N1-C2	-2.20	120.44	122.68
3	D	4494	OMG	C8-N7-C5	2.20	108.22	104.24
3	D	3825	A2M	N3-C4-N9	2.20	130.70	127.08
3	D	4499	OMG	C8-N7-C5	2.19	108.21	104.24
3	D	1534	A2M	N3-C4-N9	2.19	130.70	127.08
3	D	4523	A2M	N3-C4-N9	2.19	130.70	127.08
48	w	627	OMU	O2-C2-N1	-2.19	119.87	122.79
3	D	4420	PSU	O4'-C1'-C2'	2.19	108.23	105.14
48	w	1337	4AC	C5-C4-N4	-2.19	119.11	122.92
48	w	601	OMG	C8-N7-C5	2.19	108.20	104.24
3	D	3718	A2M	N3-C4-N9	2.18	130.68	127.08
3	D	2363	A2M	N3-C4-N9	2.18	130.68	127.08
3	D	1316	OMG	C8-N7-C5	2.18	108.19	104.24
48	w	1842	4AC	C4-N3-C2	-2.18	117.15	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	681	PSU	C6-N1-C2	-2.18	120.45	122.68
3	D	3818	UY1	O4-C4-N3	-2.18	115.94	120.12
48	w	99	A2M	C2-N1-C6	-2.17	115.03	118.77
48	w	218	PSU	C6-N1-C2	-2.17	120.46	122.68
3	D	4312	PSU	C6-N1-C2	-2.17	120.46	122.68
48	w	159	A2M	C2'-C1'-N9	-2.17	109.88	113.53
3	D	3734	PSU	C6-C5-C4	2.17	119.72	118.20
3	D	3715	PSU	C6-N1-C2	-2.17	120.47	122.68
48	w	1174	PSU	C6-N1-C2	-2.17	120.47	122.68
48	w	1850	MA6	C5-C4-N9	2.17	108.30	105.78
2	C	54	PSU	C6-N1-C2	-2.17	120.47	122.68
2	C	57	1MA	C6-C5-N7	-2.17	128.26	132.20
3	D	2787	A2M	C2-N1-C6	-2.16	115.05	118.77
48	w	668	A2M	N3-C4-N9	2.16	130.65	127.08
3	D	2508	PSU	C6-N1-C2	-2.16	120.47	122.68
3	D	3785	A2M	C2-N1-C6	-2.16	115.06	118.77
48	w	1248	B8N	C32-C33-C34	-2.16	105.16	110.30
3	D	4361	PSU	O2-C2-N1	-2.16	120.41	122.79
3	D	1524	A2M	C2'-C1'-N9	-2.16	109.90	113.53
48	w	814	PSU	C6-C5-C4	2.16	119.71	118.20
3	D	3944	OMG	C8-N7-C5	2.16	108.14	104.24
3	D	3724	A2M	N3-C4-N9	2.16	130.63	127.08
5	F	75	OMG	C8-N7-C5	2.16	108.14	104.24
48	w	99	A2M	N3-C4-N9	2.15	130.63	127.08
3	D	4392	OMG	C8-N7-C5	2.15	108.13	104.24
3	D	1744	PSU	C6-N1-C2	-2.15	120.49	122.68
48	w	866	PSU	C6-N1-C2	-2.14	120.49	122.68
48	w	668	A2M	C2-N1-C6	-2.14	115.08	118.77
2	B	6	2MG	C8-N7-C5	2.14	108.12	104.24
3	D	1760	OMG	C1'-N9-C8	2.14	132.80	126.70
3	D	2815	A2M	C2-N1-C6	-2.14	115.09	118.77
48	w	1337	4AC	C4-N3-C2	-2.14	117.20	120.12
3	D	2401	A2M	C2-N1-C6	-2.14	115.09	118.77
3	D	1326	A2M	N3-C4-N9	2.14	130.61	127.08
3	D	400	A2M	N3-C4-N9	2.14	130.61	127.08
48	w	683	OMG	C8-N7-C5	2.14	108.11	104.24
48	w	509	OMG	C1'-N9-C4	-2.14	120.15	126.50
48	w	1842	4AC	CM7-C7-N4	-2.14	111.60	115.29
3	D	1522	OMG	C8-N7-C5	2.14	108.11	104.24
3	D	4220	6MZ	C4-N9-C8	2.14	108.04	105.73
48	w	1639	G7M	CN7-N7-C8	-2.13	121.54	124.84
48	w	649	PSU	C6-N1-C2	-2.13	120.50	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1490	OMG	C1'-N9-C4	-2.13	120.17	126.50
48	w	1832	6MZ	C4-N9-C8	2.13	108.04	105.73
48	w	1678	A2M	N3-C4-N9	2.13	130.59	127.08
48	w	1639	G7M	O3'-C3'-C2'	2.13	118.71	111.82
48	w	436	OMG	C1'-N9-C8	2.13	132.75	126.70
48	w	36	PSU	C6-C5-C4	2.13	119.69	118.20
48	w	1445	PSU	C6-N1-C2	-2.13	120.51	122.68
3	D	4972	PSU	C6-N1-C2	-2.12	120.51	122.68
48	w	1248	B8N	O4'-C1'-C2'	2.12	108.14	105.14
3	D	3830	A2M	C5-C4-N3	-2.12	123.98	126.75
48	w	668	A2M	C5-C4-N3	-2.12	123.98	126.75
3	D	2351	OMC	O2-C2-N3	-2.12	118.89	122.33
2	C	47	5MC	CM5-C5-C6	-2.12	120.02	122.85
3	D	3920	PSU	C6-N1-C2	-2.12	120.52	122.68
3	D	3627	OMG	C8-N7-C5	2.12	108.07	104.24
48	w	1238	PSU	C6-N1-C2	-2.11	120.52	122.68
2	C	9	1MA	C6-C5-N7	-2.11	128.35	132.20
3	D	2401	A2M	N3-C4-N9	2.11	130.57	127.08
48	w	1244	PSU	C6-C5-C4	2.11	119.68	118.20
48	w	1045	PSU	C6-N1-C2	-2.11	120.52	122.68
48	w	1692	PSU	C6-N1-C2	-2.11	120.52	122.68
48	w	1177	PSU	C6-N1-C2	-2.11	120.53	122.68
2	B	47	5MC	CM5-C5-C6	-2.10	120.04	122.85
3	D	2364	OMG	C8-N7-C5	2.10	108.05	104.24
48	w	1490	OMG	C8-N7-C5	2.10	108.05	104.24
2	B	34	56B	C8-C7-C5	2.10	108.31	106.08
3	D	398	A2M	C2-N1-C6	-2.10	115.16	118.77
2	C	38	5MC	CM5-C5-C6	-2.10	120.04	122.85
3	D	4220	6MZ	C6-C5-N7	2.10	134.66	132.39
3	D	3851	PSU	C6-N1-C2	-2.10	120.53	122.68
3	D	3718	A2M	C2-N1-C6	-2.10	115.17	118.77
3	D	4523	A2M	C2-N1-C6	-2.10	115.17	118.77
3	D	4299	PSU	C6-N1-C2	-2.10	120.54	122.68
3	D	4499	OMG	C1'-N9-C8	2.09	132.66	126.70
3	D	4370	OMG	C1'-N9-C8	2.09	132.65	126.70
48	w	822	PSU	C6-N1-C2	-2.09	120.54	122.68
3	D	1534	A2M	O4'-C1'-C2'	-2.09	102.90	106.57
3	D	4576	PSU	C6-N1-C2	-2.09	120.55	122.68
3	D	400	A2M	C2-N1-C6	-2.09	115.18	118.77
3	D	3762	PSU	C6-C5-C4	2.09	119.66	118.20
3	D	4500	PSU	C6-C5-C4	2.09	119.66	118.20
3	D	4392	OMG	C1'-N9-C8	2.09	132.64	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1322	1MA	C6-C5-N7	-2.09	128.40	132.20
2	B	13	PSU	C6-C5-C4	2.09	119.66	118.20
3	D	4689	PSU	O2-C2-N1	-2.09	120.49	122.79
48	w	1442	OMU	O2-C2-N1	-2.09	120.01	122.79
48	w	484	A2M	C2-N1-C6	-2.08	115.19	118.77
3	D	4312	PSU	C6-C5-C4	2.08	119.66	118.20
2	B	54	PSU	C6-N1-C2	-2.08	120.55	122.68
3	D	4196	OMG	C8-N7-C5	2.08	108.00	104.24
3	D	1524	A2M	C5-C4-N3	-2.07	124.05	126.75
3	D	2508	PSU	C6-C5-C4	2.07	119.65	118.20
48	w	1445	PSU	C6-C5-C4	2.07	119.65	118.20
48	w	210	PSU	C6-N1-C2	-2.07	120.56	122.68
3	D	3853	PSU	C6-N1-C2	-2.07	120.56	122.68
3	D	4353	PSU	C6-N1-C2	-2.07	120.56	122.68
48	w	159	A2M	C2-N1-C6	-2.07	115.22	118.77
48	w	1347	PSU	C6-N1-C2	-2.06	120.57	122.68
3	D	4523	A2M	C3'-C2'-C1'	-2.06	99.01	102.89
48	w	166	A2M	C2-N1-C6	-2.06	115.23	118.77
3	D	4618	OMG	C8-N7-C5	2.06	107.97	104.24
3	D	3637	PSU	C6-C5-C4	2.06	119.64	118.20
48	w	1367	PSU	C6-N1-C2	-2.06	120.58	122.68
3	D	398	A2M	C5-C4-N3	-2.06	124.07	126.75
3	D	3744	OMG	C8-N7-C5	2.06	107.96	104.24
3	D	3825	A2M	C2'-C1'-N9	-2.05	110.07	113.53
3	D	1782	PSU	C6-N1-C2	-2.05	120.58	122.68
3	D	4618	OMG	C1'-N9-C8	2.05	132.54	126.70
3	D	4637	OMG	C8-N7-C5	2.05	107.95	104.24
3	D	1625	OMG	C8-N7-C5	2.05	107.94	104.24
48	w	509	OMG	C8-N7-C5	2.05	107.94	104.24
48	w	1625	PSU	C6-C5-C4	2.05	119.63	118.20
48	w	866	PSU	C6-C5-C4	2.04	119.63	118.20
48	w	27	A2M	C2-N1-C6	-2.04	115.26	118.77
3	D	3887	OMC	C2'-C1'-N1	-2.04	110.26	114.22
3	D	3792	OMG	C8-N7-C5	2.04	107.93	104.24
2	B	48	5MC	CM5-C5-C6	-2.04	120.13	122.85
48	w	576	A2M	C2-N1-C6	-2.04	115.27	118.77
3	D	3760	A2M	N3-C4-N9	2.03	130.43	127.08
3	D	3724	A2M	C2-N1-C6	-2.03	115.28	118.77
48	w	1244	PSU	C6-N1-C2	-2.03	120.61	122.68
3	D	4442	PSU	O4'-C1'-C2'	2.03	108.01	105.14
3	D	1760	OMG	C8-N9-C4	2.03	109.91	106.05
48	w	1804	OMU	O2-C2-N1	-2.03	120.09	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	166	A2M	C5-C4-N3	-2.03	124.11	126.75
3	D	4361	PSU	C6-N1-C2	-2.03	120.61	122.68
48	w	1337	4AC	C5-C4-N3	2.03	125.86	122.59
48	w	406	PSU	C6-N1-C2	-2.02	120.61	122.68
48	w	590	A2M	C2-N1-C6	-2.02	115.29	118.77
48	w	1383	A2M	N3-C4-N9	2.02	130.41	127.08
48	w	1367	PSU	C6-C5-C4	2.02	119.61	118.20
48	w	815	PSU	C6-N1-C2	-2.02	120.62	122.68
2	B	6	2MG	CM2-N2-C2	-2.02	119.41	123.86
3	D	4420	PSU	C6-C5-C4	2.02	119.61	118.20
3	D	3825	A2M	C2-N1-C6	-2.01	115.32	118.77
48	w	1383	A2M	C2-N1-C6	-2.01	115.32	118.77
48	w	1238	PSU	C6-C5-C4	2.01	119.60	118.20
3	D	1871	A2M	C2-N1-C6	-2.01	115.32	118.77
48	w	1383	A2M	C2'-C3'-C4'	-2.00	97.64	101.99
3	D	4972	PSU	C6-C5-C4	2.00	119.60	118.20
48	w	651	PSU	C6-N1-C2	-2.00	120.64	122.68
3	D	4530	UR3	C1'-N1-C2	2.00	120.37	116.99
48	w	801	PSU	C6-C5-C4	2.00	119.60	118.20

There are no chirality outliers.

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	34	56B	C11-C10-N10-C9
2	B	47	5MC	O4'-C4'-C5'-O5'
2	B	47	5MC	C3'-C4'-C5'-O5'
2	B	48	5MC	O4'-C4'-C5'-O5'
2	C	48	5MC	O4'-C4'-C5'-O5'
2	B	53	5MU	O4'-C4'-C5'-O5'
3	D	1534	A2M	C1'-C2'-O2'-CM'
3	D	1677	PSU	C2'-C1'-C5-C4
3	D	1760	OMG	C3'-C4'-C5'-O5'
3	D	1773	OMU	C1'-C2'-O2'-CM2
3	D	2415	OMU	C1'-C2'-O2'-CM2
3	D	2424	OMG	O4'-C4'-C5'-O5'
3	D	2424	OMG	C3'-C4'-C5'-O5'
3	D	2815	A2M	O4'-C4'-C5'-O5'
3	D	2815	A2M	C3'-C4'-C5'-O5'
3	D	3701	OMC	C2'-C1'-N1-C6
3	D	3785	A2M	O4'-C4'-C5'-O5'
3	D	3925	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
3	D	3944	OMG	O4'-C4'-C5'-O5'
3	D	3944	OMG	C3'-C4'-C5'-O5'
3	D	4196	OMG	C1'-C2'-O2'-CM2
3	D	4500	PSU	C3'-C4'-C5'-O5'
3	D	4500	PSU	O4'-C4'-C5'-O5'
3	D	4620	OMU	C1'-C2'-O2'-CM2
3	D	4637	OMG	C1'-C2'-O2'-CM2
48	w	27	A2M	C1'-C2'-O2'-CM'
48	w	34	PSU	C3'-C4'-C5'-O5'
48	w	116	OMU	C3'-C4'-C5'-O5'
48	w	116	OMU	O4'-C4'-C5'-O5'
48	w	159	A2M	O4'-C4'-C5'-O5'
48	w	159	A2M	C3'-C4'-C5'-O5'
48	w	159	A2M	C1'-C2'-O2'-CM'
48	w	166	A2M	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	512	A2M	O4'-C4'-C5'-O5'
48	w	512	A2M	C3'-C4'-C5'-O5'
48	w	576	A2M	C3'-C4'-C5'-O5'
48	w	576	A2M	C1'-C2'-O2'-CM'
48	w	627	OMU	C1'-C2'-O2'-CM2
48	w	627	OMU	O4'-C4'-C5'-O5'
48	w	668	A2M	O4'-C4'-C5'-O5'
48	w	799	OMU	C1'-C2'-O2'-CM2
48	w	1326	OMU	C1'-C2'-O2'-CM2
48	w	1639	G7M	O4'-C4'-C5'-O5'
48	w	1678	A2M	C1'-C2'-O2'-CM'
48	w	1804	OMU	C1'-C2'-O2'-CM2
48	w	1851	MA6	O4'-C4'-C5'-O5'
48	w	627	OMU	C2'-C1'-N1-C6
3	D	3701	OMC	C2'-C1'-N1-C2
2	C	34	56B	C3'-C4'-C5'-O5'
2	B	48	5MC	C3'-C4'-C5'-O5'
2	C	48	5MC	C3'-C4'-C5'-O5'
2	B	53	5MU	C3'-C4'-C5'-O5'
3	D	3818	UY1	C3'-C4'-C5'-O5'
3	D	3818	UY1	O4'-C4'-C5'-O5'
48	w	99	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
48	w	644	OMG	C3'-C4'-C5'-O5'
48	w	1851	MA6	C3'-C4'-C5'-O5'
2	C	9	1MA	O4'-C4'-C5'-O5'
2	C	34	56B	O4'-C4'-C5'-O5'
2	C	47	5MC	C3'-C4'-C5'-O5'
3	D	1760	OMG	O4'-C4'-C5'-O5'
3	D	2364	OMG	O4'-C4'-C5'-O5'
3	D	3785	A2M	C3'-C4'-C5'-O5'
48	w	34	PSU	O4'-C4'-C5'-O5'
48	w	99	A2M	C3'-C4'-C5'-O5'
48	w	166	A2M	O4'-C4'-C5'-O5'
48	w	428	OMU	C3'-C4'-C5'-O5'
48	w	428	OMU	O4'-C4'-C5'-O5'
48	w	576	A2M	O4'-C4'-C5'-O5'
48	w	627	OMU	C3'-C4'-C5'-O5'
48	w	668	A2M	C3'-C4'-C5'-O5'
48	w	799	OMU	C3'-C4'-C5'-O5'
48	w	1337	4AC	O4'-C4'-C5'-O5'
48	w	1490	OMG	C3'-C4'-C5'-O5'
48	w	1639	G7M	C3'-C4'-C5'-O5'
48	w	627	OMU	C2'-C1'-N1-C2
48	w	1238	PSU	C3'-C4'-C5'-O5'
3	D	4447	5MC	C2'-C1'-N1-C6
2	C	9	1MA	C3'-C4'-C5'-O5'
3	D	2364	OMG	C3'-C4'-C5'-O5'
3	D	3760	A2M	C3'-C4'-C5'-O5'
48	w	799	OMU	O4'-C4'-C5'-O5'
48	w	1288	OMU	C3'-C4'-C5'-O5'
3	D	1677	PSU	O4'-C4'-C5'-O5'
3	D	3760	A2M	O4'-C4'-C5'-O5'
48	w	644	OMG	O4'-C4'-C5'-O5'
48	w	1238	PSU	O4'-C4'-C5'-O5'
48	w	1490	OMG	O4'-C4'-C5'-O5'
48	w	822	PSU	C3'-C4'-C5'-O5'
48	w	1703	OMC	O4'-C4'-C5'-O5'
48	w	1490	OMG	C4'-C5'-O5'-P
3	D	1677	PSU	C3'-C4'-C5'-O5'
48	w	590	A2M	O4'-C4'-C5'-O5'
2	C	53	5MU	O4'-C4'-C5'-O5'
3	D	2787	A2M	C2'-C1'-N9-C8
3	D	1534	A2M	O4'-C4'-C5'-O5'
48	w	822	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	D	4447	5MC	C2'-C1'-N1-C2
48	w	627	OMU	O4'-C1'-N1-C6
2	B	47	5MC	C4'-C5'-O5'-P
3	D	1534	A2M	C4'-C5'-O5'-P
2	B	13	PSU	C3'-C4'-C5'-O5'
48	w	1288	OMU	O4'-C4'-C5'-O5'
3	D	3701	OMC	O4'-C1'-N1-C2
3	D	1524	A2M	C3'-C2'-O2'-CM'
3	D	1625	OMG	C3'-C2'-O2'-CM2
3	D	4494	OMG	C3'-C2'-O2'-CM2
3	D	4499	OMG	C3'-C2'-O2'-CM2
48	w	683	OMG	C3'-C2'-O2'-CM2
48	w	1326	OMU	C3'-C2'-O2'-CM2
3	D	3701	OMC	O4'-C1'-N1-C6
3	D	4447	5MC	O4'-C1'-N1-C6
3	D	3944	OMG	C4'-C5'-O5'-P
2	C	47	5MC	O4'-C4'-C5'-O5'
3	D	3851	PSU	C3'-C4'-C5'-O5'
48	w	590	A2M	C3'-C4'-C5'-O5'
48	w	1337	4AC	C3'-C4'-C5'-O5'
48	w	428	OMU	O4'-C1'-N1-C6
3	D	4500	PSU	C4'-C5'-O5'-P
48	w	627	OMU	O4'-C1'-N1-C2
48	w	1326	OMU	O4'-C1'-N1-C6
48	w	1248	B8N	C32-C33-C34-O36
48	w	1248	B8N	C32-C33-C34-O35
3	D	4447	5MC	O4'-C1'-N1-C2
48	w	34	PSU	C4'-C5'-O5'-P
48	w	1288	OMU	C4'-C5'-O5'-P
3	D	2401	A2M	C3'-C2'-O2'-CM'
48	w	644	OMG	C4'-C5'-O5'-P
3	D	2787	A2M	C2'-C1'-N9-C4
2	B	34	56B	O4'-C4'-C5'-O5'
48	w	428	OMU	O4'-C1'-N1-C2
48	w	1326	OMU	O4'-C1'-N1-C2
3	D	1677	PSU	O4'-C1'-C5-C4
3	D	3715	PSU	O4'-C1'-C5-C4
3	D	3818	UY1	O4'-C1'-C5-C4
3	D	4521	PSU	O4'-C1'-C5-C4
2	C	47	5MC	C4'-C5'-O5'-P
3	D	1322	1MA	C2'-C1'-N9-C8
3	D	3818	UY1	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
3	D	1524	A2M	O4'-C1'-N9-C8
48	w	484	A2M	O4'-C4'-C5'-O5'
48	w	1703	OMC	C3'-C4'-C5'-O5'
48	w	1442	OMU	C1'-C2'-O2'-CM2
48	w	1326	OMU	C2'-C1'-N1-C2
3	D	1322	1MA	C2'-C1'-N9-C4
2	C	53	5MU	C3'-C4'-C5'-O5'
3	D	3770	PSU	C3'-C4'-C5'-O5'
3	D	1677	PSU	O4'-C1'-C5-C6
3	D	3818	UY1	O4'-C1'-C5-C6
3	D	4521	PSU	O4'-C1'-C5-C6
48	w	1851	MA6	C4'-C5'-O5'-P
3	D	2787	A2M	O4'-C1'-N9-C8
3	D	2422	OMC	O4'-C4'-C5'-O5'
3	D	3785	A2M	C2'-C1'-N9-C8
48	w	1288	OMU	C2'-C1'-N1-C2
3	D	3944	OMG	C3'-C2'-O2'-CM2
3	D	2351	OMC	O4'-C4'-C5'-O5'
3	D	2351	OMC	C2'-C1'-N1-C2
48	w	668	A2M	C2'-C1'-N9-C8
3	D	3887	OMC	C4'-C5'-O5'-P

There are no ring outliers.

59 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	75	OMG	1	0
3	D	1773	OMU	4	0
48	w	1442	OMU	2	0
3	D	4623	OMG	2	0
48	w	1490	OMG	1	0
2	C	53	5MU	2	0
3	D	398	A2M	1	0
48	w	1232	PSU	2	0
3	D	2787	A2M	1	0
3	D	3718	A2M	2	0
2	C	6	2MG	1	0
48	w	1850	MA6	2	0
48	w	428	OMU	2	0
3	D	4494	OMG	1	0
48	w	1031	A2M	1	0
48	w	1288	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	w	1804	OMU	1	0
3	D	2815	A2M	1	0
48	w	512	A2M	2	0
3	D	3792	OMG	1	0
2	B	9	1MA	2	0
48	w	1842	4AC	1	0
48	w	1326	OMU	1	0
3	D	1326	A2M	1	0
3	D	1340	OMC	2	0
48	w	601	OMG	2	0
48	w	121	OMU	2	0
3	D	3818	UY1	1	0
2	B	53	5MU	3	0
48	w	644	OMG	1	0
48	w	116	OMU	1	0
3	D	3925	OMU	1	0
3	D	4637	OMG	2	0
48	w	1391	OMC	1	0
3	D	4457	PSU	1	0
48	w	590	A2M	2	0
3	D	4579	PSU	1	0
48	w	1639	G7M	1	0
48	w	509	OMG	3	0
3	D	2351	OMC	2	0
48	w	681	PSU	1	0
48	w	159	A2M	2	0
3	D	3944	OMG	1	0
3	D	4620	OMU	2	0
3	D	2415	OMU	1	0
48	w	799	OMU	2	0
3	D	4196	OMG	1	0
48	w	36	PSU	1	0
48	w	1678	A2M	1	0
2	C	47	5MC	1	0
48	w	651	PSU	1	0
3	D	3724	A2M	1	0
48	w	609	PSU	1	0
48	w	436	OMG	2	0
3	D	4447	5MC	1	0
48	w	27	A2M	1	0
48	w	166	A2M	3	0
3	D	4293	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	w	172	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 547 ligands modelled in this entry, 545 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
81	MAN	C	101	2	11,11,12	1.95	5 (45%)	15,15,17	1.22	1 (6%)
81	MAN	B	101	2	11,11,12	2.17	6 (54%)	15,15,17	1.10	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	MAN	C	101	2	-	2/2/19/22	0/1/1/1
81	MAN	B	101	2	-	2/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	B	101	MAN	C4-C5	3.58	1.60	1.53
81	C	101	MAN	C4-C5	3.42	1.60	1.53
81	B	101	MAN	O5-C1	-2.75	1.39	1.43
81	B	101	MAN	O2-C2	-2.71	1.37	1.43
81	B	101	MAN	O3-C3	-2.67	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	C	101	MAN	O2-C2	-2.54	1.38	1.43
81	C	101	MAN	O5-C1	-2.47	1.39	1.43
81	B	101	MAN	C1-C2	2.42	1.57	1.52
81	C	101	MAN	O3-C3	-2.27	1.37	1.43
81	B	101	MAN	O4-C4	-2.15	1.37	1.43
81	C	101	MAN	O4-C4	-2.11	1.38	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	C	101	MAN	O5-C1-C2	-2.04	107.63	110.77
81	B	101	MAN	O5-C1-C2	-2.03	107.64	110.77

There are no chirality outliers.

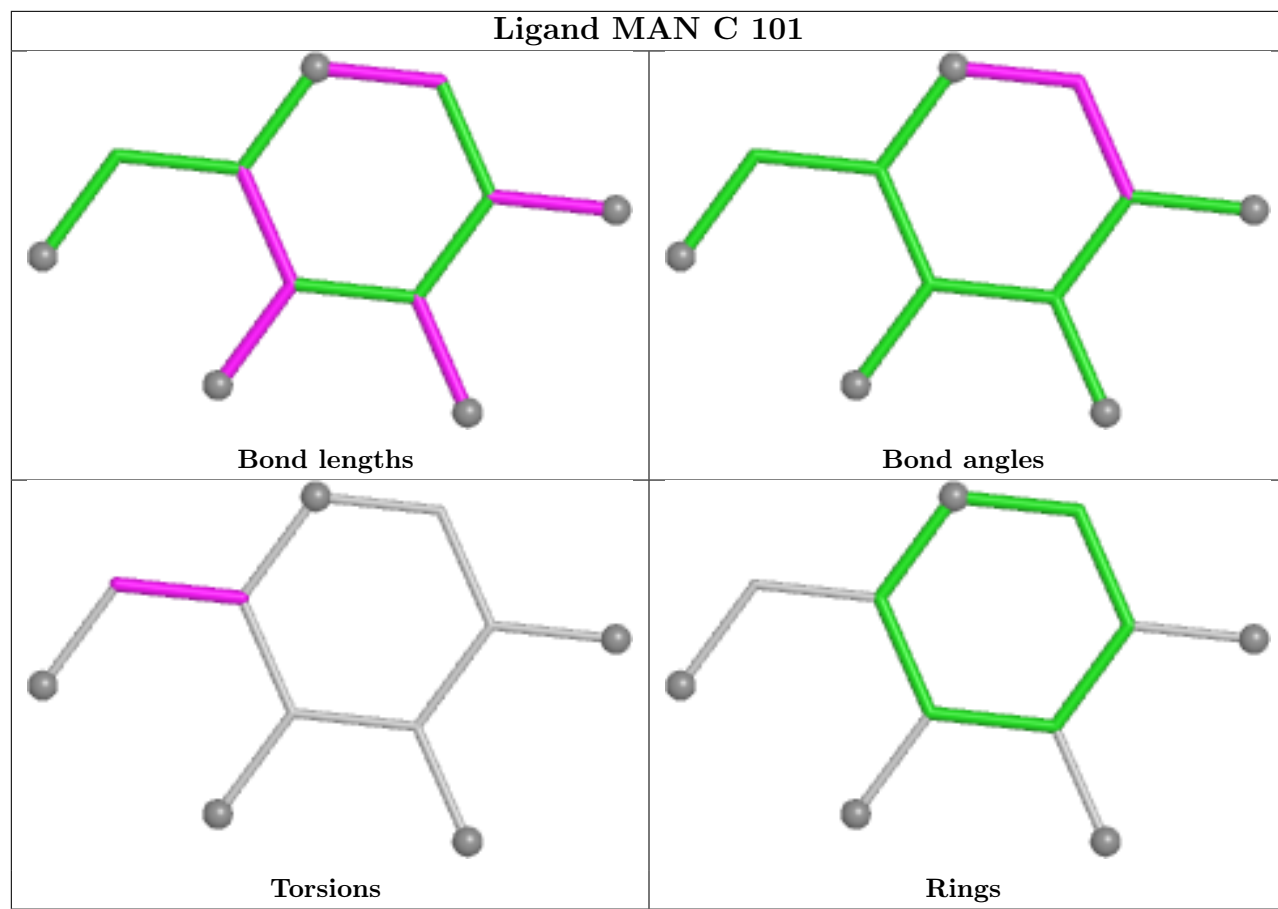
All (4) torsion outliers are listed below:

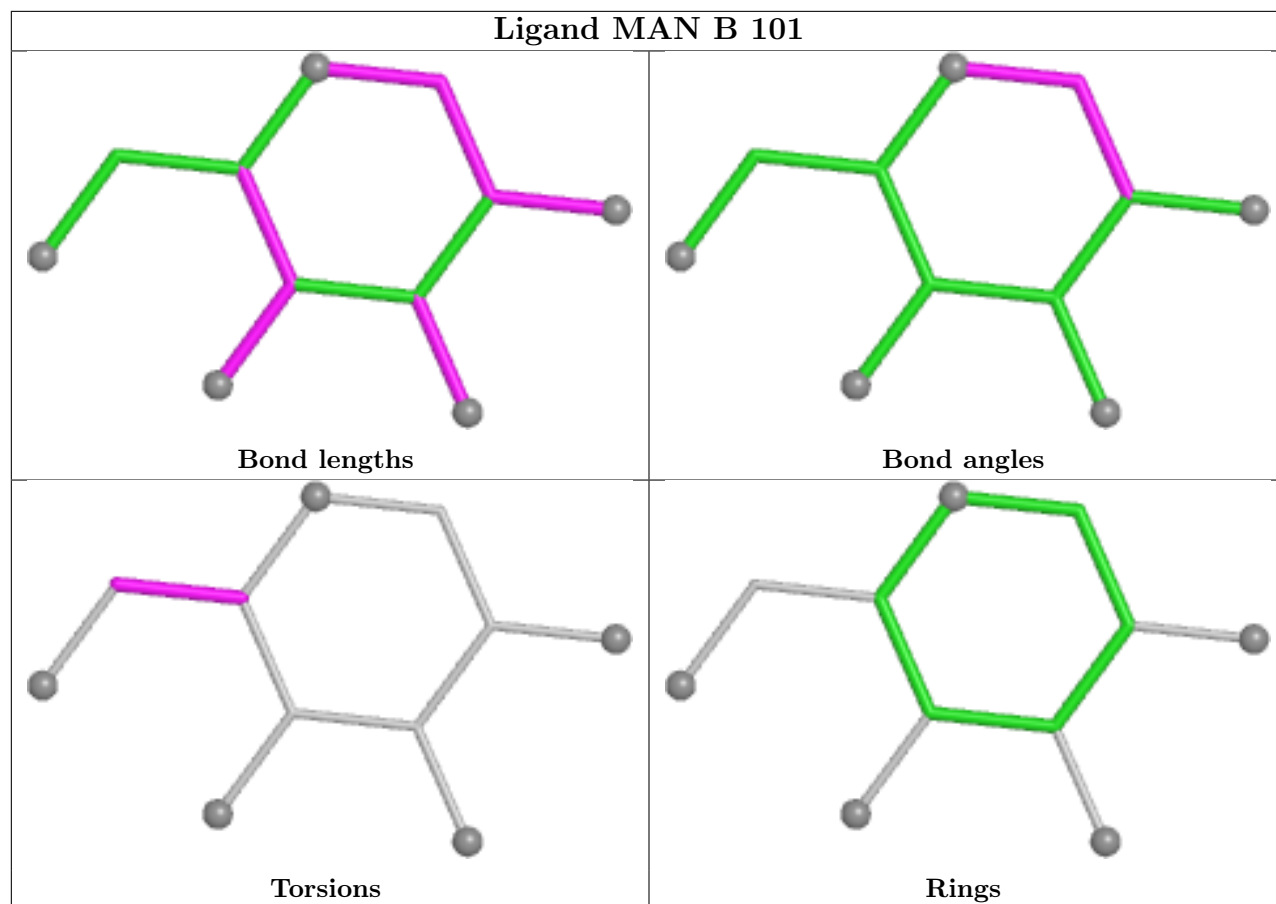
Mol	Chain	Res	Type	Atoms
81	C	101	MAN	C4-C5-C6-O6
81	C	101	MAN	O5-C5-C6-O6
81	B	101	MAN	C4-C5-C6-O6
81	B	101	MAN	O5-C5-C6-O6

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.

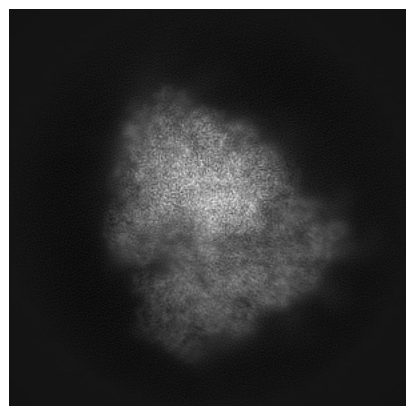
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36179. These allow visual inspection of the internal detail of the map and identification of artifacts.

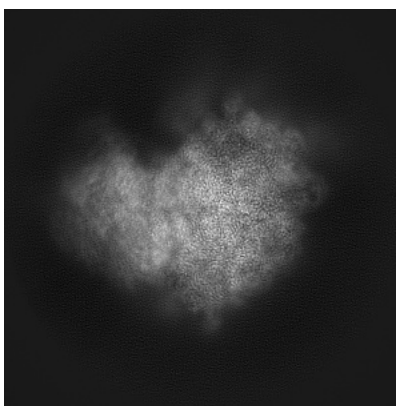
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

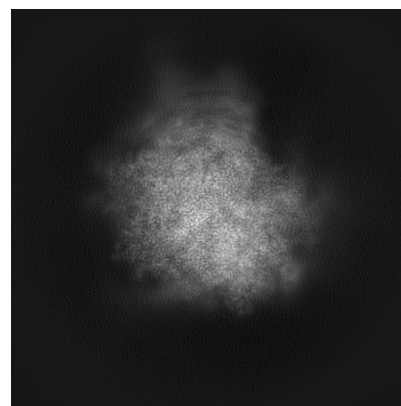
6.1.1 Primary map



X

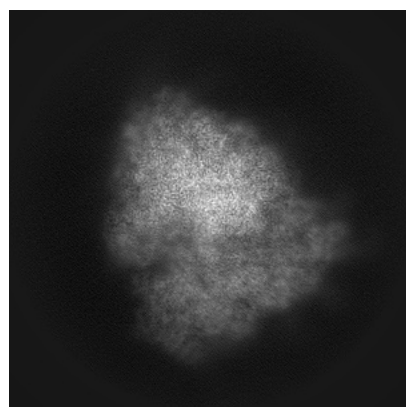


Y

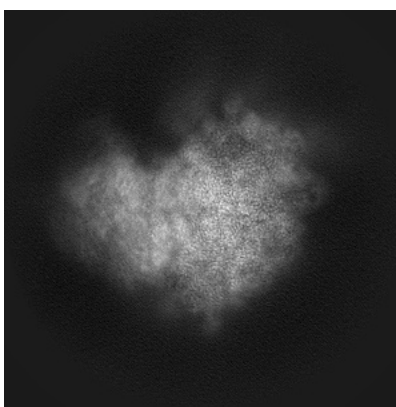


Z

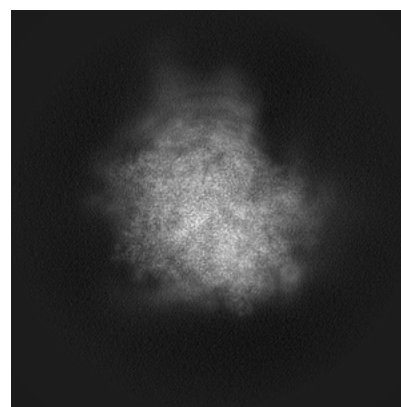
6.1.2 Raw map



X



Y

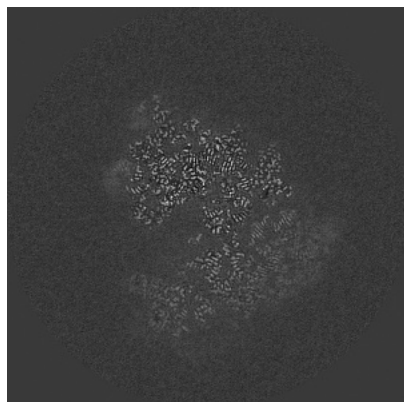


Z

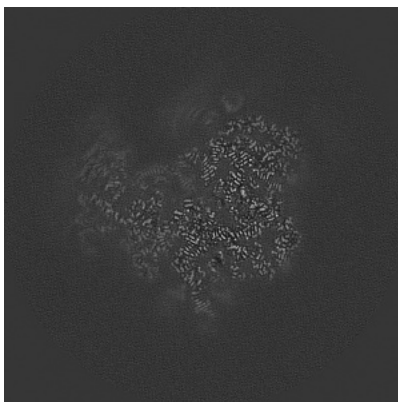
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

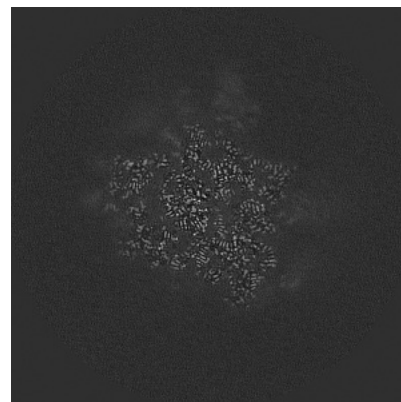
6.2.1 Primary map



X Index: 265

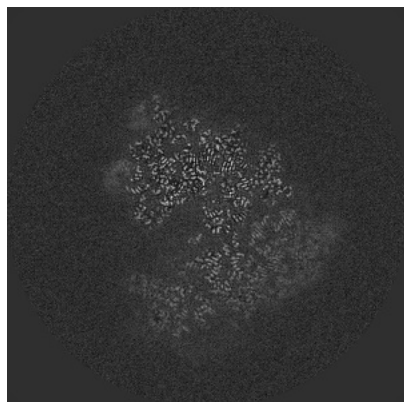


Y Index: 265

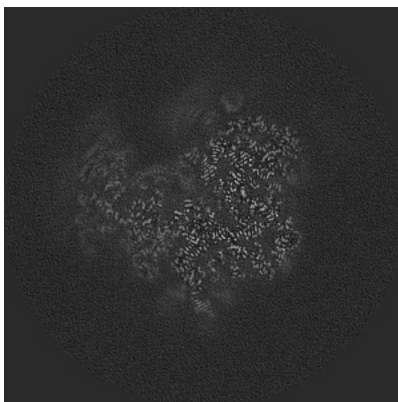


Z Index: 265

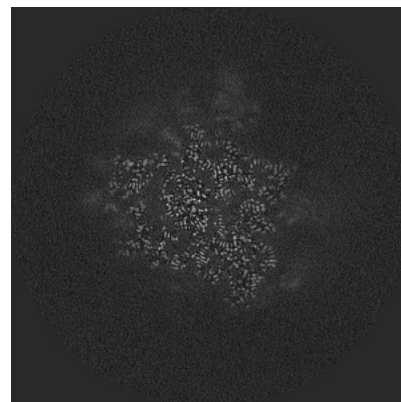
6.2.2 Raw map



X Index: 265



Y Index: 265

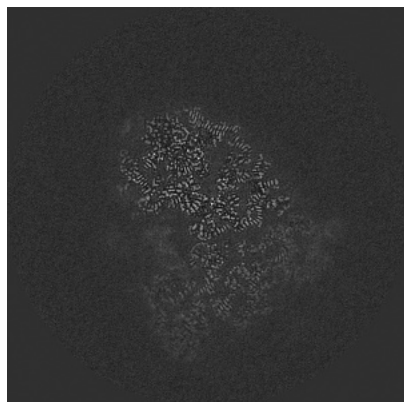


Z Index: 265

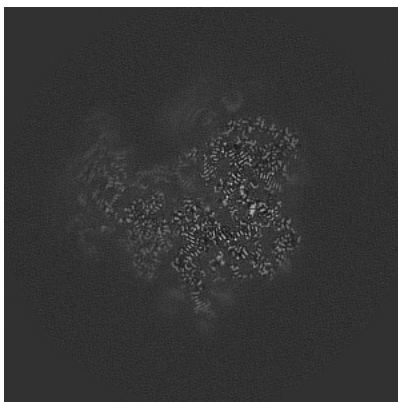
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

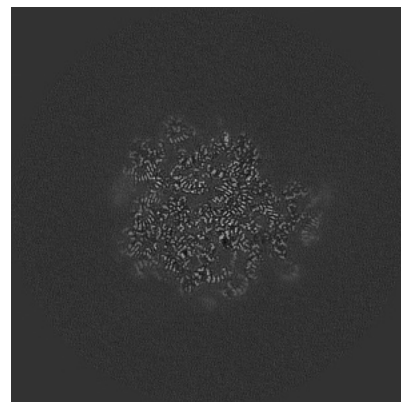
6.3.1 Primary map



X Index: 246

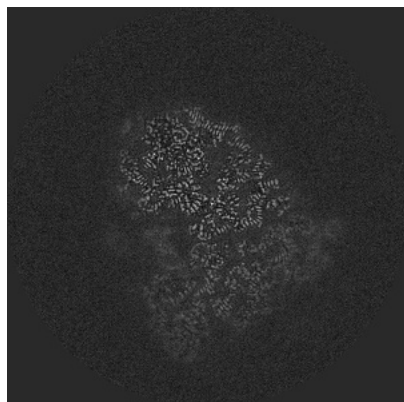


Y Index: 266

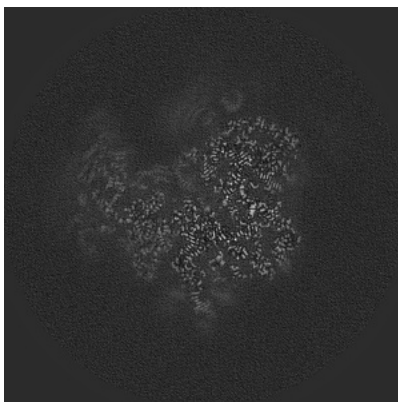


Z Index: 304

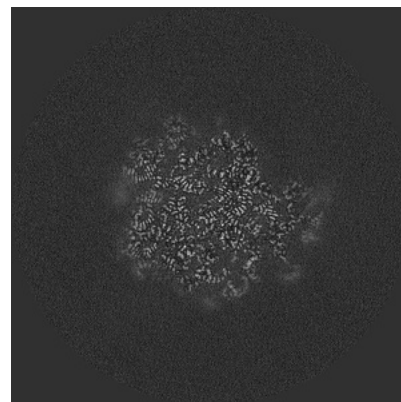
6.3.2 Raw map



X Index: 246



Y Index: 266

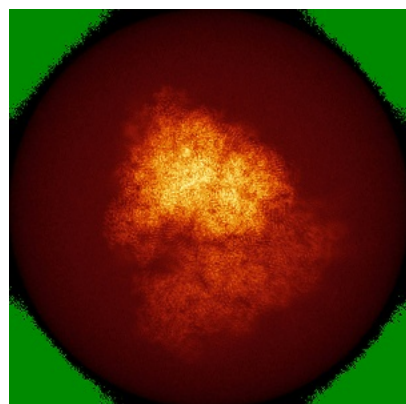


Z Index: 303

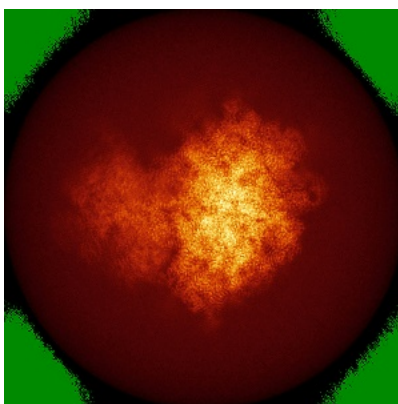
The images above show the largest variance slices of the map in three orthogonal directions.

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

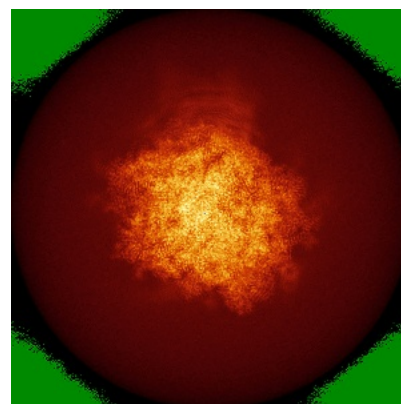
6.4.1 Primary map



X

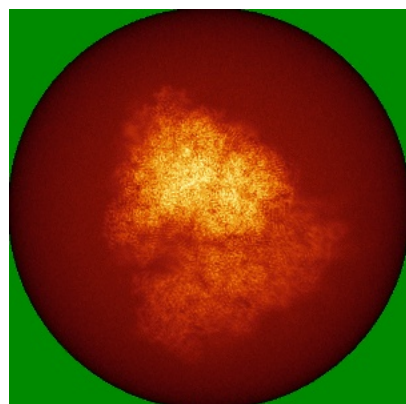


Y

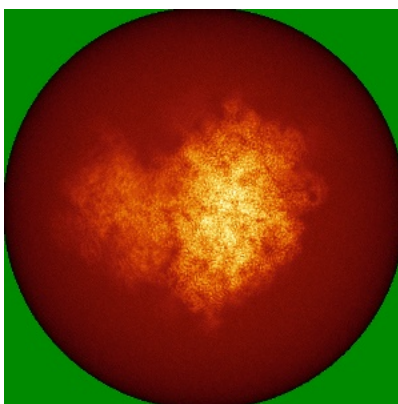


Z

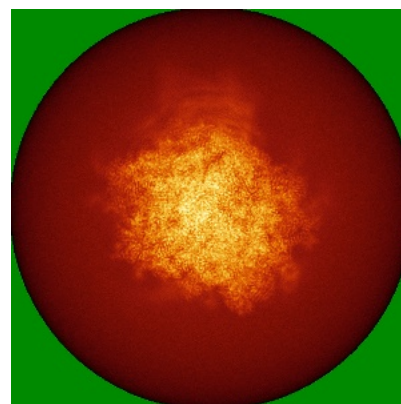
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0197. 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.

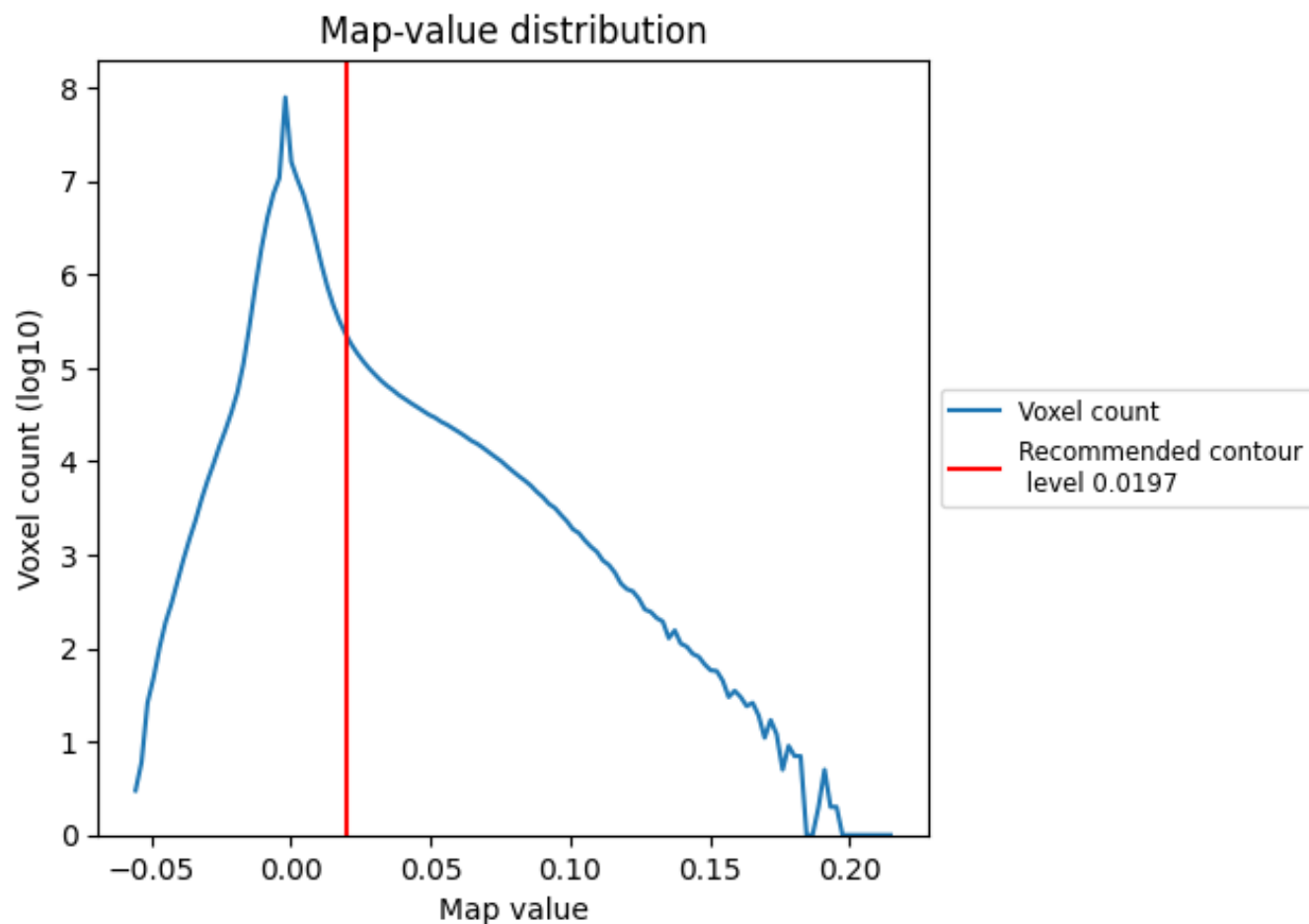
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

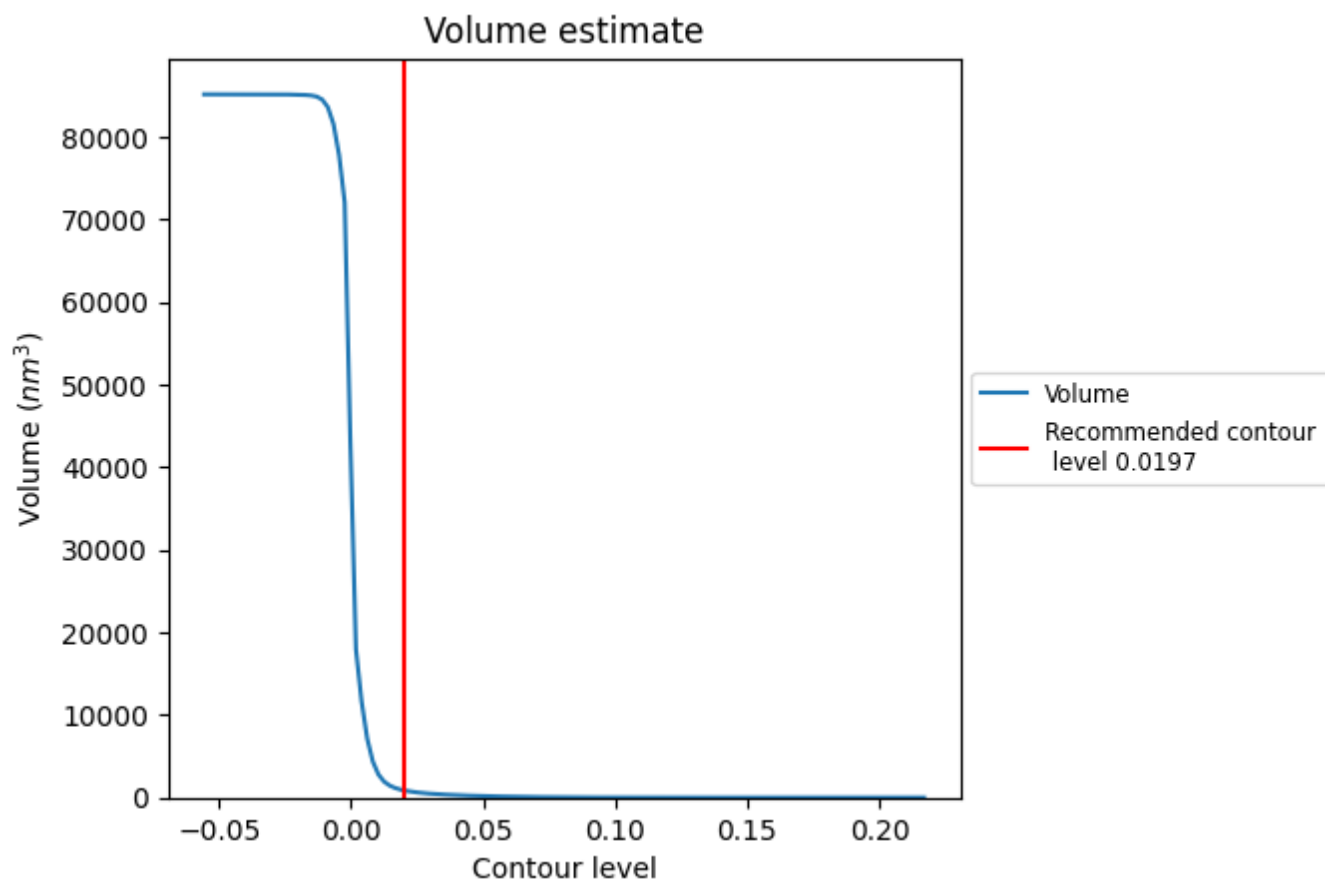
This section contains the results of statistical analysis of the map.

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.

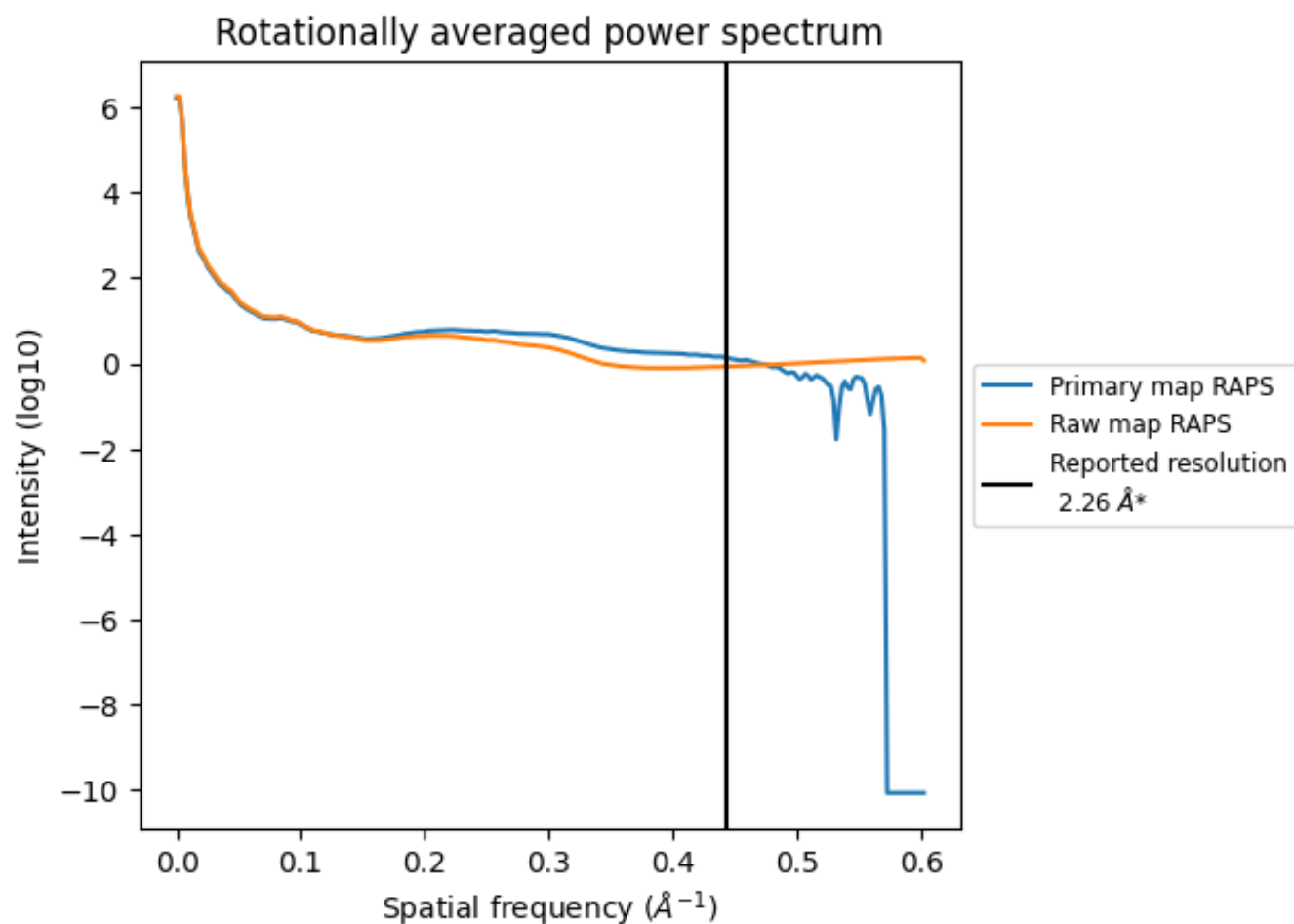
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 894 nm³; this corresponds to an approximate mass of 807 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

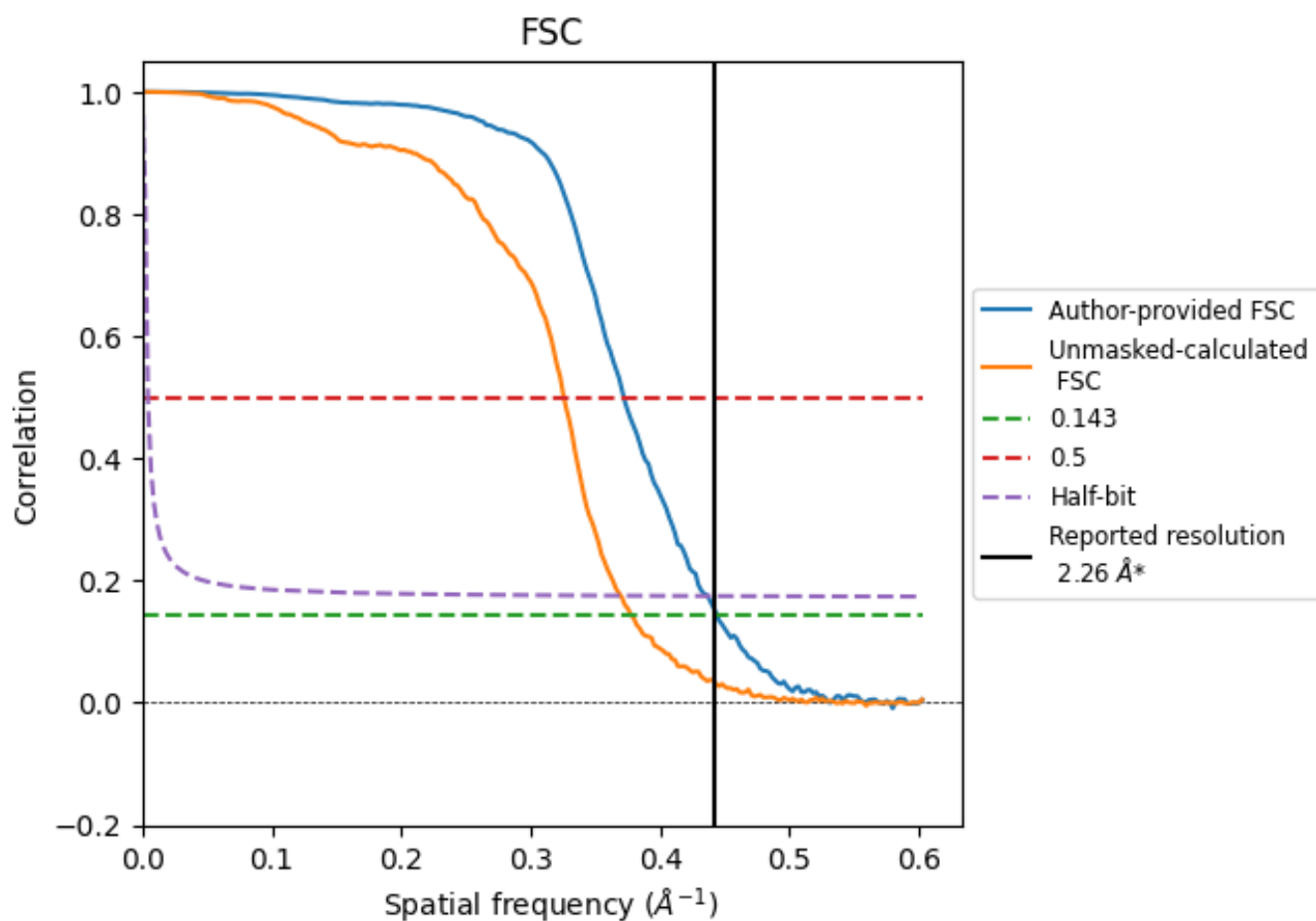


*Reported resolution corresponds to spatial frequency of 0.442 $\text{\AA}^{-1}$

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 $0.442 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

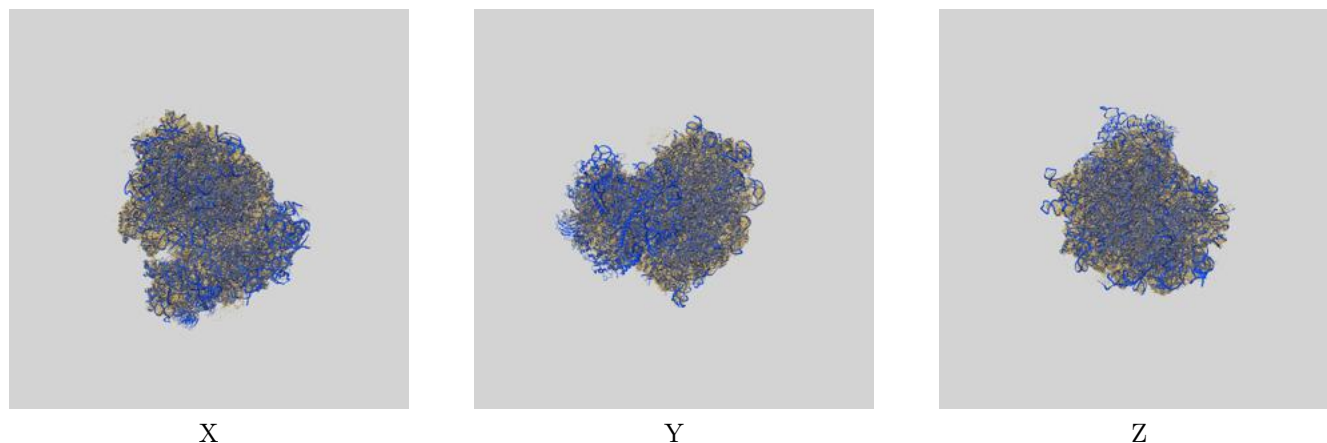
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.26	-	-
Author-provided FSC curve	2.25	2.69	2.29
Unmasked-calculated*	2.65	3.07	2.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.65 differs from the reported value 2.26 by more than 10 %

9 Map-model fit [i](#)

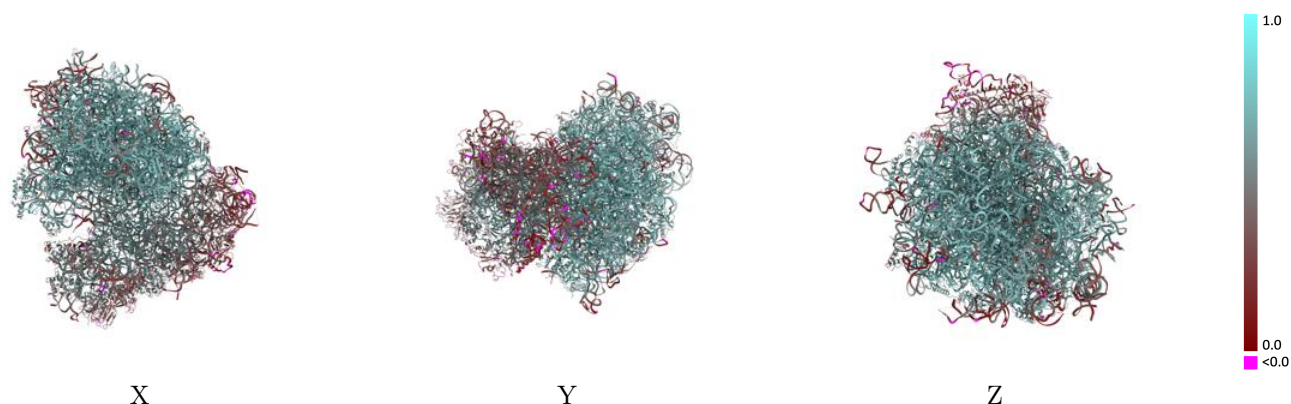
This section contains information regarding the fit between EMDB map EMD-36179 and PDB model 8JDK. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



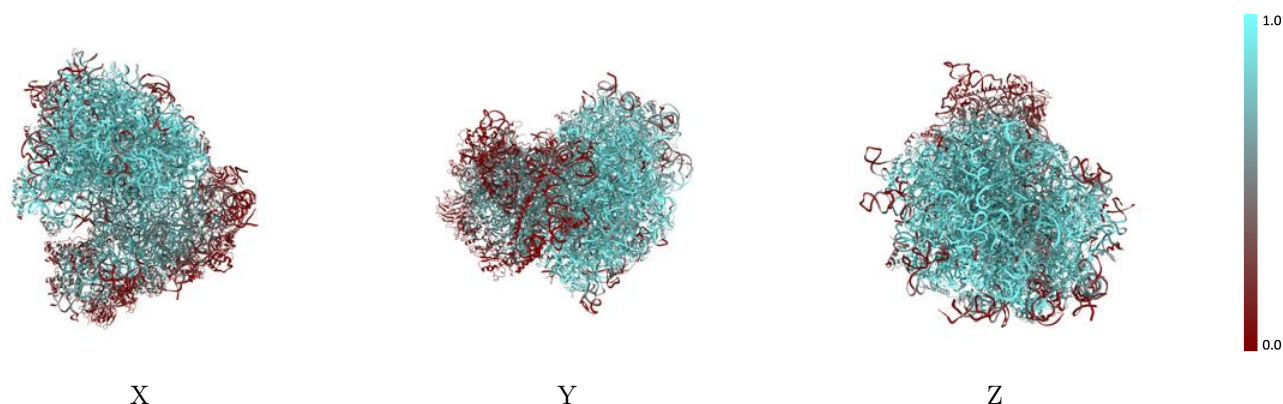
The images above show the 3D surface view of the map at the recommended contour level 0.0197 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



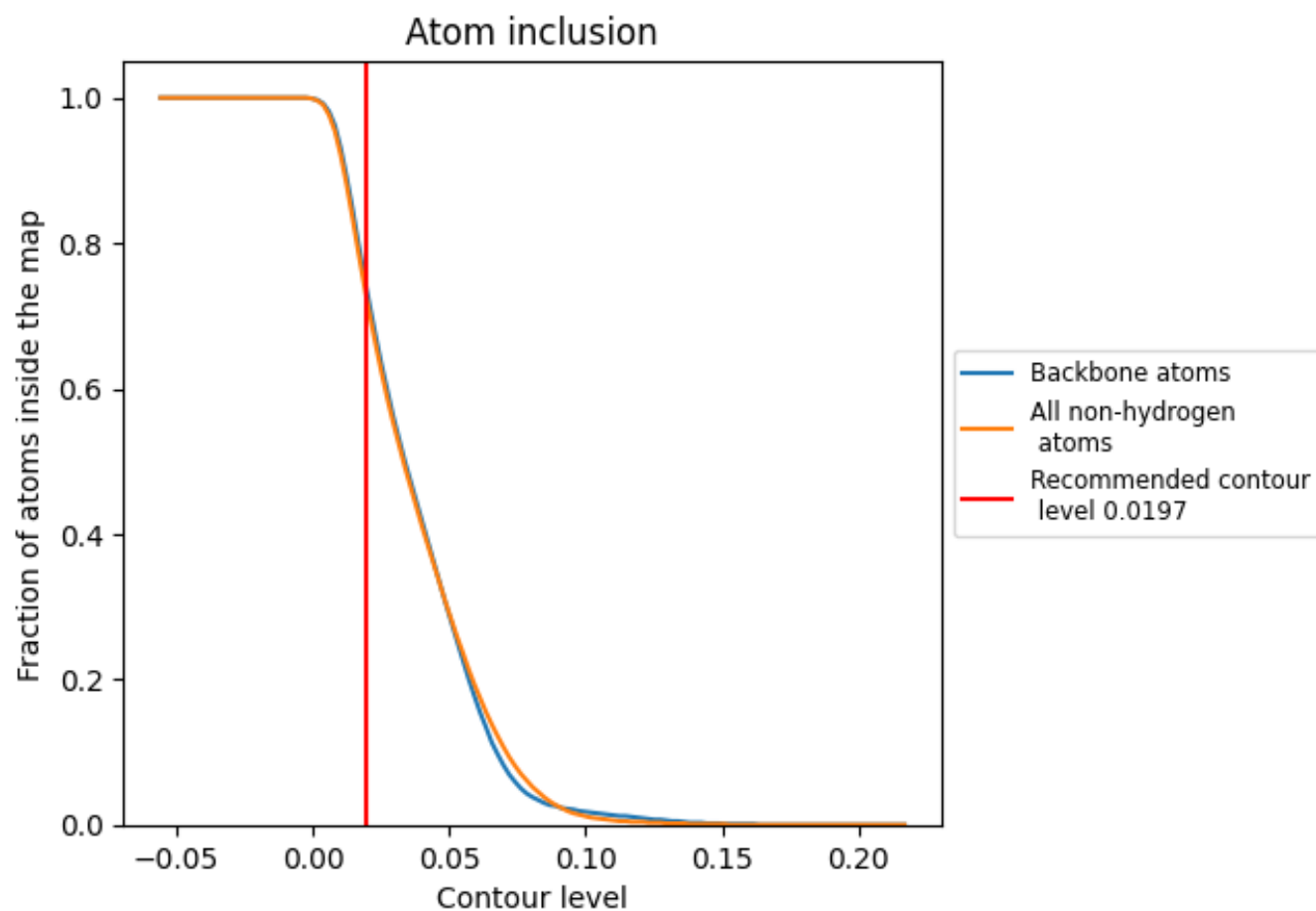
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0197).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0197) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7260	 0.5770
0	 0.3640	 0.4290
1	 0.1240	 0.2860
2	 0.4880	 0.5060
3	 0.0910	 0.2390
4	 0.1430	 0.3240
5	 0.3160	 0.3890
6	 0.1800	 0.3200
7	 0.1090	 0.3060
8	 0.4190	 0.4480
9	 0.5710	 0.5520
A	 0.6940	 0.5490
AA	 0.6370	 0.5420
AB	 0.2410	 0.3830
AC	 0.4290	 0.4810
AD	 0.2570	 0.3800
AE	 0.3610	 0.4400
AF	 0.3860	 0.4740
AG	 0.3510	 0.4170
AH	 0.3750	 0.4930
AI	 0.6210	 0.5800
AJ	 0.5650	 0.5000
AK	 0.0650	 0.2660
AL	 0.2110	 0.4050
AM	 0.6570	 0.5630
AN	 0.3360	 0.4230
AO	 0.3860	 0.4550
AP	 0.6390	 0.5390
AQ	 0.2010	 0.3240
AR	 0.0620	 0.2940
B	 0.6370	 0.5120
C	 0.4930	 0.5140
D	 0.8440	 0.6310
E	 0.9740	 0.6820
F	 0.9050	 0.6530



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Chain	Atom inclusion	Q-score
G	 0.9660	 0.7170
H	 0.9020	 0.6890
I	 0.9220	 0.6820
J	 0.7920	 0.6200
K	 0.7810	 0.6110
L	 0.9010	 0.6820
M	 0.7500	 0.6040
N	 0.8180	 0.6440
O	 0.8430	 0.6490
P	 0.6660	 0.5600
Q	 0.8220	 0.6400
R	 0.8510	 0.6410
S	 0.9740	 0.7220
T	 0.9160	 0.7040
U	 0.9020	 0.6950
V	 0.9550	 0.7130
W	 0.7870	 0.6130
X	 0.9200	 0.6860
Y	 0.8640	 0.6690
Z	 0.5380	 0.5090
a	 0.9280	 0.7030
b	 0.8840	 0.6780
c	 0.8650	 0.6590
d	 0.8540	 0.6490
e	 0.8290	 0.6360
f	 0.9260	 0.6960
g	 0.7140	 0.5710
h	 0.8370	 0.6250
i	 0.8400	 0.6580
j	 0.9480	 0.7190
k	 0.9480	 0.7000
l	 0.8700	 0.6580
m	 0.8710	 0.6530
n	 0.8170	 0.6460
o	 0.9630	 0.7150
p	 0.6530	 0.5690
q	 0.9120	 0.6750
r	 0.8220	 0.6590
s	 0.8940	 0.6830
t	 0.8390	 0.6410
u	 0.9070	 0.6810
v	 0.9090	 0.6700

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Chain	Atom inclusion	Q-score
w	 0.6580	 0.4940
x	 0.4000	 0.4960
y	 0.4980	 0.5290
z	 0.5740	 0.5410