



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 09:25 AM EDT

PDB ID : 7UCK / pdb_00007uck
EMDB ID : EMD-26445
Title : 80S translation initiation complex with ac4c(-1) mRNA and Harringtonine
Authors : Yang, R.; Arango, D.; Sturgill, D.; Oberdoerffer, S.
Deposited on : 2022-03-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

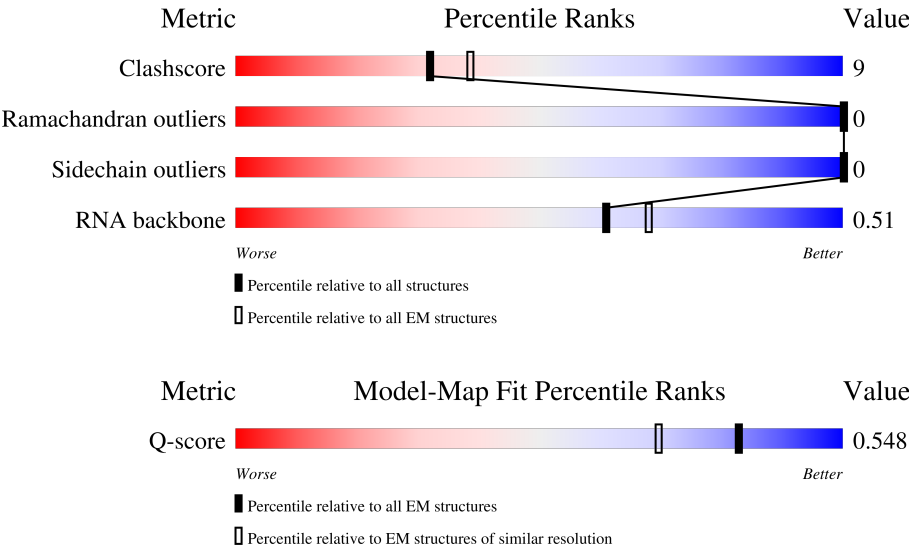
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	2	76	47% 49% 37% 9% 5%
2	1	6	67% 17% 17%
3	5	3546	10% 54% 37% 9%

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Mol	Chain	Length	Quality of chain
4	7	120	
5	8	156	
6	9	1698	
7	A	248	
8	B	394	
9	C	360	
10	D	291	
11	E	251	
12	F	225	
13	G	234	
14	H	190	
15	I	213	
16	J	170	
17	L	210	
18	M	138	
19	N	203	
20	O	199	
21	P	153	
22	Q	187	
23	R	180	
24	S	176	
25	T	159	
26	U	98	
27	V	131	
28	W	121	

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Mol	Chain	Length	Quality of chain
29	X	118	
30	Y	134	
31	Z	135	
32	a	147	
33	b	116	
34	c	98	
35	d	107	
36	e	128	
37	f	109	
38	g	114	
39	h	122	
40	i	102	
41	j	86	
42	k	69	
43	l	50	
44	m	51	
45	n	25	
46	o	103	
47	p	91	
48	r	124	
49	AA	217	
50	BB	213	
51	CC	221	
52	DD	228	
53	EE	262	

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Mol	Chain	Length	Quality of chain
54	FF	191	
55	GG	237	
56	HH	189	
57	II	206	
58	JJ	185	
59	KK	96	
60	LL	151	
61	NN	149	
62	OO	136	
63	PP	120	
64	QQ	142	
65	RR	132	
66	SS	144	
67	TT	141	
68	UU	100	
69	VV	83	
70	WW	129	
71	XX	141	
72	YY	124	
73	ZZ	75	
74	Aa	101	
75	Bb	83	
76	Cc	62	
77	Dd	55	
78	Ee	55	

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Mol	Chain	Length	Quality of chain
79	G _g	313	59% 65% 35%

2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 210046 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 P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	72	Total	C	N	O	P	0	0
			1552	694	289	498	71		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	6	Total	C	N	O	P	0	0
			133	60	25	42	6		

- Molecule 3 is a RNA chain called 28s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	3546	Total	C	N	O	P	0	0
			76153	33978	13919	24710	3546		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	2	U	N	conflict	GB X06789.1
7	36	C	N	conflict	GB X06789.1
7	102	U	N	conflict	GB X06789.1
7	112	U	N	conflict	GB X06789.1
7	114	U	N	conflict	GB X06789.1
7	119	U	C	conflict	GB X06789.1
7	120	U	N	conflict	GB X06789.1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	151	Total	C	N	O	P	0	0
			3209	1433	564	1062	150		

- Molecule 6 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	1698	Total	C	N	O	P	0	0
			36291	16217	6509	11868	1697		

- Molecule 7 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 8 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 9 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	360	Total	C	N	O	S	0	0
			2870	1806	575	475	14		

- Molecule 10 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	291	Total	C	N	O	S	0	0
			2381	1506	436	425	14		

- Molecule 11 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 12 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	227	Total	C	N	O	S	0	0
			1837	1172	354	307	4		

- Molecule 14 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 15 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 16 is a protein called 60S ribosomal protein L11.

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

- Molecule 17 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ILE	-	insertion	UNP G1TPV0
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0

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Chain	Residue	Modelled	Actual	Comment	Reference
L	52	ALA	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0

- Molecule 18 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 21 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 22 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 23 is a protein called 60S ribosomal protein L19.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	HIS	conflict	UNP G1TYL6
R	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 24 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	98	Total	C	N	O	S	0	0
			800	514	139	145	2		

- Molecule 27 is a protein called 60S ribosomal protein L23.

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

- Molecule 28 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 30 is a protein called 60S ribosomal protein L26.

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

- Molecule 31 is a protein called 60S ribosomal protein L27.

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

- Molecule 32 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 33 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 35 is a protein called 60S ribosomal protein L31.

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

- Molecule 36 is a protein called 60S ribosomal protein L32.

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

- Molecule 37 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 38 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 39 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 40 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 41 is a protein called 60S ribosomal protein L37.

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

- Molecule 42 is a protein called 60S ribosomal protein L38.

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

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 44 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	51	Total	C	N	O	S	0	0
			420	261	88	65	6		

- Molecule 45 is a protein called eL41.

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

- Molecule 46 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 47 is a protein called 60S ribosomal protein L37a.

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

- Molecule 48 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 49 is a protein called 40S_SA_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AA	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	CC	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	73	MET	VAL	conflict	UNP G1TUT9
CC	101	SER	ALA	conflict	UNP G1TUT9
CC	119	GLY	ALA	conflict	UNP G1TUT9
CC	194	ARG	HIS	conflict	UNP G1TUT9
CC	215	MET	LEU	conflict	UNP G1TUT9
CC	227	ARG	TRP	conflict	UNP G1TUT9
CC	228	GLY	SER	conflict	UNP G1TUT9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	DD	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 54 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	FF	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	GG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	HH	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	II	203	Total	C	N	O	S	0	0
			1668	1047	328	288	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	JJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
59	KK	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	LL	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	NN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
62	OO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	PP	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
64	QQ	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	RR	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
67	TT	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
68	UU	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 69 is a protein called eS21.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VV	3	ASN	SER	conflict	UNP G1TM82
VV	4	ASP	ASN	conflict	UNP G1TM82
VV	33	GLN	PRO	conflict	UNP G1TM82
VV	50	PHE	SER	conflict	UNP G1TM82
VV	75	ALA	SER	conflict	UNP G1TM82
VV	76	ASP	HIS	conflict	UNP G1TM82
VV	81	LYS	GLN	conflict	UNP G1TM82

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

Mol	Chain	Residues	Atoms					AltConf	Trace
70	WW	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	XX	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	YY	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
73	ZZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 74 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	28	ARG	CYS	conflict	UNP G1TFE8
Aa	56	ALA	VAL	conflict	UNP G1TFE8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Cc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Dd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ee	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

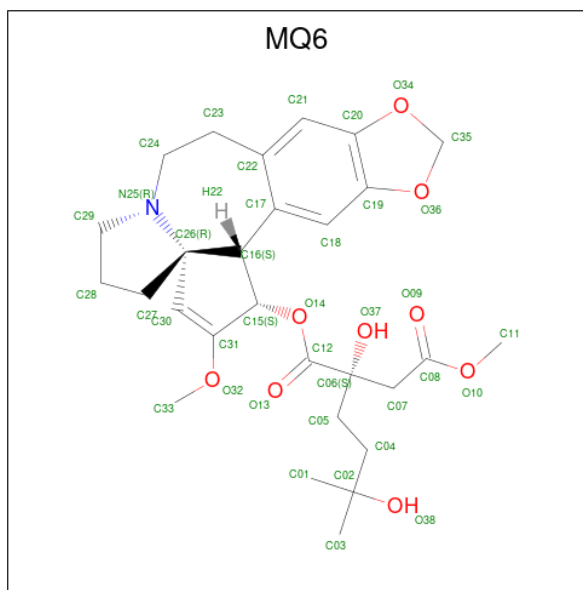
- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Gg	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	5	196	Total	Mg	0
			196	196	
80	7	7	Total	Mg	0
			7	7	
80	8	8	Total	Mg	0
			8	8	
80	9	78	Total	Mg	0
			78	78	
80	A	1	Total	Mg	0
			1	1	
80	I	1	Total	Mg	0
			1	1	
80	P	1	Total	Mg	0
			1	1	
80	V	1	Total	Mg	0
			1	1	
80	a	1	Total	Mg	0
			1	1	
80	g	1	Total	Mg	0
			1	1	
80	j	1	Total	Mg	0
			1	1	
80	LL	1	Total	Mg	0
			1	1	

- Molecule 81 is Harringtonine (CCD ID: MQ6) (formula: $C_{28}H_{37}NO_9$).



Mol	Chain	Residues	Atoms				AltConf
81	5	1	Total	C	N	O	0
			38	28	1	9	

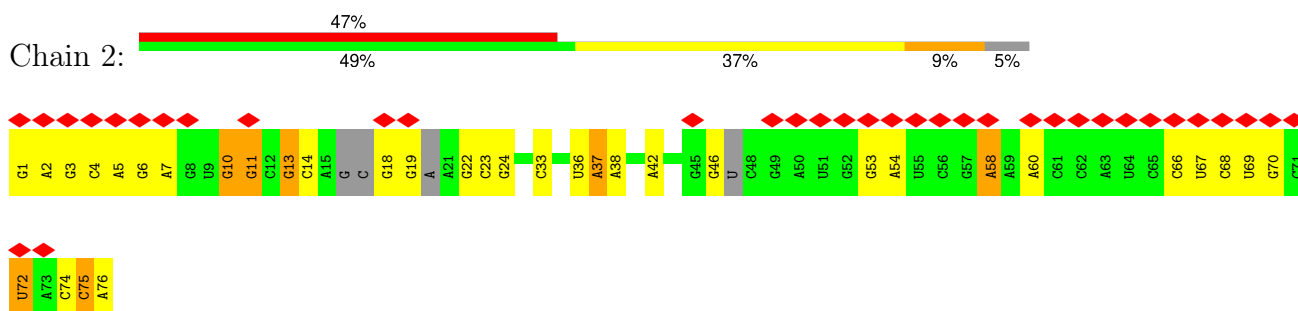
- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
82	g	1	Total	Zn	0
			1	1	
82	j	1	Total	Zn	0
			1	1	
82	m	1	Total	Zn	0
			1	1	
82	o	1	Total	Zn	0
			1	1	
82	p	1	Total	Zn	0
			1	1	
82	Aa	1	Total	Zn	0
			1	1	
82	Dd	1	Total	Zn	0
			1	1	

3 Residue-property plots

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

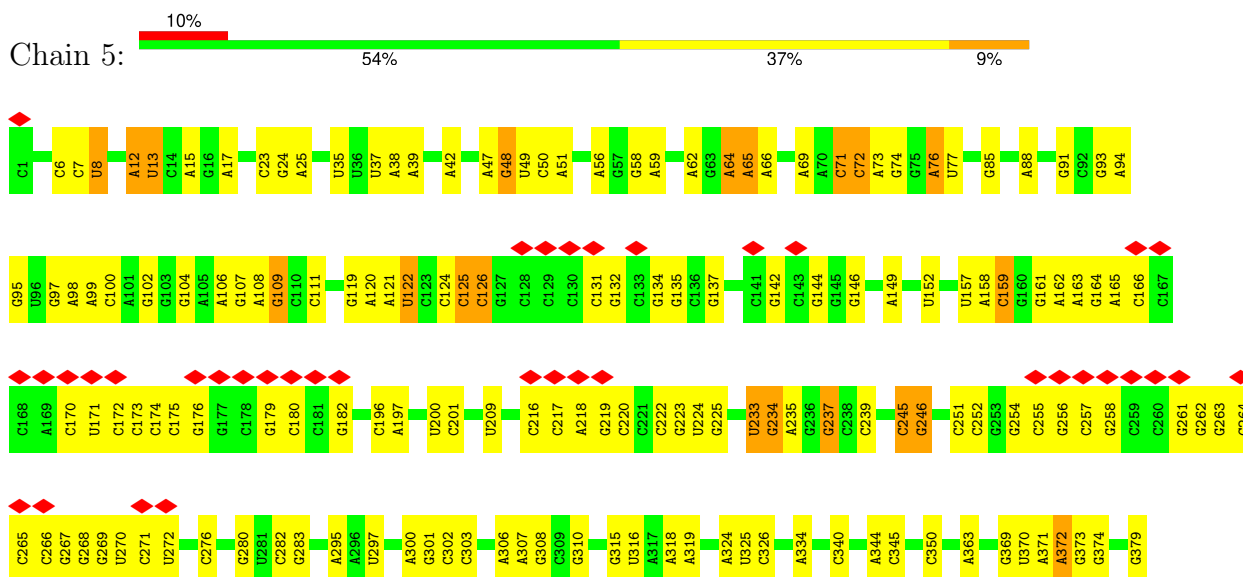
• Molecule 1: P-site tRNA

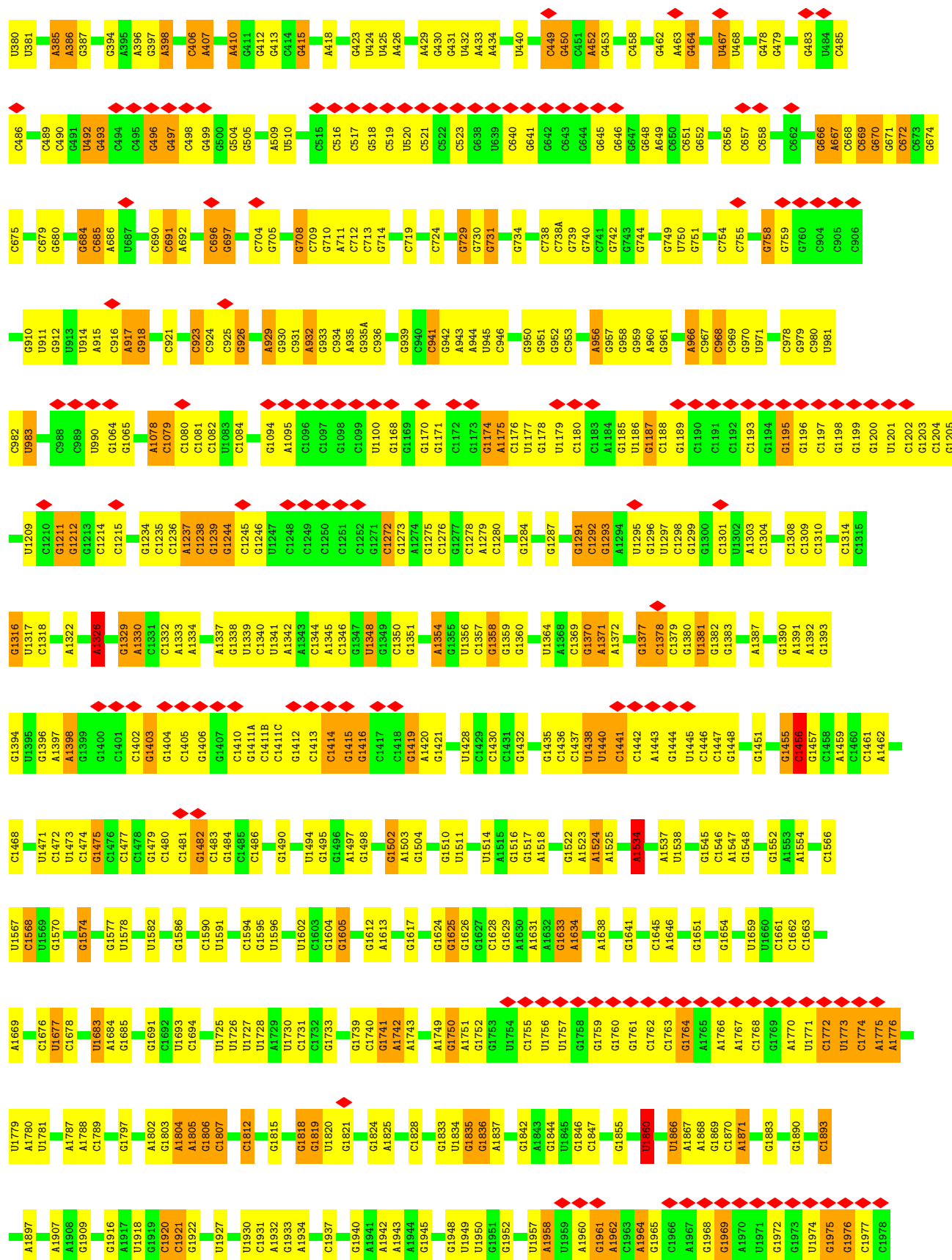


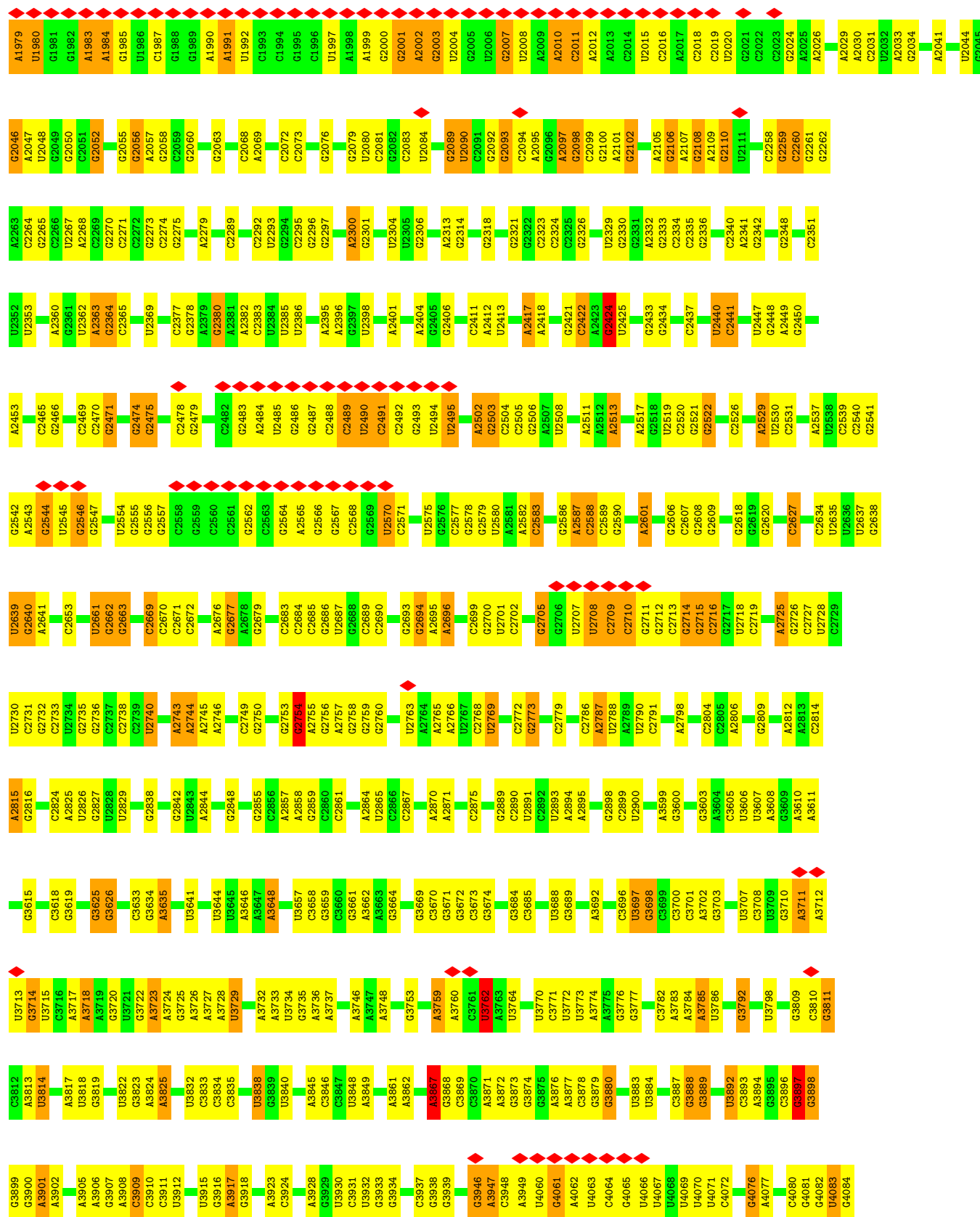
• Molecule 2: mRNA

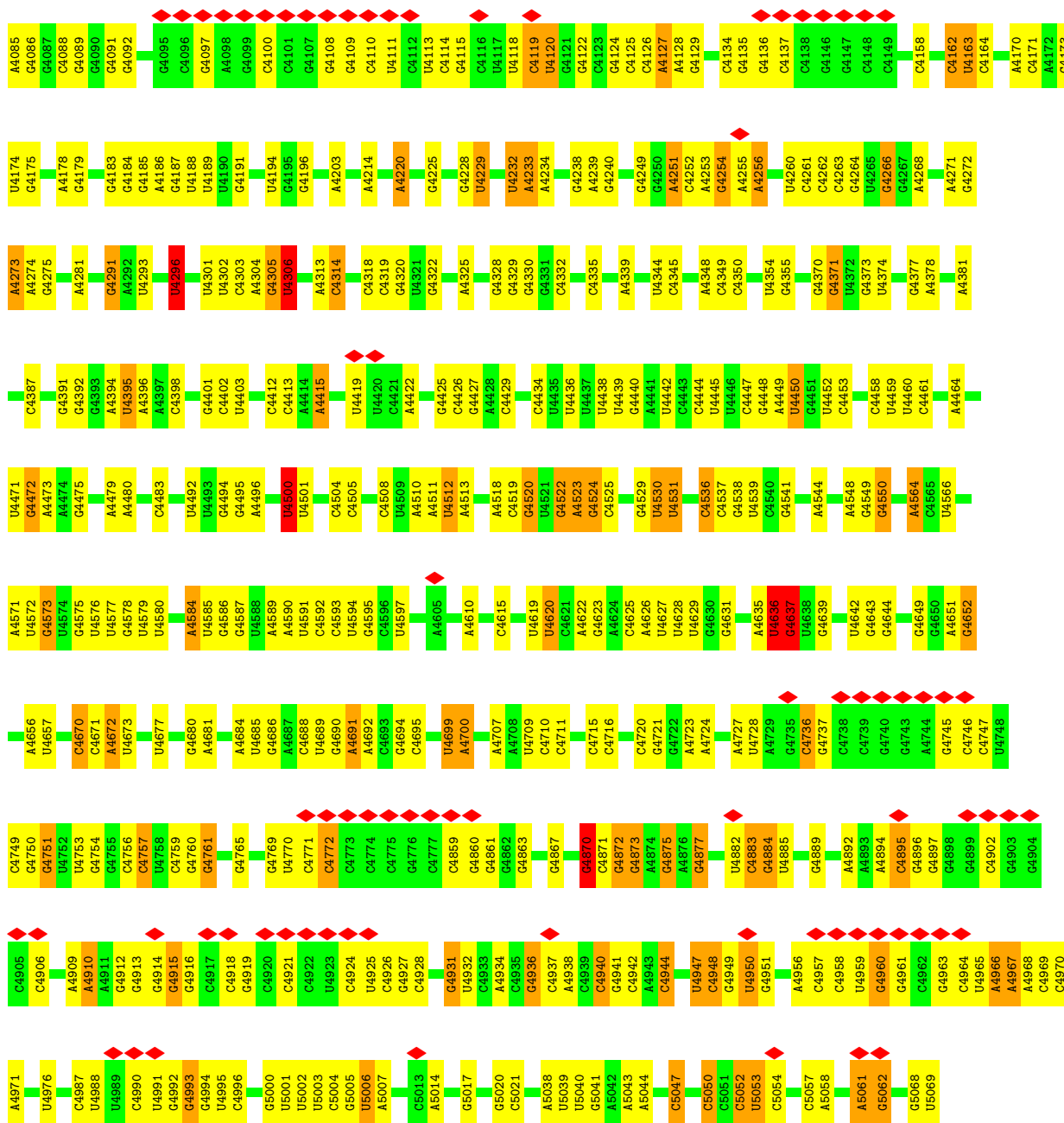


• Molecule 3: 28s rRNA

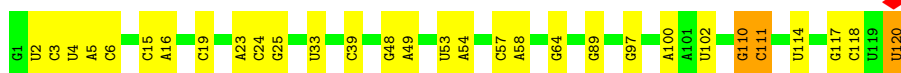
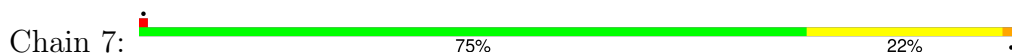






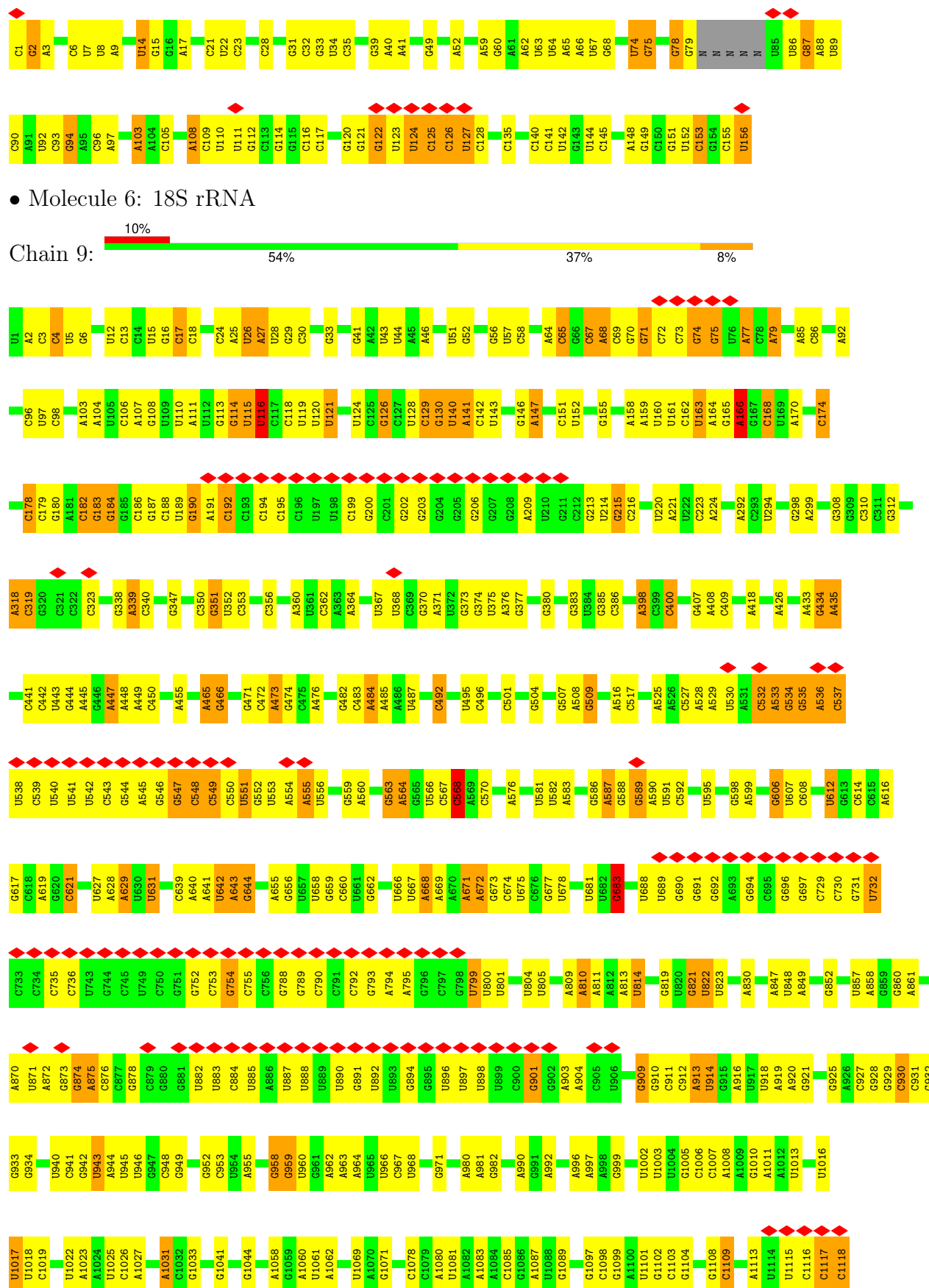


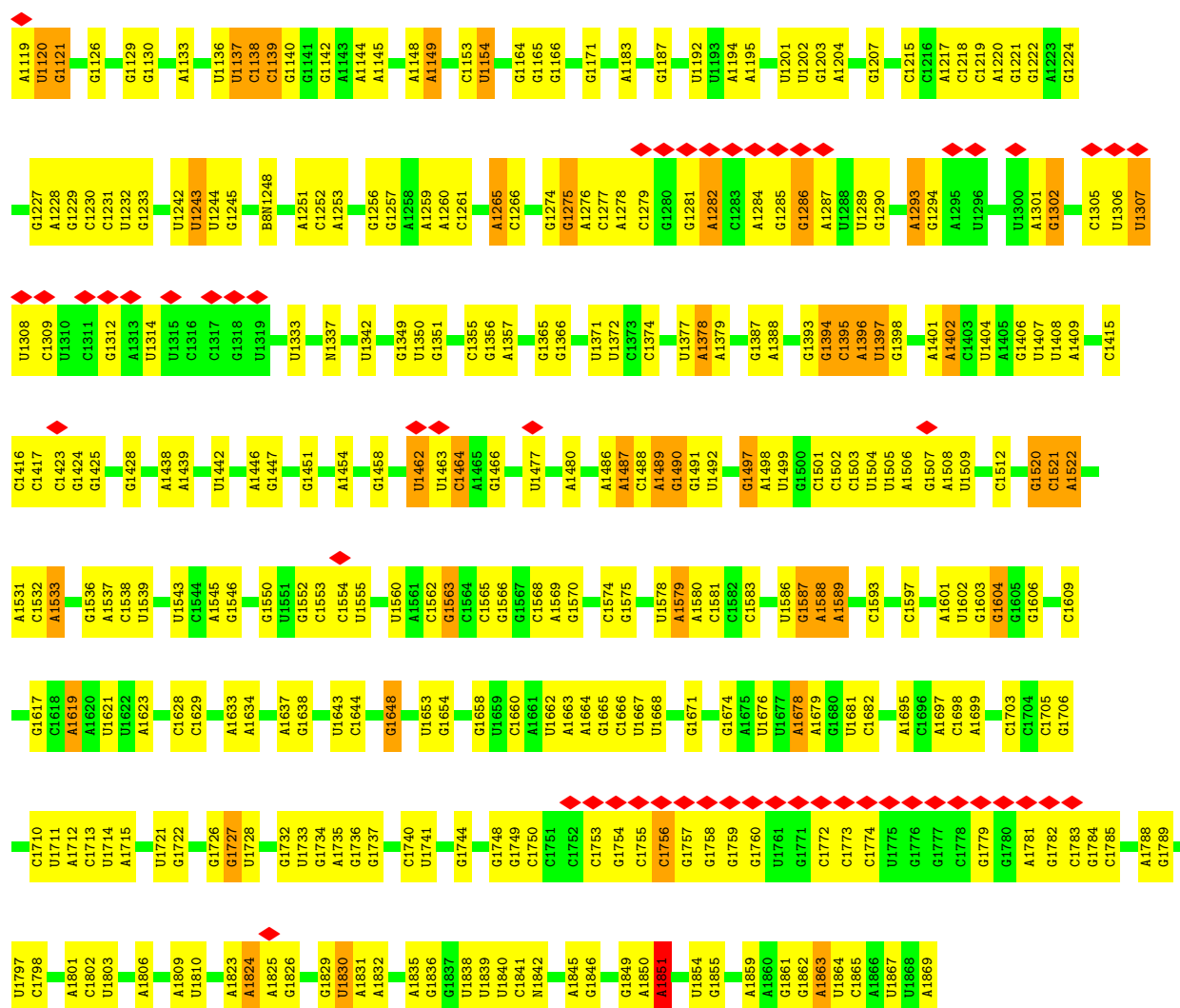
● Molecule 4: 5S rRNA



● Molecule 5: 5.8S rRNA

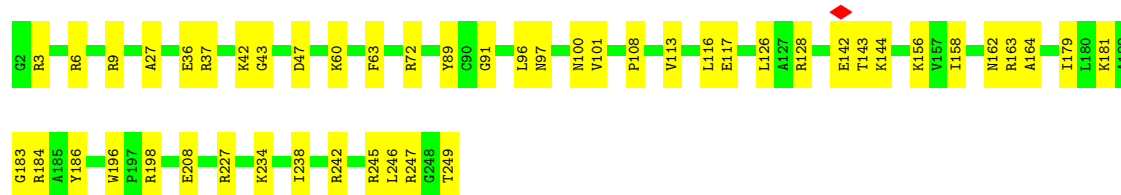






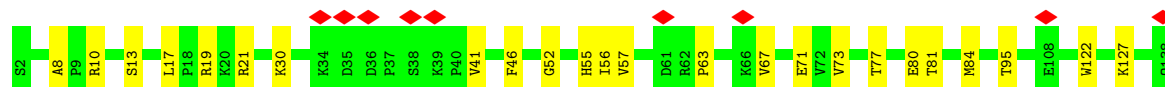
• Molecule 7: 60S ribosomal protein L8

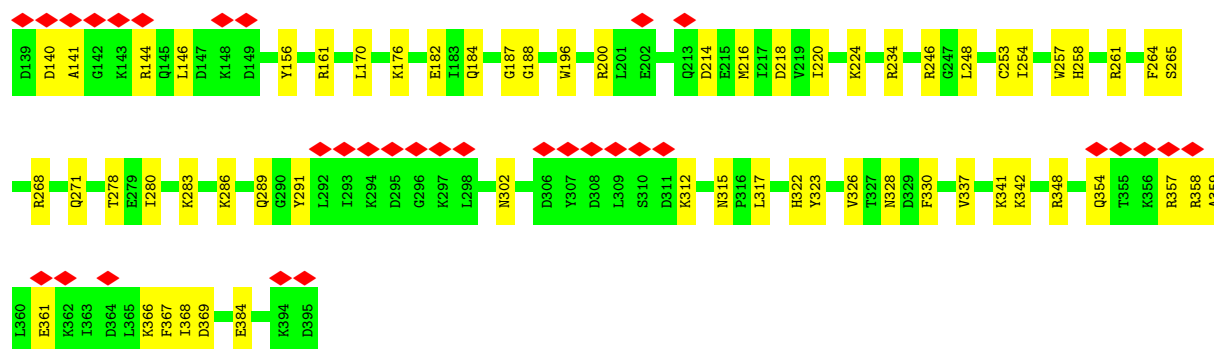
Chain A: 81% 19%



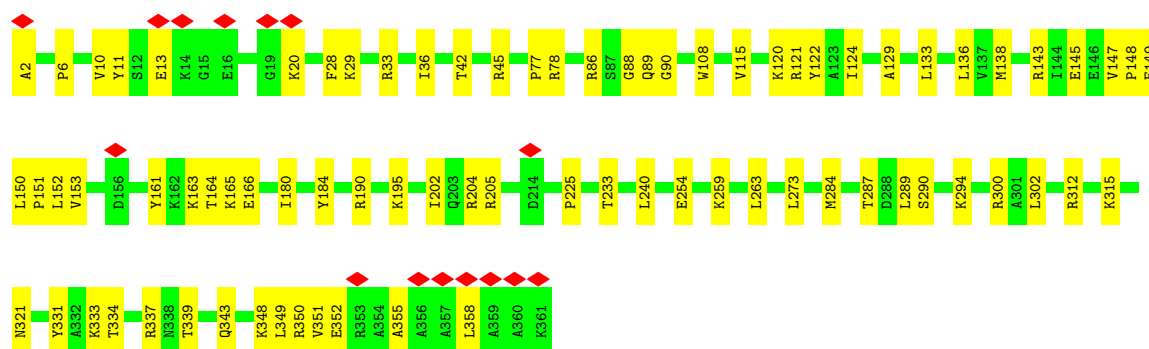
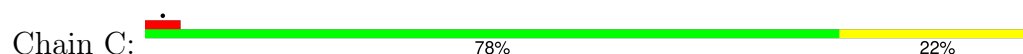
• Molecule 8: 60S ribosomal protein L3

Chain B: 11% 79% 21%

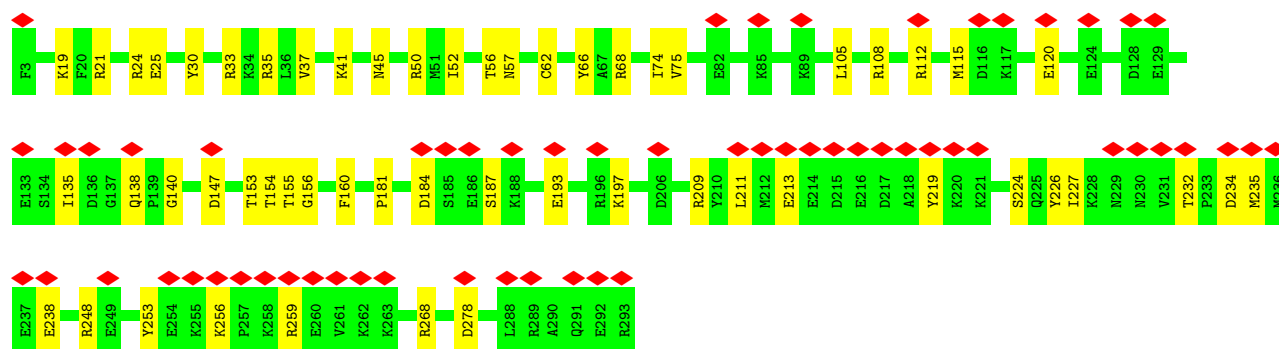
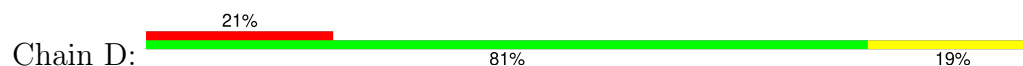




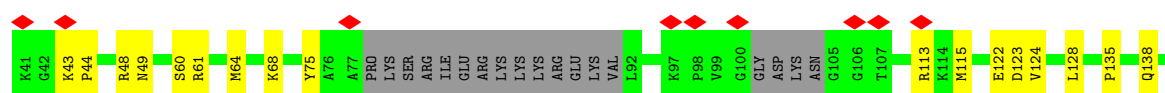
• Molecule 9: 60S ribosomal protein L4

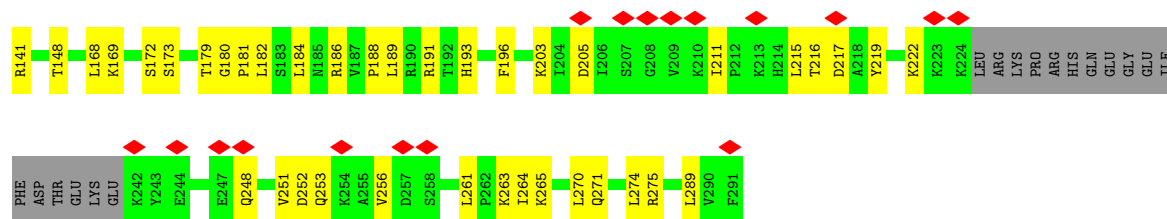


• Molecule 10: Ribosomal_L18_c domain-containing protein

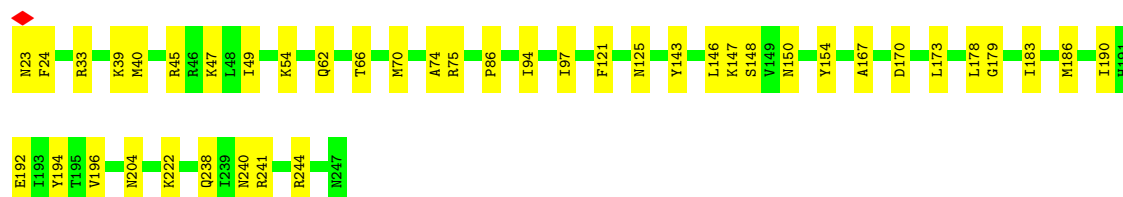
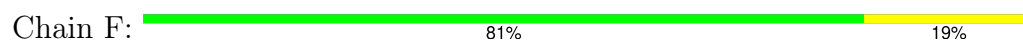


• Molecule 11: 60S ribosomal protein L6

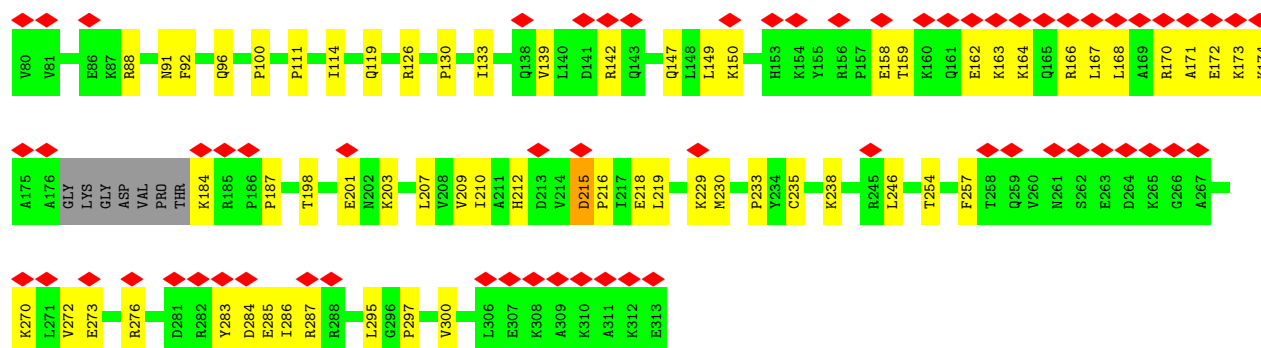




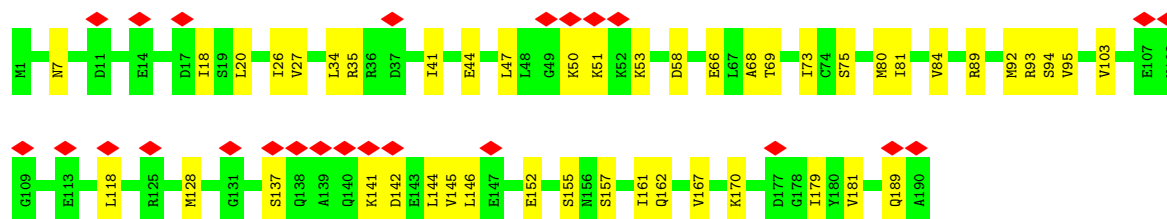
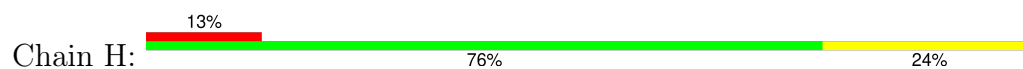
• Molecule 12: 60S ribosomal protein L7



• Molecule 13: 60S ribosomal protein L7a

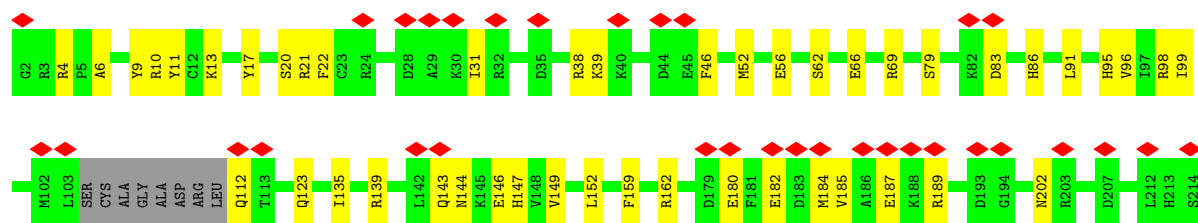


• Molecule 14: 60S ribosomal protein L9

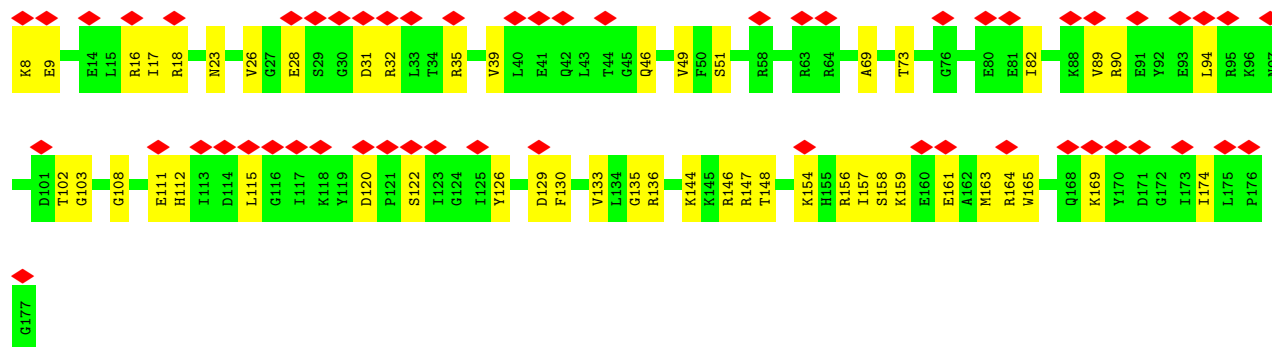


• Molecule 15: Ribosomal protein L10

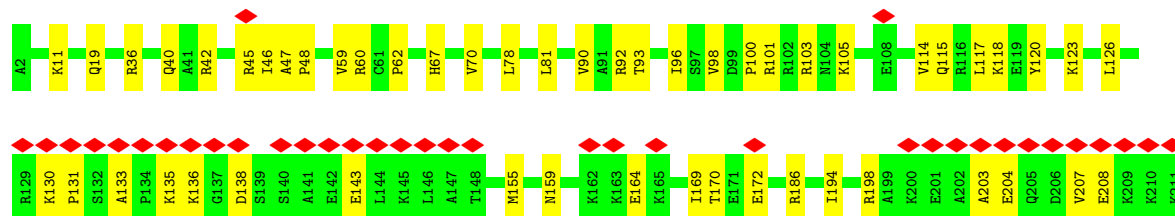
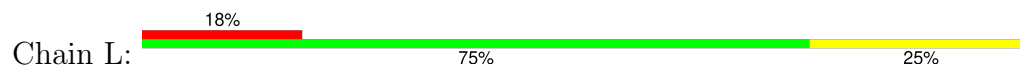




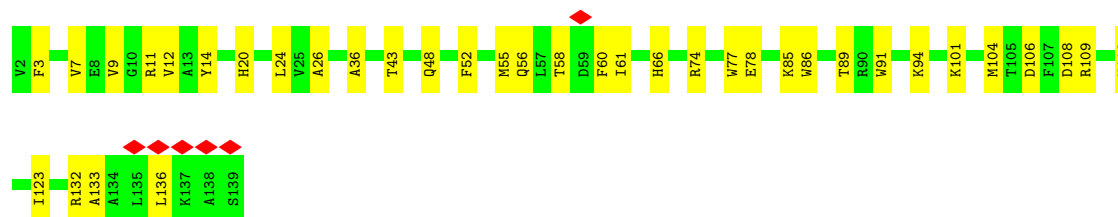
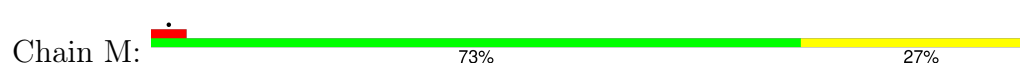
• Molecule 16: 60S ribosomal protein L11



• Molecule 17: 60S ribosomal protein L13

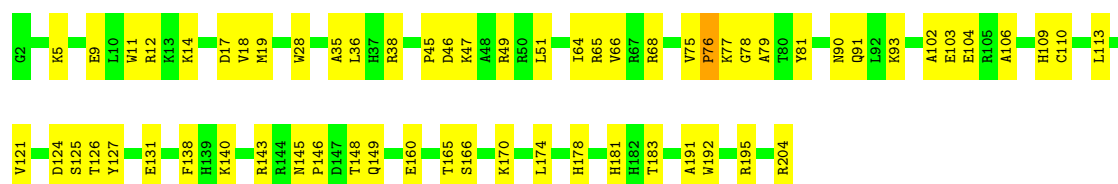


• Molecule 18: 60S ribosomal protein L14

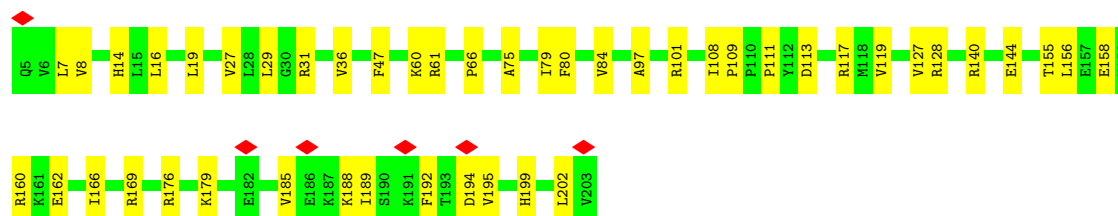
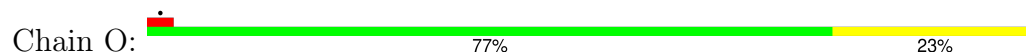


• Molecule 19: 60S ribosomal protein L15

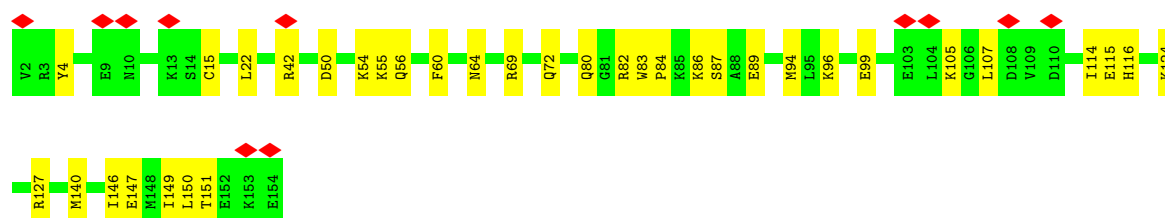
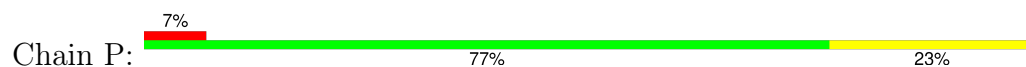




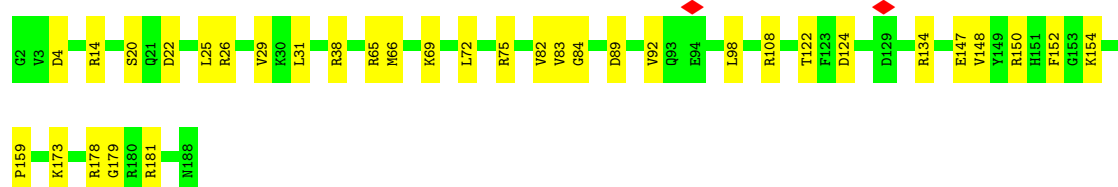
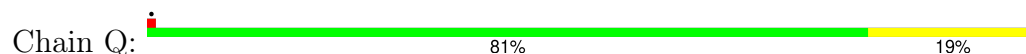
- Molecule 20: 60S ribosomal protein L13a



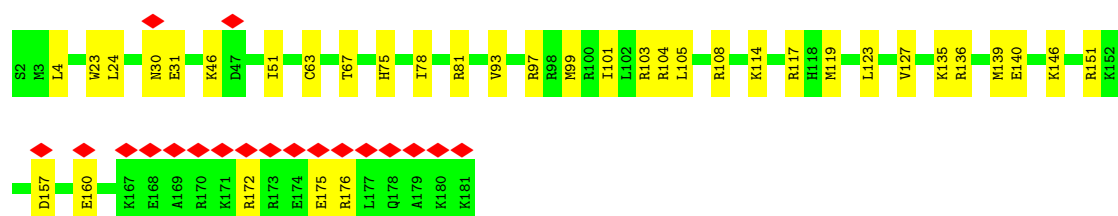
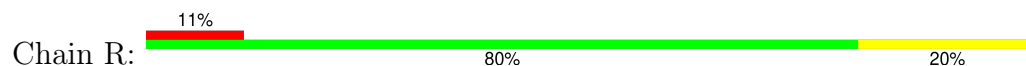
- Molecule 21: 60S ribosomal protein L17



- Molecule 22: 60S ribosomal protein L18

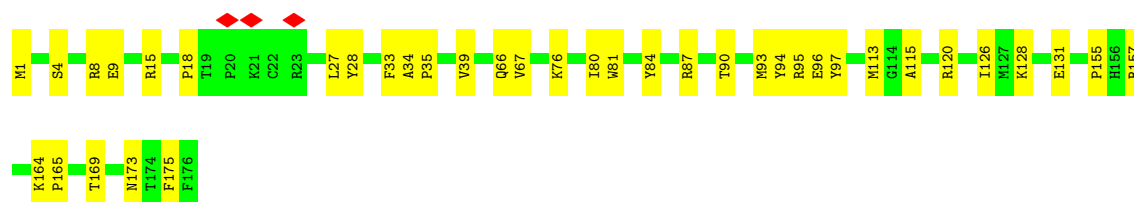


- Molecule 23: 60S ribosomal protein L19



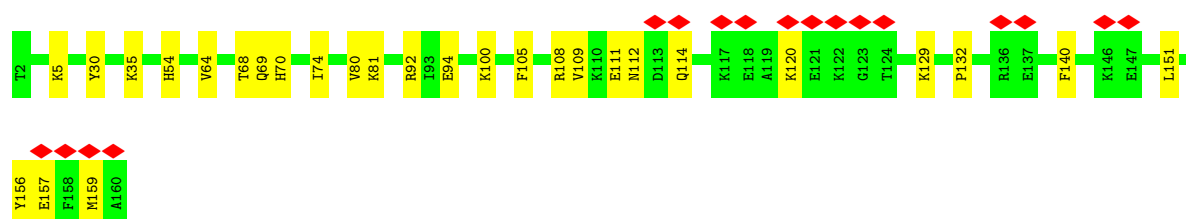
- Molecule 24: 60S ribosomal protein L18a

Chain S:  78% 22%



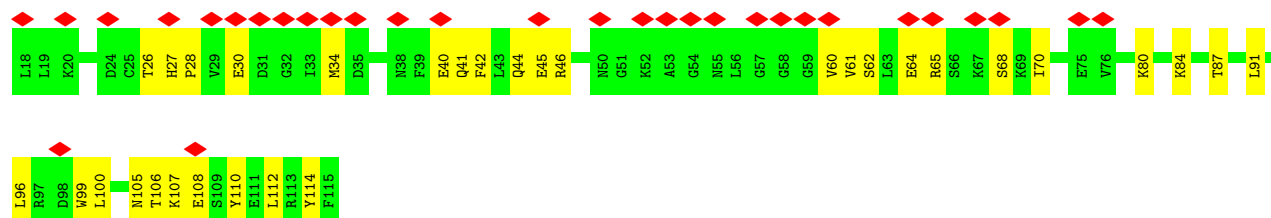
- Molecule 25: 60S ribosomal protein L21

Chain T:  11% 82% 18%



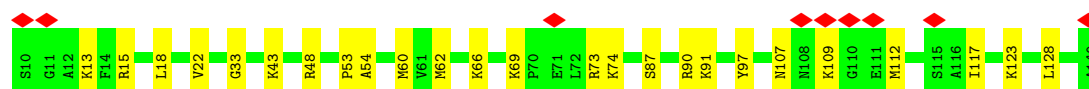
- Molecule 26: 60S ribosomal protein L22

Chain U:  32% 67% 33%



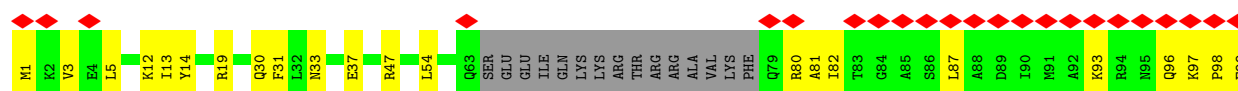
- Molecule 27: 60S ribosomal protein L23

Chain V:  7% 81% 19%



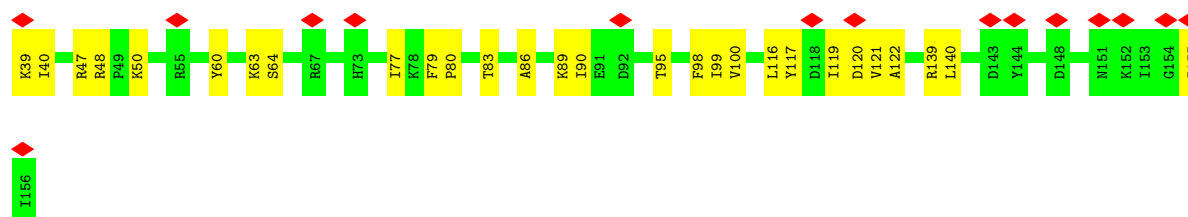
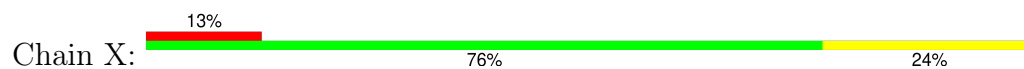
- Molecule 28: Ribosomal protein L24

Chain W:  37% 60% 28% 12%

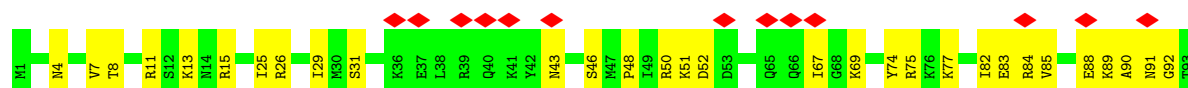




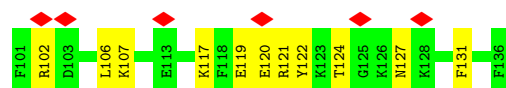
- Molecule 29: 60S ribosomal protein L23a



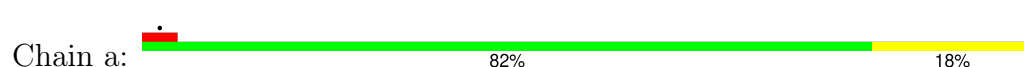
- Molecule 30: 60S ribosomal protein L26



- Molecule 31: 60S ribosomal protein L27

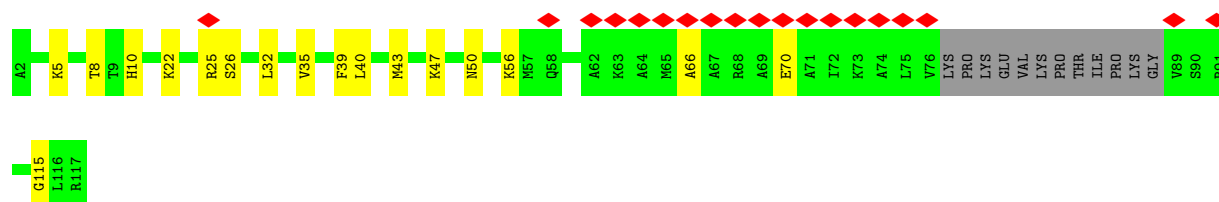


- Molecule 32: 60S ribosomal protein L27a

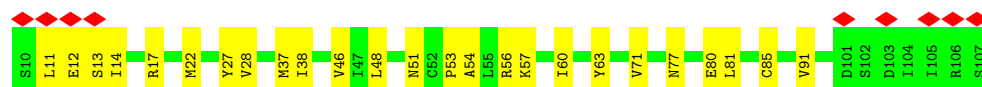
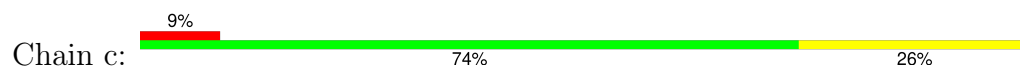


- Molecule 33: 60S ribosomal protein L29

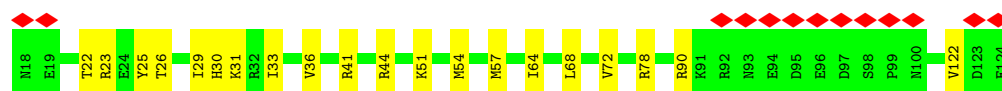
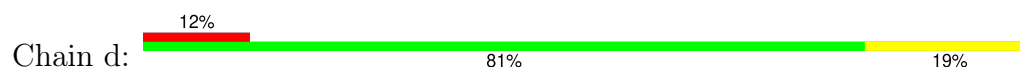




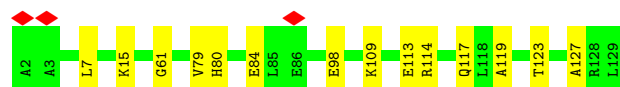
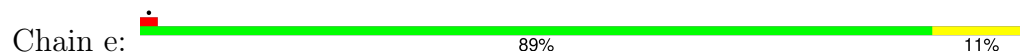
- Molecule 34: 60S ribosomal protein L30



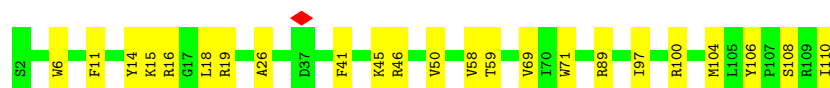
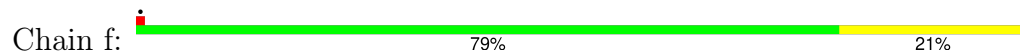
- Molecule 35: 60S ribosomal protein L31



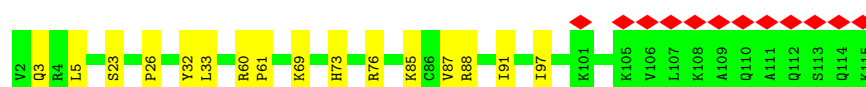
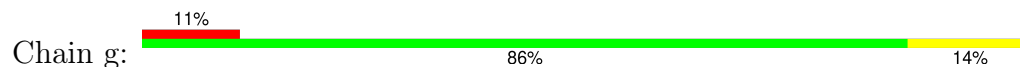
- Molecule 36: 60S ribosomal protein L32



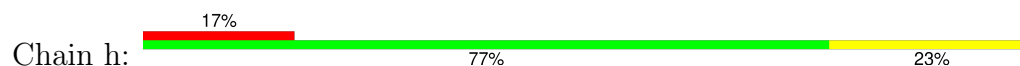
- Molecule 37: 60S ribosomal protein L35a

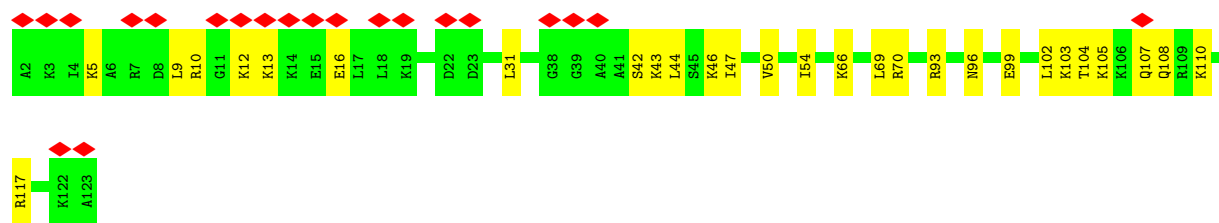


- Molecule 38: 60S ribosomal protein L34

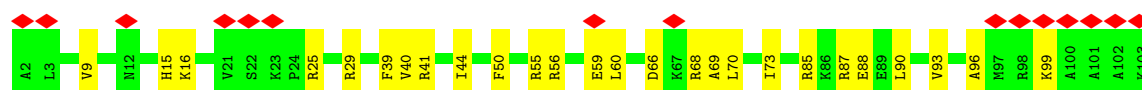
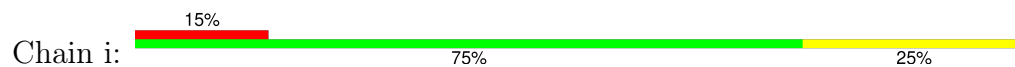


- Molecule 39: 60S ribosomal protein L35

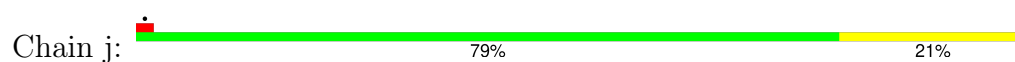




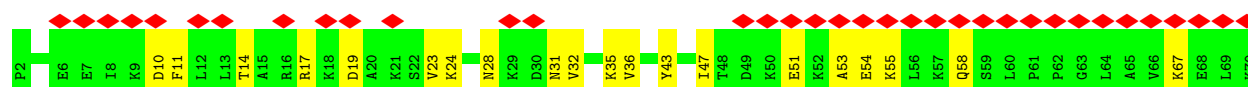
- Molecule 40: 60S ribosomal protein L36



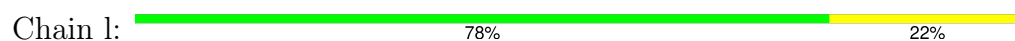
- Molecule 41: 60S ribosomal protein L37



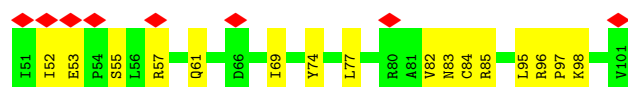
- Molecule 42: 60S ribosomal protein L38



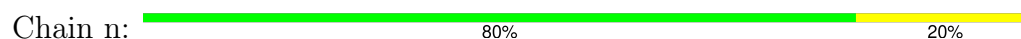
- Molecule 43: 60S ribosomal protein L39



- Molecule 44: 60S ribosomal protein L40

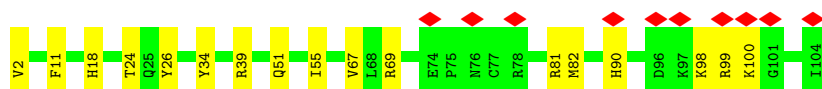
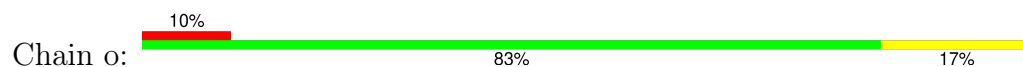


- Molecule 45: eL41

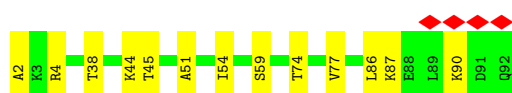
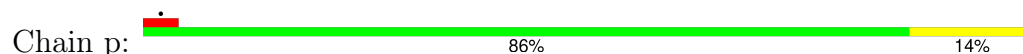




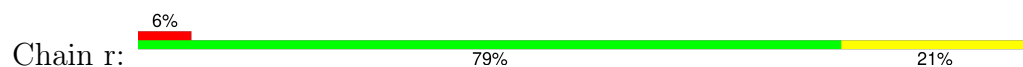
- Molecule 46: 60S ribosomal protein L36a



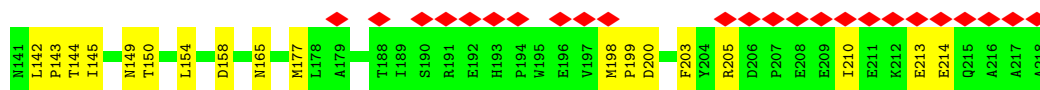
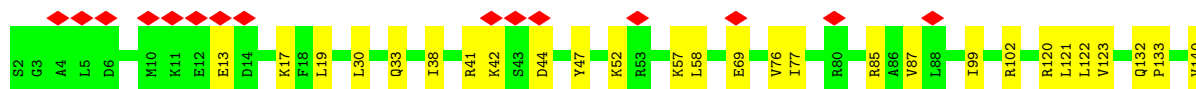
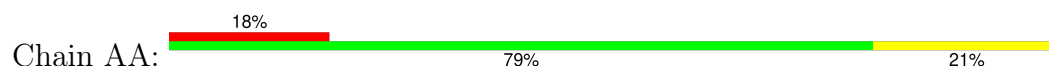
- Molecule 47: 60S ribosomal protein L37a



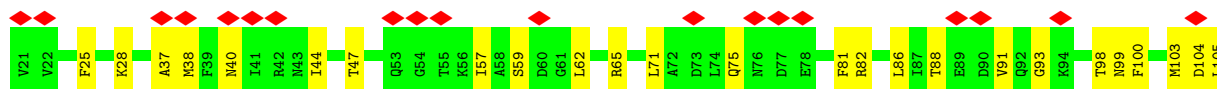
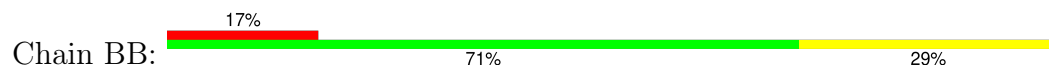
- Molecule 48: 60S ribosomal protein L28

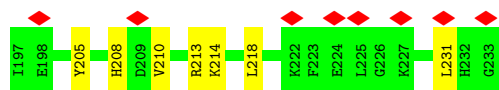


- Molecule 49: 40S_SA_C domain-containing protein

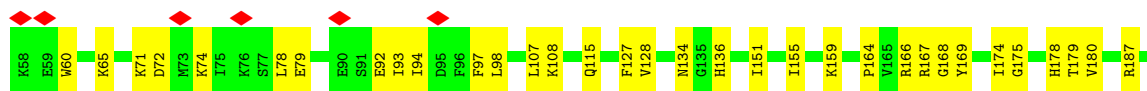
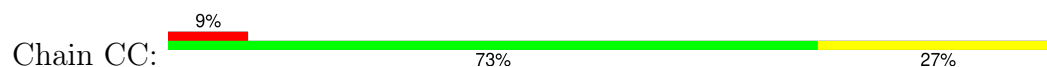


- Molecule 50: 40S ribosomal protein S3a

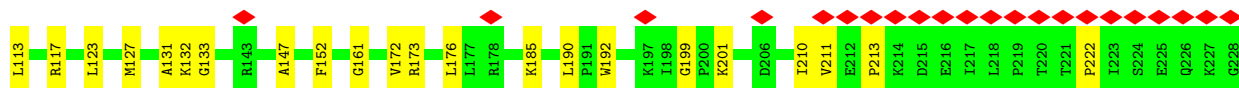
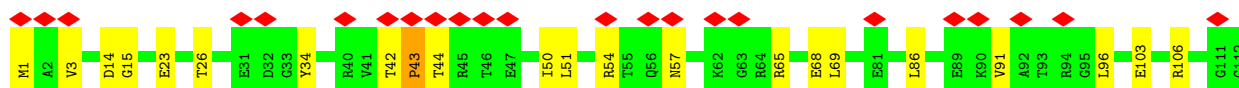
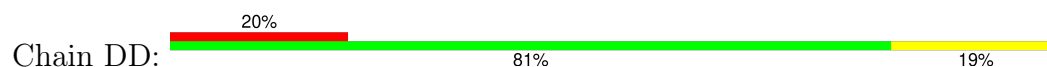




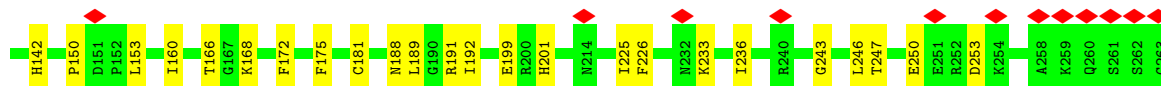
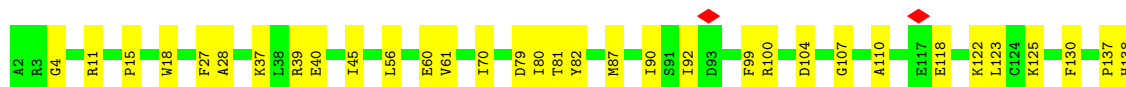
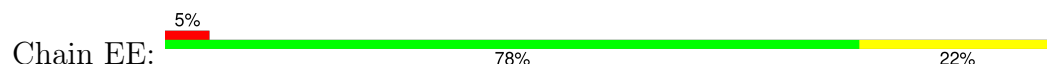
- Molecule 51: 40S ribosomal protein S2



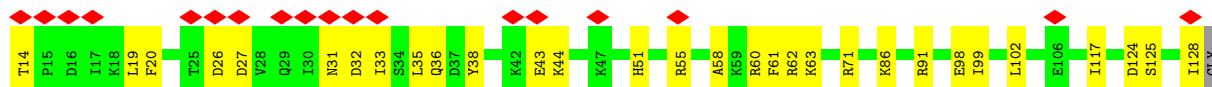
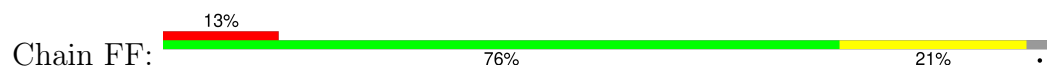
- Molecule 52: 40S ribosomal protein S3



- Molecule 53: 40S ribosomal protein S4

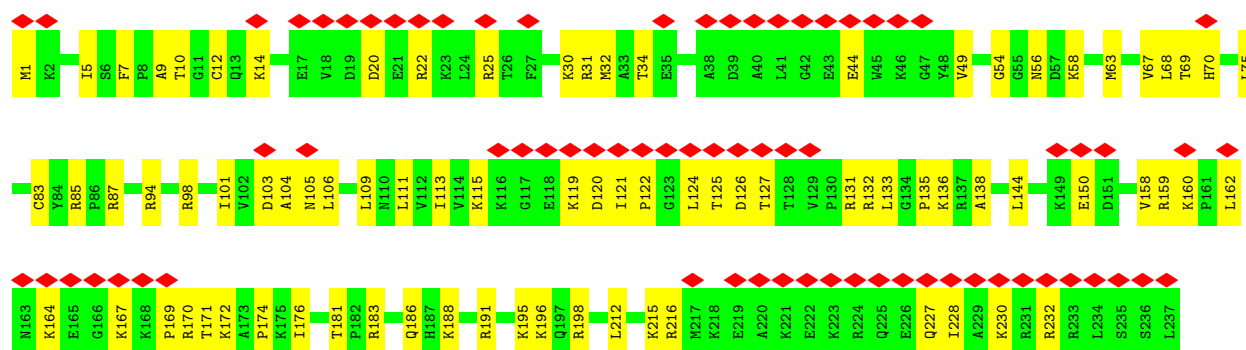


- Molecule 54: Ribosomal protein S5



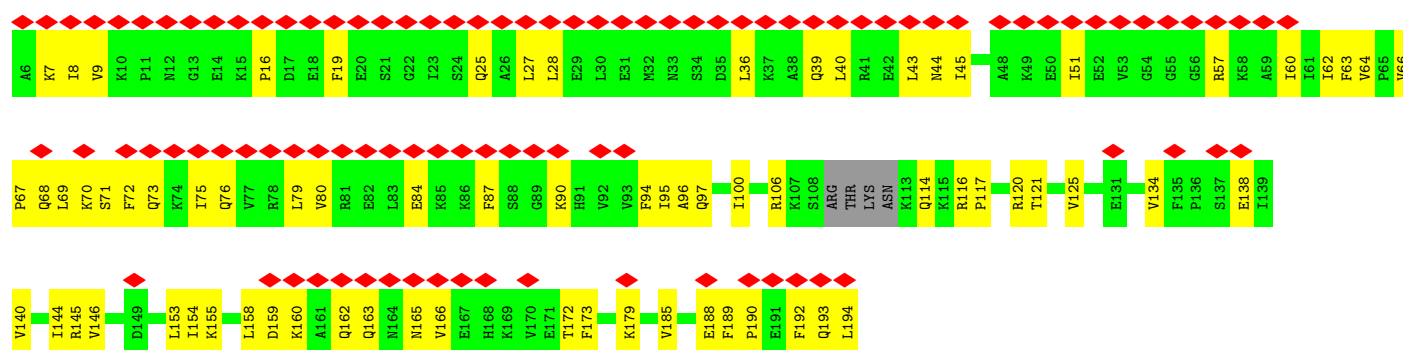
- Molecule 55: 40S ribosomal protein S6

Chain GG: 



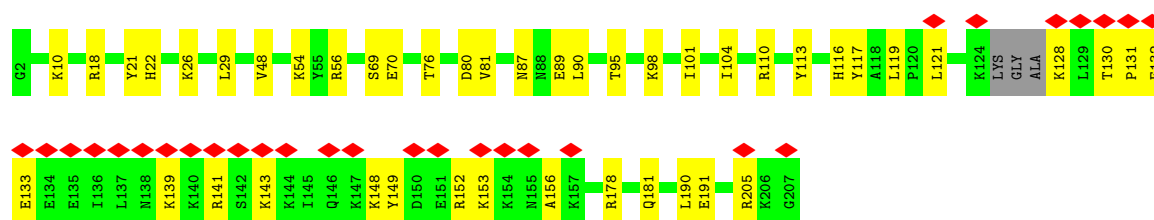
• Molecule 56: 40S ribosomal protein S7

Chain HH: 



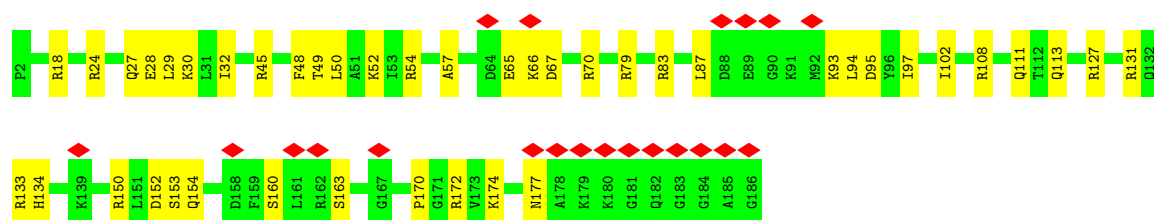
• Molecule 57: 40S ribosomal protein S8

Chain II: 

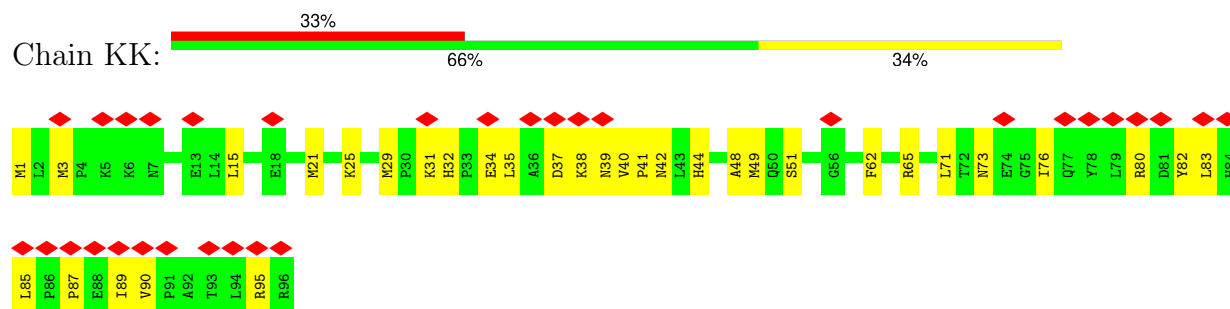


• Molecule 58: 40S ribosomal protein S9

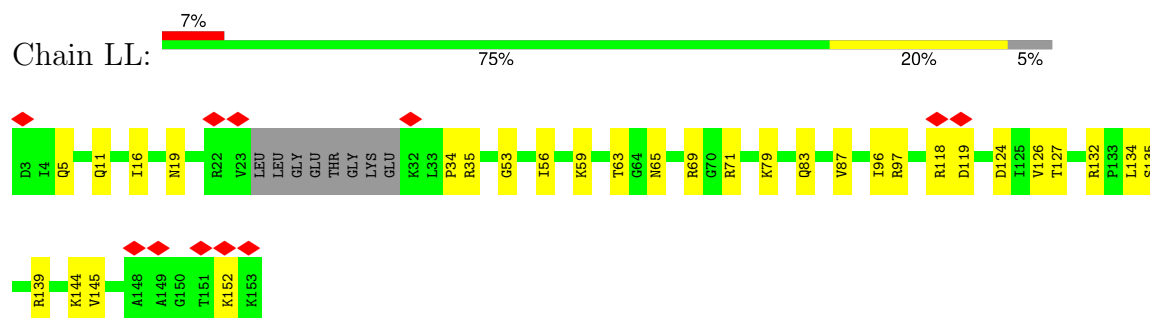
Chain JJ: 



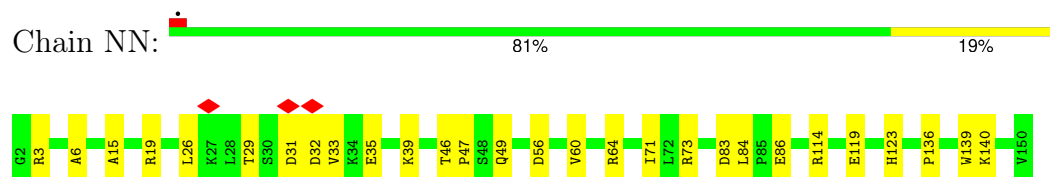
- Molecule 59: 40S ribosomal protein S10



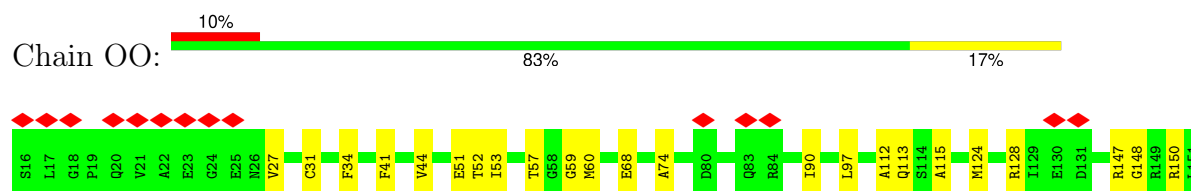
- Molecule 60: 40S ribosomal protein S11



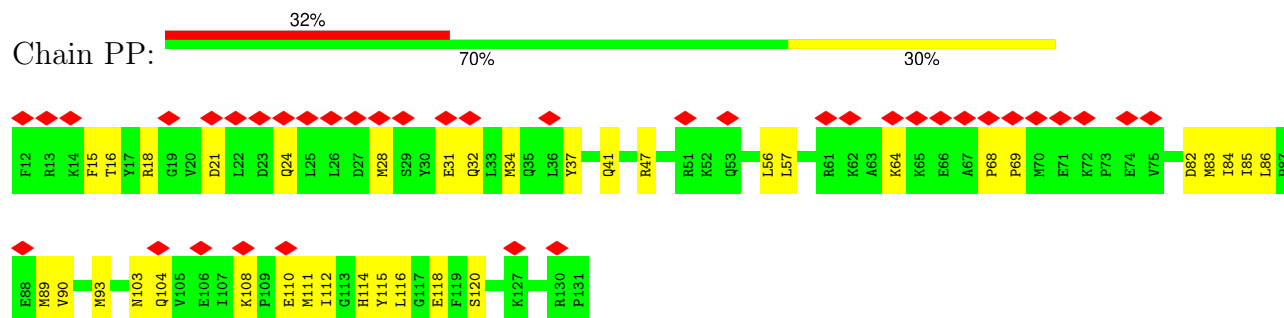
- Molecule 61: 40S ribosomal protein S13



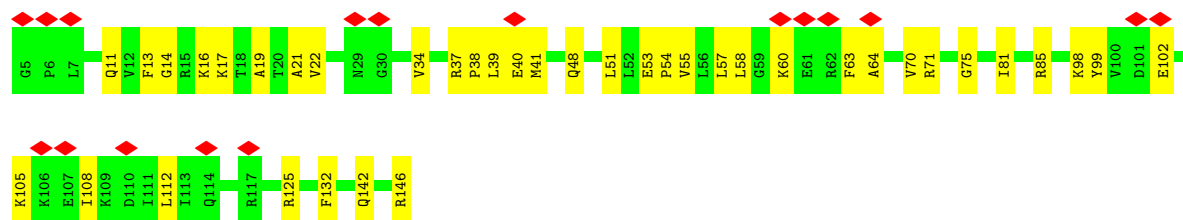
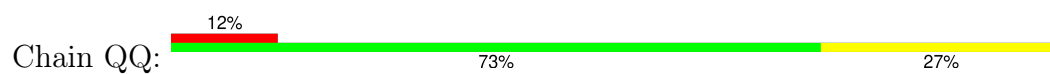
- Molecule 62: 40S ribosomal protein S14



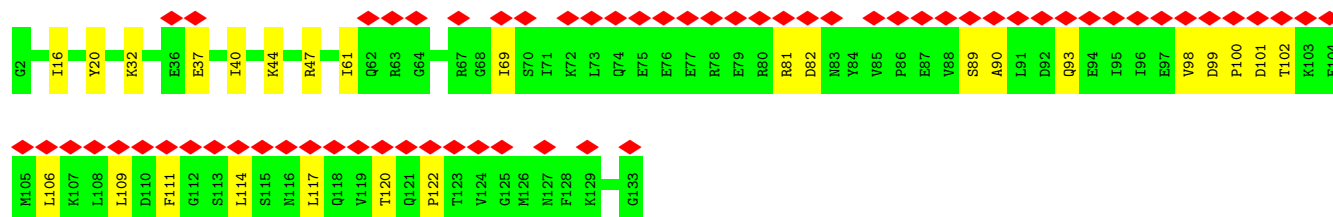
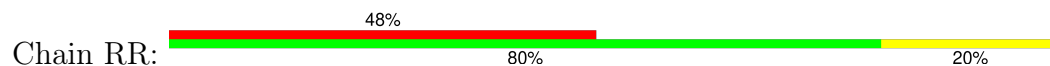
- Molecule 63: 40S ribosomal protein S15



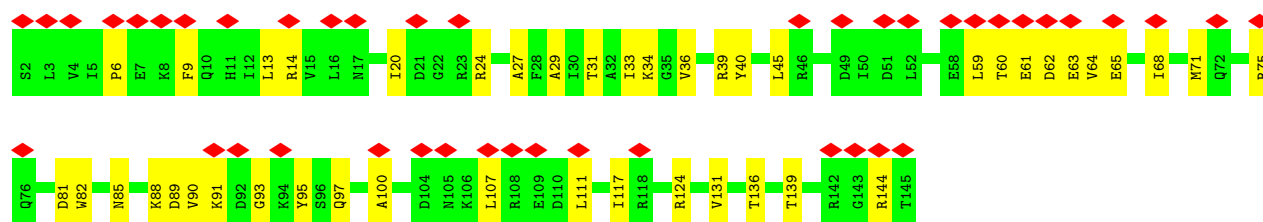
- Molecule 64: 40S ribosomal protein S16



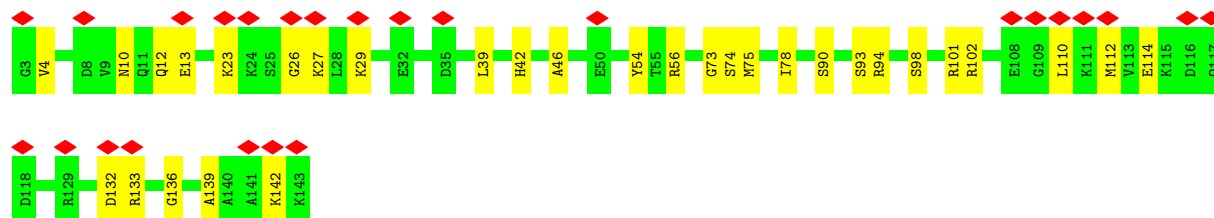
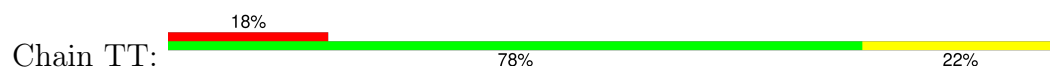
- Molecule 65: 40S ribosomal protein S17



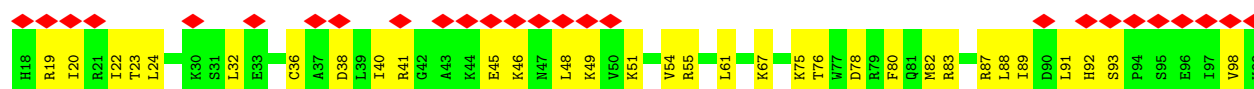
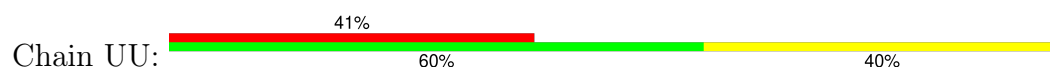
- Molecule 66: 40S ribosomal protein S18

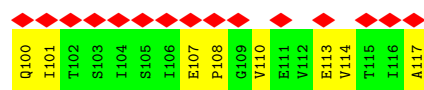


- Molecule 67: 40S ribosomal protein S19

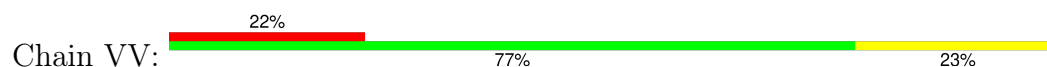


- Molecule 68: 40S ribosomal protein S20

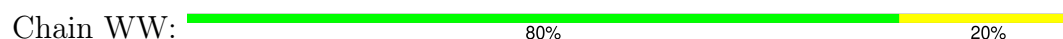




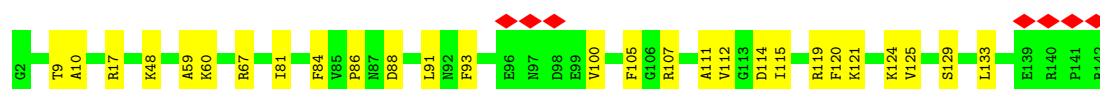
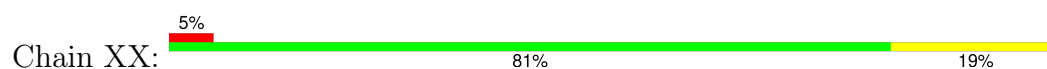
• Molecule 69: eS21



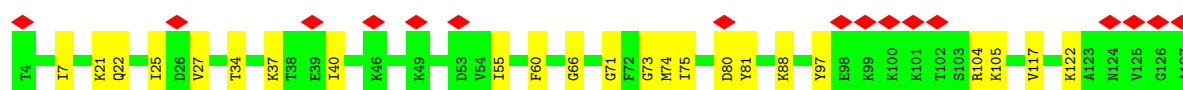
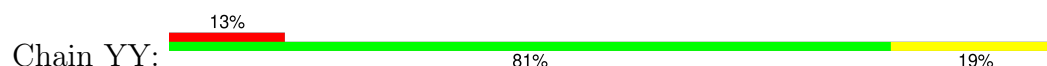
• Molecule 70: 40S ribosomal protein S15a



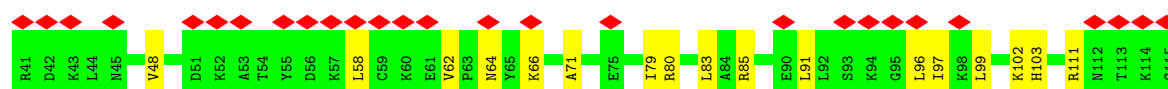
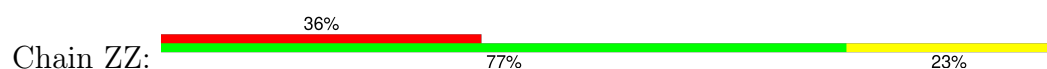
• Molecule 71: 40S ribosomal protein S23



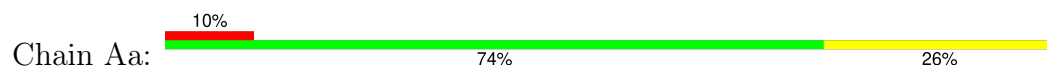
• Molecule 72: 40S ribosomal protein S24



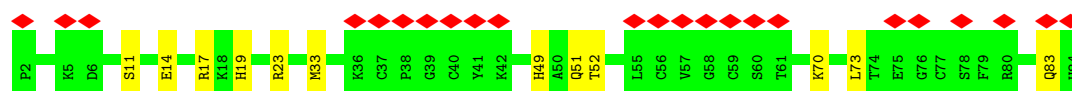
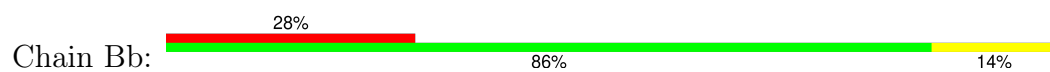
• Molecule 73: 40S ribosomal protein S25



• Molecule 74: eS26



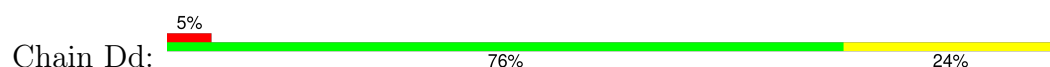
• Molecule 75: 40S ribosomal protein S27



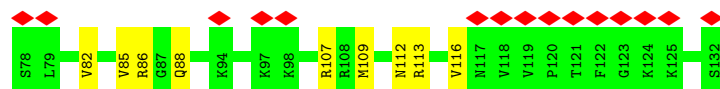
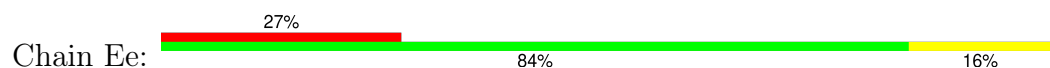
- Molecule 76: 40S ribosomal protein S28



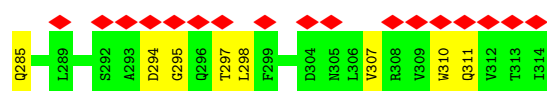
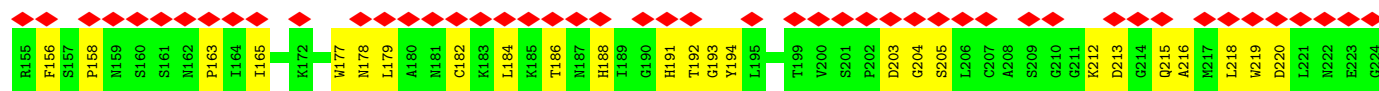
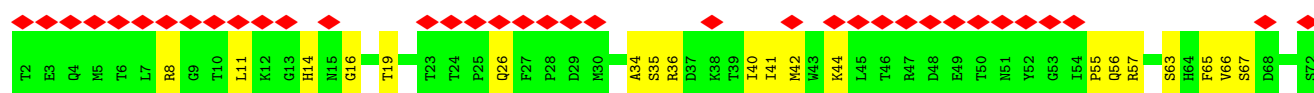
- Molecule 77: 40S ribosomal protein S29



- 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, Not provided	
Number of particles used	107057	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.037	Depositor
Map size ($\text{\AA}$)	651.84, 651.84, 651.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.358, 1.358, 1.358	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, 2MG, B8K, MLZ, MHG, OMG, 4AC, 5MU, E6G, B9H, P7G, 5MC, MMX, MA6, E7G, A2M, 6MZ, OMU, B8T, B9B, T6A, BGH, M7A, MG, MQ6, B8W, B8Q, 7MG, 1MA, PSU, I4U, ZN, P4U, OMC, B8H, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.18	1/1698 (0.1%)	0.28	0/2640
2	1	0.12	0/122	0.22	0/186
3	5	0.18	1/82609 (0.0%)	0.30	0/128762
4	7	0.14	0/2858	0.24	0/4455
5	8	0.17	0/3559	0.25	0/5543
6	9	0.18	0/39730	0.30	0/61898
7	A	0.18	0/1936	0.40	0/2596
8	B	0.18	0/3240	0.38	0/4339
9	C	0.18	0/2913	0.35	0/3913
10	D	0.15	0/2427	0.34	0/3250
11	E	0.15	0/1762	0.35	0/2362
12	F	0.18	0/1911	0.37	0/2549
13	G	0.19	0/1868	0.43	0/2514
14	H	0.18	0/1535	0.43	0/2063
15	I	0.16	0/1702	0.34	0/2272
16	J	0.17	0/1385	0.46	0/1852
17	L	0.17	0/1733	0.39	0/2316
18	M	0.20	0/1158	0.43	0/1547
19	N	0.20	0/1746	0.38	0/2338
20	O	0.20	0/1662	0.39	0/2222
21	P	0.18	0/1268	0.41	0/1700
22	Q	0.18	0/1539	0.41	1/2054 (0.0%)
23	R	0.18	0/1524	0.42	0/2013
24	S	0.17	0/1501	0.36	0/2012
25	T	0.17	0/1326	0.35	0/1770
26	U	0.18	0/814	0.53	0/1092
27	V	0.15	0/993	0.32	0/1332
28	W	0.19	0/873	0.51	0/1158
29	X	0.15	0/984	0.37	0/1323
30	Y	0.18	0/1132	0.38	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Z	0.15	0/1130	0.33	0/1507
32	a	0.18	0/1191	0.35	0/1590
33	b	0.16	0/861	0.34	0/1138
34	c	0.17	0/771	0.40	0/1034
35	d	0.16	0/903	0.35	0/1216
36	e	0.18	0/1071	0.34	0/1429
37	f	0.17	0/895	0.36	0/1198
38	g	0.16	0/916	0.34	0/1220
39	h	0.16	0/1021	0.40	0/1348
40	i	0.14	0/841	0.36	0/1112
41	j	0.17	0/720	0.38	0/952
42	k	0.17	0/575	0.37	0/761
43	l	0.19	0/459	0.40	0/608
44	m	0.16	0/415	0.44	0/550
45	n	0.25	0/240	0.57	0/305
46	o	0.15	0/855	0.31	0/1128
47	p	0.15	0/718	0.33	0/953
48	r	0.17	0/1010	0.35	0/1354
49	AA	0.15	0/1747	0.30	0/2374
50	BB	0.16	0/1756	0.33	0/2350
51	CC	0.19	0/1753	0.37	0/2369
52	DD	0.14	0/1796	0.36	1/2417 (0.0%)
53	EE	0.16	0/2118	0.33	0/2849
54	FF	0.13	0/1492	0.32	0/2005
55	GG	0.15	0/1946	0.34	1/2590 (0.0%)
56	HH	0.15	0/1510	0.35	0/2022
57	II	0.17	0/1696	0.35	0/2261
58	JJ	0.17	0/1550	0.33	0/2069
59	KK	0.15	0/834	0.33	0/1125
60	LL	0.19	0/1195	0.36	0/1597
61	NN	0.16	0/1226	0.34	0/1649
62	OO	0.16	0/1029	0.34	0/1380
63	PP	0.20	0/1017	0.39	0/1358
64	QQ	0.14	0/1146	0.33	0/1534
65	RR	0.15	0/1082	0.35	0/1452
66	SS	0.16	0/1208	0.38	0/1618
67	TT	0.14	0/1115	0.29	0/1493
68	UU	0.15	0/805	0.38	0/1081
69	VV	0.15	0/643	0.31	0/860
70	WW	0.21	0/1051	0.39	0/1406
71	XX	0.17	0/1116	0.38	0/1490
72	YY	0.17	0/1028	0.35	0/1366
73	ZZ	0.13	0/604	0.38	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Aa	0.16	0/828	0.36	0/1109
75	Bb	0.15	0/665	0.33	0/891
76	Cc	0.16	0/490	0.39	0/656
77	Dd	0.14	0/470	0.28	0/623
78	Ee	0.12	0/447	0.30	0/587
79	Gg	0.15	0/2493	0.38	0/3394
All	All	0.17	2/221956 (0.0%)	0.32	3/325763 (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
13	G	0	1
19	N	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	37	T6A	O3'-P	5.20	1.61	1.56
3	5	3785	A2M	O3'-P	5.09	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	DD	43	PRO	CA-N-CD	-7.55	101.44	112.00
22	Q	83	VAL	N-CA-C	-5.38	107.12	111.91
55	GG	169	PRO	CA-N-CD	-5.14	104.80	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	G	215	ASP	Peptide
19	N	76	PRO	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	2	1552	0	793	32	0
2	1	133	0	68	1	0
3	5	76153	0	38232	993	0
4	7	2558	0	1296	23	0
5	8	3209	0	1631	58	0
6	9	36291	0	18318	464	0
7	A	1898	0	1993	40	0
8	B	3172	0	3310	68	0
9	C	2870	0	3045	61	0
10	D	2381	0	2414	43	0
11	E	1729	0	1887	52	0
12	F	1875	0	1995	36	0
13	G	1837	0	1977	46	0
14	H	1516	0	1596	38	0
15	I	1664	0	1711	33	0
16	J	1362	0	1399	36	0
17	L	1702	0	1820	44	0
18	M	1137	0	1209	27	0
19	N	1701	0	1749	51	0
20	O	1630	0	1778	35	0
21	P	1242	0	1274	22	0
22	Q	1515	0	1634	29	0
23	R	1508	0	1664	26	0
24	S	1462	0	1508	26	0
25	T	1298	0	1366	26	0
26	U	800	0	825	21	0
27	V	979	0	1039	16	0
28	W	860	0	903	35	0
29	X	967	0	1040	20	0
30	Y	1115	0	1205	36	0
31	Z	1107	0	1182	28	0
32	a	1162	0	1209	24	0
33	b	848	0	920	11	0
34	c	761	0	794	17	0
35	d	888	0	930	13	0
36	e	1053	0	1147	9	0
37	f	876	0	912	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	g	906	0	998	12	0
39	h	1013	0	1147	22	0
40	i	830	0	916	22	0
41	j	705	0	737	13	0
42	k	569	0	637	16	0
43	l	447	0	480	9	0
44	m	420	0	453	14	0
45	n	239	0	289	4	0
46	o	842	0	912	11	0
47	p	708	0	756	9	0
48	r	994	0	1051	20	0
49	AA	1710	0	1708	37	0
50	BB	1729	0	1803	41	0
51	CC	1716	0	1806	52	0
52	DD	1768	0	1866	32	0
53	EE	2076	0	2177	39	0
54	FF	1471	0	1522	33	0
55	GG	1923	0	2089	64	0
56	HH	1488	0	1582	52	0
57	II	1668	0	1750	31	0
58	JJ	1525	0	1640	33	0
59	KK	810	0	836	26	0
60	LL	1175	0	1249	24	0
61	NN	1202	0	1289	20	0
62	OO	1016	0	1039	18	0
63	PP	997	0	1045	28	0
64	QQ	1128	0	1195	33	0
65	RR	1068	0	1121	20	0
66	SS	1190	0	1249	34	0
67	TT	1097	0	1132	22	0
68	UU	795	0	862	30	0
69	VV	636	0	637	15	0
70	WW	1034	0	1080	22	0
71	XX	1098	0	1167	21	0
72	YY	1011	0	1083	18	0
73	ZZ	598	0	656	13	0
74	Aa	814	0	863	19	0
75	Bb	651	0	672	8	0
76	Cc	488	0	514	15	0
77	Dd	459	0	449	9	0
78	Ee	443	0	492	8	0
79	Gg	2436	0	2393	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	5	196	0	0	0	0
80	7	7	0	0	0	0
80	8	8	0	0	0	0
80	9	78	0	0	0	0
80	A	1	0	0	0	0
80	I	1	0	0	0	0
80	LL	1	0	0	0	0
80	P	1	0	0	0	0
80	V	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
81	5	38	0	0	0	0
82	Aa	1	0	0	0	0
82	Dd	1	0	0	0	0
82	g	1	0	0	0	0
82	j	1	0	0	0	0
82	m	1	0	0	0	0
82	o	1	0	0	0	0
82	p	1	0	0	0	0
All	All	210046	0	155115	3102	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 9.

All (3102) 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)
3:5:4296:B8H:C5	3:5:4296:B8H:C4	1.81	1.53
3:5:3762:B8H:C4	3:5:3762:B8H:C5	1.82	1.52
3:5:1860:B8H:C4	3:5:1860:B8H:C5	1.81	1.52
3:5:2007:G:H21	3:5:2012:A:N6	1.53	1.06
3:5:2007:G:N2	3:5:2012:A:H62	1.53	1.05
3:5:1100:U:H3	3:5:1195:G:H1	1.10	0.99
3:5:1761:G:H1	3:5:1771:U:H3	0.97	0.97
3:5:2557:G:H1	3:5:2570:U:H3	1.11	0.93
3:5:179:G:N2	3:5:257:C:O2	2.05	0.89
3:5:4949:G:H4'	3:5:4950:U:H5'	1.51	0.89
6:9:1760:G:N2	6:9:1772:C:O2	2.05	0.89
6:9:1759:G:N2	6:9:1773:C:O2	2.07	0.88
30:Y:83:GLU:HG2	30:Y:84:ARG:HD3	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:164:A:H3'	6:9:165:G:H21	1.38	0.88
3:5:1759:G:H1	3:5:1773:U:H3	0.86	0.86
15:I:4:ARG:HH11	15:I:99:ILE:HG13	1.40	0.86
38:g:60:ARG:HD3	38:g:61:PRO:HD2	1.57	0.86
3:5:3722:G:H2'	3:5:3723:A2M:H8	1.55	0.86
3:5:3692:A:H62	3:5:3823:G:H21	1.23	0.85
6:9:1302:G:H1	6:9:1307:U:H3	1.25	0.85
6:9:1033:G:H1	6:9:1080:A:HO2'	1.23	0.84
76:Cc:31:ARG:HG2	76:Cc:43:ILE:HG13	1.58	0.84
6:9:1760:G:N1	6:9:1772:C:N3	2.25	0.84
79:Gg:87:LEU:HB2	79:Gg:101:PHE:HB2	1.60	0.84
6:9:696:G:N2	6:9:730:C:O2	2.09	0.84
42:k:23:VAL:HG12	42:k:36:VAL:HG12	1.58	0.83
6:9:1758:G:N2	6:9:1774:C:O2	2.11	0.83
3:5:3717:A:H2'	3:5:3718:A2M:H8	1.60	0.82
6:9:203:G:OP2	57:II:143:LYS:NZ	2.13	0.82
6:9:696:G:N1	6:9:730:C:N3	2.27	0.82
60:LL:11:GLN:HB3	60:LL:56:ILE:HD11	1.61	0.82
6:9:952:G:H21	62:OO:52:THR:HG21	1.44	0.82
50:BB:157:GLN:HB2	50:BB:160:GLN:HG3	1.62	0.82
3:5:690:C:H4'	48:r:85:ASN:HD22	1.42	0.82
54:FF:55:ARG:HE	64:QQ:125:ARG:HH21	1.28	0.81
6:9:568:MMX:N4	6:9:582:U:O2	2.13	0.81
3:5:4910:A:H4'	8:B:95:THR:HG22	1.62	0.81
79:Gg:188:HIS:HB3	79:Gg:219:TRP:HZ3	1.43	0.81
3:5:3892:U:O2'	21:P:80:GLN:NE2	2.14	0.80
8:B:289:GLN:O	8:B:302:ASN:ND2	2.15	0.80
3:5:3937:C:H1'	19:N:125:SER:HB3	1.64	0.80
6:9:1758:G:N1	6:9:1774:C:N3	2.29	0.80
28:W:82:ILE:HG22	55:GG:131:ARG:HB2	1.63	0.80
6:9:1759:G:N1	6:9:1773:C:N3	2.30	0.79
17:L:169:ILE:HG12	32:a:123:ILE:HD11	1.63	0.79
3:5:180:C:N3	3:5:256:G:N1	2.28	0.79
5:8:49:G:H5'	39:h:47:ILE:HD11	1.65	0.79
3:5:180:C:O2	3:5:256:G:N2	2.11	0.79
79:Gg:124:SER:OG	79:Gg:126:ASP:OD1	2.01	0.79
14:H:18:ILE:HG12	14:H:27:VAL:HG22	1.63	0.79
3:5:2262:G:OP2	48:r:98:ARG:NH2	2.15	0.79
3:5:159:C:H5'	40:i:25:ARG:HH21	1.49	0.78
58:JJ:134:HIS:HD1	58:JJ:163:SER:HG	1.31	0.78
63:PP:108:LYS:H	63:PP:111:MET:HE3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:2893:U:H5''	57:II:205:ARG:HH22	1.49	0.77
52:DD:50:ILE:HD11	52:DD:86:LEU:HD23	1.65	0.77
6:9:697:G:N1	6:9:729:C:N3	2.29	0.77
28:W:106:GLU:HA	28:W:109:ILE:HG12	1.67	0.77
6:9:697:G:N2	6:9:729:C:O2	2.15	0.77
3:5:667:A:O2'	9:C:29:LYS:NZ	2.18	0.77
28:W:47:ARG:HE	28:W:54:LEU:HD23	1.48	0.77
3:5:3688:U:OP2	7:A:198:ARG:NH1	2.19	0.76
6:9:1488:C:O2'	6:9:1490:G:OP2	2.03	0.76
42:k:54:GLU:O	42:k:58:GLN:NE2	2.18	0.76
7:A:97:ASN:OD1	7:A:100:ASN:ND2	2.19	0.76
3:5:1604:G:H2'	3:5:1605:7MG:H82	1.68	0.75
3:5:179:G:N1	3:5:257:C:N3	2.29	0.75
3:5:1212:G:H5''	12:F:62:GLN:HE22	1.52	0.75
36:e:98:GLU:OE2	36:e:123:THR:OG1	2.04	0.75
6:9:1664:A:O2'	6:9:1666:C:N4	2.20	0.75
3:5:2260:C:O2	48:r:99:LYS:NZ	2.18	0.75
26:U:28:PRO:HB2	26:U:34:MET:HG2	1.69	0.75
59:KK:3:MET:HE1	59:KK:48:ALA:HB2	1.67	0.75
71:XX:67:ARG:HG3	71:XX:115:ILE:HG13	1.68	0.75
6:9:1679:A:H2'	54:FF:60:ARG:HD3	1.67	0.74
11:E:189:LEU:H	11:E:253:GLN:HE22	1.35	0.74
63:PP:110:GLU:OE2	66:SS:117:ILE:HG21	1.88	0.74
3:5:464:G:O6	3:5:691:C:N4	2.17	0.74
3:5:2520:C:O2	3:5:2640:G:N2	2.19	0.74
59:KK:32:HIS:ND1	59:KK:42:ASN:OD1	2.17	0.74
3:5:262:G:H2'	3:5:263:G:H8	1.51	0.74
22:Q:154:LYS:NZ	22:Q:159:PRO:O	2.21	0.74
34:c:22:MET:HE1	34:c:85:CYS:HA	1.68	0.74
58:JJ:18:ARG:O	58:JJ:24:ARG:NH1	2.21	0.74
56:HH:117:PRO:HG2	56:HH:120:ARG:HD3	1.68	0.74
3:5:2093:G:OP1	48:r:101:LYS:NZ	2.20	0.73
22:Q:66:MET:HE3	22:Q:98:LEU:HD13	1.70	0.73
14:H:89:ARG:HH11	14:H:189:GLN:HE22	1.36	0.73
3:5:4313:A:OP1	25:T:92:ARG:NH2	2.20	0.73
79:Gg:236:ILE:HG22	79:Gg:252:THR:HG22	1.69	0.73
3:5:1199:G:H2'	3:5:1200:G:H8	1.53	0.73
3:5:2274:C:H5'	9:C:312:ARG:HB3	1.68	0.73
51:CC:166:ARG:HB2	51:CC:248:TYR:CE1	2.23	0.73
3:5:990:U:H3	3:5:1064:G:H1	1.37	0.73
6:9:352:U:O2	60:LL:71:ARG:NH1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:548:C:H5'	6:9:549:C:H5''	1.70	0.73
3:5:1552:G:O2'	3:5:1574:B9B:N2	2.22	0.73
79:Gg:247:TRP:HB3	79:Gg:258:ILE:HD11	1.71	0.73
6:9:927:C:O2	75:Bb:51:GLN:NE2	2.22	0.72
16:J:90:ARG:NH2	16:J:108:GLY:O	2.19	0.72
20:O:140:ARG:NH2	20:O:144:GLU:OE1	2.23	0.72
22:Q:178:ARG:H	32:a:51:GLY:HA2	1.54	0.72
39:h:31:LEU:HB3	39:h:47:ILE:HG22	1.72	0.72
64:QQ:39:LEU:HD22	64:QQ:51:LEU:HD23	1.71	0.72
59:KK:35:LEU:HD11	59:KK:40:VAL:HG12	1.72	0.72
13:G:170:ARG:HA	13:G:173:LYS:HG2	1.72	0.72
53:EE:87:MET:HE1	53:EE:236:ILE:HD13	1.70	0.72
1:2:6:G:H1	1:2:67:U:H3	1.36	0.71
1:2:33:C:OP2	64:QQ:146:ARG:NH1	2.23	0.71
13:G:139:VAL:HG21	13:G:238:LYS:HG2	1.71	0.71
66:SS:75:ARG:NH1	66:SS:81:ASP:OD2	2.23	0.71
7:A:36:GLU:HG3	7:A:91:GLY:HA2	1.71	0.71
6:9:318:A:N6	55:GG:186:GLN:OE1	2.23	0.71
3:5:3798:U:OP2	27:V:74:LYS:NZ	2.24	0.71
51:CC:166:ARG:HB2	51:CC:248:TYR:CD1	2.25	0.71
6:9:1192:U:OP2	71:XX:119:ARG:NH2	2.23	0.71
52:DD:127:MET:HE1	52:DD:133:GLY:HA2	1.71	0.71
29:X:77:ILE:HD11	29:X:116:LEU:HD22	1.73	0.71
79:Gg:219:TRP:HE1	79:Gg:226:HIS:HD2	1.39	0.71
3:5:4162:C:H5	13:G:126:ARG:HH12	1.37	0.70
6:9:1117:C:O2'	6:9:1118:C:O2	2.04	0.70
19:N:174:LEU:HA	19:N:183:THR:HG21	1.73	0.70
3:5:4944:C:H1'	37:f:69:VAL:HG21	1.73	0.70
3:5:2521:G:H2'	3:5:2522:7MG:H82	1.73	0.70
6:9:621:C:OP1	71:XX:107:ARG:NH1	2.24	0.70
51:CC:263:LYS:NZ	51:CC:268:GLU:HG3	2.05	0.70
16:J:161:GLU:HA	16:J:164:ARG:HG2	1.71	0.70
3:5:1870:C:H2'	3:5:1871:A2M:H8	1.73	0.70
52:DD:113:LEU:HD11	52:DD:117:ARG:HD2	1.73	0.70
3:5:4594:U:H2'	3:5:4595:G:H8	1.57	0.70
6:9:483:C:H5''	71:XX:48:LYS:HE2	1.74	0.70
3:5:1866:UR3:OP1	15:I:4:ARG:NH1	2.25	0.70
51:CC:65:LYS:HD3	51:CC:273:LEU:HD21	1.74	0.70
3:5:2493:G:H2'	3:5:2494:U:C6	2.27	0.70
49:AA:69:GLU:HG3	51:CC:270:THR:HG21	1.74	0.70
58:JJ:57:ALA:HB2	58:JJ:97:ILE:HD11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:j:2:THR:O	41:j:7:SER:OG	2.09	0.70
3:5:5047:C:O2'	3:5:5050:C:OP2	2.09	0.69
8:B:71:GLU:OE1	28:W:1:MET:N	2.20	0.69
16:J:51:SER:HB2	16:J:69:ALA:HB3	1.74	0.69
25:T:68:THR:HG22	25:T:69:GLN:H	1.57	0.69
63:PP:18:ARG:NH2	66:SS:88:LYS:O	2.24	0.69
3:5:2300:A:N7	9:C:143:ARG:NH1	2.40	0.69
53:EE:100:ARG:HH21	53:EE:118:GLU:HG2	1.57	0.69
59:KK:3:MET:HE2	59:KK:44:HIS:HB3	1.74	0.69
6:9:151:C:O2'	55:GG:132:ARG:NH2	2.26	0.69
6:9:1658:G:OP2	6:9:1660:C:N4	2.25	0.69
27:V:90:ARG:HH12	27:V:123:LYS:HB3	1.58	0.69
6:9:919:A:OP2	61:NN:64:ARG:NH2	2.26	0.69
29:X:64:SER:HB2	39:h:69:LEU:HD21	1.74	0.69
9:C:78:ARG:HB3	9:C:88:GLY:HA2	1.74	0.69
18:M:101:LYS:HG3	18:M:104:MET:HE2	1.74	0.69
6:9:190:G:O2'	6:9:209:A:N6	2.25	0.69
57:II:113:TYR:OH	57:II:156:ALA:O	2.10	0.69
3:5:3641:U:OP2	3:5:3646:A:N6	2.26	0.69
63:PP:41:GLN:HG3	63:PP:84:ILE:HD12	1.73	0.69
53:EE:15:PRO:HB3	53:EE:39:ARG:HD3	1.75	0.69
3:5:175:C:H2'	3:5:176:G:H8	1.58	0.69
14:H:26:ILE:HG12	14:H:35:ARG:HG2	1.74	0.69
62:OO:113:GLN:HE22	74:Aa:45:VAL:HA	1.58	0.69
6:9:1228:A:H2'	6:9:1229:G:C8	2.28	0.68
6:9:1536:G:H2'	6:9:1537:A:H8	1.58	0.68
8:B:286:LYS:NZ	8:B:302:ASN:O	2.21	0.68
65:RR:98:VAL:HG21	65:RR:117:LEU:HD22	1.74	0.68
6:9:681:U:H4'	71:XX:9:THR:HG22	1.75	0.68
55:GG:162:LEU:HD11	55:GG:172:LYS:HE2	1.76	0.68
68:UU:40:ILE:HD11	68:UU:89:ILE:HD12	1.75	0.68
3:5:1444:G:H22	3:5:2110:G:H1	1.38	0.68
15:I:91:LEU:HD12	15:I:135:ILE:HG23	1.75	0.68
24:S:9:GLU:HG2	24:S:67:VAL:HB	1.75	0.68
46:o:51:GLN:HG2	46:o:55:ILE:HD11	1.76	0.68
6:9:587:A:H5'	6:9:592:C:H41	1.59	0.68
18:M:14:TYR:HD2	18:M:56:GLN:HE21	1.42	0.68
3:5:1818:G:O2'	3:5:1819:G:OP1	2.11	0.68
13:G:139:VAL:HG11	13:G:238:LYS:HE3	1.76	0.68
30:Y:69:LYS:N	30:Y:83:GLU:OE1	2.26	0.68
52:DD:172:VAL:HG22	52:DD:185:LYS:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:4875:G:H2'	24:S:169:THR:HG22	1.75	0.68
3:5:1351:G:OP1	9:C:33:ARG:NH1	2.28	0.68
42:k:51:GLU:OE1	42:k:55:LYS:NZ	2.26	0.68
79:Gg:42:MET:SD	79:Gg:44:LYS:NZ	2.67	0.68
79:Gg:133:ASN:HD21	79:Gg:137:VAL:HB	1.59	0.68
1:2:13:G:O6	1:2:22:G:O6	2.12	0.67
6:9:1293:A:H61	6:9:1306:U:H3	1.41	0.67
52:DD:54:ARG:HB3	52:DD:57:ASN:HD22	1.58	0.67
6:9:925:G:H1	6:9:1017:U:H3	1.41	0.67
1:2:58:A:O2'	1:2:60:A:OP2	2.09	0.67
3:5:464:G:N1	3:5:691:C:N3	2.37	0.67
8:B:46:PHE:HE2	8:B:81:THR:OG1	1.77	0.67
3:5:308:G:OP2	3:5:308:G:N2	2.22	0.67
3:5:2745:A:H2'	3:5:2746:A:C8	2.29	0.67
15:I:39:LYS:HA	15:I:86:HIS:HD2	1.59	0.67
6:9:1154:U:OP2	51:CC:187:ARG:NH2	2.28	0.67
13:G:147:GLN:HA	13:G:150:LYS:HG2	1.76	0.67
6:9:507:G:OP2	72:YY:104:ARG:NH2	2.28	0.67
69:VV:2:GLN:HE21	69:VV:8:PHE:HE2	1.42	0.67
3:5:4884:G:N7	11:E:275:ARG:NH2	2.42	0.67
3:5:4520:G:N2	8:B:253:CYS:SG	2.68	0.67
31:Z:52:LYS:O	31:Z:65:ARG:NH2	2.20	0.67
53:EE:107:GLY:HA2	53:EE:189:LEU:HD11	1.75	0.67
63:PP:56:LEU:HD23	63:PP:83:MET:HE3	1.77	0.67
3:5:1759:G:O6	3:5:1773:U:O4	2.13	0.66
3:5:4873:G:N7	20:O:179:LYS:NZ	2.35	0.66
22:Q:82:VAL:HG12	22:Q:84:GLY:H	1.59	0.66
24:S:34:ALA:HB1	24:S:39:VAL:HG13	1.77	0.66
3:5:1398:A:H62	3:5:1419:G:N2	1.92	0.66
6:9:383:G:H4'	60:LL:132:ARG:HD2	1.75	0.66
15:I:46:PHE:HB3	15:I:139:ARG:HG2	1.75	0.66
74:Aa:51:ARG:NH2	76:Cc:39:SER:OG	2.25	0.66
5:8:75:G:OP2	30:Y:74:TYR:OH	2.12	0.66
6:9:1277:C:H2'	6:9:1278:A:H8	1.60	0.66
8:B:46:PHE:CE1	8:B:84:MET:HG3	2.29	0.66
66:SS:36:VAL:HG23	66:SS:40:TYR:HD2	1.60	0.66
10:D:33:ARG:HH21	10:D:37:VAL:HG11	1.60	0.66
28:W:117:LYS:HA	28:W:120:GLN:HG2	1.77	0.66
3:5:3946:G:H1	3:5:4067:U:H3	1.42	0.66
15:I:39:LYS:HA	15:I:86:HIS:CD2	2.31	0.66
76:Cc:29:GLN:HE22	76:Cc:67:ARG:HA	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:3717:A:H2'	3:5:3718:A2M:C8	2.26	0.66
4:7:6:C:H4'	10:D:52:ILE:HD13	1.76	0.66
38:g:69:LYS:HG2	38:g:73:HIS:CD2	2.31	0.66
51:CC:74:LYS:HB3	51:CC:269:PHE:HE1	1.61	0.66
6:9:819:G:OP1	58:JJ:79:ARG:NH2	2.28	0.66
36:e:15:LYS:NZ	36:e:61:GLY:O	2.27	0.66
56:HH:7:LYS:NZ	56:HH:40:LEU:O	2.29	0.66
79:Gg:73:SER:OG	79:Gg:117:ASN:ND2	2.28	0.66
41:j:19:CYS:HB3	41:j:27:TYR:HB2	1.77	0.66
71:XX:100:VAL:HG12	71:XX:125:VAL:HG23	1.78	0.66
3:5:4751:G:H1	3:5:4948:C:H5	1.44	0.66
13:G:111:PRO:HD2	13:G:114:ILE:HD12	1.78	0.65
6:9:1654:G:OP1	67:TT:90:SER:OG	2.14	0.65
8:B:67:VAL:HG11	27:V:91:LYS:HD2	1.77	0.65
27:V:18:LEU:HD13	27:V:54:ALA:HB3	1.78	0.65
6:9:168:C:OP1	55:GG:131:ARG:NE	2.27	0.65
6:9:1643:U:H1'	64:QQ:142:GLN:HE22	1.62	0.65
8:B:81:THR:HG22	8:B:330:PHE:HA	1.75	0.65
28:W:81:ALA:HB2	28:W:87:LEU:HB2	1.79	0.65
56:HH:43:LEU:HD13	56:HH:68:GLN:HE21	1.59	0.65
3:5:4541:G:N2	3:5:4544:A:OP2	2.26	0.65
11:E:135:PRO:HD2	11:E:138:GLN:HE21	1.59	0.65
70:WW:42:MET:HE1	70:WW:49:GLU:HA	1.77	0.65
3:5:2000:G:O2'	3:5:2001:G:N7	2.29	0.65
14:H:92:MET:HG2	14:H:181:VAL:HA	1.78	0.65
3:5:3848:U:H2'	3:5:3849:A:H8	1.62	0.65
3:5:3861:A:H2'	3:5:3862:A:C8	2.32	0.65
5:8:87:G:OP1	39:h:5:LYS:NZ	2.29	0.65
6:9:74:G:N2	6:9:77:A:OP1	2.30	0.65
6:9:848:U:H2'	6:9:849:A:H8	1.61	0.65
14:H:18:ILE:HD11	14:H:81:ILE:HD11	1.78	0.65
40:i:50:PHE:O	40:i:55:ARG:NH1	2.30	0.65
3:5:2341:A:OP2	32:a:4:ARG:NH1	2.29	0.65
11:E:43:LYS:HD3	11:E:44:PRO:HD2	1.78	0.65
19:N:103:GLU:OE2	19:N:165:THR:OG1	2.12	0.65
56:HH:69:LEU:HD22	56:HH:96:ALA:HB2	1.78	0.65
60:LL:59:LYS:HG2	60:LL:134:LEU:HD22	1.78	0.65
68:UU:38:ASP:OD1	68:UU:41:ARG:NH2	2.30	0.65
3:5:2406:G:N7	43:l:2:SER:N	2.45	0.65
3:5:2745:A:H2'	3:5:2746:A:H8	1.61	0.65
6:9:69:C:OP2	55:GG:167:LYS:NZ	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:41:LYS:NZ	25:T:30:TYR:O	2.22	0.65
19:N:75:VAL:HG22	19:N:76:PRO:HD2	1.78	0.65
30:Y:52:ASP:HB2	30:Y:110:LYS:HD2	1.77	0.65
51:CC:108:LYS:HD2	51:CC:233:LEU:HD13	1.78	0.65
3:5:1646:A:O2'	41:j:49:TRP:O	2.15	0.65
15:I:189:ARG:NH1	15:I:202:ASN:OD1	2.30	0.65
3:5:2485:U:H2'	3:5:2486:G:C8	2.33	0.64
6:9:65:C:H4'	55:GG:172:LYS:HD3	1.78	0.64
29:X:39:LYS:HG2	29:X:40:ILE:H	1.60	0.64
79:Gg:188:HIS:HB3	79:Gg:219:TRP:CZ3	2.28	0.64
31:Z:53:VAL:HG21	31:Z:62:ILE:HG23	1.79	0.64
56:HH:154:ILE:HB	56:HH:185:VAL:HG22	1.79	0.64
50:BB:28:LYS:NZ	62:OO:51:GLU:OE1	2.27	0.64
3:5:1176:C:O3'	10:D:268:ARG:NH2	2.30	0.64
6:9:495:U:O2'	53:EE:27:PHE:O	2.15	0.64
6:9:1103:C:OP1	50:BB:157:GLN:NE2	2.26	0.64
10:D:75:VAL:O	10:D:112:ARG:NH1	2.30	0.64
51:CC:74:LYS:HB3	51:CC:269:PHE:CE1	2.32	0.64
6:9:694:G:H1	6:9:732:U:H3	1.46	0.64
6:9:1597:C:OP2	73:ZZ:85:ARG:NH1	2.28	0.64
8:B:10:ARG:NH1	8:B:265:SER:O	2.28	0.64
35:d:22:THR:HG23	35:d:122:VAL:HG13	1.78	0.64
3:5:1952:G:H4'	24:S:93:MET:HG3	1.78	0.64
3:5:2579:G:N2	3:5:2582:A:OP2	2.25	0.64
3:5:4304:A:OP2	3:5:4305:G:N2	2.31	0.64
3:5:2063:G:OP1	24:S:4:SER:OG	2.13	0.64
51:CC:60:TRP:O	51:CC:71:LYS:NZ	2.28	0.64
56:HH:145:ARG:NH2	70:WW:49:GLU:OE2	2.30	0.64
3:5:4694:G:OP1	3:5:4694:G:N2	2.29	0.64
42:k:17:ARG:NH2	42:k:19:ASP:OD2	2.31	0.64
52:DD:103:GLU:OE2	52:DD:173:ARG:NH1	2.31	0.64
70:WW:111:MET:HB2	70:WW:115:GLU:OE2	1.97	0.64
15:I:79:SER:OG	15:I:147:HIS:ND1	2.31	0.64
40:i:70:LEU:HD13	40:i:87:ARG:HD2	1.80	0.64
52:DD:132:LYS:NZ	52:DD:190:LEU:O	2.30	0.64
3:5:1403:G:H2'	3:5:1404:G:C8	2.33	0.63
6:9:1536:G:H2'	6:9:1537:A:C8	2.33	0.63
13:G:284:ASP:OD1	13:G:285:GLU:N	2.30	0.63
16:J:18:ARG:HG3	16:J:135:GLY:HA3	1.81	0.63
3:5:4260:U:H2'	3:5:4261:C:H6	1.64	0.63
3:5:245:C:O2'	3:5:246:G:OP2	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:1402:A:H5'	68:UU:51:LYS:HD2	1.79	0.63
3:5:1332:C:H2'	3:5:1333:A:H8	1.63	0.63
3:5:1405:C:H2'	3:5:1406:G:C8	2.34	0.63
3:5:1975:G:N2	3:5:1983:A:OP1	2.32	0.63
3:5:3717:A:OP2	3:5:3735:G:N2	2.31	0.63
3:5:4274:A:H2'	3:5:4275:G:C8	2.34	0.63
3:5:4772:C:H41	3:5:4863:G:H1	1.45	0.63
6:9:794:A:H2'	6:9:795:A:H8	1.62	0.63
3:5:2502:A:O2'	3:5:2503:G:O5'	2.16	0.63
3:5:4115:G:OP2	3:5:4115:G:N2	2.29	0.63
3:5:4472:B8W:O2'	44:m:74:TYR:O	2.16	0.63
6:9:640:A:H2'	6:9:641:A:C8	2.33	0.63
19:N:138:PHE:HA	19:N:143:ARG:HD2	1.81	0.63
51:CC:200:ARG:O	58:JJ:54:ARG:NH1	2.32	0.63
55:GG:70:HIS:O	55:GG:98:ARG:NH1	2.29	0.63
63:PP:57:LEU:HD21	63:PP:89:MET:HE2	1.81	0.63
3:5:2627:C:H41	3:5:4649:G:H1	1.45	0.63
14:H:50:LYS:O	14:H:51:LYS:HG2	1.98	0.63
23:R:136:ARG:O	23:R:140:GLU:HG2	1.99	0.63
57:II:101:ILE:HD12	57:II:190:LEU:HD11	1.80	0.63
3:5:1984:A:N7	3:5:2010:A:O2'	2.32	0.62
6:9:885:U:O2	6:9:901:G:O6	2.16	0.62
50:BB:104:ASP:OD1	50:BB:105:LEU:N	2.32	0.62
3:5:979:G:OP1	11:E:49:ASN:ND2	2.32	0.62
3:5:1432:G:O2'	3:5:1451:G:N2	2.32	0.62
3:5:1548:G:O2'	3:5:2812:A:N3	2.30	0.62
3:5:2580:U:O2	31:Z:76:ASN:ND2	2.31	0.62
8:B:57:VAL:HG22	8:B:73:VAL:HG12	1.81	0.62
3:5:1402:C:N4	3:5:1403:G:O6	2.31	0.62
3:5:4062:A:H2'	3:5:4063:U:C6	2.34	0.62
3:5:4415:1MA:N6	3:5:4427:G:HO2'	1.98	0.62
6:9:697:G:O6	6:9:729:C:N4	2.28	0.62
55:GG:67:VAL:HG12	55:GG:69:THR:HG22	1.81	0.62
58:JJ:170:PRO:HB3	58:JJ:174:LYS:HD2	1.80	0.62
3:5:2663:G:H4'	23:R:117:ARG:HH11	1.65	0.62
3:5:4957:C:N4	3:5:4958:C:N3	2.46	0.62
53:EE:199:GLU:OE1	53:EE:201:HIS:NE2	2.31	0.62
3:5:300:A:H2'	3:5:301:G:H8	1.65	0.62
3:5:4260:U:H2'	3:5:4261:C:C6	2.35	0.62
6:9:804:U:OP1	70:WW:82:GLN:NE2	2.32	0.62
52:DD:103:GLU:OE1	52:DD:106:ARG:NH1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Gg:219:TRP:HE1	79:Gg:226:HIS:CD2	2.17	0.62
3:5:4274:A:H2'	3:5:4275:G:H8	1.63	0.62
5:8:67:U:H2'	5:8:68:G:H8	1.64	0.62
3:5:1280:C:O2'	9:C:321:ASN:OD1	2.17	0.62
3:5:1985:G:N2	3:5:2003:G:O2'	2.33	0.62
6:9:70:G:N2	6:9:71:G:O6	2.33	0.62
55:GG:58:LYS:HE2	55:GG:105:ASN:HA	1.81	0.62
68:UU:80:PHE:HB3	77:Dd:52:PHE:HB3	1.81	0.62
3:5:385:A:OP1	30:Y:77:LYS:NZ	2.32	0.62
6:9:1520:G:O2'	6:9:1521:C:OP1	2.18	0.62
17:L:186:ARG:HE	40:i:9:VAL:HG11	1.65	0.62
30:Y:11:ARG:O	30:Y:15:ARG:HG3	1.99	0.62
31:Z:87:VAL:HG12	31:Z:89:ILE:HG13	1.82	0.62
50:BB:82:ARG:NH1	50:BB:188:LEU:O	2.32	0.62
1:2:11:G:N2	1:2:24:G:H22	1.97	0.61
11:E:148:THR:OG1	11:E:203:LYS:NZ	2.33	0.61
30:Y:74:TYR:HE2	30:Y:77:LYS:HG3	1.65	0.61
19:N:91:GLN:O	19:N:93:LYS:NZ	2.33	0.61
7:A:179:ILE:HG23	7:A:184:ARG:HB2	1.82	0.61
11:E:122:GLU:HG3	36:e:7:LEU:HD22	1.83	0.61
71:XX:59:ALA:O	71:XX:60:LYS:HG3	2.00	0.61
3:5:2261:G:H4'	11:E:115:MET:HE3	1.81	0.61
3:5:4124:G:N2	13:G:96:GLN:O	2.33	0.61
9:C:124:ILE:HD11	9:C:240:LEU:HD12	1.81	0.61
14:H:118:LEU:HD11	14:H:167:VAL:HG22	1.82	0.61
49:AA:33:GLN:HB3	49:AA:154:LEU:HD12	1.82	0.61
56:HH:145:ARG:HG3	56:HH:155:LYS:NZ	2.14	0.61
6:9:981:A:H2'	6:9:982:G:C8	2.34	0.61
6:9:146:G:O2'	6:9:147:A:O5'	2.16	0.61
6:9:1183:A:OP1	45:n:15:ARG:NH1	2.34	0.61
19:N:17:ASP:OD2	19:N:18:VAL:N	2.34	0.61
3:5:261:G:H2'	3:5:262:G:C8	2.36	0.61
3:5:303:C:OP2	19:N:68:ARG:NH2	2.34	0.61
11:E:168:LEU:HD11	11:E:179:THR:HB	1.81	0.61
50:BB:144:LYS:HD3	50:BB:208:HIS:HB3	1.82	0.61
56:HH:62:ILE:HD12	56:HH:94:PHE:HE2	1.64	0.61
59:KK:1:MET:HE3	59:KK:44:HIS:HD2	1.66	0.61
6:9:72:C:H41	55:GG:170:ARG:HH11	1.46	0.61
6:9:551:U:H2'	6:9:552:G:C8	2.36	0.61
73:ZZ:58:LEU:HD21	73:ZZ:91:LEU:HD11	1.82	0.61
79:Gg:8:ARG:HD2	79:Gg:311:GLN:NE2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:4594:U:H2'	3:5:4595:G:C8	2.36	0.61
6:9:921:G:C6	70:WW:28:ARG:HD2	2.36	0.61
11:E:261:LEU:O	11:E:265:LYS:HG2	2.00	0.61
20:O:109:PRO:HB2	20:O:111:PRO:HD2	1.83	0.61
66:SS:136:THR:O	66:SS:144:ARG:NH2	2.33	0.61
3:5:3848:U:H2'	3:5:3849:A:C8	2.36	0.61
17:L:170:THR:HG22	17:L:172:GLU:H	1.66	0.61
27:V:43:LYS:HD3	27:V:60:MET:HE3	1.82	0.61
56:HH:67:PRO:O	56:HH:70:LYS:NZ	2.34	0.61
3:5:1447:C:O2'	9:C:300:ARG:NH2	2.33	0.60
3:5:4895:C:O2	18:M:132:ARG:NH1	2.27	0.60
26:U:28:PRO:HB3	26:U:100:LEU:HD21	1.82	0.60
35:d:57:MET:SD	35:d:90:ARG:NH2	2.73	0.60
64:QQ:13:PHE:HA	64:QQ:22:VAL:HA	1.83	0.60
66:SS:124:ARG:HB2	66:SS:131:VAL:HG12	1.83	0.60
5:8:8:U:H2'	5:8:9:A:H8	1.65	0.60
6:9:380:G:OP1	57:II:56:ARG:NH2	2.34	0.60
9:C:334:THR:HG22	9:C:337:ARG:HH11	1.66	0.60
31:Z:68:ILE:N	31:Z:119:GLU:OE2	2.33	0.60
59:KK:80:ARG:NH1	59:KK:87:PRO:HA	2.15	0.60
23:R:151:ARG:NH2	60:LL:119:ASP:OD1	2.35	0.60
24:S:15:ARG:HH12	24:S:18:PRO:HG3	1.66	0.60
54:FF:51:HIS:HD2	54:FF:86:LYS:HG2	1.65	0.60
68:UU:48:LEU:HD22	68:UU:93:SER:HB2	1.80	0.60
73:ZZ:79:ILE:HB	73:ZZ:83:LEU:HD23	1.83	0.60
33:b:5:LYS:HE3	33:b:8:THR:OG1	2.02	0.60
34:c:80:GLU:OE2	34:c:80:GLU:N	2.29	0.60
3:5:2007:G:H21	3:5:2012:A:H62	0.73	0.60
44:m:96:ARG:NH1	44:m:97:PRO:O	2.34	0.60
3:5:1763:C:OP2	3:5:1764:G:N2	2.34	0.60
6:9:943:U:OP1	50:BB:214:LYS:NZ	2.32	0.60
8:B:46:PHE:HE2	8:B:81:THR:HG1	1.50	0.60
27:V:66:LYS:O	27:V:73:ARG:NH1	2.33	0.60
64:QQ:16:LYS:HG3	64:QQ:17:LYS:H	1.65	0.60
1:2:53:G:H2'	1:2:54:A:H8	1.66	0.60
3:5:668:C:H4'	9:C:6:PRO:HB3	1.83	0.60
3:5:4622:A:H4'	8:B:13:SER:HB2	1.84	0.60
14:H:51:LYS:HE2	14:H:53:LYS:HD3	1.84	0.60
19:N:46:ASP:OD1	19:N:47:LYS:N	2.33	0.60
3:5:4232:U:H4'	3:5:4233:A:O5'	2.02	0.60
3:5:4254:G:O2'	3:5:4256:A:N7	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:1587:G:N1	67:TT:74:SER:OG	2.35	0.60
7:A:142:GLU:O	7:A:143:THR:OG1	2.20	0.60
11:E:141:ARG:NH1	11:E:172:SER:O	2.34	0.60
27:V:43:LYS:HD2	27:V:62:MET:HE3	1.84	0.60
34:c:81:LEU:HG	34:c:91:VAL:HG23	1.84	0.60
3:5:517:C:H2'	3:5:518:G:H8	1.67	0.60
3:5:4992:G:H2'	3:5:4993:G:C8	2.37	0.60
5:8:122:G:H21	5:8:128:C:H5	1.49	0.60
39:h:96:ASN:OD1	39:h:99:GLU:HG2	2.02	0.60
46:o:11:PHE:O	46:o:81:ARG:NH1	2.35	0.60
47:p:51:ALA:HB3	47:p:54:ILE:HD12	1.84	0.60
79:Gg:220:ASP:HB2	79:Gg:227:LEU:HD11	1.82	0.60
6:9:183:G:O2'	6:9:184:G:O5'	2.18	0.59
6:9:318:A:H3'	6:9:319:C:H5''	1.82	0.59
12:F:238:GLN:OE1	12:F:241:ARG:NH2	2.35	0.59
13:G:158:GLU:OE2	13:G:158:GLU:N	2.32	0.59
3:5:4128:A:O2'	13:G:88:ARG:NH2	2.34	0.59
49:AA:214:GLU:OE2	65:RR:81:ARG:NH2	2.35	0.59
58:JJ:65:GLU:HA	58:JJ:70:ARG:HG2	1.84	0.59
3:5:2483:G:H22	3:5:2495:U:H3	1.50	0.59
5:8:155:C:OP2	13:G:142:ARG:NH2	2.35	0.59
14:H:7:ASN:HB3	14:H:58:ASP:HB3	1.85	0.59
3:5:1369:C:OP2	3:5:1370:G:O2'	2.15	0.59
3:5:3861:A:H2'	3:5:3862:A:H8	1.67	0.59
32:a:62:HIS:CE1	32:a:64:LYS:HE2	2.37	0.59
39:h:103:LYS:HB2	39:h:107:GLN:NE2	2.17	0.59
59:KK:65:ARG:NH2	77:Dd:25:SER:OG	2.35	0.59
3:5:923:C:H5''	3:5:924:C:H5''	1.83	0.59
3:5:3928:A:OP1	19:N:90:ASN:ND2	2.36	0.59
9:C:233:THR:HA	9:C:263:LEU:HD21	1.83	0.59
13:G:163:LYS:HA	13:G:166:ARG:HG2	1.83	0.59
35:d:36:VAL:HG11	35:d:44:ARG:HD2	1.84	0.59
69:VV:42:VAL:HG23	69:VV:43:THR:HG23	1.83	0.59
70:WW:28:ARG:HB3	70:WW:29:PRO:HD3	1.85	0.59
79:Gg:101:PHE:CE2	79:Gg:136:GLY:HA2	2.37	0.59
1:2:1:G:H22	1:2:72:U:H3	1.48	0.59
3:5:125:C:H2'	3:5:126:C:H6	1.68	0.59
6:9:1228:A:H2'	6:9:1229:G:H8	1.66	0.59
26:U:40:GLU:O	26:U:44:GLN:HG2	2.02	0.59
61:NN:31:ASP:OD1	61:NN:32:ASP:N	2.35	0.59
3:5:2555:G:H2'	3:5:2556:G:H8	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:8:126:C:O2'	5:8:127:U:O5'	2.21	0.59
17:L:143:GLU:OE2	17:L:143:GLU:N	2.31	0.59
26:U:107:LYS:HG3	26:U:108:GLU:OE1	2.02	0.59
56:HH:44:ASN:OD1	56:HH:45:ILE:N	2.36	0.59
68:UU:19:ARG:O	68:UU:117:ALA:N	2.31	0.59
3:5:1244:G:N1	33:b:115:GLY:HA2	2.18	0.59
3:5:2583:C:OP2	38:g:76:ARG:NH2	2.20	0.59
50:BB:99:ASN:OD1	50:BB:100:PHE:N	2.36	0.59
59:KK:85:LEU:HB3	59:KK:89:ILE:HD11	1.85	0.59
65:RR:32:LYS:HD2	65:RR:47:ARG:HH21	1.67	0.59
3:5:1404:G:H2'	3:5:1405:C:C6	2.37	0.59
3:5:2725:A:H5''	23:R:97:ARG:HH21	1.68	0.59
14:H:93:ARG:HH21	14:H:141:LYS:HE3	1.68	0.59
3:5:2295:C:O2'	9:C:45:ARG:NH2	2.36	0.58
3:5:3873:G:H2'	3:5:3874:G:C8	2.38	0.58
3:5:4670:C:O2'	3:5:4672:A:OP2	2.17	0.58
6:9:1003:U:H5''	50:BB:165:ARG:NH2	2.17	0.58
6:9:1305:C:H2'	6:9:1306:U:C6	2.37	0.58
9:C:284:MET:HE2	9:C:287:THR:HA	1.84	0.58
52:DD:65:ARG:HA	52:DD:68:GLU:HG2	1.85	0.58
55:GG:32:MET:HE3	55:GG:54:GLY:HA3	1.85	0.58
74:Aa:87:ARG:NH2	74:Aa:94:ASP:OD2	2.36	0.58
3:5:684:G:H5'	3:5:685:C:OP2	2.04	0.58
3:5:710:G:H2'	3:5:711:A:H8	1.68	0.58
6:9:1653:U:H2'	6:9:1654:G:C8	2.37	0.58
14:H:92:MET:HE2	14:H:179:ILE:HG22	1.84	0.58
55:GG:7:PHE:HD1	55:GG:113:ILE:HB	1.68	0.58
79:Gg:133:ASN:HD22	79:Gg:139:LYS:HD3	1.67	0.58
5:8:8:U:H2'	5:8:9:A:C8	2.39	0.58
6:9:508:A:H3'	6:9:509:OMG:H8	1.67	0.58
9:C:190:ARG:O	9:C:195:LYS:NZ	2.31	0.58
17:L:204:GLU:O	17:L:207:VAL:HG22	2.03	0.58
3:5:62:A:N3	3:5:77:U:O2'	2.35	0.58
3:5:1377:G:H21	3:5:1380:G:H5''	1.67	0.58
3:5:4940:C:OP2	11:E:222:LYS:NZ	2.37	0.58
8:B:384:GLU:OE1	28:W:14:TYR:OH	2.21	0.58
34:c:53:PRO:HD2	34:c:56:ARG:HD2	1.85	0.58
1:2:69:U:H2'	1:2:70:G:H8	1.68	0.58
3:5:1391:A:H5'	22:Q:181:ARG:HH12	1.68	0.58
3:5:5006:U:H4'	3:5:5007:A:H5'	1.84	0.58
4:7:23:A:N3	4:7:118:C:O2'	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:1566:G:N7	67:TT:101:ARG:NH2	2.52	0.58
30:Y:82:ILE:HB	30:Y:85:VAL:HG22	1.86	0.58
3:5:4238:G:H2'	3:5:4239:A:H8	1.66	0.58
6:9:1758:G:O6	6:9:1774:C:N4	2.35	0.58
8:B:291:TYR:OH	8:B:315:ASN:ND2	2.36	0.58
17:L:100:PRO:O	40:i:25:ARG:NH2	2.35	0.58
18:M:123:ILE:HD11	20:O:189:ILE:HD13	1.85	0.58
39:h:66:LYS:O	39:h:70:ARG:HG3	2.03	0.58
67:TT:139:ALA:HA	67:TT:142:LYS:HE3	1.84	0.58
3:5:1503:A:H4'	3:5:1504:G:H5'	1.86	0.58
3:5:2492:C:H2'	3:5:2493:G:C8	2.38	0.58
6:9:140:U:O2'	6:9:141:A:OP1	2.22	0.58
6:9:1275:G:N2	6:9:1506:A:OP2	2.27	0.58
6:9:1458:G:OP1	79:Gg:277:THR:OG1	2.21	0.58
10:D:232:THR:HG23	10:D:234:ASP:H	1.68	0.58
32:a:75:LEU:HD13	32:a:113:GLY:HA2	1.85	0.58
66:SS:6:PRO:HG2	66:SS:9:PHE:HB2	1.85	0.58
79:Gg:219:TRP:NE1	79:Gg:226:HIS:HD2	2.02	0.58
3:5:4060:U:H2'	3:5:4061:G:C8	2.38	0.58
3:5:4584:A:H2'	3:5:4585:U:O4'	2.04	0.58
4:7:120:U:OP1	10:D:259:ARG:NH1	2.36	0.58
34:c:77:ASN:N	34:c:80:GLU:OE1	2.36	0.58
41:j:59:THR:HG22	41:j:64:MET:HE1	1.84	0.58
50:BB:163:GLN:HA	50:BB:166:LYS:HG2	1.85	0.58
53:EE:87:MET:HG2	53:EE:123:LEU:O	2.04	0.58
60:LL:79:LYS:HE2	60:LL:87:VAL:HG11	1.85	0.58
69:VV:4:ASP:OD1	69:VV:5:ALA:N	2.36	0.58
79:Gg:270:LEU:HD21	79:Gg:310:TRP:CE2	2.39	0.58
3:5:1481:C:O2'	3:5:1482:G:N3	2.31	0.58
3:5:2267:U:OP1	48:r:37:SER:OG	2.22	0.58
3:5:3657:U:H5'	7:A:246:LEU:HD23	1.85	0.58
3:5:4254:G:N3	3:5:4254:G:H2'	2.17	0.58
4:7:117:G:OP1	10:D:253:TYR:OH	2.22	0.58
6:9:551:U:H2'	6:9:552:G:H8	1.68	0.58
34:c:13:SER:OG	34:c:17:ARG:NH1	2.36	0.58
42:k:24:LYS:HG3	42:k:35:LYS:HB2	1.86	0.58
52:DD:42:THR:OG1	52:DD:43:PRO:HD3	2.03	0.58
53:EE:79:ASP:HB3	53:EE:82:TYR:HB2	1.85	0.58
79:Gg:26:GLN:NE2	79:Gg:73:SER:O	2.37	0.58
1:2:11:G:H22	1:2:24:G:H1	1.51	0.58
3:5:1195:G:H2'	3:5:1196:G:H8	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:1244:G:H2'	3:5:1245:C:C6	2.39	0.58
3:5:1481:C:O2'	3:5:1482:G:O5'	2.21	0.58
42:k:36:VAL:HG22	42:k:43:TYR:HB2	1.86	0.58
8:B:140:ASP:OD1	8:B:141:ALA:N	2.36	0.57
23:R:30:ASN:OD1	23:R:31:GLU:N	2.36	0.57
52:DD:51:LEU:HD12	52:DD:91:VAL:HG12	1.86	0.57
6:9:683:OMG:N1	6:9:1022:U:OP2	2.29	0.57
11:E:289:LEU:HD13	18:M:109:ARG:HH22	1.69	0.57
17:L:47:ALA:HB3	17:L:48:PRO:HD3	1.86	0.57
28:W:113:LYS:HA	28:W:116:LYS:HG2	1.84	0.57
1:2:2:A:H3'	1:2:3:G:H21	1.68	0.57
3:5:1961:G:N1	3:5:2024:G:O2'	2.38	0.57
3:5:2590:G:N2	3:5:2754:B9B:O2'	2.33	0.57
3:5:2718:U:H5''	3:5:2719:C:H5'	1.86	0.57
6:9:1438:A:H2'	6:9:1439:A:C8	2.39	0.57
6:9:1619:A:O2'	63:PP:82:ASP:OD2	2.22	0.57
8:B:41:VAL:HG12	8:B:188:GLY:H	1.67	0.57
9:C:339:THR:O	9:C:343:GLN:HG3	2.04	0.57
11:E:123:ASP:OD2	11:E:124:VAL:N	2.36	0.57
3:5:257:C:H2'	3:5:258:G:C8	2.39	0.57
3:5:1942:A:H2'	3:5:1943:A:C8	2.39	0.57
3:5:4619:U:H2'	3:5:4620:OMU:H6	1.86	0.57
4:7:4:U:H2'	4:7:5:A:H8	1.69	0.57
6:9:696:G:O6	6:9:730:C:N4	2.34	0.57
15:I:38:ARG:HB2	15:I:83:ASP:HB2	1.86	0.57
16:J:23:ASN:OD1	16:J:129:ASP:HB2	2.03	0.57
16:J:136:ARG:NH1	16:J:156:ARG:O	2.34	0.57
37:f:45:LYS:HE3	37:f:108:SER:HA	1.86	0.57
54:FF:99:ILE:HA	54:FF:102:LEU:HG	1.85	0.57
54:FF:128:ILE:HD12	76:Cc:22:GLY:HA2	1.87	0.57
3:5:4238:G:H2'	3:5:4239:A:C8	2.40	0.57
6:9:639:C:H2'	6:9:640:A:H8	1.68	0.57
64:QQ:40:GLU:O	64:QQ:48:GLN:NE2	2.38	0.57
3:5:1983:A:N3	3:5:2010:A:H5''	2.20	0.57
6:9:1550:G:H3'	6:9:1579:A:H61	1.70	0.57
18:M:55:MET:O	24:S:157:ARG:NH2	2.37	0.57
26:U:42:PHE:CZ	26:U:46:ARG:HD3	2.39	0.57
63:PP:86:LEU:H	63:PP:89:MET:HE3	1.70	0.57
3:5:1094:G:H2'	3:5:1095:A:H8	1.69	0.57
3:5:1459:A:OP1	22:Q:65:ARG:NH1	2.38	0.57
3:5:2588:C:OP1	3:5:2768:C:O2'	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:2756:G:O6	31:Z:51:ARG:NH2	2.32	0.57
25:T:157:GLU:HB3	25:T:159:MET:HE3	1.87	0.57
28:W:5:LEU:O	28:W:30:GLN:NE2	2.38	0.57
3:5:1398:A:H62	3:5:1419:G:H21	1.53	0.57
3:5:1420:A:N7	32:a:116:LYS:HD3	2.19	0.57
6:9:532:C:H2'	6:9:533:A:C8	2.39	0.57
8:B:322:HIS:O	8:B:342:LYS:NZ	2.34	0.57
28:W:82:ILE:HD11	55:GG:158:VAL:HG11	1.87	0.57
38:g:5:LEU:HD11	38:g:32:TYR:CE1	2.40	0.57
73:ZZ:99:LEU:HD21	73:ZZ:102:LYS:HB2	1.87	0.57
1:2:7:A:H61	1:2:66:C:H42	1.51	0.57
3:5:109:G:H5'	17:L:92:ARG:HH12	1.70	0.57
3:5:1195:G:H2'	3:5:1196:G:C8	2.40	0.57
3:5:4178:A:H2'	3:5:4179:G:H8	1.70	0.57
64:QQ:51:LEU:HD11	64:QQ:81:ILE:HD12	1.86	0.57
73:ZZ:66:LYS:HD2	73:ZZ:111:ARG:HH12	1.69	0.57
3:5:3809:G:OP2	3:5:3809:G:N2	2.30	0.57
3:5:4699:U:OP2	44:m:85:ARG:NH2	2.34	0.57
50:BB:147:ASN:OD1	50:BB:148:ASN:N	2.38	0.57
3:5:1818:G:H2'	3:5:1820:U:OP2	2.05	0.56
3:5:3911:C:H2'	3:5:3912:U:H6	1.70	0.56
5:8:97:A:OP2	39:h:66:LYS:NZ	2.34	0.56
79:Gg:228:TYR:OH	79:Gg:261:LEU:HD12	2.04	0.56
3:5:958:G:N2	11:E:128:LEU:O	2.23	0.56
3:5:4994:G:H2'	3:5:4995:U:C6	2.40	0.56
6:9:555:A:N6	6:9:589:G:N3	2.52	0.56
6:9:581:U:OP1	58:JJ:133:ARG:NH2	2.37	0.56
7:A:27:ALA:O	7:A:128:ARG:NH2	2.38	0.56
1:2:24:G:H21	3:5:3770:U:H5'	1.69	0.56
3:5:1364:U:OP2	17:L:36:ARG:NH2	2.39	0.56
3:5:2765:A:H2'	3:5:2766:A:C8	2.40	0.56
6:9:107:A:H2'	6:9:108:G:C8	2.41	0.56
6:9:804:U:H2'	6:9:805:U:C6	2.40	0.56
6:9:928:G:H2'	6:9:929:G:C8	2.40	0.56
6:9:1797:U:H2'	6:9:1798:C:C6	2.40	0.56
8:B:41:VAL:HA	8:B:187:GLY:HA3	1.87	0.56
13:G:215:ASP:OD1	13:G:216:PRO:HD2	2.05	0.56
35:d:64:ILE:HG23	35:d:68:LEU:HD23	1.88	0.56
37:f:46:ARG:HD3	37:f:106:TYR:CE1	2.41	0.56
40:i:69:ALA:O	40:i:73:ILE:HG13	2.05	0.56
50:BB:47:THR:OG1	50:BB:65:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:UU:61:LEU:HB2	68:UU:82:MET:HB3	1.87	0.56
3:5:2474:G:H5'	29:X:47:ARG:HH21	1.70	0.56
51:CC:128:VAL:HG11	51:CC:155:ILE:HG12	1.88	0.56
3:5:942:G:OP1	12:F:244:ARG:NH1	2.38	0.56
6:9:532:C:H2'	6:9:533:A:H8	1.70	0.56
29:X:79:PHE:CZ	29:X:99:ILE:HD11	2.40	0.56
34:c:54:ALA:HA	34:c:57:LYS:HG2	1.85	0.56
50:BB:129:THR:OG1	50:BB:131:ASP:O	2.23	0.56
68:UU:19:ARG:HH12	68:UU:92:HIS:HA	1.71	0.56
76:Cc:44:ARG:NH2	76:Cc:63:ARG:O	2.39	0.56
3:5:449:C:H4'	3:5:450:G:O5'	2.04	0.56
3:5:1806:G:H2'	3:5:1807:C:H6	1.69	0.56
3:5:1979:A:O2'	3:5:1980:U:OP1	2.20	0.56
9:C:36:ILE:HD11	9:C:122:TYR:CE2	2.40	0.56
19:N:146:PRO:HB2	39:h:104:THR:HG23	1.88	0.56
20:O:155:THR:O	20:O:158:GLU:HG3	2.05	0.56
20:O:166:ILE:HD13	20:O:169:ARG:HH21	1.71	0.56
74:Aa:32:LYS:O	74:Aa:37:LYS:NZ	2.33	0.56
1:2:23:C:H2'	1:2:24:G:C8	2.41	0.56
3:5:3725:G:N2	3:5:3728:A:OP2	2.32	0.56
5:8:52:A:H62	43:l:27:ILE:HD13	1.71	0.56
10:D:62:CYS:HB3	10:D:105:LEU:HD22	1.87	0.56
24:S:164:LYS:HB3	24:S:165:PRO:HD3	1.86	0.56
30:Y:67:ILE:O	30:Y:84:ARG:NH2	2.35	0.56
53:EE:137:PRO:HB2	53:EE:150:PRO:HD2	1.88	0.56
54:FF:167:LYS:HB2	54:FF:171:GLU:OE2	2.05	0.56
79:Gg:99:ARG:NH1	79:Gg:135:LEU:HA	2.20	0.56
3:5:2334:C:OP2	9:C:195:LYS:NZ	2.38	0.56
3:5:2844:A:O2'	3:5:4631:G:H4'	2.06	0.56
3:5:4348:A:O2'	3:5:4350:C:OP2	2.21	0.56
3:5:4987:C:OP1	8:B:176:LYS:NZ	2.36	0.56
8:B:196:TRP:NE1	8:B:200:ARG:HH12	2.04	0.56
31:Z:33:THR:OG1	31:Z:35:ASP:OD1	2.24	0.56
49:AA:140:VAL:HG23	49:AA:142:LEU:HD22	1.87	0.56
58:JJ:113:GLN:OE1	58:JJ:154:GLN:NE2	2.39	0.56
1:2:4:C:H2'	1:2:5:A:H8	1.70	0.56
3:5:2018:C:H2'	3:5:2019:C:C6	2.41	0.56
3:5:4936:G:C5	11:E:186:ARG:HD3	2.41	0.56
6:9:1758:G:H2'	6:9:1759:G:C8	2.41	0.56
12:F:150:ASN:HD22	12:F:190:ILE:HD13	1.70	0.56
51:CC:74:LYS:HE3	51:CC:269:PHE:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:EE:192:ILE:HG13	53:EE:243:GLY:HA3	1.88	0.56
61:NN:83:ASP:OD1	61:NN:84:LEU:N	2.38	0.56
67:TT:10:ASN:HB3	67:TT:13:GLU:OE2	2.05	0.56
74:Aa:90:GLU:OE1	74:Aa:90:GLU:N	2.32	0.56
3:5:1199:G:H2'	3:5:1200:G:C8	2.40	0.56
3:5:1354:A:OP1	22:Q:108:ARG:NH2	2.39	0.56
3:5:1518:A:H61	17:L:19:GLN:HE22	1.52	0.56
3:5:4859:C:H2'	3:5:4860:G:H8	1.71	0.56
3:5:4894:A:H3'	3:5:4895:C:H6	1.69	0.56
6:9:809:A:H2'	6:9:810:A:O4'	2.06	0.56
6:9:1714:U:H2'	6:9:1715:A:C8	2.41	0.56
16:J:31:ASP:O	16:J:35:ARG:HG3	2.07	0.56
3:5:1198:G:H2'	3:5:1199:G:C8	2.41	0.55
3:5:2411:C:H2'	3:5:2412:A:H8	1.71	0.55
3:5:4944:C:N4	37:f:58:VAL:O	2.38	0.55
6:9:1736:G:H2'	6:9:1737:G:C8	2.41	0.55
6:9:1760:G:O6	6:9:1772:C:N4	2.35	0.55
9:C:290:SER:O	9:C:294:LYS:HG2	2.06	0.55
12:F:121:PHE:O	12:F:204:ASN:ND2	2.37	0.55
51:CC:169:TYR:OH	51:CC:175:GLY:O	2.21	0.55
55:GG:5:ILE:HD13	55:GG:111:LEU:HB2	1.88	0.55
57:II:80:ASP:OD1	57:II:81:VAL:N	2.40	0.55
3:5:162:A:H2'	3:5:163:A:C8	2.42	0.55
3:5:4108:G:H2'	3:5:4109:G:C8	2.42	0.55
3:5:4239:A:H2'	3:5:4240:G:H8	1.71	0.55
9:C:263:LEU:HD12	9:C:273:LEU:HD21	1.88	0.55
15:I:112:GLN:OE1	15:I:112:GLN:N	2.39	0.55
23:R:4:LEU:HD23	23:R:24:LEU:HD23	1.88	0.55
38:g:69:LYS:HG2	38:g:73:HIS:HD2	1.71	0.55
61:NN:35:GLU:OE1	61:NN:39:LYS:NZ	2.39	0.55
3:5:4251:A:H5''	16:J:108:GLY:HA3	1.87	0.55
6:9:118:C:H1'	6:9:445:A:C5	2.42	0.55
24:S:95:ARG:NH1	24:S:97:TYR:OH	2.39	0.55
68:UU:22:ILE:HG22	68:UU:114:VAL:HG12	1.89	0.55
73:ZZ:96:LEU:HD12	73:ZZ:97:ILE:HG23	1.89	0.55
3:5:758:G:H2'	3:5:759:G:O4'	2.06	0.55
3:5:4591:U:H2'	3:5:4592:C:C6	2.41	0.55
3:5:4753:U:OP1	37:f:100:ARG:NH1	2.38	0.55
6:9:191:A:H3'	6:9:192:C:H5''	1.88	0.55
10:D:45:ASN:OD1	10:D:68:ARG:NH1	2.35	0.55
16:J:120:ASP:OD2	16:J:122:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Gg:177:TRP:HA	79:Gg:184:LEU:HA	1.87	0.55
3:5:978:C:OP2	11:E:61:ARG:NH1	2.38	0.55
3:5:1761:G:O6	3:5:1772:C:N4	2.39	0.55
5:8:23:C:OP1	30:Y:15:ARG:NH1	2.40	0.55
6:9:528:A:H2'	6:9:529:A:H8	1.71	0.55
6:9:560:A:OP2	58:JJ:177:ASN:ND2	2.39	0.55
8:B:196:TRP:CE2	8:B:200:ARG:NH1	2.74	0.55
56:HH:145:ARG:HG3	56:HH:155:LYS:HZ2	1.72	0.55
72:YY:80:ASP:OD1	72:YY:81:TYR:N	2.40	0.55
76:Cc:51:ARG:HG2	76:Cc:52:GLU:H	1.70	0.55
3:5:970:G:H2'	3:5:971:U:O4'	2.07	0.55
3:5:4896:G:H2'	3:5:4897:G:H8	1.72	0.55
4:7:4:U:H2'	4:7:5:A:C8	2.41	0.55
6:9:17:C:O2'	6:9:1194:A:N1	2.38	0.55
6:9:1491:G:H2'	6:9:1492:U:C6	2.42	0.55
6:9:1533:A:H2	6:9:1536:G:N3	2.05	0.55
48:r:82:ILE:HG22	48:r:89:THR:HG22	1.88	0.55
60:LL:126:VAL:HG12	60:LL:145:VAL:HG12	1.89	0.55
3:5:4680:G:H2'	3:5:4681:A:C8	2.42	0.55
6:9:942:G:H2'	6:9:943:U:C6	2.42	0.55
6:9:1568:C:H2'	6:9:1569:A:C8	2.41	0.55
7:A:116:LEU:HB3	7:A:126:LEU:HB2	1.89	0.55
28:W:97:LYS:HD2	28:W:98:PRO:CD	2.37	0.55
51:CC:134:ASN:HB2	51:CC:167:ARG:HH12	1.71	0.55
3:5:152:U:P	19:N:49:ARG:HH12	2.30	0.55
3:5:1414:C:N4	3:5:1415:G:O6	2.39	0.55
6:9:1678:A2M:OP2	54:FF:63:LYS:NZ	2.40	0.55
16:J:146:ARG:HD3	16:J:147:ARG:HG3	1.88	0.55
24:S:35:PRO:HD2	24:S:39:VAL:HG11	1.87	0.55
55:GG:227:GLN:HA	55:GG:230:LYS:HE3	1.88	0.55
59:KK:37:ASP:OD1	59:KK:38:LYS:N	2.38	0.55
3:5:519:C:O2'	17:L:115:GLN:NE2	2.40	0.55
3:5:2475:G:O6	29:X:48:ARG:NH2	2.40	0.55
3:5:4272:G:OP2	3:5:4272:G:N2	2.24	0.55
3:5:4736:C:H2'	3:5:4737:G:H8	1.72	0.55
7:A:108:PRO:HD3	47:p:90:LYS:HD3	1.89	0.55
58:JJ:65:GLU:OE1	58:JJ:66:LYS:HG2	2.07	0.55
63:PP:85:ILE:HD11	63:PP:111:MET:O	2.07	0.55
79:Gg:34:ALA:HB1	79:Gg:66:VAL:HG13	1.89	0.55
3:5:709:C:H1'	3:5:4942:C:H5	1.71	0.55
3:5:4537:C:H2'	3:5:4538:G:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:4915:G:H2'	3:5:4916:G:C8	2.42	0.55
15:I:52:MET:HE1	15:I:159:PHE:HE1	1.72	0.55
54:FF:71:ARG:NH1	54:FF:148:ASN:OD1	2.40	0.55
63:PP:16:THR:HA	63:PP:21:ASP:HA	1.88	0.55
66:SS:60:THR:O	66:SS:64:VAL:HG23	2.07	0.55
3:5:233:U:H2'	3:5:234:G:C8	2.41	0.54
3:5:1100:U:O4	3:5:1195:G:O6	2.25	0.54
3:5:1976:G:O6	3:5:1991:A:N7	2.41	0.54
3:5:4135:G:H2'	3:5:4136:G:H8	1.72	0.54
3:5:4459:U:H2'	3:5:4460:U:C6	2.42	0.54
15:I:9:TYR:OH	15:I:98:ARG:O	2.15	0.54
28:W:97:LYS:HE3	28:W:99:GLU:HB2	1.88	0.54
59:KK:15:LEU:HG	59:KK:71:LEU:HD22	1.89	0.54
63:PP:64:LYS:NZ	63:PP:90:VAL:O	2.38	0.54
79:Gg:107:ASP:OD1	79:Gg:108:VAL:N	2.40	0.54
3:5:520:U:H2'	3:5:521:C:C6	2.43	0.54
6:9:1217:A:H2'	6:9:1218:C:C6	2.42	0.54
44:m:53:GLU:OE1	44:m:55:SER:OG	2.19	0.54
68:UU:46:LYS:HE2	68:UU:100:GLN:HE22	1.72	0.54
73:ZZ:91:LEU:HD22	73:ZZ:96:LEU:HD11	1.88	0.54
3:5:72:C:N3	17:L:60:ARG:NH2	2.47	0.54
3:5:4322:G:N2	3:5:4325:A:OP2	2.39	0.54
6:9:678:U:OP2	6:9:1026:C:N4	2.32	0.54
6:9:788:G:H2'	6:9:789:G:C8	2.42	0.54
6:9:1306:U:H2'	6:9:1307:U:O4'	2.06	0.54
32:a:132:ARG:O	32:a:136:LYS:HG3	2.07	0.54
53:EE:87:MET:SD	53:EE:100:ARG:HD3	2.47	0.54
79:Gg:108:VAL:HA	79:Gg:124:SER:HA	1.88	0.54
3:5:651:C:H2'	3:5:652:G:H8	1.73	0.54
3:5:1237:A:H8	12:F:47:LYS:HG3	1.72	0.54
3:5:1339:U:H2'	3:5:1340:C:C6	2.42	0.54
3:5:3713:U:H3'	3:5:3714:G:H5''	1.90	0.54
15:I:17:TYR:O	15:I:96:VAL:HG12	2.07	0.54
54:FF:58:ALA:HB3	54:FF:62:ARG:HH11	1.72	0.54
65:RR:100:PRO:HG2	65:RR:122:PRO:HD3	1.90	0.54
3:5:196:C:H4'	30:Y:126:ARG:HG2	1.88	0.54
3:5:2097:A:H3'	3:5:2098:G:H5'	1.89	0.54
3:5:2539:C:H2'	3:5:2540:C:C6	2.42	0.54
3:5:4188:U:H2'	3:5:4189:U:C6	2.43	0.54
6:9:183:G:O2'	6:9:184:G:O4'	2.26	0.54
11:E:264:ILE:HB	11:E:270:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:41:ILE:HD11	14:H:69:THR:HB	1.89	0.54
51:CC:65:LYS:HG3	51:CC:273:LEU:HD11	1.89	0.54
67:TT:110:LEU:HD12	67:TT:112:MET:HG2	1.90	0.54
72:YY:60:PHE:CD2	72:YY:71:GLY:HA3	2.42	0.54
3:5:239:C:OP1	30:Y:46:SER:OG	2.26	0.54
3:5:1332:C:H2'	3:5:1333:A:C8	2.41	0.54
6:9:1714:U:H2'	6:9:1715:A:H8	1.72	0.54
14:H:44:GLU:HB3	14:H:58:ASP:OD1	2.08	0.54
20:O:158:GLU:O	20:O:162:GLU:OE1	2.26	0.54
38:g:87:VAL:O	38:g:91:ILE:HG13	2.08	0.54
49:AA:42:LYS:HE2	65:RR:99:ASP:OD2	2.08	0.54
50:BB:37:ALA:N	50:BB:231:LEU:O	2.33	0.54
76:Cc:15:THR:HG23	76:Cc:33:GLU:OE1	2.08	0.54
79:Gg:254:PRO:HA	79:Gg:285:GLN:HA	1.90	0.54
3:5:121:A:OP1	13:G:163:LYS:NZ	2.35	0.54
3:5:1398:A:N6	3:5:1419:G:H21	2.05	0.54
3:5:1824:G:H5''	25:T:35:LYS:HE2	1.88	0.54
3:5:2083:C:OP2	22:Q:14:ARG:NH2	2.41	0.54
3:5:4135:G:H2'	3:5:4136:G:C8	2.43	0.54
3:5:4314:C:H4'	25:T:68:THR:HG21	1.89	0.54
16:J:112:HIS:HD2	16:J:126:TYR:H	1.54	0.54
20:O:36:VAL:HG12	20:O:108:ILE:HG12	1.90	0.54
59:KK:32:HIS:CD2	59:KK:34:GLU:HG3	2.43	0.54
68:UU:20:ILE:HD11	68:UU:91:LEU:HD12	1.90	0.54
74:Aa:46:GLU:CD	74:Aa:47:ALA:H	2.15	0.54
79:Gg:14:HIS:CE1	79:Gg:41:ILE:HD12	2.42	0.54
3:5:2608:G:H2'	3:5:2609:G:H8	1.73	0.54
6:9:1407:U:H2'	6:9:1408:U:C6	2.43	0.54
16:J:112:HIS:CD2	16:J:126:TYR:H	2.25	0.54
19:N:18:VAL:HG12	19:N:19:MET:HE2	1.90	0.54
19:N:191:ALA:O	19:N:195:ARG:HG3	2.06	0.54
35:d:29:ILE:O	35:d:33:ILE:HG12	2.07	0.54
55:GG:56:ASN:O	55:GG:106:LEU:HB2	2.08	0.54
65:RR:90:ALA:O	65:RR:93:GLN:NE2	2.24	0.54
71:XX:124:LYS:HG2	71:XX:129:SER:HA	1.89	0.54
75:Bb:14:GLU:HA	75:Bb:17:ARG:HE	1.71	0.54
3:5:1185:G:O2'	10:D:278:ASP:OD2	2.25	0.54
3:5:1405:C:H2'	3:5:1406:G:H8	1.73	0.54
3:5:1484:G:O2'	3:5:1486:C:OP2	2.25	0.54
3:5:1867:A:H2'	3:5:1868:A:C8	2.42	0.54
3:5:4691:A:O2'	14:H:68:ALA:O	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:948:C:H2'	6:9:949:G:H8	1.73	0.54
22:Q:122:THR:OG1	22:Q:124:ASP:OD1	2.19	0.54
50:BB:71:LEU:HD23	50:BB:82:ARG:HG3	1.90	0.54
59:KK:31:LYS:NZ	59:KK:39:ASN:HB3	2.23	0.54
72:YY:7:ILE:HG22	72:YY:27:VAL:HG22	1.90	0.54
3:5:267:G:H2'	3:5:268:G:H8	1.71	0.54
3:5:1634:A:H62	7:A:3:ARG:HH12	1.54	0.54
3:5:2296:G:O4'	9:C:45:ARG:NH2	2.41	0.54
8:B:312:LYS:NZ	8:B:368:ILE:O	2.25	0.54
66:SS:139:THR:O	66:SS:144:ARG:NH2	2.40	0.54
72:YY:88:LYS:HB3	72:YY:97:TYR:CE1	2.43	0.54
3:5:406:C:O2'	3:5:407:A:OP1	2.24	0.53
3:5:1317:U:H2'	3:5:1318:C:C6	2.43	0.53
3:5:1629:G:N1	7:A:208:GLU:OE1	2.35	0.53
3:5:4392:G:N2	3:5:4395:U:O2	2.37	0.53
6:9:128:U:H3'	6:9:129:C:C6	2.43	0.53
9:C:13:GLU:OE1	9:C:161:TYR:OH	2.21	0.53
69:VV:66:ASP:OD1	69:VV:67:ASP:N	2.41	0.53
74:Aa:38:LYS:HB2	74:Aa:71:LEU:HB2	1.91	0.53
75:Bb:33:MET:HE1	75:Bb:73:LEU:HD11	1.90	0.53
3:5:942:G:H3'	12:F:147:LYS:HD2	1.88	0.53
3:5:2448:G:H2'	3:5:2449:A:C8	2.44	0.53
13:G:229:LYS:HZ3	40:i:39:PHE:HE1	1.56	0.53
23:R:23:TRP:CE3	23:R:51:ILE:HG12	2.44	0.53
69:VV:82:ASN:OD1	69:VV:83:PHE:N	2.41	0.53
3:5:398:A2M:O5'	3:5:398:A2M:H8	2.07	0.53
3:5:1174:G:H2'	3:5:1175:A:C8	2.44	0.53
3:5:1846:G:H2'	3:5:1847:C:H6	1.73	0.53
3:5:2404:A:H61	3:5:2787:A:H61	1.55	0.53
3:5:2696:A:H62	42:k:35:LYS:NZ	2.07	0.53
3:5:2765:A:H2'	3:5:2766:A:H8	1.73	0.53
6:9:51:U:H2'	6:9:52:G:C8	2.44	0.53
13:G:218:GLU:OE1	19:N:11:TRP:NE1	2.41	0.53
22:Q:178:ARG:N	32:a:51:GLY:HA2	2.22	0.53
23:R:78:ILE:HD13	23:R:81:ARG:HH21	1.74	0.53
51:CC:209:VAL:HG23	51:CC:210:PRO:HD3	1.91	0.53
55:GG:31:ARG:HG2	55:GG:101:ILE:HG22	1.90	0.53
61:NN:26:LEU:HD21	61:NN:60:VAL:HG12	1.91	0.53
3:5:711:A:H2'	3:5:712:C:C6	2.43	0.53
3:5:1991:A:H4'	3:5:1991:A:OP1	2.07	0.53
6:9:375:U:H2'	6:9:376:A:H8	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:789:G:H2'	6:9:790:C:C6	2.43	0.53
6:9:1227:G:C2	6:9:1228:A:C8	2.95	0.53
6:9:1356:G:H2'	6:9:1357:A:C8	2.43	0.53
60:LL:127:THR:HB	60:LL:144:LYS:HG2	1.90	0.53
67:TT:73:GLY:O	67:TT:94:ARG:NH2	2.42	0.53
3:5:3692:A:H62	3:5:3823:G:N2	2.00	0.53
3:5:3710:G:N2	3:5:3711:A:N1	2.56	0.53
9:C:302:LEU:HD22	22:Q:38:ARG:HB3	1.91	0.53
11:E:248:GLN:HA	11:E:251:VAL:HG22	1.90	0.53
53:EE:104:ASP:HB3	53:EE:110:ALA:HB2	1.90	0.53
79:Gg:11:LEU:HB2	79:Gg:307:VAL:HB	1.90	0.53
3:5:1308:C:H2'	3:5:1309:C:C6	2.43	0.53
6:9:67:C:H2'	55:GG:167:LYS:HZ2	1.73	0.53
6:9:1462:U:H2'	6:9:1464:C:C4	2.44	0.53
21:P:86:LYS:HA	21:P:89:GLU:HG3	1.91	0.53
3:5:1836:G:O5'	25:T:129:LYS:NZ	2.41	0.53
3:5:2486:G:H2'	3:5:2487:G:C8	2.44	0.53
3:5:3897:B8K:O2'	3:5:3898:G:OP2	2.26	0.53
6:9:1712:A:H2'	6:9:1713:C:C6	2.44	0.53
14:H:95:VAL:HG22	44:m:52:ILE:HD11	1.91	0.53
51:CC:179:THR:HG21	51:CC:198:ALA:H	1.74	0.53
53:EE:160:ILE:HG22	53:EE:172:PHE:HB3	1.89	0.53
3:5:162:A:H2'	3:5:163:A:H8	1.71	0.53
3:5:1617:G:H1'	3:5:2513:A:N6	2.24	0.53
3:5:5057:C:H2'	3:5:5058:A:C8	2.44	0.53
6:9:507:G:O6	72:YY:105:LYS:NZ	2.42	0.53
6:9:945:U:H2'	6:9:946:U:C6	2.44	0.53
6:9:1593:C:O2	67:TT:12:GLN:NE2	2.40	0.53
7:A:234:LYS:HG3	7:A:238:ILE:HD12	1.90	0.53
53:EE:153:LEU:HD23	55:GG:216:ARG:HE	1.73	0.53
69:VV:21:ASN:HB3	70:WW:67:GLY:HA3	1.90	0.53
69:VV:60:ARG:HA	69:VV:65:SER:HB2	1.91	0.53
79:Gg:244:ASN:OD1	79:Gg:245:ARG:N	2.42	0.53
3:5:2661:U:O3'	3:5:2662:G:H4'	2.09	0.53
6:9:1697:A:N3	51:CC:115:GLN:NE2	2.57	0.53
32:a:132:ARG:HA	32:a:135:GLU:HG2	1.91	0.53
3:5:1435:G:O2'	3:5:2105:A:N1	2.37	0.53
3:5:1479:G:H2'	3:5:1480:C:C6	2.44	0.53
3:5:1762:C:H2'	3:5:1763:C:C6	2.43	0.53
3:5:4872:2MG:HM21	20:O:202:LEU:HA	1.91	0.53
6:9:1781:A:H2'	6:9:1782:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:165:TRP:CZ2	16:J:169:LYS:HD3	2.44	0.53
17:L:92:ARG:HH21	17:L:98:VAL:HB	1.74	0.53
25:T:64:VAL:HA	25:T:74:ILE:HG22	1.91	0.53
56:HH:25:GLN:HA	56:HH:28:LEU:HB3	1.91	0.53
58:JJ:48:PHE:CE2	58:JJ:52:LYS:HE2	2.44	0.53
61:NN:119:GLU:O	61:NN:123:HIS:ND1	2.42	0.53
3:5:2046:G:H5'	20:O:60:LYS:HE3	1.90	0.52
3:5:2404:A:H61	3:5:2787:A:N6	2.08	0.52
3:5:3720:G:H22	3:5:3733:A:H2	1.57	0.52
3:5:4178:A:H2'	3:5:4179:G:C8	2.43	0.52
6:9:1398:G:H1'	79:Gg:63:SER:HB3	1.91	0.52
6:9:1643:U:H2'	6:9:1644:C:C6	2.44	0.52
6:9:1824:A:O2'	6:9:1825:A:H5''	2.09	0.52
8:B:17:LEU:O	8:B:19:ARG:N	2.42	0.52
23:R:136:ARG:HA	23:R:139:MET:HG2	1.90	0.52
26:U:91:LEU:HD22	26:U:96:LEU:HD11	1.91	0.52
52:DD:1:MET:HE1	52:DD:3:VAL:HG12	1.91	0.52
63:PP:83:MET:HB3	63:PP:116:LEU:HG	1.92	0.52
77:Dd:30:LEU:HA	77:Dd:39:CYS:HA	1.91	0.52
3:5:1844:G:OP1	33:b:22:LYS:NZ	2.39	0.52
3:5:2318:G:N2	3:5:2321:G:OP2	2.25	0.52
3:5:4504:C:H2'	3:5:4505:C:C6	2.44	0.52
5:8:155:C:H2'	5:8:156:U:O4'	2.09	0.52
6:9:848:U:H2'	6:9:849:A:C8	2.44	0.52
6:9:960:U:O2'	6:9:962:A:N7	2.37	0.52
6:9:1013:U:OP1	6:9:1129:G:O2'	2.28	0.52
8:B:46:PHE:CE2	8:B:81:THR:OG1	2.60	0.52
10:D:37:VAL:HG12	10:D:50:ARG:HD3	1.89	0.52
18:M:26:ALA:HB2	18:M:77:TRP:HZ3	1.74	0.52
21:P:64:ASN:HB2	21:P:80:GLN:OE1	2.09	0.52
53:EE:175:PHE:HE2	53:EE:225:ILE:HG21	1.74	0.52
3:5:85:G:O2'	3:5:97:G:O6	2.23	0.52
3:5:1442:C:H2'	3:5:1443:A:C8	2.45	0.52
3:5:1999:A:O2'	3:5:2000:G:O4'	2.22	0.52
6:9:691:G:H2'	6:9:692:G:C8	2.43	0.52
6:9:1424:G:H2'	6:9:1425:G:H8	1.74	0.52
41:j:52:LYS:O	41:j:56:ARG:HG3	2.10	0.52
44:m:77:LEU:HD12	44:m:95:LEU:HD11	1.91	0.52
79:Gg:216:ALA:HB3	79:Gg:230:LEU:HB2	1.90	0.52
3:5:2543:A:H2	3:5:2773:OMG:HN21	1.57	0.52
3:5:4673:U:OP2	27:V:15:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:1220:A:H2'	6:9:1221:G:O4'	2.09	0.52
6:9:1286:G:N2	6:9:1312:G:O2'	2.43	0.52
6:9:1737:G:OP1	55:GG:94:ARG:NH2	2.42	0.52
6:9:1788:A:H2'	6:9:1789:G:O4'	2.10	0.52
8:B:63:PRO:HD2	8:B:357:ARG:NH2	2.25	0.52
17:L:42:ARG:HA	17:L:45:ARG:HG2	1.90	0.52
19:N:178:HIS:HA	19:N:181:HIS:CE1	2.44	0.52
51:CC:78:LEU:HB3	51:CC:97:PHE:CD2	2.45	0.52
3:5:1812:C:H5'	33:b:56:LYS:HE2	1.92	0.52
3:5:2492:C:H2'	3:5:2493:G:H8	1.74	0.52
3:5:2555:G:H2'	3:5:2556:G:C8	2.44	0.52
3:5:3659:G:H4'	7:A:227:ARG:HH22	1.74	0.52
6:9:163:U:O3'	55:GG:83:CYS:HA	2.09	0.52
6:9:1854:U:H2'	6:9:1855:G:H8	1.75	0.52
8:B:214:ASP:OD1	8:B:283:LYS:NZ	2.41	0.52
43:l:36:ARG:HG3	43:l:37:TYR:CD1	2.44	0.52
50:BB:121:ILE:HD12	50:BB:161:VAL:HG13	1.92	0.52
51:CC:168:GLY:HA2	69:VV:1:MET:HE1	1.90	0.52
56:HH:134:VAL:HG12	56:HH:173:PHE:CE2	2.45	0.52
71:XX:105:PHE:HD1	71:XX:121:LYS:HB2	1.75	0.52
3:5:2562:G:N2	3:5:2565:A:OP2	2.38	0.52
3:5:2640:G:H2'	3:5:2641:A:H8	1.74	0.52
3:5:3633:C:H2'	3:5:3634:G:C8	2.45	0.52
6:9:1588:A:H2'	6:9:1589:A:C8	2.44	0.52
14:H:94:SER:HB3	14:H:142:ASP:HB3	1.91	0.52
20:O:194:ASP:OD1	20:O:195:VAL:N	2.42	0.52
24:S:94:TYR:OH	24:S:96:GLU:OE2	2.12	0.52
56:HH:19:PHE:HZ	56:HH:60:ILE:HD12	1.74	0.52
56:HH:140:VAL:HG11	56:HH:159:ASP:HB3	1.91	0.52
59:KK:41:PRO:HD2	59:KK:44:HIS:ND1	2.24	0.52
3:5:161:G:H2'	3:5:162:A:H8	1.75	0.52
3:5:1188:C:H2'	3:5:1189:G:H8	1.75	0.52
3:5:1415:G:H2'	3:5:1416:G:C8	2.44	0.52
3:5:1942:A:H2'	3:5:1943:A:H8	1.75	0.52
3:5:2003:G:H22	3:5:2016:C:H42	1.57	0.52
3:5:2011:C:H3'	3:5:2012:A:H8	1.74	0.52
3:5:2696:A:H62	42:k:35:LYS:HZ2	1.58	0.52
3:5:4291:G:HO2'	3:5:4328:G:HO2'	1.50	0.52
3:5:4537:C:H2'	3:5:4538:G:H8	1.74	0.52
6:9:656:G:H5'	6:9:662:G:N2	2.25	0.52
6:9:1201:U:H2'	6:9:1202:U:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:115:VAL:O	9:C:120:LYS:NZ	2.42	0.52
15:I:52:MET:HE1	15:I:159:PHE:CE1	2.45	0.52
19:N:79:ALA:HB1	19:N:81:TYR:CZ	2.45	0.52
31:Z:92:ASP:HB3	31:Z:95:VAL:HG12	1.92	0.52
54:FF:91:ARG:HD2	73:ZZ:103:HIS:CE1	2.45	0.52
1:2:38:A:O2'	6:9:1058:A:OP1	2.28	0.52
3:5:1438:U:O2'	3:5:1440:U:OP2	2.23	0.52
3:5:1537:A:H2'	3:5:1538:U:C6	2.45	0.52
3:5:2029:A:H2'	3:5:2030:A:C8	2.45	0.52
6:9:943:U:C2	6:9:944:A:C8	2.98	0.52
53:EE:181:CYS:SG	53:EE:225:ILE:HG23	2.50	0.52
59:KK:15:LEU:HD22	59:KK:49:MET:HE3	1.92	0.52
62:OO:147:ARG:HA	74:Aa:28:ARG:HH11	1.74	0.52
3:5:1846:G:H2'	3:5:1847:C:C6	2.45	0.52
3:5:4518:A:OP2	8:B:258:HIS:HB2	2.10	0.52
11:E:216:THR:H	11:E:219:TYR:HB3	1.75	0.52
12:F:154:TYR:CE1	12:F:186:MET:HG2	2.45	0.52
28:W:97:LYS:HG3	28:W:99:GLU:H	1.75	0.52
52:DD:26:THR:HA	52:DD:34:TYR:HD2	1.75	0.52
54:FF:31:ASN:OD1	54:FF:32:ASP:N	2.43	0.52
57:II:113:TYR:CD1	57:II:121:LEU:HD22	2.45	0.52
66:SS:33:ILE:HD11	66:SS:71:MET:HE1	1.92	0.52
3:5:669:C:O2'	3:5:670:G:H8	1.93	0.52
3:5:1802:A:H5''	3:5:1803:G:H5'	1.90	0.52
3:5:4088:C:H2'	3:5:4089:G:C8	2.45	0.52
6:9:1396:A:O2'	6:9:1398:G:N7	2.37	0.52
6:9:1520:G:N3	6:9:1520:G:H2'	2.24	0.52
26:U:87:THR:O	26:U:91:LEU:HG	2.10	0.52
40:i:66:ASP:HB3	40:i:87:ARG:HH22	1.74	0.52
50:BB:82:ARG:HH11	50:BB:103:MET:HE1	1.75	0.52
53:EE:37:LYS:HB2	53:EE:40:GLU:HG2	1.92	0.52
56:HH:66:VAL:HG22	56:HH:96:ALA:HB1	1.92	0.52
57:II:90:LEU:HD22	57:II:95:THR:HG21	1.91	0.52
62:OO:34:PHE:HB3	62:OO:41:PHE:HB2	1.90	0.52
79:Gg:255:SER:HB3	79:Gg:271:LYS:HD2	1.92	0.52
1:2:36:U:H2'	1:2:37:T6A:C8	2.45	0.51
3:5:318:A:H2'	3:5:319:A:C8	2.45	0.51
3:5:369:G:N2	3:5:372:A:OP2	2.33	0.51
3:5:651:C:H2'	3:5:652:G:C8	2.44	0.51
3:5:1094:G:H2'	3:5:1095:A:C8	2.45	0.51
3:5:1245:C:N4	3:5:1246:G:O6	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:1730:U:H4'	25:T:100:LYS:HB2	1.92	0.51
13:G:207:LEU:HG	13:G:257:PHE:HB2	1.90	0.51
37:f:50:VAL:HG22	37:f:69:VAL:HG22	1.92	0.51
51:CC:166:ARG:H	51:CC:247:THR:CG2	2.22	0.51
72:YY:25:ILE:HD11	72:YY:73:GLY:HA3	1.91	0.51
3:5:1804:A:H4'	3:5:1805:A:O5'	2.09	0.51
6:9:115:U:H2'	6:9:116:OMU:C6	2.40	0.51
10:D:50:ARG:NH2	10:D:147:ASP:OD2	2.43	0.51
23:R:99:MET:O	23:R:103:ARG:HG2	2.09	0.51
33:b:32:LEU:HD13	33:b:43:MET:HE1	1.91	0.51
51:CC:179:THR:OG1	51:CC:221:ASP:OD2	2.25	0.51
52:DD:43:PRO:O	52:DD:43:PRO:HD2	2.09	0.51
56:HH:138:GLU:OE1	61:NN:19:ARG:NH2	2.41	0.51
57:II:139:LYS:HG2	57:II:141:ARG:HH21	1.73	0.51
11:E:181:PRO:HG2	11:E:184:LEU:HD22	1.92	0.51
17:L:203:ALA:O	17:L:207:VAL:HG13	2.10	0.51
22:Q:154:LYS:NZ	22:Q:158:THR:HG22	2.26	0.51
74:Aa:7:ASN:ND2	74:Aa:10:ARG:O	2.42	0.51
3:5:980:C:OP2	11:E:68:LYS:HE2	2.10	0.51
3:5:2491:C:H2'	3:5:2492:C:C6	2.45	0.51
3:5:4691:A:OP1	14:H:75:SER:OG	2.21	0.51
3:5:4915:G:H2'	3:5:4916:G:H8	1.75	0.51
5:8:32:C:H2'	5:8:33:G:O4'	2.10	0.51
6:9:375:U:H2'	6:9:376:A:C8	2.45	0.51
6:9:903:A:H2'	6:9:904:A:C8	2.45	0.51
21:P:55:LYS:C	21:P:72:GLN:HE22	2.19	0.51
58:JJ:108:ARG:HH22	58:JJ:154:GLN:HG3	1.73	0.51
79:Gg:193:GLY:HA3	79:Gg:212:LYS:HB3	1.92	0.51
3:5:1204:C:H2'	3:5:1205:G:H8	1.76	0.51
3:5:1333:A:H2'	3:5:1334:A:C8	2.45	0.51
3:5:2475:G:C6	29:X:50:LYS:HD3	2.46	0.51
3:5:2542:G:H2'	3:5:2543:A:C8	2.46	0.51
21:P:114:ILE:HA	21:P:150:LEU:HD23	1.92	0.51
23:R:63:CYS:O	23:R:67:THR:HG23	2.10	0.51
31:Z:121:ARG:O	31:Z:124:THR:OG1	2.23	0.51
46:o:34:TYR:O	46:o:39:ARG:NH1	2.42	0.51
50:BB:189:ILE:HB	50:BB:190:PRO:HD3	1.91	0.51
51:CC:164:PRO:HG2	51:CC:248:TYR:CE2	2.44	0.51
77:Dd:6:LEU:HA	77:Dd:9:SER:HB3	1.92	0.51
1:2:11:G:N2	1:2:24:G:H1	2.08	0.51
3:5:670:G:H2'	3:5:671:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:1806:G:H2'	3:5:1807:C:C6	2.44	0.51
3:5:1907:A:H4'	12:F:222:LYS:HE3	1.92	0.51
3:5:4252:C:OP2	3:5:4253:A:O2'	2.22	0.51
3:5:4966:A:H2'	3:5:4967:A:O4'	2.10	0.51
3:5:4967:A:H2'	3:5:4968:A:C8	2.46	0.51
5:8:67:U:H2'	5:8:68:G:C8	2.45	0.51
8:B:122:TRP:CE2	8:B:127:LYS:HE3	2.46	0.51
9:C:315:LYS:HD2	12:F:167:ALA:HB1	1.93	0.51
18:M:108:ASP:HB2	20:O:199:HIS:NE2	2.26	0.51
42:k:10:ASP:OD1	42:k:11:PHE:N	2.43	0.51
50:BB:176:VAL:HG23	50:BB:184:VAL:HG21	1.92	0.51
53:EE:70:ILE:HD13	53:EE:92:ILE:HG12	1.92	0.51
1:2:4:C:H2'	1:2:5:A:C8	2.46	0.51
3:5:4626:A:OP2	8:B:224:LYS:HE2	2.11	0.51
6:9:106:C:H2'	6:9:107:A:H8	1.75	0.51
13:G:159:THR:HB	13:G:162:GLU:HG3	1.93	0.51
13:G:210:ILE:HG23	13:G:254:THR:HG22	1.92	0.51
17:L:194:ILE:O	17:L:198:ARG:HG3	2.11	0.51
19:N:145:ASN:HB3	19:N:148:THR:HG22	1.92	0.51
25:T:105:PHE:HD1	25:T:108:ARG:HH21	1.58	0.51
46:o:26:TYR:CG	46:o:82:MET:HE1	2.45	0.51
48:r:63:VAL:HG22	48:r:79:ARG:HG2	1.92	0.51
50:BB:82:ARG:NH1	50:BB:103:MET:HE1	2.26	0.51
57:II:132:GLU:OE1	57:II:132:GLU:N	2.29	0.51
64:QQ:98:LYS:HD3	64:QQ:99:TYR:CZ	2.45	0.51
68:UU:49:LYS:HE3	68:UU:92:HIS:HB2	1.93	0.51
72:YY:55:ILE:HD12	72:YY:75:ILE:HD12	1.92	0.51
3:5:1683:PSU:OP1	32:a:44:ASN:ND2	2.44	0.51
6:9:126:G:H5''	55:GG:195:LYS:HE3	1.93	0.51
6:9:792:C:H2'	6:9:793:G:H8	1.76	0.51
6:9:1277:C:H2'	6:9:1278:A:C8	2.43	0.51
6:9:1619:A:OP1	63:PP:47:ARG:NE	2.33	0.51
6:9:1727:G:H2'	6:9:1728:U:C6	2.45	0.51
10:D:184:ASP:OD2	10:D:187:SER:OG	2.29	0.51
51:CC:179:THR:HG22	51:CC:180:VAL:N	2.25	0.51
52:DD:192:TRP:NE1	52:DD:201:LYS:O	2.38	0.51
60:LL:35:ARG:HH21	60:LL:63:THR:HG21	1.75	0.51
75:Bb:49:HIS:HD2	75:Bb:70:LYS:HA	1.76	0.51
79:Gg:165:ILE:CG1	79:Gg:177:TRP:HB2	2.40	0.51
3:5:2019:C:H2'	3:5:2020:U:C6	2.46	0.51
3:5:3700:C:H2'	3:5:3746:A:H61	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:4239:A:H2'	3:5:4240:G:C8	2.45	0.51
3:5:4302:U:H4'	25:T:5:LYS:HD2	1.92	0.51
3:5:4522:G:O2'	3:5:4525:C:OP2	2.24	0.51
3:5:4578:G:H2'	3:5:4579:U:C6	2.45	0.51
3:5:5001:U:H5''	8:B:317:LEU:HD23	1.93	0.51
6:9:1139:C:H5	6:9:1149:A:H62	1.57	0.51
45:n:18:ARG:O	45:n:22:GLN:OE1	2.29	0.51
79:Gg:83:TRP:HA	79:Gg:107:ASP:OD1	2.11	0.51
3:5:35:U:O2'	3:5:1525:A:N1	2.43	0.51
3:5:1212:G:H5''	12:F:62:GLN:NE2	2.25	0.51
3:5:1412:G:H2'	3:5:1413:C:C6	2.45	0.51
3:5:1480:C:O2'	3:5:1482:G:OP2	2.28	0.51
3:5:2705:G:O6	23:R:46:LYS:NZ	2.44	0.51
3:5:4896:G:N2	3:5:4927:G:O6	2.31	0.51
6:9:170:A:H4'	55:GG:136:LYS:HD3	1.93	0.51
6:9:434:G:H2'	6:9:435:A:C8	2.45	0.51
9:C:10:VAL:HG21	9:C:254:GLU:HG3	1.92	0.51
21:P:84:PRO:HB2	21:P:87:SER:HB3	1.92	0.51
24:S:15:ARG:HB3	24:S:27:LEU:HD13	1.92	0.51
59:KK:80:ARG:HH11	59:KK:87:PRO:HA	1.76	0.51
79:Gg:19:THR:HG21	79:Gg:67:SER:HA	1.93	0.51
4:7:24:C:H2'	4:7:25:G:O4'	2.11	0.50
6:9:533:A:H2'	6:9:534:G:C8	2.45	0.50
6:9:1394:G:O2'	6:9:1395:C:OP1	2.20	0.50
3:5:2791:C:OP1	43:l:48:LYS:NZ	2.35	0.50
3:5:4859:C:H2'	3:5:4860:G:C8	2.46	0.50
6:9:67:C:OP1	55:GG:160:LYS:NZ	2.36	0.50
6:9:1098:C:H2'	6:9:1099:G:C8	2.46	0.50
6:9:1221:G:O2'	6:9:1676:U:O2	2.27	0.50
6:9:1489:A:H4'	6:9:1490:G:OP2	2.11	0.50
6:9:1845:A:H2'	6:9:1846:G:C8	2.46	0.50
8:B:55:HIS:HB2	8:B:369:ASP:HB3	1.92	0.50
16:J:35:ARG:O	16:J:39:VAL:HG23	2.11	0.50
17:L:103:ARG:HE	17:L:105:LYS:HD2	1.76	0.50
27:V:107:ASN:HD21	27:V:109:LYS:HE3	1.75	0.50
42:k:31:ASN:OD1	42:k:32:VAL:N	2.43	0.50
50:BB:138:PHE:O	50:BB:213:ARG:N	2.43	0.50
3:5:407:A:O2'	3:5:410:A:OP1	2.18	0.50
3:5:2362:U:H2'	3:5:2363:A2M:H8	1.93	0.50
3:5:4460:U:H2'	3:5:4461:C:H6	1.76	0.50
19:N:5:LYS:O	19:N:9:GLU:OE1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:R:151:ARG:HH12	60:LL:118:ARG:HG2	1.75	0.50
35:d:23:ARG:NH1	35:d:25:TYR:OH	2.36	0.50
50:BB:25:PHE:HZ	62:OO:53:ILE:HA	1.76	0.50
3:5:197:A:H5''	30:Y:130:LYS:NZ	2.26	0.50
3:5:517:C:H2'	3:5:518:G:C8	2.47	0.50
6:9:126:G:O6	55:GG:196:LYS:HE3	2.11	0.50
6:9:126:G:OP1	55:GG:198:ARG:NH1	2.33	0.50
6:9:581:U:H4'	72:YY:66:GLY:HA2	1.93	0.50
17:L:42:ARG:O	17:L:46:ILE:HG12	2.11	0.50
47:p:38:THR:HA	47:p:45:THR:HA	1.94	0.50
54:FF:35:LEU:HD21	54:FF:146:ARG:HD3	1.94	0.50
79:Gg:241:PHE:CE1	79:Gg:248:LEU:HD12	2.47	0.50
3:5:1645:C:H2'	3:5:1646:A:C8	2.47	0.50
3:5:2562:G:N2	3:5:2564:G:H3'	2.27	0.50
3:5:3718:A2M:H2	3:5:3934:G:O4'	2.11	0.50
3:5:4938:A:H1'	11:E:188:PRO:HG3	1.93	0.50
6:9:371:A:OP2	57:II:10:LYS:HB2	2.11	0.50
31:Z:47:ASP:HB3	31:Z:69:LYS:HG2	1.94	0.50
37:f:6:TRP:HB3	37:f:104:MET:SD	2.52	0.50
46:o:99:ARG:NH2	46:o:100:LYS:O	2.45	0.50
52:DD:14:ASP:OD2	52:DD:15:GLY:N	2.45	0.50
54:FF:138:ALA:O	76:Cc:63:ARG:NH2	2.45	0.50
55:GG:1:MET:HE2	55:GG:109:LEU:HB2	1.92	0.50
78:Ee:112:ASN:HA	78:Ee:116:VAL:HG22	1.93	0.50
3:5:690:C:H2'	3:5:691:C:H6	1.76	0.50
3:5:739:G:H2'	3:5:740:G:H8	1.77	0.50
3:5:1209:U:O2'	3:5:1211:G:H5'	2.11	0.50
3:5:3888:G:O2'	3:5:3889:G:OP1	2.28	0.50
6:9:1736:G:H2'	6:9:1737:G:H8	1.76	0.50
6:9:1759:G:O6	6:9:1773:C:N4	2.43	0.50
11:E:113:ARG:NH1	11:E:113:ARG:HA	2.27	0.50
11:E:189:LEU:H	11:E:253:GLN:NE2	2.05	0.50
15:I:146:GLU:HA	15:I:149:VAL:HG12	1.93	0.50
21:P:94:MET:HE1	21:P:146:ILE:HB	1.92	0.50
25:T:111:GLU:O	25:T:114:GLN:HG3	2.11	0.50
26:U:41:GLN:O	26:U:45:GLU:OE1	2.29	0.50
27:V:13:LYS:HD3	27:V:128:LEU:HD11	1.93	0.50
31:Z:35:ASP:OD1	31:Z:36:ARG:N	2.45	0.50
50:BB:81:PHE:CD2	50:BB:109:LYS:HD3	2.47	0.50
68:UU:19:ARG:NH1	68:UU:92:HIS:HA	2.26	0.50
3:5:254:G:H2'	3:5:255:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:708:G:H5'	37:f:89:ARG:HH22	1.77	0.50
3:5:1170:G:H2'	3:5:1171:G:H8	1.77	0.50
3:5:4088:C:H2'	3:5:4089:G:H8	1.77	0.50
7:A:186:TYR:HB2	7:A:196:TRP:CZ3	2.47	0.50
8:B:141:ALA:HA	8:B:144:ARG:HG2	1.94	0.50
49:AA:57:LYS:HD3	69:VV:70:LEU:HD13	1.94	0.50
3:5:37:U:H4'	32:a:32:ARG:HG3	1.94	0.50
3:5:2715:G:H5'	3:5:2716:C:OP2	2.11	0.50
3:5:2889:G:OP1	23:R:75:HIS:ND1	2.44	0.50
3:5:4473:A:OP1	44:m:98:LYS:NZ	2.36	0.50
6:9:1393:G:H2'	6:9:1394:G:C8	2.47	0.50
6:9:1423:C:H2'	6:9:1424:G:O4'	2.11	0.50
6:9:1545:A:H2'	6:9:1546:G:C8	2.46	0.50
7:A:47:ASP:HB2	7:A:60:LYS:HB3	1.92	0.50
10:D:193:GLU:O	10:D:197:LYS:HG2	2.11	0.50
15:I:99:ILE:HB	15:I:123:GLN:OE1	2.12	0.50
30:Y:91:ASN:OD1	30:Y:92:GLY:N	2.44	0.50
66:SS:27:ALA:HA	66:SS:45:LEU:HD21	1.94	0.50
3:5:99:A:H2'	3:5:100:C:O2	2.12	0.50
3:5:223:G:H2'	9:C:164:THR:HG21	1.93	0.50
3:5:667:A:N7	9:C:2:ALA:N	2.60	0.50
3:5:1577:G:O2'	3:5:1612:G:H4'	2.12	0.50
6:9:566:U:H2'	6:9:567:C:O4'	2.12	0.50
6:9:619:A:N6	71:XX:114:ASP:OD2	2.41	0.50
6:9:860:G:H21	70:WW:107:SER:HB3	1.76	0.50
6:9:910:G:OP1	23:R:176:ARG:NH1	2.30	0.50
6:9:1101:U:H2'	6:9:1102:G:H8	1.77	0.50
6:9:1119:A:H8	6:9:1119:A:O5'	1.93	0.50
10:D:33:ARG:NH2	10:D:37:VAL:HG11	2.26	0.50
19:N:138:PHE:HZ	39:h:93:ARG:HG3	1.77	0.50
23:R:119:MET:O	23:R:123:LEU:HD23	2.11	0.50
29:X:122:ALA:N	29:X:139:ARG:O	2.43	0.50
30:Y:50:ARG:HG2	30:Y:51:LYS:H	1.77	0.50
40:i:66:ASP:HB3	40:i:87:ARG:NH2	2.27	0.50
40:i:96:ALA:HA	40:i:99:LYS:NZ	2.27	0.50
49:AA:41:ARG:HD2	49:AA:47:TYR:CZ	2.47	0.50
55:GG:7:PHE:CE2	55:GG:9:ALA:HB3	2.46	0.50
56:HH:162:GLN:OE1	56:HH:165:ASN:ND2	2.34	0.50
61:NN:114:ARG:HG2	61:NN:114:ARG:HH21	1.77	0.50
3:5:271:C:H2'	3:5:272:U:C6	2.47	0.49
3:5:1410:C:H2'	3:5:1411(A):G:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:51:U:H2'	6:9:52:G:H8	1.77	0.49
6:9:484:A2M:H8	6:9:484:A2M:O5'	2.12	0.49
14:H:103:VAL:HG11	14:H:144:LEU:HD21	1.93	0.49
29:X:77:ILE:HA	29:X:100:VAL:HG12	1.94	0.49
51:CC:253:PRO:HA	51:CC:256:TRP:CE2	2.47	0.49
55:GG:63:MET:HG2	55:GG:98:ARG:HD2	1.93	0.49
64:QQ:58:LEU:HD11	64:QQ:112:LEU:HD11	1.94	0.49
3:5:175:C:H2'	3:5:176:G:C8	2.41	0.49
3:5:4076:G:OP1	13:G:126:ARG:NE	2.26	0.49
3:5:4549:G:H2'	3:5:4550:7MG:H82	1.92	0.49
6:9:12:U:H2'	6:9:13:C:C6	2.47	0.49
6:9:555:A:C6	6:9:589:G:H1'	2.47	0.49
6:9:996:A:H2'	6:9:997:A:C8	2.47	0.49
23:R:105:LEU:HD12	23:R:135:LYS:HE3	1.95	0.49
28:W:97:LYS:HD2	28:W:98:PRO:HD2	1.93	0.49
42:k:36:VAL:CG2	42:k:43:TYR:HB2	2.41	0.49
49:AA:17:LYS:NZ	49:AA:199:PRO:HG3	2.27	0.49
49:AA:149:ASN:HB2	49:AA:165:ASN:OD1	2.12	0.49
51:CC:60:TRP:HZ3	51:CC:71:LYS:HB2	1.78	0.49
51:CC:196:ILE:HB	51:CC:223:TYR:HB2	1.93	0.49
62:OO:97:LEU:HD11	62:OO:112:ALA:HB1	1.94	0.49
1:2:69:U:H2'	1:2:70:G:C8	2.46	0.49
3:5:308:G:H2'	40:i:41:ARG:HH12	1.77	0.49
3:5:1613:A:H5''	7:A:183:GLY:HA2	1.94	0.49
3:5:1727:U:H2'	3:5:1728:U:C6	2.48	0.49
3:5:3607:U:H2'	3:5:3608:A:C8	2.47	0.49
3:5:4173:G:H2'	3:5:4174:U:H6	1.77	0.49
6:9:544:G:H2'	6:9:545:A:C8	2.47	0.49
6:9:658:U:H1'	71:XX:17:ARG:NH2	2.26	0.49
6:9:1016:U:H5'	61:NN:15:ALA:O	2.13	0.49
6:9:1388:A:H61	52:DD:161:GLY:HA3	1.77	0.49
6:9:1628:C:H2'	6:9:1629:C:C6	2.48	0.49
26:U:105:ASN:OD1	26:U:106:THR:N	2.43	0.49
30:Y:26:ARG:NH1	30:Y:75:ARG:O	2.46	0.49
49:AA:76:VAL:HG23	49:AA:123:VAL:HG23	1.94	0.49
55:GG:164:LYS:HD3	55:GG:167:LYS:HD2	1.93	0.49
58:JJ:111:GLN:NE2	58:JJ:127:ARG:HB2	2.27	0.49
66:SS:31:THR:HA	66:SS:36:VAL:HG13	1.94	0.49
3:5:1188:C:H2'	3:5:1189:G:C8	2.47	0.49
3:5:1448:G:H5'	9:C:300:ARG:HH21	1.76	0.49
3:5:3932:U:H2'	3:5:3933:G:H8	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:1749:G:H2'	6:9:1750:C:H6	1.77	0.49
27:V:33:GLY:HA3	27:V:69:LYS:HE3	1.94	0.49
54:FF:33:ILE:HA	54:FF:36:GLN:HG2	1.95	0.49
58:JJ:24:ARG:O	58:JJ:28:GLU:HG2	2.13	0.49
3:5:674:G:H2'	3:5:675:C:C6	2.47	0.49
3:5:710:G:H2'	3:5:711:A:C8	2.48	0.49
3:5:2520:C:H2'	3:5:2521:G:H8	1.76	0.49
3:5:3732:A:H2'	3:5:3733:A:C8	2.47	0.49
3:5:4413:C:H5	3:5:4429:C:H42	1.59	0.49
3:5:4994:G:H2'	3:5:4995:U:H6	1.76	0.49
6:9:1497:G:N7	59:KK:25:LYS:NZ	2.56	0.49
6:9:1749:G:H2'	6:9:1750:C:C6	2.48	0.49
8:B:358:ARG:HA	8:B:361:GLU:HG3	1.95	0.49
11:E:215:LEU:O	11:E:215:LEU:HD12	2.12	0.49
30:Y:4:ASN:HB3	30:Y:7:VAL:HG22	1.95	0.49
31:Z:50:PRO:HD3	31:Z:68:ILE:HG12	1.94	0.49
34:c:53:PRO:HB2	34:c:56:ARG:HG2	1.93	0.49
41:j:21:ARG:HG3	41:j:39:TYR:HD1	1.77	0.49
51:CC:60:TRP:CD1	51:CC:92:GLU:HG2	2.46	0.49
51:CC:151:ILE:O	51:CC:155:ILE:HG13	2.12	0.49
56:HH:43:LEU:HD11	56:HH:71:SER:HB2	1.95	0.49
66:SS:24:ARG:HD2	66:SS:29:ALA:HA	1.94	0.49
79:Gg:256:ILE:HG13	79:Gg:270:LEU:HB3	1.93	0.49
3:5:691:C:H2'	3:5:692:A:C8	2.46	0.49
3:5:1100:U:O2'	3:5:1168:G:OP2	2.26	0.49
3:5:3845:A:H2'	3:5:3846:C:H6	1.77	0.49
17:L:169:ILE:HD13	32:a:142:GLY:HA2	1.94	0.49
51:CC:72:ASP:OD2	51:CC:272:HIS:NE2	2.44	0.49
53:EE:87:MET:HG3	53:EE:122:LYS:HB2	1.94	0.49
56:HH:76:GLN:NE2	56:HH:94:PHE:HB2	2.28	0.49
58:JJ:32:ILE:HD13	78:Ee:107:ARG:HD2	1.93	0.49
72:YY:117:VAL:O	72:YY:122:LYS:HE2	2.13	0.49
3:5:93:G:H2'	3:5:94:A:C8	2.48	0.49
3:5:713:C:H2'	3:5:714:G:H8	1.78	0.49
3:5:4610:A:H2	14:H:170:LYS:HE3	1.77	0.49
10:D:135:ILE:HG23	10:D:138:GLN:HB2	1.95	0.49
14:H:34:LEU:HD12	14:H:80:MET:HE3	1.94	0.49
14:H:41:ILE:HG21	14:H:73:ILE:HD11	1.95	0.49
20:O:14:HIS:HE1	20:O:119:VAL:HG23	1.78	0.49
20:O:14:HIS:HD2	20:O:19:LEU:HD13	1.76	0.49
23:R:151:ARG:NH1	60:LL:118:ARG:HG2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:100:LEU:HD23	26:U:112:LEU:HD23	1.94	0.49
57:II:116:HIS:CE1	57:II:152:ARG:HH21	2.29	0.49
79:Gg:178:ASN:O	79:Gg:182:CYS:HA	2.12	0.49
3:5:467:U:H3	3:5:685:C:H42	1.60	0.49
3:5:1174:G:H2'	3:5:1175:A:H8	1.77	0.49
3:5:2708:U:O2'	3:5:2709:C:O5'	2.24	0.49
3:5:3633:C:H2'	3:5:3634:G:H8	1.77	0.49
3:5:4113:U:H2'	3:5:4114:C:C6	2.46	0.49
3:5:4756:C:H5'	3:5:4757:C:OP1	2.13	0.49
3:5:5068:G:N2	3:5:5069:U:O4	2.32	0.49
6:9:1007:C:H2'	6:9:1008:A:C8	2.48	0.49
6:9:1531:A:H2'	6:9:1532:C:C6	2.47	0.49
18:M:12:VAL:HG22	18:M:60:PHE:HB2	1.94	0.49
48:r:108:MET:SD	48:r:111:ILE:HD11	2.53	0.49
53:EE:45:ILE:HD12	53:EE:61:VAL:HG11	1.95	0.49
55:GG:68:LEU:O	55:GG:68:LEU:HD23	2.12	0.49
64:QQ:53:GLU:HG3	64:QQ:85:ARG:HH11	1.78	0.49
3:5:1237:A:C8	12:F:47:LYS:HG3	2.47	0.49
5:8:142:U:OP1	19:N:38:ARG:NH2	2.43	0.49
5:8:142:U:P	19:N:38:ARG:HH22	2.35	0.49
6:9:16:G:H2'	6:9:17:C:C6	2.48	0.49
6:9:178:C:H2'	6:9:179:C:C6	2.48	0.49
6:9:532:C:HO2'	6:9:533:A:P	2.36	0.49
6:9:952:G:H2'	6:9:953:C:C6	2.48	0.49
15:I:52:MET:HB2	15:I:152:LEU:HD22	1.95	0.49
21:P:116:HIS:HB3	21:P:149:ILE:HB	1.93	0.49
58:JJ:87:LEU:HD22	58:JJ:97:ILE:HG22	1.95	0.49
65:RR:61:ILE:HD11	65:RR:69:ILE:HD11	1.94	0.49
3:5:2411:C:O2'	3:5:2526:C:O2	2.25	0.49
3:5:2640:G:H2'	3:5:2641:A:C8	2.48	0.49
3:5:4071:U:H2'	3:5:4072:C:C6	2.48	0.49
6:9:15:U:H2'	6:9:16:G:O4'	2.13	0.49
17:L:114:VAL:HG12	17:L:118:LYS:HE2	1.94	0.49
19:N:126:THR:HG23	19:N:127:TYR:CD2	2.48	0.49
43:l:2:SER:O	43:l:5:LYS:NZ	2.32	0.49
59:KK:90:VAL:O	59:KK:95:ARG:NH1	2.41	0.49
3:5:2411:C:H2'	3:5:2412:A:C8	2.48	0.48
3:5:2465:C:H2'	3:5:2466:G:O4'	2.13	0.48
3:5:2899:C:H2'	3:5:2900:U:C6	2.47	0.48
3:5:3897:B8K:C4'	8:B:254:ILE:HG13	2.43	0.48
6:9:152:U:H5'	55:GG:132:ARG:HH22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:1863:A:OP2	74:Aa:4:LYS:NZ	2.43	0.48
59:KK:82:TYR:HD2	59:KK:83:LEU:HD12	1.77	0.48
63:PP:111:MET:O	63:PP:114:HIS:ND1	2.37	0.48
3:5:165:A:H2'	3:5:166:C:C6	2.48	0.48
3:5:2529:A:O2'	3:5:2531:C:OP2	2.31	0.48
3:5:4635:A:H3'	3:5:4636:PSU:H4'	1.94	0.48
5:8:103:A:OP1	41:j:21:ARG:NH2	2.46	0.48
6:9:536:A:H3'	6:9:537:C:H5''	1.94	0.48
6:9:570:C:O2'	72:YY:34:THR:O	2.26	0.48
6:9:1378:A:OP2	49:AA:102:ARG:NH1	2.46	0.48
15:I:20:SER:OG	15:I:21:ARG:N	2.43	0.48
50:BB:81:PHE:CG	50:BB:109:LYS:HD3	2.47	0.48
3:5:174:C:H2'	3:5:175:C:C6	2.49	0.48
3:5:308:G:O6	19:N:12:ARG:NH2	2.46	0.48
3:5:696:C:H4'	3:5:697:G:O5'	2.13	0.48
3:5:1411(C):C:N4	3:5:1412:G:O6	2.45	0.48
3:5:1484:G:H2'	3:5:1484:G:N3	2.28	0.48
3:5:1964:A:H3'	3:5:1965:G:H8	1.79	0.48
3:5:2587:A:H5''	3:5:2588:C:C5	2.48	0.48
3:5:3641:U:H5	3:5:3646:A:N7	2.10	0.48
3:5:4750:G:H2'	3:5:4751:G:C8	2.48	0.48
6:9:674:C:H2'	6:9:675:U:C6	2.48	0.48
11:E:189:LEU:N	11:E:253:GLN:HE22	2.08	0.48
17:L:135:LYS:N	17:L:138:ASP:OD2	2.44	0.48
18:M:20:HIS:CD2	18:M:48:GLN:HE22	2.31	0.48
39:h:103:LYS:HB2	39:h:107:GLN:HE21	1.76	0.48
61:NN:46:THR:OG1	61:NN:49:GLN:OE1	2.30	0.48
62:OO:57:THR:OG1	62:OO:60:MET:HE3	2.13	0.48
63:PP:86:LEU:HB2	63:PP:89:MET:HE3	1.95	0.48
66:SS:13:LEU:HB2	66:SS:20:ILE:HB	1.95	0.48
66:SS:59:LEU:HB2	66:SS:63:GLU:OE2	2.13	0.48
74:Aa:45:VAL:HG11	74:Aa:53:ILE:HD13	1.95	0.48
3:5:1371:A:N1	5:8:28:C:O2'	2.45	0.48
3:5:1442:C:H2'	3:5:1443:A:H8	1.77	0.48
3:5:1725:U:H2'	3:5:1726:U:H6	1.79	0.48
3:5:2258:C:H5''	3:5:2259:G:C8	2.48	0.48
3:5:2323:C:H2'	3:5:2324:C:H6	1.77	0.48
3:5:4136:G:H2'	3:5:4137:C:C6	2.48	0.48
7:A:117:GLU:O	7:A:162:ASN:ND2	2.45	0.48
8:B:80:GLU:OE2	8:B:323:TYR:OH	2.17	0.48
15:I:31:ILE:HG22	15:I:62:SER:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:9:VAL:HG11	18:M:66:HIS:HA	1.94	0.48
54:FF:38:TYR:CE2	54:FF:144:LEU:HB2	2.49	0.48
57:II:178:ARG:NH1	57:II:181:GLN:OE1	2.46	0.48
61:NN:136:PRO:HG2	61:NN:139:TRP:HB2	1.95	0.48
3:5:109:G:H5'	17:L:92:ARG:NH1	2.28	0.48
3:5:2072:C:H2'	3:5:2073:C:H6	1.78	0.48
3:5:4871:C:OP1	18:M:94:LYS:HD2	2.13	0.48
9:C:20:LYS:HE3	9:C:20:LYS:HB2	1.68	0.48
52:DD:172:VAL:O	52:DD:173:ARG:HD3	2.14	0.48
55:GG:181:THR:HG22	55:GG:183:ARG:H	1.78	0.48
61:NN:56:ASP:OD2	75:Bb:52:THR:OG1	2.25	0.48
68:UU:19:ARG:NE	68:UU:19:ARG:HA	2.28	0.48
71:XX:105:PHE:CD2	71:XX:112:VAL:HB	2.48	0.48
3:5:1333:A:H2'	3:5:1334:A:H8	1.78	0.48
5:8:122:G:H2'	5:8:123:U:O4'	2.14	0.48
6:9:65:C:C4	55:GG:133:LEU:HD12	2.49	0.48
6:9:443:U:H2'	6:9:444:G:O4'	2.13	0.48
22:Q:154:LYS:HZ3	22:Q:158:THR:HG22	1.78	0.48
34:c:22:MET:HG2	34:c:27:TYR:CD2	2.48	0.48
43:l:24:PRO:HG2	43:l:27:ILE:HD12	1.96	0.48
79:Gg:114:SER:HA	79:Gg:156:PHE:HD2	1.78	0.48
1:2:69:U:C2	1:2:70:G:C8	3.02	0.48
3:5:2749:C:H2'	3:5:2750:G:H8	1.79	0.48
3:5:3658:C:H2'	3:5:3659:G:H8	1.79	0.48
3:5:4173:G:H2'	3:5:4174:U:C6	2.49	0.48
3:5:4947:U:O2'	3:5:4948:C:OP1	2.28	0.48
6:9:1281:G:H3'	6:9:1282:A:H8	1.79	0.48
6:9:1416:C:H5''	67:TT:133:ARG:NH1	2.29	0.48
8:B:56:ILE:O	8:B:73:VAL:HA	2.14	0.48
12:F:39:LYS:HD2	12:F:40:MET:HE2	1.95	0.48
13:G:164:LYS:HA	13:G:167:LEU:HG	1.95	0.48
13:G:171:ALA:O	13:G:174:LYS:HG3	2.14	0.48
44:m:57:ARG:O	44:m:61:GLN:HG2	2.13	0.48
55:GG:212:LEU:O	55:GG:216:ARG:HG2	2.14	0.48
57:II:76:THR:HG21	57:II:104:ILE:HB	1.96	0.48
79:Gg:252:THR:HG21	79:Gg:257:LYS:HE3	1.95	0.48
3:5:1238:C:HO2'	3:5:1239:G:P	2.35	0.48
3:5:2749:C:H2'	3:5:2750:G:C8	2.49	0.48
3:5:2757:A:H2'	3:5:2758:G:C8	2.49	0.48
3:5:4967:A:H2'	3:5:4968:A:H8	1.78	0.48
6:9:17:C:H2'	6:9:18:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:442:C:H2'	6:9:443:U:C6	2.49	0.48
6:9:544:G:H2'	6:9:545:A:H8	1.79	0.48
6:9:1101:U:H2'	6:9:1102:G:C8	2.48	0.48
6:9:1851:MA6:OP1	45:n:9:ARG:NH1	2.39	0.48
9:C:108:TRP:O	19:N:204:ARG:NH2	2.47	0.48
15:I:184:MET:HB3	15:I:189:ARG:HB3	1.96	0.48
24:S:76:LYS:HD2	24:S:131:GLU:HG3	1.94	0.48
34:c:51:ASN:ND2	34:c:77:ASN:HB2	2.28	0.48
43:l:9:ILE:O	43:l:13:LEU:HG	2.14	0.48
48:r:47:LYS:HB2	48:r:102:TYR:CZ	2.48	0.48
53:EE:15:PRO:HG2	53:EE:18:TRP:CE2	2.47	0.48
56:HH:87:PHE:HB3	56:HH:90:LYS:HG3	1.96	0.48
79:Gg:44:LYS:HD3	79:Gg:56:GLN:HB2	1.96	0.48
79:Gg:256:ILE:HD11	79:Gg:270:LEU:HD13	1.95	0.48
3:5:2056:G:C8	3:5:2058:G:C8	3.02	0.48
3:5:4948:C:O2	3:5:4949:G:H2'	2.14	0.48
6:9:433:A:H5''	57:II:22:HIS:HB3	1.96	0.48
6:9:639:C:H2'	6:9:640:A:C8	2.48	0.48
6:9:1010:G:H2'	6:9:1011:A:C8	2.49	0.48
12:F:97:ILE:HD12	22:Q:4:ASP:HB2	1.95	0.48
13:G:218:GLU:CD	19:N:11:TRP:HE1	2.21	0.48
30:Y:118:ILE:O	30:Y:122:LYS:HG3	2.14	0.48
35:d:51:LYS:HA	35:d:54:MET:HE2	1.96	0.48
79:Gg:42:MET:HE2	79:Gg:92:LEU:HD12	1.96	0.48
79:Gg:156:PHE:CD1	79:Gg:165:ILE:HG22	2.49	0.48
3:5:71:C:H1'	17:L:62:PRO:O	2.14	0.48
3:5:519:C:H2'	3:5:520:U:C6	2.48	0.48
3:5:1633:G:H5'	3:5:1634:A:OP1	2.13	0.48
3:5:2264:C:H2'	3:5:2265:G:O4'	2.12	0.48
3:5:2335:C:H2'	3:5:2336:G:H8	1.79	0.48
3:5:2669:C:H2'	3:5:2670:C:O4'	2.14	0.48
3:5:3845:A:H2'	3:5:3846:C:C6	2.49	0.48
3:5:4186:A:H2'	3:5:4187:G:C8	2.49	0.48
6:9:28:U:H2'	6:9:29:G:H8	1.79	0.48
6:9:1003:U:H5''	50:BB:165:ARG:HH22	1.77	0.48
6:9:1740:C:H2'	6:9:1741:U:C6	2.48	0.48
26:U:27:HIS:HB3	26:U:114:TYR:HE1	1.78	0.48
30:Y:115:ARG:O	30:Y:119:LEU:HD23	2.14	0.48
52:DD:123:LEU:HD22	52:DD:152:PHE:HB3	1.95	0.48
64:QQ:14:GLY:N	64:QQ:21:ALA:O	2.46	0.48
3:5:137:G:OP1	19:N:140:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:734:G:H1	3:5:929:A:H62	1.61	0.47
3:5:2738:C:O2'	3:5:2740:U:O2	2.31	0.47
6:9:1217:A:H2'	6:9:1218:C:H6	1.79	0.47
6:9:1578:U:H5''	6:9:1579:A:O4'	2.14	0.47
9:C:10:VAL:HA	9:C:153:VAL:HG13	1.96	0.47
12:F:192:GLU:O	12:F:196:VAL:HA	2.15	0.47
13:G:270:LYS:O	13:G:273:GLU:HG3	2.14	0.47
16:J:82:ILE:HG22	16:J:130:PHE:HE2	1.79	0.47
18:M:36:ALA:HB2	18:M:52:PHE:CZ	2.48	0.47
23:R:172:ARG:O	23:R:175:GLU:HG3	2.14	0.47
28:W:19:ARG:HB2	28:W:37:GLU:OE2	2.14	0.47
51:CC:174:ILE:HG12	69:VV:4:ASP:OD2	2.14	0.47
62:OO:31:CYS:HB3	62:OO:44:VAL:HG22	1.95	0.47
63:PP:31:GLU:HA	63:PP:34:MET:HG2	1.96	0.47
63:PP:37:TYR:HB3	63:PP:41:GLN:HB2	1.95	0.47
74:Aa:45:VAL:HG23	74:Aa:50:VAL:HG12	1.95	0.47
3:5:1440:U:HO2'	3:5:1441:C:P	2.37	0.47
3:5:1472:C:H2'	3:5:1473:U:C6	2.50	0.47
3:5:1733:G:N3	3:5:4214:A:H2'	2.29	0.47
3:5:1990:A:H3'	3:5:1991:A:H5''	1.96	0.47
3:5:2098:G:OP2	3:5:2098:G:H8	1.97	0.47
3:5:2484:A:H2'	3:5:2485:U:C6	2.48	0.47
3:5:3911:C:H2'	3:5:3912:U:C6	2.48	0.47
3:5:4625:C:O2'	3:5:4626:A:H5'	2.13	0.47
6:9:374:G:H2'	6:9:375:U:C6	2.49	0.47
6:9:1554:C:OP2	6:9:1555:U:O2'	2.29	0.47
13:G:130:PRO:HG2	13:G:133:ILE:HD12	1.95	0.47
29:X:117:TYR:O	29:X:119:ILE:HG23	2.14	0.47
33:b:25:ARG:HE	33:b:26:SER:H	1.62	0.47
44:m:69:ILE:HD11	44:m:96:ARG:CZ	2.44	0.47
55:GG:121:ILE:HG13	55:GG:122:PRO:HD2	1.95	0.47
63:PP:115:TYR:HB2	63:PP:118:GLU:HG3	1.96	0.47
3:5:1554:A:OP2	47:p:4:ARG:NE	2.42	0.47
3:5:1774:C:H2'	3:5:1775:A:O4'	2.14	0.47
3:5:2377:C:H2'	3:5:2378:G:O4'	2.13	0.47
3:5:2725:A:H1'	23:R:93:VAL:HG21	1.96	0.47
3:5:4699:U:H1'	3:5:4700:A:H5''	1.95	0.47
6:9:1395:C:O2'	6:9:1396:A:H5''	2.14	0.47
6:9:1756:C:H2'	6:9:1757:G:C8	2.49	0.47
14:H:20:LEU:HD13	14:H:47:LEU:HD22	1.97	0.47
20:O:14:HIS:CE1	20:O:119:VAL:HG23	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:R:97:ARG:O	23:R:101:ILE:HG12	2.14	0.47
23:R:151:ARG:CZ	60:LL:118:ARG:HE	2.27	0.47
50:BB:40:ASN:HB2	50:BB:75:GLN:HA	1.95	0.47
79:Gg:203:ASP:OD1	79:Gg:205:SER:N	2.41	0.47
3:5:180:C:N4	3:5:256:G:O6	2.31	0.47
3:5:1278:C:H2'	3:5:1279:A:O4'	2.15	0.47
3:5:1890:G:OP2	3:5:1890:G:N2	2.40	0.47
3:5:2732:G:H2'	3:5:2733:C:C6	2.49	0.47
3:5:4061:G:H2'	3:5:4062:A:C8	2.49	0.47
3:5:4263:C:H2'	3:5:4264:G:O4'	2.13	0.47
3:5:4715:C:H5''	8:B:278:THR:HG21	1.96	0.47
3:5:5004:C:H2'	3:5:5005:G:O4'	2.14	0.47
13:G:216:PRO:HG2	13:G:219:LEU:HD13	1.96	0.47
22:Q:147:GLU:HG2	22:Q:150:ARG:HH21	1.78	0.47
48:r:107:ARG:HG3	48:r:108:MET:N	2.28	0.47
56:HH:62:ILE:HB	56:HH:94:PHE:HD2	1.79	0.47
60:LL:96:ILE:HD12	71:XX:10:ALA:HB1	1.96	0.47
65:RR:111:PHE:HB3	65:RR:114:LEU:HD21	1.96	0.47
79:Gg:79:LEU:HB2	79:Gg:113:PHE:CZ	2.49	0.47
3:5:95:G:OP2	17:L:11:LYS:NZ	2.44	0.47
3:5:2033:A:OP1	15:I:162:ARG:NH1	2.48	0.47
3:5:2079:G:H2'	3:5:2080:U:C6	2.49	0.47
3:5:2098:G:H2'	3:5:2099:C:C6	2.50	0.47
3:5:2848:G:O2'	3:5:3838:U:O4	2.20	0.47
4:7:57:C:H2'	4:7:58:A:H8	1.79	0.47
11:E:265:LYS:HE3	11:E:271:GLN:OE1	2.14	0.47
17:L:204:GLU:O	17:L:208:GLU:OE1	2.32	0.47
28:W:19:ARG:HD3	28:W:37:GLU:OE2	2.14	0.47
53:EE:153:LEU:HG	55:GG:216:ARG:HH11	1.80	0.47
54:FF:51:HIS:CD2	54:FF:86:LYS:HG2	2.48	0.47
57:II:48:VAL:HG11	57:II:54:LYS:HE2	1.96	0.47
57:II:117:TYR:HB3	57:II:119:LEU:HD13	1.97	0.47
63:PP:28:MET:HA	63:PP:32:GLN:HE21	1.80	0.47
79:Gg:249:CYS:HB3	79:Gg:258:ILE:HD13	1.95	0.47
3:5:161:G:H2'	3:5:162:A:C8	2.50	0.47
3:5:251:C:H2'	3:5:252:C:C6	2.49	0.47
3:5:1771:U:H2'	3:5:1772:C:C6	2.50	0.47
3:5:2437:C:N3	29:X:89:LYS:NZ	2.62	0.47
3:5:2578:G:OP1	31:Z:107:LYS:HD3	2.15	0.47
3:5:2607:C:H2'	3:5:2608:G:H8	1.79	0.47
5:8:141:C:H2'	5:8:142:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:398:A:H5''	6:9:400:C:H5'	1.97	0.47
6:9:1333:U:H5'	52:DD:147:ALA:HB2	1.96	0.47
6:9:1753:C:H2'	6:9:1754:G:C8	2.49	0.47
7:A:113:VAL:CG1	7:A:164:ALA:HB1	2.44	0.47
10:D:108:ARG:NH2	10:D:253:TYR:HB2	2.29	0.47
13:G:212:HIS:ND1	13:G:238:LYS:HA	2.29	0.47
18:M:11:ARG:NH1	18:M:61:ILE:HD11	2.30	0.47
40:i:85:ARG:O	40:i:88:GLU:HG3	2.15	0.47
40:i:90:LEU:HA	40:i:93:VAL:HG12	1.95	0.47
55:GG:22:ARG:NH2	55:GG:25:ARG:HG3	2.29	0.47
64:QQ:19:ALA:HB2	64:QQ:75:GLY:HA3	1.97	0.47
64:QQ:108:ILE:O	64:QQ:112:LEU:HD13	2.14	0.47
67:TT:42:HIS:HB3	67:TT:93:SER:OG	2.15	0.47
3:5:163:A:H2'	3:5:164:G:H8	1.78	0.47
3:5:270:U:H2'	3:5:271:C:C6	2.49	0.47
3:5:917:A:H2'	3:5:918:G:O4'	2.15	0.47
3:5:1272:C:OP2	12:F:33:ARG:NH1	2.42	0.47
3:5:1669:A:H4'	3:5:1685:G:N2	2.30	0.47
3:5:1949:U:H2'	3:5:1950:U:C6	2.48	0.47
3:5:1999:A:H2'	3:5:2000:G:C4	2.50	0.47
3:5:4525:C:OP1	8:B:246:ARG:NH1	2.48	0.47
3:5:4700:A:H2	14:H:69:THR:HG22	1.79	0.47
6:9:29:G:H2'	6:9:30:C:C6	2.50	0.47
6:9:128:U:H3'	6:9:129:C:H6	1.79	0.47
6:9:465:A:H4'	6:9:466:G:O5'	2.15	0.47
6:9:694:G:H22	6:9:732:U:H3	1.62	0.47
6:9:1597:C:H4'	6:9:1603:G:O6	2.15	0.47
6:9:1629:C:OP1	66:SS:39:ARG:HD3	2.15	0.47
6:9:1845:A:H2'	6:9:1846:G:H8	1.79	0.47
8:B:170:LEU:O	8:B:328:ASN:ND2	2.47	0.47
9:C:77:PRO:O	9:C:90:GLY:HA2	2.14	0.47
10:D:209:ARG:O	10:D:213:GLU:HG2	2.15	0.47
11:E:193:HIS:HB3	11:E:196:PHE:HD2	1.80	0.47
14:H:162:GLN:HG3	14:H:179:ILE:O	2.15	0.47
15:I:180:GLU:OE1	15:I:184:MET:HE2	2.15	0.47
19:N:64:ILE:HD11	19:N:102:ALA:HB1	1.97	0.47
21:P:55:LYS:O	21:P:72:GLN:NE2	2.48	0.47
28:W:114:GLU:HA	28:W:117:LYS:HG2	1.97	0.47
38:g:85:LYS:O	38:g:88:ARG:HG2	2.14	0.47
41:j:33:THR:HG22	41:j:40:PRO:HG2	1.96	0.47
53:EE:80:ILE:HG13	53:EE:81:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:EE:246:LEU:HD12	53:EE:250:GLU:HG3	1.96	0.47
65:RR:101:ASP:OD1	65:RR:102:THR:N	2.47	0.47
79:Gg:232:GLY:HA2	79:Gg:257:LYS:HE2	1.96	0.47
3:5:2730:U:H2'	3:5:2731:C:C6	2.50	0.47
3:5:3734:U:H2'	3:5:3735:G:O4'	2.15	0.47
6:9:98:C:OP2	6:9:426:A:O2'	2.26	0.47
6:9:114:G:OP1	60:LL:69:ARG:NH1	2.48	0.47
6:9:1643:U:H1'	64:QQ:142:GLN:NE2	2.27	0.47
9:C:86:ARG:HA	9:C:89:GLN:OE1	2.15	0.47
16:J:46:GLN:NE2	16:J:73:THR:O	2.44	0.47
18:M:24:LEU:O	18:M:43:THR:HG21	2.14	0.47
19:N:11:TRP:O	19:N:14:LYS:NZ	2.47	0.47
19:N:121:VAL:HG11	19:N:131:GLU:HG3	1.96	0.47
19:N:166:SER:OG	19:N:170:LYS:NZ	2.47	0.47
26:U:80:LYS:HG2	26:U:110:TYR:CE1	2.50	0.47
48:r:32:LEU:HD12	48:r:106:LEU:HD13	1.96	0.47
53:EE:188:ASN:HB3	53:EE:191:ARG:HD3	1.97	0.47
57:II:191:GLU:HG3	60:LL:19:ASN:OD1	2.14	0.47
61:NN:140:LYS:HA	61:NN:140:LYS:HD3	1.75	0.47
79:Gg:131:LEU:HD21	79:Gg:140:TYR:HB3	1.97	0.47
79:Gg:297:THR:HA	79:Gg:311:GLN:HA	1.97	0.47
3:5:462:G:H2'	3:5:463:A:C8	2.50	0.47
3:5:2894:A:H2'	3:5:2895:A:C8	2.49	0.47
3:5:4572:U:H2'	3:5:4573:G:C8	2.50	0.47
6:9:455:A:O2'	6:9:1735:A:N3	2.41	0.47
6:9:555:A:H61	6:9:589:G:H21	1.63	0.47
6:9:1562:C:H2'	6:9:1563:G:H8	1.80	0.47
16:J:159:LYS:HG2	16:J:163:MET:HE2	1.97	0.47
22:Q:179:GLY:H	32:a:51:GLY:H	1.62	0.47
28:W:107:GLN:O	28:W:110:ARG:HD3	2.15	0.47
34:c:48:LEU:HD11	34:c:60:ILE:HG21	1.96	0.47
35:d:68:LEU:O	35:d:72:VAL:HG23	2.15	0.47
51:CC:79:GLU:OE1	69:VV:11:LEU:HG	2.15	0.47
51:CC:166:ARG:H	51:CC:247:THR:HG23	1.80	0.47
56:HH:36:LEU:HB3	56:HH:40:LEU:HD13	1.95	0.47
77:Dd:33:LYS:HE2	77:Dd:34:TYR:CZ	2.50	0.47
79:Gg:163:PRO:C	79:Gg:179:LEU:HD23	2.39	0.47
3:5:458:C:H4'	11:E:113:ARG:HH22	1.80	0.47
3:5:640:C:H2'	3:5:641:G:C8	2.50	0.47
3:5:2639:U:O2	38:g:26:PRO:HB3	2.15	0.47
6:9:75:G:O2'	6:9:77:A:OP1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:560:A:H5'	58:JJ:174:LYS:HB2	1.97	0.47
6:9:875:A:C1'	56:HH:114:GLN:HE22	2.28	0.47
6:9:1010:G:H2'	6:9:1011:A:H8	1.80	0.47
9:C:121:ARG:O	9:C:124:ILE:HG22	2.15	0.47
16:J:89:VAL:HG21	16:J:115:LEU:HD22	1.97	0.47
19:N:5:LYS:HG2	40:i:40:VAL:HG11	1.97	0.47
19:N:146:PRO:HA	19:N:149:GLN:HG2	1.97	0.47
3:5:23:C:H2'	3:5:24:G:O4'	2.15	0.46
3:5:516:C:H2'	3:5:517:C:C6	2.50	0.46
3:5:1683:PSU:H2'	3:5:1684:A:C8	2.50	0.46
3:5:1803:G:C6	25:T:109:VAL:HG23	2.51	0.46
6:9:57:U:OP1	6:9:504:G:O2'	2.28	0.46
6:9:916:A:C5	61:NN:73:ARG:HD3	2.49	0.46
6:9:1512:C:H5''	77:Dd:8:TRP:HZ3	1.79	0.46
10:D:30:TYR:HA	10:D:33:ARG:HB3	1.96	0.46
14:H:89:ARG:HA	14:H:146:LEU:O	2.15	0.46
16:J:158:SER:HB2	16:J:161:GLU:HG3	1.97	0.46
31:Z:76:ASN:HD22	31:Z:79:HIS:CD2	2.33	0.46
47:p:74:THR:HA	47:p:77:VAL:HG22	1.98	0.46
74:Aa:4:LYS:HD3	74:Aa:5:ARG:HH12	1.80	0.46
3:5:1326:A2M:OP2	3:5:4445:U:O2'	2.32	0.46
3:5:2484:A:H2'	3:5:2485:U:H6	1.80	0.46
3:5:3910:C:H2'	3:5:3911:C:C6	2.50	0.46
3:5:4460:U:H2'	3:5:4461:C:C6	2.50	0.46
5:8:120:G:C2	5:8:121:G:C8	3.03	0.46
6:9:883:U:H2'	6:9:884:C:C6	2.50	0.46
6:9:929:G:H2'	6:9:930:C:O4'	2.16	0.46
8:B:52:GLY:HA2	8:B:341:LYS:HE3	1.97	0.46
10:D:33:ARG:NH2	10:D:37:VAL:HG21	2.30	0.46
24:S:173:ASN:ND2	24:S:175:PHE:O	2.48	0.46
36:e:114:ARG:NH1	36:e:117:GLN:OE1	2.48	0.46
42:k:47:ILE:HD11	42:k:53:ALA:HA	1.96	0.46
51:CC:268:GLU:HG2	51:CC:269:PHE:CD2	2.50	0.46
56:HH:69:LEU:O	56:HH:73:GLN:HG2	2.15	0.46
1:2:18:G:H21	1:2:58:A:H5'	1.81	0.46
3:5:2689:C:H2'	3:5:2690:C:C6	2.50	0.46
3:5:4615:C:H5''	8:B:357:ARG:NH1	2.31	0.46
3:5:4769:G:H5'	20:O:176:ARG:HD3	1.98	0.46
4:7:89:G:N2	15:I:56:GLU:OE2	2.48	0.46
6:9:495:U:H2'	6:9:496:C:O4'	2.15	0.46
11:E:179:THR:HG23	11:E:180:GLY:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:36:ARG:O	17:L:40:GLN:HG3	2.16	0.46
20:O:61:ARG:HD3	20:O:66:PRO:HG3	1.98	0.46
21:P:4:TYR:HA	21:P:147:GLU:OE2	2.15	0.46
31:Z:87:VAL:HG13	31:Z:127:ASN:ND2	2.30	0.46
49:AA:132:GLN:HB3	49:AA:133:PRO:HD3	1.97	0.46
51:CC:60:TRP:CZ3	51:CC:71:LYS:HB2	2.50	0.46
64:QQ:38:PRO:HG2	64:QQ:41:MET:SD	2.55	0.46
70:WW:90:GLN:HB2	70:WW:94:LEU:HD12	1.97	0.46
1:2:68:C:H2'	1:2:69:U:H6	1.81	0.46
3:5:271:C:H2'	3:5:272:U:H6	1.80	0.46
3:5:648:G:H2'	3:5:649:A:H8	1.80	0.46
3:5:1396:G:HO2'	3:5:1468:C:HO2'	1.48	0.46
3:5:1825:A:H4'	33:b:39:PHE:HZ	1.80	0.46
3:5:2894:A:H2'	3:5:2895:A:H8	1.81	0.46
3:5:4114:C:H3'	3:5:4115:G:H21	1.79	0.46
3:5:5052:C:H2'	3:5:5053:U:O4'	2.15	0.46
6:9:43:U:OP2	6:9:485:A:N6	2.45	0.46
6:9:612:PSU:H4'	78:Ee:88:GLN:NE2	2.31	0.46
6:9:1144:A:H5'	6:9:1355:C:H41	1.80	0.46
15:I:182:GLU:HA	15:I:185:VAL:HG12	1.97	0.46
17:L:70:VAL:HG22	17:L:159:ASN:HB3	1.96	0.46
23:R:123:LEU:O	23:R:127:VAL:HG23	2.14	0.46
49:AA:17:LYS:HZ1	49:AA:199:PRO:HG3	1.79	0.46
49:AA:144:THR:O	49:AA:158:ASP:HB2	2.14	0.46
54:FF:124:ASP:OD2	54:FF:125:SER:N	2.47	0.46
54:FF:144:LEU:HD23	76:Cc:49:PRO:HG2	1.97	0.46
64:QQ:34:VAL:HG22	64:QQ:70:VAL:HB	1.97	0.46
66:SS:85:ASN:OD1	66:SS:97:GLN:NE2	2.49	0.46
1:2:36:U:H2'	1:2:37:T6A:H8	1.81	0.46
3:5:1398:A:H61	3:5:1419:G:H2'	1.81	0.46
3:5:3607:U:H2'	3:5:3608:A:H8	1.79	0.46
6:9:5:U:H2'	6:9:6:G:H8	1.81	0.46
30:Y:8:THR:HG21	30:Y:13:LYS:HD2	1.97	0.46
46:o:2:VAL:N	46:o:90:HIS:O	2.49	0.46
50:BB:172:MET:O	50:BB:176:VAL:HG12	2.16	0.46
56:HH:80:VAL:O	56:HH:84:GLU:HG2	2.15	0.46
60:LL:5:GLN:NE2	60:LL:11:GLN:O	2.36	0.46
60:LL:135:SER:O	60:LL:139:ARG:NH1	2.48	0.46
3:5:125:C:H2'	3:5:126:C:C6	2.47	0.46
3:5:1177:U:H2'	3:5:1178:G:C8	2.51	0.46
3:5:1204:C:H2'	3:5:1205:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:2353:U:H5''	9:C:89:GLN:HE21	1.81	0.46
3:5:2639:U:HO2'	3:5:2640:G:P	2.38	0.46
3:5:4301:U:H4'	25:T:54:HIS:CE1	2.50	0.46
3:5:4500:PSU:H2'	3:5:4501:U:C6	2.51	0.46
3:5:4688:C:O2'	14:H:155:SER:OG	2.33	0.46
5:8:60:G:O6	5:8:96:C:O2'	2.30	0.46
5:8:135:C:OP1	29:X:63:LYS:NZ	2.49	0.46
6:9:352:U:H2'	6:9:353:C:C6	2.51	0.46
10:D:35:ARG:HH11	10:D:35:ARG:HG3	1.80	0.46
14:H:152:GLU:OE1	14:H:152:GLU:HA	2.15	0.46
17:L:164:GLU:HG3	32:a:100:ILE:HG13	1.98	0.46
19:N:36:LEU:HD21	19:N:109:HIS:CG	2.50	0.46
22:Q:148:VAL:HG22	22:Q:152:PHE:CZ	2.51	0.46
28:W:105:ARG:HH11	55:GG:150:GLU:HB2	1.80	0.46
30:Y:100:HIS:ND1	30:Y:102:SER:OG	2.42	0.46
55:GG:103:ASP:CG	55:GG:104:ALA:H	2.23	0.46
56:HH:9:VAL:HB	56:HH:44:ASN:HD21	1.81	0.46
58:JJ:131:ARG:HA	58:JJ:131:ARG:HD2	1.66	0.46
78:Ee:109:MET:HE3	78:Ee:113:ARG:HH21	1.80	0.46
79:Gg:165:ILE:HG12	79:Gg:177:TRP:HB2	1.96	0.46
3:5:223:G:H4'	3:5:225:G:N7	2.31	0.46
3:5:2003:G:H22	3:5:2016:C:N4	2.13	0.46
3:5:2421:G:H4'	21:P:127:ARG:HH12	1.81	0.46
3:5:2440:U:O2'	3:5:2441:C:OP1	2.31	0.46
3:5:2447:U:H2'	3:5:2448:G:H8	1.81	0.46
3:5:4504:C:H2'	3:5:4505:C:H6	1.80	0.46
3:5:4508:C:H5''	27:V:43:LYS:HG2	1.97	0.46
6:9:142:C:OP2	55:GG:188:LYS:NZ	2.44	0.46
6:9:1349:G:H2'	6:9:1350:U:C6	2.51	0.46
6:9:1365:G:H2'	6:9:1366:G:H8	1.80	0.46
6:9:1406:G:H2'	6:9:1407:U:C6	2.50	0.46
6:9:1648:G:N7	64:QQ:17:LYS:HE2	2.30	0.46
16:J:161:GLU:O	16:J:164:ARG:HG2	2.16	0.46
19:N:75:VAL:CG2	19:N:76:PRO:HD2	2.43	0.46
28:W:93:LYS:HA	28:W:96:GLN:HE22	1.81	0.46
31:Z:122:TYR:HB2	31:Z:131:PHE:CE2	2.51	0.46
48:r:107:ARG:NH2	48:r:108:MET:HG2	2.30	0.46
51:CC:74:LYS:HE3	51:CC:269:PHE:CE1	2.51	0.46
55:GG:69:THR:O	55:GG:101:ILE:HG12	2.16	0.46
62:OO:27:VAL:HG23	62:OO:90:ILE:HA	1.98	0.46
62:OO:90:ILE:HG22	62:OO:124:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:XX:81:ILE:HD12	71:XX:120:PHE:CD2	2.50	0.46
72:YY:40:ILE:HD11	72:YY:60:PHE:CZ	2.51	0.46
73:ZZ:64:ASN:HA	73:ZZ:111:ARG:HD3	1.97	0.46
3:5:74:G:H5'	17:L:59:VAL:HG13	1.98	0.46
3:5:1415:G:H2'	3:5:1416:G:H8	1.80	0.46
3:5:1524:A2M:H62	3:5:1651:G:H22	1.64	0.46
3:5:1968:G:H2'	3:5:1969:G:C8	2.51	0.46
3:5:2539:C:H2'	3:5:2540:C:H6	1.81	0.46
3:5:3896:C:O2'	8:B:268:ARG:NH2	2.48	0.46
3:5:4941:G:OP2	11:E:191:ARG:NH1	2.48	0.46
4:7:117:G:H5'	10:D:256:LYS:HD2	1.97	0.46
6:9:164:A:H3'	6:9:165:G:N2	2.19	0.46
6:9:801:U:O4	56:HH:106:ARG:NH1	2.49	0.46
6:9:931:C:H2'	6:9:932:G:C8	2.51	0.46
6:9:1144:A:H2'	6:9:1145:A:C8	2.51	0.46
8:B:257:TRP:CD1	8:B:257:TRP:C	2.93	0.46
12:F:148:SER:OG	12:F:244:ARG:NH2	2.48	0.46
16:J:39:VAL:HG21	16:J:126:TYR:HD2	1.81	0.46
18:M:86:TRP:O	18:M:89:THR:OG1	2.34	0.46
49:AA:154:LEU:HD13	69:VV:66:ASP:OD2	2.16	0.46
53:EE:11:ARG:HA	53:EE:28:ALA:HB2	1.98	0.46
54:FF:55:ARG:HG2	64:QQ:125:ARG:NH2	2.30	0.46
70:WW:102:ILE:H	70:WW:113:HIS:CD2	2.33	0.46
79:Gg:194:TYR:CE1	79:Gg:212:LYS:HD3	2.51	0.46
2:1:46:A:O2'	6:9:1830:UR3:OP2	2.32	0.46
3:5:385:A:H4'	3:5:386:A:OP1	2.16	0.46
3:5:1345:A:H2'	3:5:1346:C:C6	2.51	0.46
3:5:3893:C:H2'	3:5:3894:A:H8	1.81	0.46
3:5:3946:G:H2'	3:5:3947:A:C8	2.51	0.46
3:5:4637:OMG:HM23	3:5:4637:OMG:H1'	1.79	0.46
6:9:535:G:H2'	6:9:536:A:C8	2.51	0.46
6:9:563:G:O2'	6:9:564:A:H8	1.98	0.46
6:9:1522:A:OP2	66:SS:144:ARG:HD2	2.15	0.46
11:E:64:MET:HE3	11:E:64:MET:HB3	1.73	0.46
25:T:92:ARG:HG2	25:T:94:GLU:OE2	2.16	0.46
28:W:99:GLU:HA	28:W:102:LYS:HG2	1.98	0.46
30:Y:50:ARG:HD3	30:Y:110:LYS:HD3	1.98	0.46
48:r:97:ILE:HG21	48:r:107:ARG:HB3	1.98	0.46
50:BB:25:PHE:CZ	62:OO:53:ILE:HA	2.51	0.46
52:DD:43:PRO:O	52:DD:44:THR:OG1	2.29	0.46
55:GG:122:PRO:HA	55:GG:126:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:SS:90:VAL:O	66:SS:91:LYS:HE2	2.16	0.46
3:5:37:U:H2'	3:5:38:A:O4'	2.16	0.46
3:5:1770:A:H2'	3:5:1771:U:H6	1.80	0.46
3:5:1788:A:H2'	15:I:22:PHE:CZ	2.51	0.46
3:5:2106:G:O2'	3:5:2108:G:H5''	2.16	0.46
3:5:4080:C:H2'	3:5:4081:G:H8	1.81	0.46
3:5:4860:G:H2'	3:5:4861:G:H8	1.80	0.46
5:8:121:G:C5	5:8:122:G:N7	2.84	0.46
6:9:538:U:H2'	6:9:539:C:C6	2.51	0.46
6:9:671:A:H4'	6:9:672:A:H5''	1.98	0.46
6:9:1759:G:H2'	6:9:1760:G:C8	2.51	0.46
26:U:40:GLU:OE2	26:U:65:ARG:HG3	2.16	0.46
26:U:60:VAL:HG13	26:U:61:VAL:HG23	1.98	0.46
34:c:38:ILE:HG21	34:c:63:TYR:HB3	1.98	0.46
55:GG:138:ALA:HA	55:GG:176:ILE:HD11	1.97	0.46
73:ZZ:48:VAL:HG12	73:ZZ:80:ARG:HG3	1.97	0.46
79:Gg:163:PRO:HB2	79:Gg:179:LEU:HB2	1.97	0.46
3:5:12:A:H5'	3:5:13:U:OP2	2.15	0.45
3:5:257:C:H2'	3:5:258:G:H8	1.81	0.45
3:5:713:C:H2'	3:5:714:G:C8	2.51	0.45
3:5:969:C:H42	3:5:2095:A:H61	1.63	0.45
3:5:1329:G:O2'	3:5:1330:A:OP1	2.31	0.45
3:5:3832:U:H2'	3:5:3833:C:H6	1.81	0.45
3:5:4077:A:N1	3:5:4171:C:N4	2.62	0.45
3:5:4576:U:H2'	3:5:4577:U:C6	2.51	0.45
6:9:444:G:N1	6:9:447:A:OP2	2.48	0.45
6:9:1018:U:H5''	61:NN:71:ILE:HD12	1.98	0.45
6:9:1438:A:H2'	6:9:1439:A:H8	1.81	0.45
7:A:6:ARG:HH22	7:A:198:ARG:CZ	2.29	0.45
7:A:242:ARG:NH2	7:A:246:LEU:HD22	2.31	0.45
11:E:48:ARG:HB2	11:E:64:MET:HE1	1.96	0.45
14:H:128:MET:HE2	14:H:146:LEU:HD11	1.98	0.45
15:I:79:SER:HG	15:I:147:HIS:HD1	1.62	0.45
28:W:104:GLN:O	28:W:107:GLN:HG3	2.16	0.45
51:CC:98:LEU:HD21	51:CC:136:HIS:CD2	2.51	0.45
56:HH:64:VAL:O	56:HH:97:GLN:N	2.42	0.45
3:5:307:A:N3	3:5:310:G:O2'	2.48	0.45
3:5:423:G:H2'	3:5:424:U:C6	2.50	0.45
3:5:2424:OMG:OP2	3:5:2424:OMG:H8	1.99	0.45
3:5:2606:G:H2'	3:5:2607:C:C6	2.51	0.45
3:5:2735:G:H2'	3:5:2736:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:2743:A:H2'	3:5:2744:A:C8	2.51	0.45
3:5:4082:G:H2'	3:5:4083:5MU:C6	2.51	0.45
3:5:4233:A:H4'	46:o:98:LYS:HE2	1.99	0.45
3:5:4538:G:H2'	3:5:4539:U:C6	2.51	0.45
3:5:4769:G:H2'	3:5:4770:U:O4'	2.16	0.45
3:5:4894:A:H5''	3:5:4895:C:H2'	1.98	0.45
6:9:96:C:H2'	6:9:97:U:C6	2.51	0.45
6:9:120:U:H2'	6:9:121:OMU:H6	1.98	0.45
6:9:1499:U:H4'	52:DD:176:LEU:HD13	1.97	0.45
6:9:1754:G:H2'	6:9:1755:C:H6	1.80	0.45
9:C:334:THR:HG22	9:C:337:ARG:NH1	2.31	0.45
10:D:66:TYR:HE1	10:D:68:ARG:HE	1.64	0.45
10:D:115:MET:HE1	10:D:140:GLY:O	2.16	0.45
12:F:66:THR:O	12:F:70:MET:HG2	2.16	0.45
16:J:8:LYS:NZ	16:J:9:GLU:O	2.48	0.45
19:N:64:ILE:HD13	19:N:106:ALA:HB2	1.98	0.45
19:N:110:CYS:HB3	19:N:113:LEU:HD12	1.99	0.45
31:Z:120:GLU:O	31:Z:124:THR:HG23	2.17	0.45
57:II:130:THR:OG1	57:II:133:GLU:HG3	2.16	0.45
79:Gg:40:ILE:HD11	79:Gg:66:VAL:HG21	1.98	0.45
79:Gg:101:PHE:HE2	79:Gg:136:GLY:HA2	1.79	0.45
3:5:394:G:N2	3:5:397:G:OP2	2.37	0.45
3:5:956:A:H8	3:5:957:G:C8	2.34	0.45
3:5:1309:C:H2'	3:5:1310:C:C6	2.52	0.45
5:8:64:U:C2	5:8:65:A:C8	3.05	0.45
5:8:122:G:C6	5:8:123:U:C2	3.05	0.45
5:8:148:A:H2'	5:8:149:G:C8	2.52	0.45
6:9:202:G:O5'	57:II:143:LYS:HE3	2.16	0.45
6:9:813:A:C8	6:9:814:5MU:H73	2.52	0.45
6:9:821:G:C6	58:JJ:150:ARG:HG3	2.52	0.45
12:F:23:ASN:OD1	12:F:24:PHE:N	2.50	0.45
13:G:119:GLN:HG3	19:N:28:TRP:HH2	1.81	0.45
20:O:7:LEU:HB2	20:O:31:ARG:NH2	2.31	0.45
21:P:115:GLU:HB2	21:P:151:THR:HG22	1.97	0.45
40:i:96:ALA:HA	40:i:99:LYS:HZ2	1.80	0.45
50:BB:143:THR:HB	50:BB:205:TYR:CE1	2.50	0.45
51:CC:178:HIS:HB2	51:CC:220:ASP:OD1	2.17	0.45
55:GG:12:CYS:SG	55:GG:127:THR:HG23	2.56	0.45
61:NN:29:THR:O	61:NN:33:VAL:HG23	2.17	0.45
63:PP:24:GLN:O	63:PP:28:MET:HG3	2.17	0.45
64:QQ:41:MET:O	64:QQ:41:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:TT:29:LYS:O	67:TT:29:LYS:HD3	2.16	0.45
76:Cc:68:LEU:HD23	76:Cc:68:LEU:H	1.81	0.45
3:5:270:U:H2'	3:5:271:C:H6	1.81	0.45
3:5:467:U:H3	3:5:685:C:N4	2.14	0.45
3:5:729:2MG:N2	24:S:66:GLN:O	2.44	0.45
3:5:1382:G:H2'	3:5:1383:G:H8	1.81	0.45
3:5:2052:G:O2'	3:5:2057:A:N1	2.42	0.45
3:5:2517:A:N3	3:5:2539:C:O2'	2.49	0.45
3:5:2759:G:O2'	3:5:2760:G:O4'	2.28	0.45
3:5:4306:OMU:HM23	3:5:4306:OMU:H1'	1.56	0.45
3:5:4471:U:H2'	3:5:4472:B8W:C8	2.47	0.45
6:9:616:A:N3	78:Ee:85:VAL:HG21	2.31	0.45
6:9:874:G:O2'	6:9:875:A:OP1	2.25	0.45
6:9:896:U:H2'	6:9:897:U:C6	2.52	0.45
6:9:1579:A:O2'	6:9:1581:C:OP2	2.25	0.45
9:C:259:LYS:HG2	9:C:263:LEU:HD13	1.99	0.45
29:X:119:ILE:HD12	29:X:140:LEU:HD22	1.99	0.45
31:Z:100:VAL:HG23	31:Z:106:LEU:HB3	1.98	0.45
36:e:80:HIS:N	36:e:84:GLU:OE2	2.38	0.45
48:r:41:ASN:OD1	48:r:44:ILE:HG12	2.16	0.45
50:BB:136:ARG:NE	50:BB:218:LEU:HD11	2.31	0.45
51:CC:79:GLU:OE1	69:VV:12:TYR:HD1	2.00	0.45
68:UU:46:LYS:HE2	68:UU:100:GLN:NE2	2.31	0.45
3:5:1743:A:N1	3:5:1789:C:O2'	2.46	0.45
3:5:2412:A:H2'	3:5:2413:U:C6	2.52	0.45
3:5:3923:A:H2'	3:5:3924:C:C6	2.51	0.45
4:7:39:C:C6	16:J:49:VAL:HG21	2.52	0.45
6:9:874:G:HO2'	6:9:875:A:P	2.38	0.45
6:9:1446:A:N3	68:UU:55:ARG:HD2	2.31	0.45
6:9:1597:C:H4'	6:9:1603:G:C6	2.52	0.45
8:B:196:TRP:CD1	8:B:200:ARG:HH12	2.35	0.45
12:F:170:ASP:OD1	12:F:173:LEU:HG	2.17	0.45
15:I:6:ALA:O	15:I:10:ARG:HB3	2.16	0.45
20:O:108:ILE:HD12	20:O:160:ARG:CZ	2.45	0.45
26:U:62:SER:OG	26:U:64:GLU:OE2	2.24	0.45
34:c:12:GLU:HG2	34:c:13:SER:N	2.32	0.45
39:h:43:LYS:O	39:h:47:ILE:HG23	2.17	0.45
41:j:51:ALA:O	41:j:55:ARG:HG3	2.16	0.45
49:AA:205:ARG:HE	49:AA:210:ILE:HG12	1.82	0.45
52:DD:23:GLU:O	52:DD:26:THR:HG22	2.17	0.45
55:GG:14:LYS:HG2	55:GG:124:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:GG:159:ARG:HD3	55:GG:171:THR:OG1	2.17	0.45
56:HH:166:VAL:HG23	56:HH:189:PHE:HZ	1.81	0.45
67:TT:23:LYS:HG3	67:TT:54:TYR:CE2	2.50	0.45
72:YY:21:LYS:HG3	72:YY:75:ILE:HB	1.98	0.45
1:2:2:A:H3'	1:2:3:G:N2	2.31	0.45
3:5:261:G:H2'	3:5:262:G:H8	1.79	0.45
3:5:679:C:H2'	3:5:680:G:H8	1.81	0.45
3:5:2890:C:H2'	3:5:2891:U:C6	2.52	0.45
3:5:3727:A:H2'	3:5:3728:A:C8	2.51	0.45
3:5:4877:G:OP1	18:M:101:LYS:HE2	2.16	0.45
3:5:5002:U:H2'	3:5:5003:U:C6	2.52	0.45
3:5:5043:A:H2'	3:5:5044:A:C8	2.51	0.45
5:8:31:G:H2'	5:8:32:C:O4'	2.16	0.45
6:9:104:A:H62	6:9:356:C:H5	1.64	0.45
6:9:1203:G:H2'	6:9:1204:A:C8	2.52	0.45
6:9:1773:C:H2'	6:9:1774:C:C6	2.51	0.45
9:C:133:LEU:HB2	9:C:136:LEU:HD12	1.97	0.45
9:C:331:TYR:CE1	12:F:54:LYS:HG3	2.52	0.45
10:D:21:ARG:NH1	10:D:25:GLU:OE1	2.45	0.45
13:G:168:LEU:O	13:G:172:GLU:OE1	2.34	0.45
34:c:22:MET:CE	34:c:85:CYS:HA	2.42	0.45
36:e:109:LYS:O	36:e:113:GLU:OE1	2.34	0.45
49:AA:76:VAL:HG13	49:AA:87:VAL:HG13	1.99	0.45
49:AA:122:LEU:HD13	49:AA:142:LEU:HD11	1.99	0.45
57:II:110:ARG:HG2	57:II:121:LEU:HD21	1.98	0.45
63:PP:110:GLU:OE2	66:SS:117:ILE:HD13	2.17	0.45
66:SS:62:ASP:O	66:SS:65:GLU:HG3	2.16	0.45
79:Gg:270:LEU:HD21	79:Gg:310:TRP:CZ2	2.52	0.45
3:5:131:C:H2'	3:5:132:G:C8	2.51	0.45
3:5:325:U:H2'	3:5:326:C:C6	2.51	0.45
3:5:429:A:H2'	3:5:430:G:C8	2.52	0.45
3:5:968:C:H2'	3:5:969:C:C6	2.52	0.45
3:5:1440:U:O2'	3:5:1441:C:OP1	2.28	0.45
3:5:1835:G:OP2	3:5:1835:G:N2	2.40	0.45
3:5:2015:U:H2'	3:5:2016:C:C6	2.52	0.45
3:5:2060:G:N2	24:S:115:ALA:HB2	2.32	0.45
3:5:4344:U:H2'	3:5:4345:C:C6	2.50	0.45
3:5:4438:U:H2'	3:5:4439:U:O4'	2.16	0.45
5:8:14:OMU:C4	5:8:15:G:C6	3.00	0.45
6:9:794:A:H2'	6:9:795:A:C8	2.48	0.45
15:I:10:ARG:HG3	15:I:11:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:159:LYS:O	16:J:163:MET:HG3	2.17	0.45
24:S:80:ILE:HG23	24:S:126:ILE:HD11	1.98	0.45
33:b:35:VAL:HG21	33:b:40:LEU:HD13	1.99	0.45
34:c:46:VAL:HB	34:c:71:VAL:HG12	1.99	0.45
39:h:9:LEU:HD23	39:h:12:LYS:HD2	1.98	0.45
53:EE:125:LYS:O	53:EE:142:HIS:N	2.50	0.45
53:EE:130:PHE:O	53:EE:138:HIS:N	2.44	0.45
58:JJ:70:ARG:NH1	58:JJ:94:LEU:HD21	2.32	0.45
70:WW:3:ARG:HH21	70:WW:28:ARG:NH2	2.15	0.45
72:YY:37:LYS:HG2	72:YY:60:PHE:CE1	2.52	0.45
72:YY:88:LYS:HB3	72:YY:97:TYR:CD1	2.51	0.45
3:5:106:A:H2'	3:5:107:G:O4'	2.17	0.45
3:5:295:A:OP2	46:o:39:ARG:NE	2.36	0.45
3:5:509:A:C6	32:a:105:ARG:HD3	2.51	0.45
3:5:754:C:H2'	3:5:755:C:H6	1.82	0.45
3:5:910:G:H2'	3:5:911:U:H6	1.81	0.45
3:5:1404:G:H2'	3:5:1405:C:H6	1.80	0.45
3:5:1613:A:H5''	7:A:183:GLY:CA	2.47	0.45
3:5:1749:A:H2'	3:5:1750:G:C8	2.50	0.45
3:5:2478:C:H2'	3:5:2479:G:O4'	2.17	0.45
3:5:2744:A:H2'	3:5:2745:A:C8	2.52	0.45
3:5:2815:A:H2'	3:5:2816:G:C8	2.50	0.45
3:5:4564:M7A:O2'	8:B:261:ARG:HB3	2.17	0.45
4:7:2:U:H2'	4:7:3:C:H6	1.82	0.45
4:7:15:C:H2'	4:7:16:A:H8	1.82	0.45
5:8:6:C:H2'	5:8:7:U:H6	1.81	0.45
5:8:40:A:H2'	5:8:41:A:C8	2.52	0.45
6:9:527:C:H2'	6:9:528:A:H8	1.82	0.45
6:9:1681:U:H2'	6:9:1682:C:C6	2.52	0.45
9:C:349:LEU:O	9:C:352:GLU:HG3	2.17	0.45
20:O:75:ALA:O	20:O:79:ILE:HG13	2.16	0.45
28:W:97:LYS:NZ	28:W:98:PRO:HG2	2.31	0.45
39:h:117:ARG:HA	39:h:117:ARG:HD2	1.71	0.45
56:HH:72:PHE:O	56:HH:76:GLN:N	2.49	0.45
79:Gg:256:ILE:HG12	79:Gg:270:LEU:HD22	1.98	0.45
3:5:1177:U:H2'	3:5:1178:G:H8	1.82	0.45
3:5:1445:U:H2'	3:5:1446:C:C6	2.52	0.45
3:5:1759:G:H2'	3:5:1760:G:H8	1.82	0.45
3:5:2469:C:H5	3:5:2471:G:H1	1.65	0.45
3:5:2713:C:H2'	3:5:2714:G:O4'	2.17	0.45
3:5:4566:U:O2'	8:B:234:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:4910:A:C4	20:O:156:LEU:HD23	2.52	0.45
6:9:71:G:H2'	6:9:72:C:C6	2.52	0.45
6:9:532:C:O2'	6:9:533:A:OP1	2.30	0.45
6:9:540:U:O2'	6:9:543:C:N4	2.49	0.45
6:9:644:OMG:HM23	6:9:644:OMG:H1'	1.64	0.45
6:9:1679:A:OP2	54:FF:60:ARG:HD2	2.17	0.45
9:C:147:VAL:HG13	9:C:152:LEU:HD22	1.99	0.45
11:E:205:ASP:OD1	11:E:263:LYS:HD2	2.17	0.45
29:X:80:PRO:HA	29:X:98:PHE:HA	1.99	0.45
36:e:79:VAL:HG13	36:e:84:GLU:HG3	1.99	0.45
49:AA:120:ARG:NH2	51:CC:267:GLN:HB2	2.32	0.45
53:EE:166:THR:HG23	53:EE:168:LYS:H	1.81	0.45
66:SS:107:LEU:O	66:SS:111:LEU:HG	2.17	0.45
68:UU:54:VAL:HG22	68:UU:88:LEU:HB2	1.98	0.45
71:XX:93:PHE:CD1	71:XX:133:LEU:HD23	2.52	0.45
71:XX:111:ALA:HB2	71:XX:119:ARG:HH12	1.82	0.45
79:Gg:16:GLY:HA3	79:Gg:36:ARG:HB2	1.99	0.45
3:5:318:A:H2'	3:5:319:A:H8	1.82	0.45
3:5:730:G:OP2	12:F:75:ARG:NE	2.46	0.45
3:5:1291:G:O2'	3:5:1292:C:OP1	2.25	0.45
3:5:4969:C:H2'	3:5:4970:C:H6	1.81	0.45
6:9:963:A:H2'	6:9:964:A:C8	2.52	0.45
6:9:1069:U:H4'	7:A:247:ARG:HB3	1.99	0.45
6:9:1662:U:O4	6:9:1663:A:N6	2.50	0.45
6:9:1674:G:N7	64:QQ:17:LYS:NZ	2.57	0.45
9:C:150:LEU:HB3	9:C:151:PRO:HD3	1.98	0.45
11:E:181:PRO:HB3	11:E:261:LEU:HD21	1.99	0.45
13:G:164:LYS:HD2	13:G:167:LEU:HD11	1.98	0.45
14:H:66:GLU:HA	14:H:69:THR:HG23	1.99	0.45
21:P:54:LYS:HA	21:P:83:TRP:CD1	2.52	0.45
26:U:99:TRP:HB2	26:U:100:LEU:HD12	1.98	0.45
66:SS:88:LYS:HB2	66:SS:95:TYR:CZ	2.51	0.45
79:Gg:76:GLN:C	79:Gg:92:LEU:HD23	2.42	0.45
79:Gg:133:ASN:OD1	79:Gg:136:GLY:N	2.47	0.45
79:Gg:144:ASP:OD1	79:Gg:145:GLU:N	2.50	0.45
1:2:1:G:H2'	1:2:2:A:C8	2.52	0.44
3:5:729:2MG:HM23	3:5:729:2MG:OP1	2.16	0.44
3:5:1893:C:H1'	3:5:1937:C:O2	2.17	0.44
3:5:2483:G:H1	3:5:2495:U:H3	1.65	0.44
3:5:2566:G:H2'	3:5:2567:G:C8	2.52	0.44
3:5:3635:A:C8	3:5:3692:A:C8	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:3811:G:O2'	3:5:3814:U:OP2	2.28	0.44
3:5:3909:OMC:HM22	3:5:3910:C:H5'	1.99	0.44
3:5:4716:C:OP2	8:B:30:LYS:HG3	2.17	0.44
5:8:121:G:C6	5:8:122:G:C5	3.05	0.44
6:9:194:C:H2'	6:9:195:C:H6	1.81	0.44
6:9:1533:A:N7	6:9:1604:G:H1'	2.31	0.44
6:9:1589:A:N3	6:9:1653:U:O2'	2.42	0.44
12:F:240:ASN:O	12:F:244:ARG:HG2	2.17	0.44
14:H:92:MET:SD	14:H:161:ILE:HD11	2.57	0.44
14:H:128:MET:CE	14:H:157:SER:HB3	2.47	0.44
17:L:42:ARG:O	17:L:45:ARG:HG2	2.17	0.44
19:N:104:GLU:HA	19:N:160:GLU:HG3	1.99	0.44
20:O:47:PHE:CE1	20:O:140:ARG:HG2	2.52	0.44
29:X:80:PRO:HG2	29:X:155:ILE:HG21	1.99	0.44
29:X:89:LYS:HG2	29:X:95:THR:OG1	2.17	0.44
42:k:24:LYS:HA	42:k:67:LYS:O	2.16	0.44
50:BB:57:ILE:HG22	50:BB:59:SER:H	1.81	0.44
56:HH:57:ARG:NH1	56:HH:172:THR:OG1	2.49	0.44
76:Cc:51:ARG:HG2	76:Cc:52:GLU:N	2.32	0.44
3:5:72:C:C5	17:L:67:HIS:HD2	2.36	0.44
3:5:124:C:H2'	3:5:125:C:C6	2.52	0.44
3:5:233:U:O2'	3:5:2304:U:O4	2.31	0.44
3:5:1766:A:H2'	3:5:1767:A:O4'	2.17	0.44
3:5:2292:C:H2'	3:5:2293:U:C6	2.53	0.44
3:5:3723:A2M:H2'	3:5:3724:A:H8	1.82	0.44
3:5:4261:C:O2'	16:J:102:THR:HG21	2.17	0.44
3:5:4736:C:H2'	3:5:4737:G:C8	2.52	0.44
6:9:121:OMU:H1'	6:9:121:OMU:HM23	1.66	0.44
6:9:1113:A:C6	6:9:1121:G:C6	3.06	0.44
6:9:1839:U:H2'	6:9:1840:U:C6	2.53	0.44
10:D:153:THR:HB	10:D:160:PHE:HZ	1.82	0.44
21:P:96:LYS:O	21:P:99:GLU:HG3	2.17	0.44
22:Q:22:ASP:O	22:Q:26:ARG:HG3	2.17	0.44
22:Q:69:LYS:O	22:Q:75:ARG:HD2	2.16	0.44
30:Y:112:ASP:OD2	30:Y:114:ASP:N	2.50	0.44
39:h:13:LYS:HB3	39:h:16:GLU:OE1	2.16	0.44
51:CC:211:LYS:HG2	51:CC:215:MET:HE3	2.00	0.44
54:FF:61:PHE:HB3	76:Cc:51:ARG:HH22	1.82	0.44
68:UU:67:LYS:NZ	68:UU:78:ASP:OD1	2.36	0.44
70:WW:24:GLN:NE2	70:WW:64:ASN:OD1	2.35	0.44
73:ZZ:66:LYS:HD2	73:ZZ:111:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:102:G:O2'	3:5:1381:U:O2'	2.33	0.44
3:5:2710:C:N4	3:5:2712:G:N7	2.64	0.44
3:5:3867:A2M:HM'3	3:5:3867:A2M:H1'	1.80	0.44
3:5:4684:A:H2'	3:5:4685:U:O4'	2.18	0.44
6:9:106:C:H2'	6:9:107:A:C8	2.52	0.44
6:9:166:A2M:H8	6:9:166:A2M:H5''	1.98	0.44
6:9:911:C:O2'	6:9:912:C:H5'	2.17	0.44
6:9:1265:A:H5''	6:9:1266:C:OP2	2.17	0.44
6:9:1416:C:H2'	6:9:1417:C:C6	2.52	0.44
17:L:126:LEU:HD12	17:L:126:LEU:HA	1.89	0.44
30:Y:88:GLU:OE2	30:Y:92:GLY:HA2	2.17	0.44
31:Z:99:ASP:HA	31:Z:102:ARG:NH2	2.32	0.44
36:e:119:ALA:HB2	48:r:119:ARG:NH1	2.33	0.44
43:l:41:ARG:HD2	43:l:41:ARG:HA	1.84	0.44
44:m:82:VAL:O	44:m:83:ASN:ND2	2.50	0.44
46:o:67:VAL:HG11	46:o:82:MET:HE3	1.99	0.44
56:HH:27:LEU:HD11	56:HH:79:LEU:HD21	1.98	0.44
67:TT:98:SER:O	67:TT:102:ARG:HG2	2.18	0.44
75:Bb:11:SER:HB3	75:Bb:14:GLU:OE1	2.17	0.44
3:5:163:A:H2'	3:5:164:G:C8	2.53	0.44
3:5:1211:G:HO2'	3:5:1212:G:P	2.38	0.44
3:5:1358:G:O2'	3:5:1360:G:O6	2.31	0.44
3:5:1577:G:C5	7:A:181:LYS:HB2	2.53	0.44
3:5:1927:U:OP1	3:5:1949:U:O2'	2.32	0.44
3:5:2079:G:H2'	3:5:2080:U:H6	1.82	0.44
3:5:3707:U:H2'	3:5:3708:C:C6	2.53	0.44
3:5:4458:C:H2'	3:5:4459:U:C6	2.52	0.44
3:5:4970:C:C2	3:5:4971:A:C8	3.06	0.44
6:9:1103:C:H2'	6:9:1104:G:C8	2.52	0.44
6:9:1289:U:H2'	6:9:1290:G:C8	2.52	0.44
6:9:1733:U:H2'	6:9:1734:G:O4'	2.16	0.44
6:9:1802:C:H2'	6:9:1803:U:H6	1.83	0.44
9:C:184:TYR:CE1	9:C:225:PRO:HG3	2.52	0.44
16:J:17:ILE:O	16:J:17:ILE:HG13	2.16	0.44
28:W:80:ARG:HG2	28:W:81:ALA:N	2.33	0.44
40:i:15:HIS:HD2	40:i:16:LYS:N	2.16	0.44
53:EE:233:LYS:HA	53:EE:233:LYS:HE3	1.99	0.44
55:GG:49:VAL:HG22	55:GG:115:LYS:HB3	1.97	0.44
57:II:148:LYS:O	57:II:152:ARG:HG3	2.18	0.44
64:QQ:60:LYS:O	64:QQ:64:ALA:N	2.50	0.44
3:5:7:C:H2'	3:5:8:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:302:C:H2'	3:5:303:C:H6	1.83	0.44
3:5:981:U:H2'	3:5:982:C:C6	2.52	0.44
3:5:1078:A:H3'	3:5:1079:C:H5''	1.99	0.44
3:5:1197:C:H2'	3:5:1198:G:C8	2.52	0.44
3:5:2034:G:OP1	24:S:87:ARG:HD3	2.17	0.44
3:5:4088:C:OP1	7:A:37:ARG:NH2	2.43	0.44
4:7:23:A:H2'	4:7:24:C:C6	2.53	0.44
6:9:223:C:H2'	6:9:224:A:C8	2.53	0.44
10:D:33:ARG:O	10:D:37:VAL:HG22	2.18	0.44
13:G:203:LYS:NZ	13:G:230:MET:O	2.49	0.44
14:H:27:VAL:HG12	14:H:84:VAL:HG11	1.98	0.44
29:X:120:ASP:OD1	29:X:121:VAL:N	2.50	0.44
37:f:11:PHE:CE2	37:f:97:ILE:HD13	2.53	0.44
50:BB:44:ILE:HD11	50:BB:86:LEU:HD12	1.98	0.44
51:CC:263:LYS:HZ2	51:CC:268:GLU:HG3	1.80	0.44
54:FF:99:ILE:HD11	54:FF:171:GLU:HA	1.99	0.44
56:HH:160:LYS:O	56:HH:163:GLN:HB2	2.17	0.44
3:5:1298:C:H2'	3:5:1299:G:H8	1.83	0.44
3:5:1455:G:O2'	3:5:1456:B8Q:OP1	2.31	0.44
3:5:2382:A:N1	3:5:2829:U:O2'	2.46	0.44
3:5:3723:A2M:H1'	3:5:3723:A2M:HM'3	1.70	0.44
3:5:3893:C:H2'	3:5:3894:A:C8	2.53	0.44
3:5:4688:C:H2'	3:5:4689:U:C6	2.53	0.44
4:7:110:G:H2'	4:7:111:C:C6	2.53	0.44
5:8:6:C:H2'	5:8:7:U:C6	2.52	0.44
5:8:86:U:OP2	30:Y:113:LYS:NZ	2.50	0.44
6:9:174:OMC:HM23	6:9:174:OMC:H1'	1.76	0.44
6:9:1705:C:H2'	6:9:1706:G:C8	2.52	0.44
19:N:146:PRO:HG3	39:h:102:LEU:HD12	2.00	0.44
20:O:127:VAL:HG12	20:O:128:ARG:HD2	2.00	0.44
20:O:162:GLU:O	20:O:166:ILE:HG12	2.17	0.44
23:R:114:LYS:O	23:R:146:LYS:NZ	2.36	0.44
24:S:90:THR:HG23	25:T:156:TYR:CD2	2.52	0.44
40:i:68:ARG:HD3	40:i:68:ARG:HA	1.74	0.44
49:AA:13:GLU:CD	49:AA:13:GLU:H	2.26	0.44
52:DD:65:ARG:O	52:DD:69:LEU:HG	2.18	0.44
52:DD:211:VAL:O	65:RR:20:TYR:OH	2.27	0.44
61:NN:32:ASP:HA	61:NN:35:GLU:HG3	2.00	0.44
64:QQ:55:VAL:HA	64:QQ:63:PHE:CE2	2.53	0.44
70:WW:52:ILE:HG22	70:WW:61:ILE:HG12	1.99	0.44
79:Gg:192:THR:OG1	79:Gg:213:ASP:OD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:74:C:O2'	1:2:75:C:H5'	2.17	0.44
3:5:374:G:OP2	41:j:56:ARG:NH2	2.45	0.44
3:5:731:G:C6	3:5:932:A:C4	3.06	0.44
3:5:950:G:H2'	3:5:951:G:H8	1.83	0.44
3:5:1202:C:H2'	3:5:1203:G:H8	1.83	0.44
3:5:1326:A2M:HM'3	3:5:1326:A2M:H1'	1.71	0.44
3:5:3871:A:H2'	3:5:3872:A:C8	2.53	0.44
3:5:4110:C:H2'	3:5:4111:U:C6	2.52	0.44
5:8:14:OMU:HM23	5:8:14:OMU:H1'	1.47	0.44
6:9:65:C:C6	55:GG:174:PRO:HB3	2.53	0.44
6:9:539:C:H2'	6:9:540:U:O4'	2.17	0.44
6:9:1841:C:H3'	45:n:2:ARG:HH11	1.83	0.44
7:A:101:VAL:HG22	7:A:163:ARG:HB3	1.99	0.44
26:U:42:PHE:O	26:U:46:ARG:HG2	2.17	0.44
29:X:86:ALA:O	29:X:90:ILE:HG23	2.17	0.44
52:DD:190:LEU:HD23	52:DD:199:GLY:HA2	1.98	0.44
65:RR:99:ASP:HA	65:RR:120:THR:HG22	1.99	0.44
79:Gg:36:ARG:HH21	79:Gg:65:PHE:HE2	1.65	0.44
3:5:6:C:H2'	3:5:7:C:C6	2.53	0.44
3:5:667:A:H5''	3:5:668:C:H5	1.82	0.44
3:5:724:C:OP1	9:C:350:ARG:HD2	2.18	0.44
3:5:1445:U:H2'	3:5:1446:C:H6	1.82	0.44
3:5:1867:A:OP1	15:I:13:LYS:NZ	2.27	0.44
3:5:2089:G:H1'	3:5:2090:U:OP2	2.17	0.44
3:5:2779:C:O2'	5:8:112:G:OP1	2.25	0.44
3:5:3658:C:H5''	7:A:242:ARG:O	2.18	0.44
3:5:4266:G:N3	3:5:4266:G:H2'	2.32	0.44
3:5:4895:C:H1'	18:M:132:ARG:NH1	2.33	0.44
6:9:1407:U:H4'	64:QQ:71:ARG:NH2	2.33	0.44
10:D:19:LYS:HB2	10:D:24:ARG:HG3	2.00	0.44
11:E:184:LEU:HD23	11:E:274:LEU:HB2	2.00	0.44
14:H:34:LEU:HD11	14:H:80:MET:HG2	2.00	0.44
21:P:50:ASP:HB3	21:P:56:GLN:HG3	1.98	0.44
24:S:1:MET:HE1	24:S:33:PHE:O	2.18	0.44
54:FF:167:LYS:HA	73:ZZ:71:ALA:HB1	1.99	0.44
57:II:87:ASN:ND2	57:II:89:GLU:HB2	2.33	0.44
58:JJ:29:LEU:HA	58:JJ:32:ILE:HG22	2.00	0.44
3:5:2015:U:H2'	3:5:2016:C:H6	1.83	0.44
3:5:2634:C:H2'	3:5:2635:U:H6	1.83	0.44
3:5:4889:G:C6	3:5:4931:G:C6	3.06	0.44
6:9:441:C:H2'	6:9:442:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:1278:A:H2'	6:9:1279:C:C6	2.53	0.44
6:9:1772:C:H2'	6:9:1773:C:C6	2.53	0.44
9:C:150:LEU:O	9:C:152:LEU:N	2.51	0.44
23:R:157:ASP:HA	23:R:160:GLU:HG3	2.00	0.44
35:d:36:VAL:HG23	35:d:41:ARG:HG2	1.99	0.44
66:SS:68:ILE:H	66:SS:68:ILE:HD12	1.82	0.44
3:5:450:G:H1	3:5:1297:U:H3	1.66	0.43
3:5:1356:U:H2'	3:5:1357:C:C6	2.53	0.43
3:5:1510:G:H2'	3:5:1511:U:C6	2.53	0.43
3:5:1567:U:H2'	3:5:1568:C:C6	2.53	0.43
3:5:1949:U:H2'	3:5:1950:U:H6	1.83	0.43
3:5:2270:G:H2'	3:5:2271:C:C6	2.53	0.43
3:5:3910:C:H2'	3:5:3911:C:H6	1.82	0.43
3:5:4254:G:H3'	3:5:4256:A:OP2	2.18	0.43
6:9:501:C:O2	6:9:501:C:H2'	2.17	0.43
6:9:528:A:H2'	6:9:529:A:C8	2.51	0.43
16:J:31:ASP:OD1	16:J:32:ARG:N	2.51	0.43
19:N:47:LYS:NZ	19:N:51:LEU:HD21	2.33	0.43
20:O:97:ALA:O	20:O:101:ARG:HG2	2.18	0.43
39:h:50:VAL:O	39:h:54:ILE:HG12	2.18	0.43
54:FF:35:LEU:HD12	54:FF:117:ILE:HG12	2.00	0.43
56:HH:63:PHE:CE1	56:HH:95:ILE:HD11	2.53	0.43
66:SS:36:VAL:HG23	66:SS:40:TYR:CD2	2.46	0.43
74:Aa:42:ARG:O	74:Aa:67:LEU:N	2.51	0.43
79:Gg:298:LEU:N	79:Gg:310:TRP:O	2.30	0.43
1:2:5:A:H61	1:2:68:C:H42	1.65	0.43
3:5:69:A:N1	3:5:324:A:O2'	2.48	0.43
3:5:754:C:H2'	3:5:755:C:C6	2.53	0.43
3:5:1472:C:H2'	3:5:1473:U:H6	1.82	0.43
3:5:1662:C:H2'	3:5:1663:C:C6	2.54	0.43
3:5:2412:A:H2'	3:5:2413:U:H6	1.83	0.43
3:5:2693:G:H2'	3:5:2694:G:N2	2.34	0.43
3:5:3949:A:N6	3:5:4064:C:N3	2.61	0.43
3:5:4657:U:H4'	35:d:78:ARG:HH12	1.83	0.43
6:9:116:OMU:HM23	6:9:116:OMU:H1'	1.69	0.43
6:9:677:G:N1	6:9:1027:A:OP2	2.27	0.43
6:9:1538:C:H2'	6:9:1539:U:C6	2.53	0.43
7:A:196:TRP:O	7:A:198:ARG:N	2.51	0.43
10:D:235:MET:O	10:D:238:GLU:HG3	2.17	0.43
18:M:74:ARG:HG2	18:M:78:GLU:OE1	2.18	0.43
22:Q:89:ASP:O	22:Q:92:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Q:178:ARG:HB2	32:a:53:PHE:O	2.18	0.43
31:Z:41:ALA:HB2	31:Z:77:TYR:HE1	1.83	0.43
32:a:74:ASN:HA	32:a:112:LEU:O	2.18	0.43
50:BB:123:ALA:HB1	50:BB:169:MET:HG3	2.00	0.43
53:EE:45:ILE:CD1	53:EE:61:VAL:HG11	2.48	0.43
57:II:69:SER:OG	57:II:70:GLU:OE1	2.27	0.43
76:Cc:36:ASP:OD2	76:Cc:37:ASP:N	2.51	0.43
79:Gg:194:TYR:CZ	79:Gg:212:LYS:HD3	2.54	0.43
3:5:492:U:H4'	3:5:493:G:OP2	2.17	0.43
3:5:4691:A:H2'	3:5:4692:A:O4'	2.17	0.43
3:5:4760:G:H2'	3:5:4761:G:O4'	2.18	0.43
3:5:5003:U:H2'	3:5:5004:C:C6	2.54	0.43
4:7:49:A:H5''	10:D:224:SER:OG	2.18	0.43
5:8:66:A:H2'	5:8:67:U:C6	2.53	0.43
6:9:373:G:H21	60:LL:83:GLN:NE2	2.16	0.43
6:9:1365:G:H2'	6:9:1366:G:C8	2.52	0.43
7:A:156:LYS:HE2	7:A:158:ILE:HD11	1.99	0.43
9:C:138:MET:HE1	9:C:145:GLU:OE2	2.18	0.43
15:I:187:GLU:OE2	15:I:189:ARG:HB2	2.18	0.43
37:f:14:TYR:O	37:f:16:ARG:HG2	2.18	0.43
40:i:29:ARG:O	40:i:29:ARG:HG2	2.17	0.43
51:CC:179:THR:HG22	51:CC:180:VAL:H	1.83	0.43
53:EE:125:LYS:HB2	53:EE:226:PHE:CD1	2.54	0.43
57:II:10:LYS:O	57:II:18:ARG:NH1	2.52	0.43
63:PP:15:PHE:CZ	63:PP:110:GLU:HA	2.53	0.43
71:XX:105:PHE:CD1	71:XX:121:LYS:HB2	2.53	0.43
79:Gg:203:ASP:OD1	79:Gg:204:GLY:N	2.51	0.43
3:5:48:G:H5'	19:N:192:TRP:NE1	2.33	0.43
3:5:1291:G:HO2'	3:5:1292:C:P	2.39	0.43
3:5:2340:C:H4'	9:C:42:THR:HG23	2.00	0.43
3:5:2758:G:O2'	3:5:2765:A:N3	2.38	0.43
3:5:4412:C:H2'	3:5:4413:C:O2	2.18	0.43
6:9:220:U:H2'	6:9:221:A:H8	1.83	0.43
6:9:1244:U:H2'	6:9:1245:G:H8	1.84	0.43
6:9:1387:G:H2'	6:9:1388:A:O4'	2.19	0.43
6:9:1712:A:H2'	6:9:1713:C:H6	1.81	0.43
6:9:1809:A:H2'	6:9:1810:U:C6	2.53	0.43
8:B:71:GLU:OE2	8:B:366:LYS:HE2	2.19	0.43
9:C:190:ARG:HB2	9:C:202:ILE:HG23	2.00	0.43
12:F:74:ALA:HB2	25:T:140:PHE:HE1	1.84	0.43
19:N:77:LYS:HG3	19:N:78:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:76:ASN:HB2	31:Z:79:HIS:CD2	2.52	0.43
44:m:69:ILE:HD11	44:m:96:ARG:NH2	2.32	0.43
50:BB:38:MET:HE1	50:BB:231:LEU:HD22	2.01	0.43
52:DD:213:PRO:HB3	65:RR:20:TYR:CE1	2.53	0.43
58:JJ:83:ARG:HG2	58:JJ:150:ARG:HD3	1.99	0.43
58:JJ:152:ASP:OD1	58:JJ:153:SER:N	2.51	0.43
60:LL:124:ASP:OD1	60:LL:124:ASP:N	2.41	0.43
66:SS:82:TRP:CD1	66:SS:82:TRP:H	2.36	0.43
68:UU:24:LEU:HB3	68:UU:32:LEU:HD11	2.00	0.43
68:UU:107:GLU:HB3	68:UU:110:VAL:HG23	1.99	0.43
3:5:325:U:H2'	3:5:326:C:H6	1.83	0.43
3:5:710:G:H4'	11:E:193:HIS:NE2	2.32	0.43
3:5:956:A:H1'	3:5:2076:G:H5''	2.00	0.43
3:5:1308:C:H2'	3:5:1309:C:H6	1.84	0.43
3:5:1933:G:H2'	3:5:1934:A:C8	2.54	0.43
3:5:3722:G:H2'	3:5:3723:A2M:C8	2.40	0.43
3:5:4578:G:H2'	3:5:4579:U:H6	1.83	0.43
3:5:5043:A:H2'	3:5:5044:A:H8	1.84	0.43
4:7:2:U:H2'	4:7:3:C:C6	2.53	0.43
4:7:3:C:H2'	4:7:4:U:H6	1.82	0.43
5:8:7:U:H2'	5:8:8:U:C6	2.54	0.43
6:9:92:A:O2'	53:EE:4:GLY:HA3	2.19	0.43
6:9:160:U:O2'	6:9:161:U:H3'	2.19	0.43
6:9:1543:U:H5''	64:QQ:37:ARG:HH12	1.83	0.43
6:9:1633:A:H2'	6:9:1634:A:C8	2.53	0.43
7:A:96:LEU:O	47:p:87:LYS:HD3	2.18	0.43
7:A:116:LEU:HD12	7:A:117:GLU:H	1.83	0.43
8:B:77:THR:HG21	8:B:337:VAL:HG22	2.00	0.43
9:C:149:GLU:HG2	9:C:151:PRO:HD2	1.99	0.43
11:E:261:LEU:HD13	11:E:264:ILE:HD11	1.99	0.43
13:G:91:ASN:ND2	13:G:96:GLN:OE1	2.52	0.43
50:BB:169:MET:O	50:BB:173:THR:HG23	2.19	0.43
51:CC:191:VAL:HG11	51:CC:236:PHE:HD1	1.83	0.43
53:EE:56:LEU:N	53:EE:60:GLU:OE1	2.51	0.43
57:II:149:TYR:O	57:II:153:LYS:HG2	2.18	0.43
72:YY:60:PHE:CE2	72:YY:71:GLY:HA3	2.54	0.43
3:5:396:A:H2'	3:5:397:G:C8	2.54	0.43
3:5:1920:C:H3'	3:5:1921:C:H5''	2.01	0.43
3:5:2727:C:H2'	3:5:2728:U:C6	2.54	0.43
3:5:4587:G:OP1	20:O:61:ARG:NH1	2.52	0.43
3:5:4883:C:H5	11:E:275:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:8:144:U:H2'	5:8:145:C:C6	2.53	0.43
6:9:885:U:O2	6:9:901:G:C6	2.72	0.43
6:9:1711:U:H2'	6:9:1712:A:H8	1.84	0.43
8:B:248:LEU:HD23	8:B:248:LEU:H	1.82	0.43
9:C:163:LYS:HB2	9:C:166:GLU:HG2	2.00	0.43
10:D:52:ILE:HA	10:D:147:ASP:HB3	2.01	0.43
17:L:123:LYS:HB2	17:L:123:LYS:HE2	1.80	0.43
20:O:16:LEU:HD12	20:O:80:PHE:HD1	1.83	0.43
27:V:87:SER:HA	27:V:97:TYR:HB3	2.01	0.43
28:W:102:LYS:O	28:W:106:GLU:OE1	2.36	0.43
33:b:47:LYS:HA	33:b:50:ASN:OD1	2.18	0.43
37:f:71:TRP:HB2	37:f:89:ARG:HH11	1.83	0.43
59:KK:21:MET:HG2	59:KK:49:MET:SD	2.59	0.43
61:NN:3:ARG:HB2	61:NN:6:ALA:HB3	1.99	0.43
3:5:497:G:O6	3:5:658:C:N4	2.51	0.43
3:5:924:C:OP1	3:5:926:G:O2'	2.35	0.43
3:5:983:U:OP1	11:E:75:TYR:OH	2.28	0.43
3:5:3888:G:HO2'	3:5:3889:G:P	2.42	0.43
3:5:4615:C:H5''	8:B:357:ARG:HH11	1.83	0.43
3:5:5002:U:H2'	3:5:5003:U:H6	1.84	0.43
3:5:5061:A:H3'	3:5:5062:G:H5'	2.00	0.43
6:9:96:C:O2	6:9:473:A:O2'	2.33	0.43
6:9:1171:G:O2'	6:9:1187:G:O6	2.25	0.43
6:9:1560:U:O2'	6:9:1583:C:O2'	2.23	0.43
6:9:1754:G:H2'	6:9:1755:C:C6	2.54	0.43
31:Z:61:LYS:HG2	31:Z:65:ARG:HD2	1.99	0.43
32:a:28:HIS:CD2	32:a:32:ARG:HD3	2.53	0.43
39:h:105:LYS:HA	39:h:108:GLN:HG2	2.00	0.43
42:k:28:ASN:OD1	42:k:31:ASN:HB3	2.19	0.43
54:FF:14:THR:HG22	64:QQ:57:LEU:HA	2.01	0.43
56:HH:51:ILE:HG12	56:HH:179:LYS:HG2	2.00	0.43
66:SS:61:GLU:CD	66:SS:61:GLU:H	2.27	0.43
67:TT:26:GLY:C	67:TT:27:LYS:HD3	2.44	0.43
79:Gg:191:HIS:NE2	79:Gg:215:GLN:O	2.50	0.43
3:5:50:C:C2	3:5:51:A:C8	3.07	0.43
3:5:64:A:H1'	3:5:76:A:H1'	2.01	0.43
3:5:952:G:H2'	3:5:953:C:C6	2.53	0.43
3:5:978:C:H4'	9:C:333:MLZ:HCM1	2.01	0.43
3:5:1461:C:H2'	3:5:1462:A:H8	1.83	0.43
3:5:2637:U:HO2'	3:5:2718:U:HO2'	1.65	0.43
3:5:3599:A:H2'	3:5:3600:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:4109:G:H2'	3:5:4110:C:H6	1.84	0.43
3:5:4960:G:H2'	3:5:4961:G:C8	2.53	0.43
6:9:754:G:H2'	6:9:755:C:C6	2.52	0.43
6:9:1451:G:N7	65:RR:44:LYS:NZ	2.56	0.43
6:9:1617:G:N2	6:9:1619:A:H3'	2.34	0.43
10:D:211:LEU:HG	10:D:219:TYR:HB2	2.01	0.43
11:E:252:ASP:O	11:E:256:VAL:HG23	2.19	0.43
13:G:283:TYR:HA	13:G:286:ILE:HB	2.00	0.43
27:V:112:MET:HE1	27:V:117:ILE:HD11	2.01	0.43
28:W:107:GLN:HA	28:W:110:ARG:CD	2.49	0.43
31:Z:95:VAL:HG13	31:Z:96:VAL:HG23	2.00	0.43
55:GG:228:ILE:O	55:GG:232:ARG:N	2.42	0.43
56:HH:146:VAL:O	70:WW:49:GLU:HB2	2.19	0.43
70:WW:31:SER:O	70:WW:35:VAL:HG23	2.19	0.43
73:ZZ:58:LEU:O	73:ZZ:62:VAL:HB	2.19	0.43
3:5:520:U:H2'	3:5:521:C:H6	1.84	0.43
3:5:2489:C:O2'	3:5:2491:C:N4	2.51	0.43
3:5:2683:C:H2'	3:5:2684:C:H6	1.83	0.43
3:5:3736:A:H2'	3:5:3737:A:C8	2.53	0.43
3:5:4401:G:H2'	3:5:4402:C:H6	1.83	0.43
6:9:799:U:H2'	6:9:800:U:C6	2.54	0.43
6:9:1397:U:H5	64:QQ:11:GLN:O	2.01	0.43
8:B:161:ARG:HG2	8:B:184:GLN:HA	2.00	0.43
10:D:219:TYR:CE1	10:D:227:ILE:HD11	2.53	0.43
13:G:198:THR:HA	13:G:201:GLU:HG2	2.00	0.43
20:O:27:VAL:HG13	20:O:101:ARG:HG3	2.00	0.43
22:Q:25:LEU:O	22:Q:29:VAL:HG23	2.18	0.43
22:Q:72:LEU:HD23	22:Q:72:LEU:HA	1.87	0.43
31:Z:73:LYS:HD2	31:Z:75:TYR:CZ	2.54	0.43
37:f:41:PHE:HE2	37:f:110:ILE:HD11	1.84	0.43
49:AA:121:LEU:HD13	49:AA:143:PRO:HG2	2.00	0.43
50:BB:91:VAL:HG12	50:BB:93:GLY:H	1.83	0.43
54:FF:98:GLU:OE1	54:FF:98:GLU:HA	2.18	0.43
55:GG:20:ASP:OD2	55:GG:22:ARG:HB3	2.18	0.43
61:NN:46:THR:HB	61:NN:86:GLU:OE1	2.18	0.43
67:TT:4:VAL:HG21	67:TT:136:GLY:HA2	1.99	0.43
3:5:246:G:OP1	30:Y:132:LYS:NZ	2.39	0.43
3:5:1209:U:O2'	3:5:1211:G:H8	2.01	0.43
3:5:1346:C:OP1	22:Q:148:VAL:HG23	2.18	0.43
3:5:2809:G:O2'	3:5:4644:G:OP1	2.35	0.43
3:5:4629:U:O3'	28:W:19:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:4892:A:H5''	20:O:188:LYS:HD3	2.01	0.43
3:5:4927:G:H3'	3:5:4928:C:O2	2.19	0.43
5:8:78:G:H2'	5:8:79:G:C8	2.53	0.43
5:8:108:A:C2	5:8:112:G:C6	3.07	0.43
6:9:4:C:H4'	51:CC:207:ALA:HB2	2.01	0.43
6:9:599:A:H2'	6:9:606:G:N2	2.34	0.43
6:9:1276:A:O2'	59:KK:51:SER:HA	2.18	0.43
6:9:1406:G:H2'	6:9:1407:U:H6	1.83	0.43
6:9:1758:G:H2'	6:9:1759:G:H8	1.83	0.43
13:G:92:PHE:CD2	13:G:100:PRO:HD3	2.53	0.43
13:G:209:VAL:HG22	13:G:235:CYS:SG	2.59	0.43
16:J:161:GLU:CA	16:J:164:ARG:HG2	2.45	0.43
17:L:78:LEU:HD13	17:L:100:PRO:HA	2.01	0.43
41:j:20:ARG:NH1	41:j:39:TYR:OH	2.52	0.43
49:AA:210:ILE:O	49:AA:213:GLU:HG3	2.18	0.43
3:5:121:A:H5'	3:5:122:U:OP2	2.19	0.42
3:5:1430:C:OP1	22:Q:134:ARG:HB2	2.19	0.42
3:5:2342:G:OP2	32:a:2:PRO:HA	2.19	0.42
3:5:2545:U:H5''	3:5:2546:G:OP2	2.19	0.42
3:5:2701:U:H2'	3:5:2702:C:C6	2.54	0.42
3:5:3689:G:O2'	3:5:3818:U:OP2	2.34	0.42
3:5:3893:C:H1'	21:P:69:ARG:NH2	2.34	0.42
3:5:3930:U:H2'	3:5:3931:C:C6	2.54	0.42
3:5:4134:C:H2'	3:5:4135:G:H8	1.84	0.42
3:5:4522:G:H5''	3:5:4524:G:N7	2.34	0.42
3:5:4536:OMC:HM22	3:5:4537:C:O4'	2.19	0.42
6:9:213:G:H2'	6:9:214:U:O4'	2.19	0.42
6:9:629:A:O2'	6:9:631:U:OP1	2.36	0.42
6:9:1232:U:H2'	6:9:1233:G:C8	2.54	0.42
6:9:1446:A:O2'	6:9:1447:G:H5''	2.18	0.42
9:C:348:LYS:O	9:C:351:VAL:HG12	2.19	0.42
11:E:181:PRO:HB2	11:E:184:LEU:HD13	2.00	0.42
20:O:185:VAL:O	20:O:189:ILE:HG12	2.19	0.42
22:Q:20:SER:O	22:Q:26:ARG:NH1	2.52	0.42
31:Z:46:ILE:HA	31:Z:70:SER:HA	2.01	0.42
48:r:108:MET:O	48:r:112:ARG:HG2	2.19	0.42
55:GG:120:ASP:OD1	55:GG:125:THR:HB	2.19	0.42
64:QQ:38:PRO:HB2	64:QQ:40:GLU:OE1	2.19	0.42
67:TT:56:ARG:HA	67:TT:56:ARG:HD3	1.84	0.42
71:XX:91:LEU:HD23	78:Ee:82:VAL:HG11	2.01	0.42
76:Cc:18:LEU:HD21	76:Cc:31:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:76:A:H5'	17:L:101:ARG:NH2	2.34	0.42
3:5:1662:C:H2'	3:5:1663:C:H6	1.84	0.42
3:5:2685:C:H2'	3:5:2686:G:O4'	2.19	0.42
3:5:2768:C:H5'	3:5:2769:U:OP1	2.18	0.42
3:5:4523:A2M:H5''	3:5:4524:G:H5'	2.01	0.42
6:9:68:A:OP2	55:GG:164:LYS:NZ	2.52	0.42
6:9:85:A:H2'	6:9:86:C:H6	1.84	0.42
12:F:125:ASN:ND2	25:T:132:PRO:HG2	2.34	0.42
13:G:147:GLN:OE1	13:G:147:GLN:N	2.47	0.42
14:H:95:VAL:CG2	44:m:52:ILE:HD11	2.49	0.42
17:L:120:TYR:HA	17:L:155:MET:HE1	2.00	0.42
18:M:7:VAL:HG11	18:M:52:PHE:CE1	2.53	0.42
19:N:9:GLU:HB2	40:i:44:ILE:HG13	2.01	0.42
20:O:113:ASP:OD1	20:O:113:ASP:N	2.49	0.42
24:S:28:TYR:CD1	25:T:151:LEU:HD11	2.54	0.42
30:Y:25:ILE:O	30:Y:29:ILE:HG13	2.19	0.42
40:i:60:LEU:HD23	40:i:60:LEU:HA	1.92	0.42
49:AA:85:ARG:NH2	65:RR:82:ASP:O	2.43	0.42
53:EE:87:MET:HE3	53:EE:123:LEU:HB2	1.99	0.42
68:UU:107:GLU:CD	68:UU:108:PRO:HD2	2.44	0.42
79:Gg:218:LEU:HD11	79:Gg:248:LEU:HD13	2.01	0.42
3:5:246:G:H4'	30:Y:132:LYS:HE2	2.00	0.42
3:5:690:C:H2'	3:5:691:C:C6	2.55	0.42
3:5:910:G:H2'	3:5:911:U:C6	2.53	0.42
3:5:1064:G:H2'	3:5:1065:G:H8	1.84	0.42
3:5:2068:C:OP1	37:f:15:LYS:HE2	2.18	0.42
6:9:533:A:H2'	6:9:534:G:H8	1.84	0.42
6:9:1031:A2M:H1'	6:9:1031:A2M:HM'3	1.82	0.42
9:C:263:LEU:HG	9:C:273:LEU:HD11	2.01	0.42
13:G:215:ASP:OD1	13:G:216:PRO:CD	2.67	0.42
16:J:94:LEU:O	16:J:174:ILE:HA	2.19	0.42
18:M:108:ASP:O	18:M:112:VAL:HG23	2.18	0.42
31:Z:91:LEU:HD22	31:Z:117:LYS:HD2	2.02	0.42
48:r:32:LEU:C	48:r:34:ALA:H	2.28	0.42
52:DD:96:LEU:HD21	52:DD:131:ALA:HB2	2.01	0.42
56:HH:116:ARG:NH1	56:HH:121:THR:HG22	2.35	0.42
56:HH:158:LEU:O	56:HH:190:PRO:HD2	2.19	0.42
62:OO:59:GLY:HA2	62:OO:68:GLU:HG2	2.00	0.42
66:SS:39:ARG:HH22	67:TT:46:ALA:HB2	1.84	0.42
66:SS:89:ASP:OD1	66:SS:93:GLY:N	2.51	0.42
3:5:2326:G:H5''	36:e:127:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:2699:C:H2'	3:5:2700:G:H8	1.84	0.42
3:5:3670:C:H2'	3:5:3671:G:C8	2.55	0.42
3:5:4642:U:H2'	3:5:4643:G:C8	2.54	0.42
3:5:4651:A:H2'	3:5:4652:G:O4'	2.18	0.42
3:5:4699:U:H4'	3:5:4700:A:OP1	2.19	0.42
3:5:4746:C:H2'	3:5:4747:C:H6	1.85	0.42
6:9:730:C:H2'	6:9:731:G:C8	2.54	0.42
6:9:1164:G:O2'	6:9:1165:G:H5'	2.20	0.42
6:9:1565:C:OP2	67:TT:101:ARG:NH1	2.52	0.42
8:B:146:LEU:HD23	8:B:146:LEU:HA	1.87	0.42
8:B:220:ILE:HD11	8:B:348:ARG:HD3	2.01	0.42
17:L:186:ARG:NE	40:i:9:VAL:HG11	2.34	0.42
21:P:124:LYS:HB3	21:P:140:MET:HE3	2.02	0.42
33:b:8:THR:HG22	33:b:10:HIS:H	1.84	0.42
41:j:14:LYS:HE2	41:j:14:LYS:HB3	1.77	0.42
51:CC:107:LEU:HB2	51:CC:127:PHE:HB2	2.01	0.42
53:EE:250:GLU:HA	53:EE:253:ASP:HB2	2.01	0.42
55:GG:44:GLU:HA	55:GG:119:LYS:HE2	2.01	0.42
56:HH:8:ILE:HD13	56:HH:16:PRO:HG3	2.02	0.42
60:LL:35:ARG:NH1	60:LL:53:GLY:O	2.51	0.42
63:PP:93:MET:HE1	63:PP:104:GLN:HE21	1.84	0.42
67:TT:39:LEU:HA	67:TT:39:LEU:HD12	1.81	0.42
74:Aa:46:GLU:CD	74:Aa:47:ALA:N	2.77	0.42
3:5:656:C:H2'	3:5:657:C:C6	2.54	0.42
3:5:1341:U:H2'	3:5:1342:A:H8	1.84	0.42
3:5:1344:C:H2'	3:5:1345:A:H8	1.84	0.42
3:5:1590:C:H4'	3:5:2857:A:H5'	2.01	0.42
3:5:3658:C:H2'	3:5:3659:G:C8	2.53	0.42
3:5:3917:A:H2'	3:5:3918:G:H8	1.84	0.42
3:5:4495:G:C2	3:5:4496:A:N7	2.88	0.42
5:8:140:C:H2'	5:8:141:C:H6	1.84	0.42
6:9:69:C:P	55:GG:167:LYS:HZ1	2.42	0.42
6:9:1005:G:H2'	6:9:1006:C:H6	1.84	0.42
10:D:56:THR:HG22	10:D:57:ASN:N	2.35	0.42
39:h:42:SER:O	39:h:46:LYS:HG2	2.20	0.42
49:AA:19:LEU:HD11	65:RR:106:LEU:HD11	2.02	0.42
49:AA:77:ILE:HG13	49:AA:99:ILE:HB	2.01	0.42
51:CC:94:ILE:HG13	51:CC:159:LYS:O	2.20	0.42
58:JJ:67:ASP:HB3	58:JJ:70:ARG:CB	2.50	0.42
58:JJ:70:ARG:HH12	58:JJ:94:LEU:HD21	1.84	0.42
62:OO:128:ARG:HG2	74:Aa:59:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:UU:67:LYS:HG2	68:UU:78:ASP:OD2	2.19	0.42
70:WW:28:ARG:HH11	70:WW:28:ARG:HG2	1.84	0.42
3:5:379:G:O2'	3:5:380:U:H5'	2.19	0.42
3:5:433:A:H2'	3:5:434:A:O4'	2.19	0.42
3:5:2002:A:N3	3:5:2002:A:H2'	2.34	0.42
3:5:2676:A:C4	3:5:2677:G:C8	3.07	0.42
3:5:4273:A:H2'	3:5:4274:A:C8	2.55	0.42
3:5:4344:U:H2'	3:5:4345:C:H6	1.84	0.42
3:5:4710:C:H2'	3:5:4711:C:C6	2.54	0.42
3:5:4749:C:H2'	3:5:4750:G:O4'	2.20	0.42
5:8:93:C:HO2'	5:8:94:G:H8	1.66	0.42
6:9:298:G:C2	6:9:299:A:C8	3.07	0.42
6:9:492:C:H5	72:YY:104:ARG:HH22	1.68	0.42
6:9:1727:G:H2'	6:9:1728:U:H6	1.84	0.42
7:A:42:LYS:HB3	7:A:89:TYR:CE1	2.54	0.42
12:F:70:MET:HE3	25:T:140:PHE:CZ	2.55	0.42
14:H:146:LEU:HA	14:H:146:LEU:HD13	1.78	0.42
17:L:90:VAL:O	17:L:93:THR:HG22	2.20	0.42
28:W:105:ARG:NH1	55:GG:150:GLU:HB2	2.34	0.42
30:Y:31:SER:HA	30:Y:48:PRO:HA	2.02	0.42
30:Y:43:ASN:OD1	30:Y:126:ARG:NH1	2.49	0.42
38:g:3:GLN:HE22	38:g:5:LEU:HB3	1.84	0.42
49:AA:30:LEU:HA	49:AA:150:THR:O	2.19	0.42
54:FF:43:GLU:HG2	54:FF:44:LYS:N	2.34	0.42
54:FF:176:GLU:OE1	54:FF:187:SER:HB2	2.20	0.42
71:XX:88:ASP:OD2	78:Ee:86:ARG:HB2	2.18	0.42
79:Gg:186:THR:HG22	79:Gg:188:HIS:CD2	2.55	0.42
1:2:68:C:H2'	1:2:69:U:C6	2.55	0.42
3:5:124:C:H2'	3:5:125:C:H6	1.84	0.42
3:5:496:G:H2'	3:5:497:G:H5'	2.01	0.42
3:5:516:C:H2'	3:5:517:C:H6	1.84	0.42
3:5:671:G:H2'	3:5:672:C:C6	2.55	0.42
3:5:2434:G:H5'	29:X:83:THR:HG21	2.02	0.42
3:5:2520:C:H2'	3:5:2521:G:C8	2.55	0.42
3:5:2671:C:H2'	3:5:2672:C:C6	2.55	0.42
3:5:4136:G:H2'	3:5:4137:C:H6	1.85	0.42
3:5:4260:U:O2'	16:J:133:VAL:HG11	2.20	0.42
3:5:4580:U:O2'	8:B:182:GLU:OE2	2.29	0.42
3:5:4637:OMG:OP1	35:d:30:HIS:NE2	2.47	0.42
5:8:126:C:O2'	5:8:127:U:H6	2.02	0.42
6:9:735:C:H2'	6:9:736:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:918:U:H2'	6:9:919:A:O4'	2.20	0.42
6:9:980:A:H2'	6:9:981:A:C8	2.55	0.42
6:9:1139:C:H2'	6:9:1140:G:O4'	2.20	0.42
6:9:1648:G:H5''	64:QQ:125:ARG:HB2	2.02	0.42
18:M:58:THR:HG22	18:M:91:TRP:CZ3	2.55	0.42
21:P:15:CYS:SG	21:P:150:LEU:HB2	2.60	0.42
28:W:33:ASN:O	28:W:37:GLU:HG3	2.20	0.42
31:Z:66:SER:HB2	31:Z:122:TYR:HE2	1.84	0.42
33:b:66:ALA:O	33:b:70:GLU:OE1	2.38	0.42
41:j:64:MET:O	41:j:68:LYS:HG2	2.20	0.42
56:HH:144:ILE:O	70:WW:51:GLU:HG3	2.19	0.42
63:PP:103:ASN:HD21	63:PP:120:SER:HA	1.84	0.42
3:5:268:G:H2'	3:5:269:G:H8	1.85	0.42
3:5:1378:C:H4'	3:5:1379:C:H5'	2.02	0.42
3:5:1739:G:H2'	3:5:1740:C:C6	2.55	0.42
3:5:2493:G:H2'	3:5:2494:U:H6	1.81	0.42
3:5:2566:G:H2'	3:5:2567:G:H8	1.85	0.42
3:5:3610:A:H2'	3:5:3611:A:C8	2.53	0.42
3:5:4319:C:H2'	3:5:4320:G:H8	1.85	0.42
3:5:4479:A:H2'	3:5:4480:A:O4'	2.20	0.42
3:5:4944:C:N4	37:f:59:THR:HA	2.35	0.42
6:9:547:G:O2'	6:9:548:C:O4'	2.36	0.42
6:9:586:G:C6	58:JJ:172:ARG:HD3	2.55	0.42
6:9:1628:C:H2'	6:9:1629:C:H6	1.85	0.42
7:A:245:ARG:HA	7:A:245:ARG:HD2	1.91	0.42
8:B:216:MET:SD	8:B:359:ALA:HA	2.59	0.42
12:F:70:MET:HE3	25:T:140:PHE:HZ	1.84	0.42
17:L:81:LEU:HD12	17:L:117:LEU:HD21	2.01	0.42
24:S:120:ARG:HH11	24:S:120:ARG:HG3	1.85	0.42
49:AA:52:LYS:HB2	65:RR:109:LEU:HD21	2.02	0.42
50:BB:86:LEU:HB3	50:BB:98:THR:HB	2.00	0.42
51:CC:134:ASN:HB2	51:CC:167:ARG:NH1	2.35	0.42
53:EE:90:ILE:HB	53:EE:99:PHE:HB2	2.02	0.42
56:HH:134:VAL:HG23	56:HH:134:VAL:O	2.19	0.42
70:WW:36:ARG:HG2	70:WW:110:ILE:HB	2.02	0.42
3:5:197:A:N1	3:5:225:G:O2'	2.50	0.42
3:5:489:C:H2'	3:5:490:C:C6	2.55	0.42
3:5:1186:U:H2'	3:5:1187:G:N3	2.35	0.42
3:5:2474:G:H1'	3:5:2475:G:OP1	2.18	0.42
3:5:2683:C:H2'	3:5:2684:C:C6	2.54	0.42
3:5:3669:G:H21	3:5:3672:G:N2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:4870:OMG:H5''	18:M:91:TRP:CD2	2.55	0.42
5:8:92:U:H2'	5:8:93:C:O4'	2.19	0.42
6:9:380:G:P	57:II:56:ARG:HH22	2.42	0.42
6:9:540:U:H2'	6:9:542:U:OP2	2.18	0.42
6:9:792:C:H2'	6:9:793:G:C8	2.54	0.42
6:9:882:U:H2'	6:9:883:U:C6	2.55	0.42
6:9:1533:A:N3	6:9:1533:A:H2'	2.35	0.42
16:J:144:LYS:O	16:J:148:THR:OG1	2.34	0.42
25:T:80:VAL:O	25:T:81:LYS:C	2.62	0.42
30:Y:117:LYS:O	30:Y:120:GLU:HG3	2.20	0.42
32:a:132:ARG:O	32:a:135:GLU:HG2	2.18	0.42
52:DD:222:PRO:HG2	79:Gg:226:HIS:CE1	2.55	0.42
54:FF:19:LEU:HG	54:FF:20:PHE:CD2	2.55	0.42
56:HH:134:VAL:HG12	56:HH:173:PHE:CD2	2.54	0.42
57:II:128:LYS:NZ	57:II:131:PRO:HD3	2.35	0.42
62:OO:148:GLY:O	62:OO:150:ARG:NH2	2.53	0.42
63:PP:64:LYS:HE2	63:PP:64:LYS:HB2	1.87	0.42
79:Gg:127:LYS:HE3	79:Gg:149:GLU:HA	2.01	0.42
3:5:263:G:C6	3:5:264:C:N4	2.88	0.42
3:5:302:C:H2'	3:5:303:C:C6	2.54	0.42
3:5:324:A:H2'	3:5:325:U:C6	2.55	0.42
3:5:1341:U:H2'	3:5:1342:A:C8	2.55	0.42
3:5:1983:A:C4	3:5:2010:A:H5''	2.55	0.42
3:5:2041:A:N7	3:5:4434:C:O2'	2.52	0.42
3:5:2329:U:H2'	3:5:2330:G:O4'	2.19	0.42
3:5:2838:G:OP1	8:B:248:LEU:N	2.51	0.42
3:5:3648:A:H1'	3:5:3785:A2M:N6	2.35	0.42
3:5:3867:A2M:H2'	3:5:3868:G:C8	2.54	0.42
3:5:3883:U:H2'	3:5:3884:U:C6	2.55	0.42
3:5:4070:U:H2'	3:5:4071:U:C6	2.54	0.42
3:5:4091:G:H2'	3:5:4092:G:O4'	2.20	0.42
3:5:4318:C:O2'	46:o:18:HIS:ND1	2.39	0.42
5:8:74:U:C4	30:Y:74:TYR:HD1	2.38	0.42
6:9:96:C:H2'	6:9:97:U:H6	1.85	0.42
6:9:182:C:H4'	6:9:183:G:O5'	2.19	0.42
6:9:215:G:H2'	6:9:216:C:C6	2.55	0.42
6:9:659:G:H21	71:XX:17:ARG:HH12	1.68	0.42
6:9:966:U:H2'	6:9:967:C:C6	2.55	0.42
6:9:1018:U:H2'	6:9:1019:C:C6	2.55	0.42
6:9:1137:U:O2'	6:9:1138:C:OP1	2.27	0.42
7:A:101:VAL:HG23	7:A:164:ALA:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:137:SER:HB2	14:H:145:VAL:HG23	2.01	0.42
14:H:141:LYS:HD2	14:H:142:ASP:N	2.35	0.42
17:L:130:LYS:HD3	17:L:131:PRO:HD2	2.01	0.42
18:M:3:PHE:CE1	24:S:155:PRO:HA	2.55	0.42
20:O:80:PHE:O	20:O:84:VAL:HG23	2.20	0.42
24:S:81:TRP:HB2	24:S:128:LYS:HB3	2.02	0.42
42:k:51:GLU:HA	42:k:54:GLU:HG3	2.02	0.42
56:HH:160:LYS:H	56:HH:194:LEU:C	2.28	0.42
58:JJ:93:LYS:HG3	58:JJ:95:ASP:OD1	2.19	0.42
67:TT:75:MET:HA	67:TT:78:ILE:HG22	2.02	0.42
68:UU:98:VAL:HA	68:UU:101:ILE:HD12	2.02	0.42
70:WW:28:ARG:HG2	70:WW:28:ARG:NH1	2.35	0.42
74:Aa:22:ARG:NH1	74:Aa:27:ALA:O	2.52	0.42
77:Dd:43:PHE:O	77:Dd:47:ALA:N	2.52	0.42
3:5:65:A:N1	3:5:76:A:H5''	2.35	0.41
3:5:750:U:H1'	3:5:917:A:C8	2.55	0.41
3:5:1209:U:HO2'	3:5:1211:G:H5'	1.84	0.41
3:5:2102:G:C2	12:F:179:GLY:HA3	2.55	0.41
3:5:2601:A:N6	3:5:2743:A:H3'	2.35	0.41
6:9:294:U:C4	60:LL:65:ASN:HB3	2.55	0.41
6:9:338:G:H2'	6:9:339:A:C8	2.55	0.41
6:9:1025:U:O3'	6:9:1089:G:N2	2.52	0.41
6:9:1136:U:H2'	6:9:1137:U:C6	2.54	0.41
6:9:1533:A:C8	6:9:1604:G:H1'	2.55	0.41
8:B:216:MET:HB2	8:B:354:GLN:OE1	2.20	0.41
31:Z:21:ARG:NH2	31:Z:47:ASP:OD1	2.52	0.41
40:i:56:ARG:O	40:i:59:GLU:HG3	2.19	0.41
49:AA:123:VAL:HG12	49:AA:145:ILE:HB	2.01	0.41
49:AA:158:ASP:OD1	69:VV:32:ILE:HD13	2.20	0.41
51:CC:210:PRO:HD3	51:CC:236:PHE:CE2	2.54	0.41
64:QQ:102:GLU:OE2	79:Gg:55:PRO:HB2	2.19	0.41
70:WW:18:GLU:HG2	70:WW:69:LEU:HB3	2.02	0.41
79:Gg:294:ASP:OD1	79:Gg:295:GLY:N	2.52	0.41
3:5:197:A:H5''	30:Y:130:LYS:HZ2	1.83	0.41
3:5:282:C:H2'	3:5:283:G:O4'	2.20	0.41
3:5:690:C:OP1	48:r:87:ARG:NH1	2.53	0.41
3:5:750:U:C2	3:5:751:G:C8	3.08	0.41
3:5:1316:OMG:H1'	3:5:1316:OMG:HM23	1.79	0.41
3:5:1344:C:H2'	3:5:1345:A:C8	2.55	0.41
3:5:3697:U:O2'	3:5:3698:G:OP2	2.33	0.41
3:5:4220:6MZ:O5'	3:5:4220:6MZ:H8	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:57:C:H2'	4:7:58:A:C8	2.55	0.41
5:8:124:U:H4'	5:8:125:C:O5'	2.20	0.41
6:9:70:G:O2'	6:9:79:A:N6	2.49	0.41
6:9:616:A:H1'	78:Ee:85:VAL:HG23	2.01	0.41
8:B:80:GLU:HG3	8:B:326:VAL:HG13	2.01	0.41
13:G:297:PRO:HA	13:G:300:VAL:HG12	2.01	0.41
17:L:130:LYS:HB3	17:L:133:ALA:HB3	2.01	0.41
32:a:36:GLY:HA3	32:a:40:HIS:CE1	2.55	0.41
52:DD:14:ASP:OD2	52:DD:14:ASP:C	2.63	0.41
55:GG:135:PRO:HG2	55:GG:144:LEU:HD22	2.02	0.41
63:PP:68:PRO:HA	63:PP:69:PRO:HD3	1.93	0.41
65:RR:37:GLU:HG2	79:Gg:150:TRP:HZ2	1.84	0.41
1:2:10:G:H2'	1:2:11:G:C8	2.55	0.41
3:5:88:A:N7	22:Q:173:LYS:NZ	2.68	0.41
3:5:170:C:H5''	17:L:136:LYS:NZ	2.36	0.41
3:5:176:G:C6	3:5:261:G:N1	2.89	0.41
3:5:645:G:H2'	3:5:646:G:H8	1.85	0.41
3:5:1833:G:OP1	25:T:120:LYS:NZ	2.53	0.41
3:5:2639:U:O2'	3:5:2640:G:O5'	2.36	0.41
3:5:3610:A:H2'	3:5:3611:A:H8	1.85	0.41
5:8:21:C:N4	5:8:22:U:O4	2.52	0.41
6:9:1394:G:HO2'	6:9:1395:C:P	2.40	0.41
6:9:1486:A:H2'	6:9:1487:A:O4'	2.20	0.41
7:A:43:GLY:HA3	7:A:63:PHE:CD1	2.56	0.41
8:B:218:ASP:HB2	8:B:348:ARG:CG	2.50	0.41
10:D:120:GLU:O	10:D:248:ARG:NH2	2.40	0.41
10:D:153:THR:HB	10:D:160:PHE:CZ	2.55	0.41
11:E:169:LYS:HD2	11:E:211:ILE:CD1	2.50	0.41
11:E:179:THR:HG23	11:E:180:GLY:H	1.85	0.41
13:G:283:TYR:O	13:G:287:ARG:HG2	2.20	0.41
19:N:66:VAL:HG21	19:N:102:ALA:HB2	2.02	0.41
28:W:31:PHE:CD1	28:W:37:GLU:HG2	2.55	0.41
32:a:8:THR:HG23	32:a:9:ARG:HD2	2.02	0.41
47:p:44:LYS:NZ	47:p:59:SER:OG	2.50	0.41
48:r:54:ALA:HA	48:r:61:VAL:HG23	2.02	0.41
49:AA:38:ILE:HD11	49:AA:150:THR:HG22	2.03	0.41
68:UU:55:ARG:HG2	68:UU:87:ARG:HD3	2.02	0.41
72:YY:22:GLN:HA	72:YY:74:MET:HA	2.02	0.41
3:5:381:U:H4'	3:5:415:G:H5'	2.01	0.41
3:5:670:G:H2'	3:5:671:G:C8	2.52	0.41
3:5:941:C:OP2	12:F:241:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:1760:G:H2'	3:5:1761:G:O4'	2.21	0.41
3:5:2519:U:H1'	3:5:2520:C:C6	2.56	0.41
3:5:4076:G:OP2	3:5:4163:U:N3	2.39	0.41
3:5:4253:A:H5'	3:5:4254:G:C8	2.56	0.41
3:5:4301:U:OP2	3:5:4303:C:N4	2.54	0.41
3:5:4593:C:H2'	3:5:4594:U:H6	1.86	0.41
6:9:5:U:H2'	6:9:6:G:C8	2.56	0.41
6:9:339:A:H2'	6:9:340:C:C5	2.56	0.41
7:A:142:GLU:C	7:A:144:LYS:H	2.28	0.41
11:E:113:ARG:HA	11:E:113:ARG:HH11	1.84	0.41
20:O:8:VAL:HG12	20:O:117:ARG:HG3	2.03	0.41
28:W:105:ARG:O	28:W:109:ILE:HG23	2.21	0.41
38:g:97:ILE:HD13	38:g:97:ILE:HA	1.95	0.41
50:BB:149:GLN:HE22	50:BB:154:SER:HB2	1.85	0.41
64:QQ:54:PRO:O	64:QQ:58:LEU:HD13	2.21	0.41
3:5:158:A:N1	3:5:276:C:O2'	2.50	0.41
3:5:1502:G:H1	22:Q:89:ASP:HA	1.85	0.41
3:5:1570:G:O6	47:p:2:ALA:N	2.54	0.41
3:5:1683:PSU:H2'	3:5:1684:A:H8	1.85	0.41
3:5:1727:U:H2'	3:5:1728:U:H6	1.85	0.41
3:5:2080:U:H2'	3:5:2081:C:C6	2.55	0.41
3:5:2864:A:H2'	3:5:2865:U:C6	2.56	0.41
3:5:4126:C:H5''	3:5:4127:A:H5''	2.02	0.41
5:8:88:A:H2'	5:8:89:U:O4'	2.21	0.41
6:9:909:G:H2'	6:9:910:G:C8	2.55	0.41
6:9:1119:A:H2'	6:9:1120:U:C6	2.55	0.41
12:F:74:ALA:HB2	25:T:140:PHE:CE1	2.56	0.41
12:F:94:ILE:HG22	12:F:222:LYS:HG3	2.01	0.41
13:G:233:PRO:HG2	13:G:272:VAL:HG13	2.03	0.41
16:J:103:GLY:HA3	16:J:157:ILE:HG22	2.03	0.41
17:L:90:VAL:HA	17:L:93:THR:HG22	2.02	0.41
18:M:106:ASP:O	18:M:109:ARG:HG2	2.21	0.41
25:T:108:ARG:HD2	25:T:112:ASN:ND2	2.35	0.41
46:o:24:THR:HG23	46:o:69:ARG:HB3	2.02	0.41
47:p:86:LEU:HD23	47:p:86:LEU:HA	1.90	0.41
62:OO:74:ALA:HB1	62:OO:115:ALA:HB2	2.03	0.41
68:UU:36:CYS:O	68:UU:40:ILE:HG12	2.20	0.41
69:VV:70:LEU:HG	69:VV:74:LYS:NZ	2.35	0.41
3:5:370:U:H4'	3:5:1534:A2M:H61	1.84	0.41
3:5:2385:U:H2'	3:5:2386:U:C6	2.56	0.41
3:5:3625:G:O2'	3:5:3626:G:OP1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:4261:C:H2'	3:5:4262:C:H6	1.85	0.41
3:5:4727:A:H2'	3:5:4728:U:O4'	2.20	0.41
3:5:5038:A:H2'	3:5:5039:U:C6	2.56	0.41
4:7:3:C:H2'	4:7:4:U:C6	2.55	0.41
6:9:351:G:C2	6:9:352:U:C6	3.09	0.41
6:9:914:U:OP1	56:HH:67:PRO:HG3	2.20	0.41
6:9:1117:C:O2'	6:9:1118:C:O5'	2.38	0.41
6:9:1221:G:H2'	6:9:1222:G:C8	2.55	0.41
6:9:1232:U:H2'	6:9:1233:G:H8	1.85	0.41
6:9:1377:U:H3'	49:AA:102:ARG:HH11	1.86	0.41
6:9:1415:C:O2'	67:TT:132:ASP:OD2	2.31	0.41
6:9:1801:A:H2'	6:9:1802:C:C6	2.56	0.41
11:E:182:LEU:HD13	11:E:186:ARG:HA	2.02	0.41
19:N:35:ALA:HB2	19:N:65:ARG:NH1	2.36	0.41
24:S:8:ARG:O	24:S:33:PHE:HA	2.20	0.41
26:U:27:HIS:O	26:U:30:GLU:HG3	2.20	0.41
28:W:3:VAL:HG13	28:W:13:ILE:O	2.21	0.41
37:f:18:LEU:HD23	37:f:19:ARG:NH1	2.36	0.41
51:CC:234:GLY:O	51:CC:238:LYS:HG2	2.21	0.41
53:EE:107:GLY:HA2	53:EE:189:LEU:CD1	2.45	0.41
56:HH:192:PHE:CD2	56:HH:193:GLN:HB2	2.56	0.41
59:KK:73:ASN:HA	59:KK:76:ILE:HG12	2.02	0.41
66:SS:62:ASP:OD1	66:SS:62:ASP:N	2.52	0.41
68:UU:23:THR:OG1	68:UU:113:GLU:OE1	2.39	0.41
1:2:10:G:H2'	1:2:11:G:H8	1.85	0.41
3:5:1411(B):C:H2'	3:5:1411(C):C:C6	2.56	0.41
3:5:1461:C:H2'	3:5:1462:A:C8	2.56	0.41
3:5:1567:U:H2'	3:5:1568:C:H6	1.86	0.41
3:5:1739:G:N3	3:5:1742:A:N6	2.69	0.41
3:5:1779:U:H2'	3:5:1780:A:C8	2.55	0.41
3:5:2544:G:H2'	3:5:2545:U:O4'	2.21	0.41
3:5:3702:A:C6	3:5:3703:G:C8	3.09	0.41
3:5:3726:A:H2'	3:5:3727:A:C8	2.55	0.41
3:5:4228:G:H5''	3:5:4229:U:O4'	2.21	0.41
3:5:4619:U:H2'	3:5:4620:OMU:C6	2.49	0.41
3:5:4996:C:OP2	35:d:31:LYS:NZ	2.48	0.41
3:5:5020:G:H2'	3:5:5021:C:C6	2.56	0.41
6:9:912:C:H3'	6:9:913:A:H5''	2.03	0.41
6:9:1261:C:O2	77:Dd:10:HIS:NE2	2.53	0.41
6:9:1503:C:H2'	6:9:1504:U:C6	2.55	0.41
10:D:41:LYS:HE2	10:D:41:LYS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:17:TYR:H	15:I:95:HIS:HD2	1.69	0.41
19:N:45:PRO:O	19:N:49:ARG:HG3	2.20	0.41
20:O:192:PHE:HA	20:O:195:VAL:HG12	2.03	0.41
48:r:65:LYS:O	48:r:102:TYR:OH	2.31	0.41
49:AA:58:LEU:HD21	49:AA:177:MET:HG3	2.03	0.41
50:BB:140:VAL:O	50:BB:210:VAL:HA	2.21	0.41
54:FF:26:ASP:OD1	54:FF:27:ASP:N	2.49	0.41
54:FF:33:ILE:HD11	76:Cc:11:LEU:HD11	2.02	0.41
56:HH:155:LYS:HD3	56:HH:188:GLU:OE1	2.19	0.41
57:II:21:TYR:CZ	57:II:22:HIS:HD2	2.39	0.41
58:JJ:160:SER:OG	58:JJ:163:SER:HB2	2.21	0.41
70:WW:42:MET:HE2	70:WW:42:MET:HB2	1.94	0.41
3:5:1693:U:H2'	3:5:1694:C:O4'	2.20	0.41
3:5:2540:C:H2'	3:5:2541:G:H8	1.86	0.41
3:5:2824:C:H2'	3:5:2825:A:C8	2.56	0.41
3:5:4084:G:O6	7:A:72:ARG:NH2	2.54	0.41
3:5:4119:C:O2'	3:5:4120:U:OP1	2.31	0.41
3:5:4492:U:O2'	3:5:4512:U:O2	2.27	0.41
4:7:48:G:H5'	10:D:226:TYR:HE1	1.85	0.41
5:8:140:C:H2'	5:8:141:C:C6	2.55	0.41
5:8:152:U:H2'	5:8:153:C:O4'	2.20	0.41
6:9:377:G:H5'	57:II:98:LYS:HD3	2.03	0.41
6:9:940:U:H3	6:9:1002:U:H3	1.68	0.41
8:B:57:VAL:HB	8:B:367:PHE:HB3	2.02	0.41
9:C:28:PHE:HA	9:C:129:ALA:HA	2.03	0.41
12:F:86:PRO:HG3	12:F:143:TYR:CD2	2.55	0.41
13:G:149:LEU:HD22	13:G:246:LEU:HD21	2.03	0.41
18:M:85:LYS:O	18:M:89:THR:HG23	2.21	0.41
21:P:105:LYS:HD2	21:P:107:LEU:HD11	2.03	0.41
55:GG:191:ARG:O	55:GG:195:LYS:HG3	2.21	0.41
58:JJ:50:LEU:HD13	58:JJ:102:ILE:HG22	2.01	0.41
59:KK:29:MET:HG2	59:KK:42:ASN:ND2	2.36	0.41
60:LL:16:ILE:HG21	60:LL:34:PRO:O	2.21	0.41
64:QQ:105:LYS:O	64:QQ:108:ILE:HG22	2.20	0.41
64:QQ:132:PHE:CE2	68:UU:76:THR:HA	2.55	0.41
66:SS:34:LYS:HB2	66:SS:100:ALA:HA	2.01	0.41
1:2:5:A:H2'	1:2:6:G:H8	1.86	0.41
3:5:98:A:OP1	19:N:195:ARG:HD3	2.21	0.41
3:5:197:A:N3	3:5:222:C:O2'	2.51	0.41
3:5:222:C:H2'	3:5:223:G:O4'	2.19	0.41
3:5:267:G:H2'	3:5:268:G:C8	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:418:A:C2	5:8:17:A:H1'	2.56	0.41
3:5:1065:G:OP2	11:E:43:LYS:NZ	2.47	0.41
3:5:1340:C:H2'	3:5:1341:U:C6	2.55	0.41
3:5:1392:A:H2'	3:5:1393:G:C8	2.55	0.41
3:5:1762:C:H2'	3:5:1763:C:H6	1.85	0.41
3:5:2273:G:H2'	3:5:2274:C:C6	2.56	0.41
3:5:2487:G:O6	3:5:2489:C:H1'	2.21	0.41
3:5:2756:G:H2'	3:5:2757:A:C8	2.55	0.41
3:5:2858:A:H2'	3:5:2859:G:O4'	2.20	0.41
3:5:3825:A2M:HM'3	3:5:3825:A2M:H1'	1.83	0.41
3:5:4174:U:H2'	3:5:4175:G:H8	1.85	0.41
3:5:4314:C:OP1	25:T:70:HIS:N	2.48	0.41
3:5:4425:G:OP1	44:m:74:TYR:OH	2.30	0.41
5:8:116:C:H2'	5:8:117:C:C6	2.55	0.41
6:9:186:C:H2'	6:9:187:G:H8	1.86	0.41
6:9:861:A:N3	56:HH:106:ARG:NH2	2.69	0.41
6:9:955:A:N1	6:9:968:U:O2'	2.49	0.41
6:9:1609:C:OP1	66:SS:131:VAL:HG22	2.21	0.41
9:C:204:ARG:HG2	9:C:205:ARG:N	2.36	0.41
9:C:337:ARG:NH2	11:E:60:SER:HA	2.36	0.41
9:C:355:ALA:O	9:C:358:LEU:HG	2.20	0.41
10:D:154:THR:HG22	10:D:155:THR:H	1.85	0.41
10:D:232:THR:HG22	10:D:235:MET:HE2	2.03	0.41
11:E:173:SER:OG	11:E:217:ASP:OD2	2.25	0.41
11:E:265:LYS:HB3	11:E:265:LYS:HE2	1.77	0.41
12:F:178:LEU:HD13	12:F:183:ILE:HD11	2.02	0.41
13:G:295:LEU:HD23	13:G:295:LEU:HA	1.96	0.41
14:H:128:MET:HE1	14:H:157:SER:HB3	2.02	0.41
15:I:143:GLN:NE2	15:I:144:ASN:OD1	2.54	0.41
16:J:16:ARG:O	16:J:135:GLY:N	2.54	0.41
16:J:111:GLU:HB3	66:SS:14:ARG:HH11	1.85	0.41
19:N:68:ARG:NH1	19:N:124:ASP:O	2.51	0.41
21:P:60:PHE:CE2	21:P:82:ARG:HB2	2.56	0.41
30:Y:112:ASP:OD2	30:Y:112:ASP:C	2.64	0.41
32:a:132:ARG:HG3	32:a:132:ARG:HH11	1.85	0.41
55:GG:215:LYS:NZ	55:GG:216:ARG:HH21	2.18	0.41
56:HH:145:ARG:HB2	56:HH:153:LEU:HB3	2.02	0.41
58:JJ:45:ARG:O	58:JJ:49:THR:HG23	2.21	0.41
59:KK:29:MET:HG2	59:KK:42:ASN:HD22	1.86	0.41
62:OO:60:MET:HE2	62:OO:60:MET:HB3	1.89	0.41
68:UU:45:GLU:OE2	68:UU:46:LYS:NZ	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:WW:111:MET:HE1	70:WW:119:LYS:HD2	2.03	0.41
75:Bb:83:GLN:OE1	75:Bb:83:GLN:N	2.54	0.41
79:Gg:109:LEU:N	79:Gg:123:GLY:O	2.39	0.41
3:5:710:G:H4'	11:E:193:HIS:HE2	1.86	0.41
3:5:966:A:H1'	3:5:968:C:N4	2.36	0.41
3:5:1211:G:O2'	3:5:1212:G:OP1	2.31	0.41
3:5:1297:U:H2'	3:5:1298:C:H6	1.85	0.41
3:5:1317:U:OP1	32:a:21:ARG:NH1	2.43	0.41
3:5:1962:A:N3	3:5:1962:A:H2'	2.35	0.41
3:5:2520:C:H1'	3:5:2640:G:H21	1.86	0.41
3:5:4685:U:H2'	3:5:4686:G:C8	2.56	0.41
3:5:4991:U:H2'	3:5:4992:G:H8	1.86	0.41
4:7:114:U:O2	10:D:74:ILE:HD12	2.20	0.41
5:8:1:C:H2'	5:8:2:G:H5'	2.03	0.41
5:8:65:A:O2'	39:h:10:ARG:NH2	2.54	0.41
5:8:93:C:O2'	5:8:94:G:H8	2.04	0.41
6:9:891:G:N3	6:9:891:G:H2'	2.36	0.41
6:9:1351:G:O2'	6:9:1378:A:N1	2.48	0.41
6:9:1667:U:H2'	6:9:1668:U:C6	2.55	0.41
9:C:11:TYR:CZ	9:C:148:PRO:HB2	2.56	0.41
12:F:146:LEU:HD12	12:F:194:TYR:CE2	2.56	0.41
13:G:119:GLN:HG3	19:N:28:TRP:CH2	2.56	0.41
34:c:11:LEU:HA	34:c:14:ILE:HG22	2.02	0.41
49:AA:33:GLN:HA	49:AA:33:GLN:OE1	2.21	0.41
49:AA:42:LYS:HB3	49:AA:44:ASP:H	1.86	0.41
49:AA:198:MET:HG3	49:AA:199:PRO:HD2	2.03	0.41
54:FF:179:ASN:HB3	54:FF:187:SER:HB3	2.02	0.41
59:KK:34:GLU:OE2	59:KK:35:LEU:HD23	2.21	0.41
65:RR:40:ILE:HG13	65:RR:40:ILE:O	2.21	0.41
66:SS:40:TYR:CZ	66:SS:97:GLN:HG2	2.56	0.41
68:UU:83:ARG:HH12	77:Dd:55:LEU:HD13	1.84	0.41
3:5:17:A:OP2	29:X:60:TYR:OH	2.27	0.40
3:5:425:U:H2'	3:5:426:A:H8	1.86	0.40
3:5:1494:U:H2'	3:5:1495:G:C8	2.56	0.40
3:5:1545:G:H2'	3:5:1546:C:C6	2.55	0.40
3:5:1594:C:H2'	3:5:1595:G:O4'	2.21	0.40
3:5:1628:C:OP2	7:A:9:ARG:HD2	2.21	0.40
3:5:2489:C:H4'	3:5:2490:U:H5	1.86	0.40
3:5:3771:C:H2'	3:5:3772:U:O4'	2.21	0.40
3:5:3785:A2M:H8	3:5:3785:A2M:H2'	1.90	0.40
3:5:4069:U:H2'	3:5:4070:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:4413:C:H5	3:5:4429:C:N4	2.19	0.40
4:7:19:C:OP2	16:J:154:LYS:NZ	2.44	0.40
6:9:26:U:H2'	6:9:27:A2M:H8	2.03	0.40
6:9:873:G:C2	60:LL:152:LYS:HD3	2.56	0.40
6:9:941:C:H2'	6:9:942:G:C8	2.56	0.40
6:9:952:G:N2	62:OO:52:THR:HG21	2.23	0.40
6:9:958:G:H3'	6:9:959:G:H8	1.85	0.40
6:9:1142:G:N2	6:9:1145:A:OP2	2.43	0.40
6:9:1619:A:H8	6:9:1619:A:OP2	2.04	0.40
9:C:165:LYS:HE2	9:C:165:LYS:HB2	1.86	0.40
16:J:26:VAL:HG13	16:J:28:GLU:H	1.86	0.40
28:W:3:VAL:HG11	28:W:12:LYS:NZ	2.35	0.40
44:m:77:LEU:HD11	44:m:84:CYS:HA	2.03	0.40
49:AA:200:ASP:OD2	65:RR:89:SER:HA	2.21	0.40
56:HH:100:ILE:HG12	56:HH:125:VAL:HG11	2.03	0.40
71:XX:84:PHE:CE2	71:XX:86:PRO:HA	2.55	0.40
1:2:37:T6A:N1	1:2:37:T6A:N11	2.64	0.40
3:5:165:A:H2'	3:5:166:C:H6	1.84	0.40
3:5:371:A:O2'	3:5:372:A:H5'	2.21	0.40
3:5:452:A:H62	3:5:1293:G:H5''	1.87	0.40
3:5:1350:C:H2'	3:5:1351:G:C8	2.56	0.40
3:5:1741:G:H3'	3:5:1742:A:C5'	2.51	0.40
3:5:3661:G:O2'	7:A:156:LYS:HD2	2.22	0.40
3:5:3736:A:H2'	3:5:3737:A:H8	1.86	0.40
5:8:52:A:O5'	43:l:21:ARG:HD3	2.21	0.40
6:9:852:G:H8	60:LL:97:ARG:NH1	2.19	0.40
6:9:1108:G:H2'	6:9:1109:C:H5''	2.02	0.40
6:9:1867:U:C4	74:Aa:84:VAL:HG12	2.57	0.40
8:B:8:ALA:HB1	27:V:48:ARG:HH22	1.86	0.40
8:B:63:PRO:HD2	8:B:357:ARG:HH21	1.87	0.40
19:N:17:ASP:OD2	19:N:17:ASP:C	2.64	0.40
26:U:40:GLU:OE2	26:U:70:ILE:HG13	2.21	0.40
30:Y:89:LYS:HG2	30:Y:90:ALA:H	1.85	0.40
42:k:14:THR:O	42:k:17:ARG:HB2	2.21	0.40
55:GG:75:LEU:O	55:GG:94:ARG:HA	2.22	0.40
56:HH:43:LEU:HD13	56:HH:68:GLN:NE2	2.33	0.40
63:PP:93:MET:HE1	63:PP:104:GLN:NE2	2.36	0.40
67:TT:114:GLU:N	67:TT:114:GLU:OE1	2.54	0.40
74:Aa:66:LYS:HB2	74:Aa:68:TYR:CE1	2.56	0.40
79:Gg:14:HIS:ND1	79:Gg:35:SER:HB2	2.36	0.40
79:Gg:57:ARG:HD3	79:Gg:95:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Gg:114:SER:OG	79:Gg:116:ASP:OD1	2.37	0.40
79:Gg:158:PRO:HD2	79:Gg:204:GLY:HA2	2.03	0.40
79:Gg:177:TRP:CE3	79:Gg:184:LEU:N	2.89	0.40
79:Gg:262:GLU:HG2	79:Gg:263:GLY:N	2.36	0.40
3:5:478:G:H2'	3:5:479:G:C8	2.56	0.40
3:5:489:C:H2'	3:5:490:C:H6	1.87	0.40
3:5:1340:C:H2'	3:5:1341:U:H6	1.86	0.40
3:5:1975:G:O4'	3:5:1984:A:H1'	2.21	0.40
3:5:2417:A:C4	3:5:2418:A:C8	3.09	0.40
3:5:2870:A:H2'	3:5:2871:A:H8	1.87	0.40
3:5:3684:G:H2'	3:5:3685:C:C6	2.56	0.40
3:5:3834:C:H2'	3:5:3835:C:C6	2.57	0.40
3:5:3902:A:OP1	3:5:4450:PSU:H4'	2.22	0.40
3:5:4918:C:H2'	3:5:4919:G:C8	2.56	0.40
3:5:4931:G:C6	3:5:4932:U:C4	3.09	0.40
6:9:1378:A:H4'	6:9:1379:A:O5'	2.20	0.40
8:B:21:ARG:HG2	8:B:271:GLN:HG2	2.03	0.40
9:C:289:LEU:HD11	22:Q:31:LEU:HB2	2.02	0.40
12:F:147:LYS:HD3	12:F:244:ARG:HH11	1.86	0.40
15:I:66:GLU:OE2	15:I:69:ARG:NH2	2.54	0.40
26:U:84:LYS:HB2	26:U:110:TYR:CE1	2.56	0.40
27:V:22:VAL:HG23	27:V:53:PRO:O	2.21	0.40
28:W:113:LYS:HA	28:W:116:LYS:HE3	2.03	0.40
37:f:11:PHE:HE1	37:f:26:ALA:HB1	1.85	0.40
38:g:23:SER:OG	38:g:33:LEU:HD23	2.21	0.40
38:g:60:ARG:CD	38:g:61:PRO:HD2	2.39	0.40
50:BB:62:LEU:O	50:BB:88:THR:OG1	2.31	0.40
50:BB:127:VAL:HG11	50:BB:176:VAL:HG11	2.02	0.40
51:CC:93:ILE:HD12	51:CC:93:ILE:H	1.86	0.40
55:GG:85:ARG:O	55:GG:87:ARG:NH1	2.53	0.40
58:JJ:24:ARG:O	58:JJ:27:GLN:HG3	2.21	0.40
58:JJ:30:LYS:HE3	58:JJ:30:LYS:HB3	1.90	0.40
59:KK:21:MET:HB3	59:KK:49:MET:HE1	2.04	0.40
59:KK:25:LYS:HD2	59:KK:62:PHE:CE2	2.57	0.40
3:5:6:C:H2'	3:5:7:C:H6	1.86	0.40
3:5:666:G:H4'	3:5:667:A:H5'	2.04	0.40
3:5:1201:U:H2'	3:5:1202:C:H6	1.87	0.40
3:5:1390:G:N2	3:5:1393:G:OP2	2.46	0.40
3:5:3900:G:H5''	3:5:3901:A:H4'	2.03	0.40
3:5:4723:A:H2'	3:5:4724:A:C8	2.57	0.40
6:9:667:U:H5''	6:9:1087:A:C5	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:1230:C:H2'	6:9:1231:C:H6	1.87	0.40
8:B:17:LEU:HD21	8:B:264:PHE:HD2	1.87	0.40
8:B:218:ASP:OD1	8:B:280:ILE:HA	2.21	0.40
10:D:156:GLY:HA2	10:D:181:PRO:HD3	2.04	0.40
13:G:184:LYS:HZ1	13:G:187:PRO:HD3	1.87	0.40
13:G:273:GLU:HA	13:G:276:ARG:HG2	2.03	0.40
17:L:96:ILE:HD13	17:L:117:LEU:HD11	2.03	0.40
20:O:29:LEU:HD23	20:O:29:LEU:HA	1.89	0.40
21:P:22:LEU:HD12	21:P:146:ILE:HD13	2.03	0.40
24:S:84:TYR:CG	24:S:113:MET:HE1	2.56	0.40
49:AA:85:ARG:HD3	49:AA:203:PHE:O	2.22	0.40
55:GG:30:LYS:HB3	55:GG:34:THR:HG21	2.02	0.40
56:HH:39:GLN:OE1	56:HH:75:ILE:HG21	2.21	0.40
63:PP:85:ILE:HG13	63:PP:112:ILE:HA	2.04	0.40
75:Bb:19:HIS:O	75:Bb:23:ARG:HD2	2.22	0.40
3:5:111:C:OP1	39:h:110:LYS:HE3	2.21	0.40
3:5:424:U:H2'	3:5:425:U:C6	2.56	0.40
3:5:911:U:H2'	3:5:912:G:O4'	2.21	0.40
3:5:1238:C:O2'	3:5:1239:G:OP1	2.29	0.40
3:5:1338:G:H4'	3:5:1339:U:C6	2.57	0.40
3:5:1471:U:H2'	3:5:1472:C:H6	1.86	0.40
3:5:1475:G:N2	3:5:1490:G:C4	2.90	0.40
3:5:1759:G:N2	3:5:1773:U:O2	2.33	0.40
3:5:1776:A:N3	3:5:1776:A:H2'	2.37	0.40
3:5:1958:A:H5'	3:5:1962:A:O2'	2.22	0.40
3:5:3759:A:O2'	6:9:1826:G:O2'	2.27	0.40
3:5:4909:A:H2'	8:B:156:TYR:CE1	2.56	0.40
3:5:4996:C:H4'	35:d:26:THR:HG23	2.02	0.40
3:5:5000:G:H2'	3:5:5001:U:O4'	2.20	0.40
6:9:130:G:H2'	6:9:130:G:N3	2.36	0.40
6:9:199:C:H2'	6:9:200:G:O4'	2.22	0.40
6:9:642:U:H4'	6:9:643:A:OP1	2.21	0.40
6:9:857:U:H2'	6:9:858:A:C8	2.57	0.40
6:9:1044:G:C8	7:A:249:THR:HG22	2.57	0.40
6:9:1252:C:OP1	68:UU:75:LYS:NZ	2.50	0.40
6:9:1501:C:H2'	6:9:1502:C:H6	1.86	0.40
6:9:1678:A2M:HM'3	6:9:1678:A2M:H1'	1.63	0.40
7:A:158:ILE:CG2	7:A:162:ASN:HD21	2.34	0.40
9:C:180:ILE:HD12	9:C:180:ILE:H	1.87	0.40
12:F:45:ARG:O	12:F:49:ILE:HG23	2.21	0.40
18:M:133:ALA:O	18:M:136:LEU:HG	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:42:ARG:HD3	21:P:42:ARG:HA	1.73	0.40
23:R:104:ARG:O	23:R:108:ARG:HG2	2.21	0.40
26:U:26:THR:HA	26:U:68:SER:OG	2.21	0.40
28:W:107:GLN:HA	28:W:110:ARG:NE	2.37	0.40
30:Y:112:ASP:H	30:Y:115:ARG:HB2	1.87	0.40
34:c:28:VAL:HG21	34:c:37:MET:HG3	2.03	0.40
39:h:44:LEU:O	39:h:47:ILE:HG12	2.21	0.40
52:DD:123:LEU:HD12	52:DD:123:LEU:HA	1.96	0.40
52:DD:210:ILE:HD12	65:RR:16:ILE:HG12	2.03	0.40
53:EE:247:THR:OG1	53:EE:250:GLU:OE1	2.40	0.40
54:FF:175:ASP:OD2	54:FF:176:GLU:N	2.54	0.40
55:GG:7:PHE:HE2	55:GG:10:THR:HG23	1.86	0.40
57:II:26:LYS:O	57:II:29:LEU:HD22	2.21	0.40
61:NN:47:PRO:HD2	61:NN:86:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	A	246/248 (99%)	228 (93%)	18 (7%)	0	100	100
8	B	392/394 (100%)	378 (96%)	14 (4%)	0	100	100
9	C	357/360 (99%)	347 (97%)	10 (3%)	0	100	100
10	D	289/291 (99%)	280 (97%)	9 (3%)	0	100	100
11	E	208/251 (83%)	198 (95%)	10 (5%)	0	100	100
12	F	223/225 (99%)	211 (95%)	12 (5%)	0	100	100
13	G	223/234 (95%)	215 (96%)	8 (4%)	0	100	100
14	H	188/190 (99%)	177 (94%)	11 (6%)	0	100	100
15	I	201/213 (94%)	195 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	J	168/170 (99%)	163 (97%)	5 (3%)	0	100	100
17	L	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
18	M	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
19	N	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
20	O	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
21	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
22	Q	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
23	R	178/180 (99%)	171 (96%)	7 (4%)	0	100	100
24	S	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
25	T	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
26	U	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
27	V	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
28	W	102/121 (84%)	99 (97%)	3 (3%)	0	100	100
29	X	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
30	Y	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
31	Z	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
32	a	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
33	b	100/116 (86%)	97 (97%)	3 (3%)	0	100	100
34	c	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	d	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
36	e	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
37	f	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
38	g	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
39	h	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
40	i	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
41	j	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
42	k	67/69 (97%)	67 (100%)	0	0	100	100
43	l	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
44	m	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
45	n	23/25 (92%)	23 (100%)	0	0	100	100
46	o	101/103 (98%)	100 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	p	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
48	r	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
49	AA	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
50	BB	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
51	CC	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
52	DD	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
53	EE	260/262 (99%)	255 (98%)	5 (2%)	0	100	100
54	FF	181/191 (95%)	166 (92%)	15 (8%)	0	100	100
55	GG	235/237 (99%)	229 (97%)	6 (3%)	0	100	100
56	HH	181/189 (96%)	171 (94%)	10 (6%)	0	100	100
57	II	199/206 (97%)	190 (96%)	9 (4%)	0	100	100
58	JJ	183/185 (99%)	178 (97%)	5 (3%)	0	100	100
59	KK	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
60	LL	139/151 (92%)	134 (96%)	5 (4%)	0	100	100
61	NN	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
62	OO	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
63	PP	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
64	QQ	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
65	RR	130/132 (98%)	129 (99%)	1 (1%)	0	100	100
66	SS	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
67	TT	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
68	UU	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
69	VV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
70	WW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
71	XX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
72	YY	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
73	ZZ	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
74	Aa	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
75	Bb	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
76	Cc	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
77	Dd	53/55 (96%)	50 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	Ee	53/55 (96%)	53 (100%)	0	0	100	100
79	Gg	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
All	All	10973/11241 (98%)	10587 (96%)	386 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	
7	A	190/190 (100%)	190 (100%)	0	100	100
8	B	342/342 (100%)	342 (100%)	0	100	100
9	C	299/299 (100%)	299 (100%)	0	100	100
10	D	247/247 (100%)	247 (100%)	0	100	100
11	E	190/223 (85%)	190 (100%)	0	100	100
12	F	196/196 (100%)	196 (100%)	0	100	100
13	G	196/201 (98%)	196 (100%)	0	100	100
14	H	169/169 (100%)	169 (100%)	0	100	100
15	I	175/180 (97%)	175 (100%)	0	100	100
16	J	143/143 (100%)	143 (100%)	0	100	100
17	L	175/175 (100%)	175 (100%)	0	100	100
18	M	117/117 (100%)	117 (100%)	0	100	100
19	N	171/171 (100%)	171 (100%)	0	100	100
20	O	171/171 (100%)	171 (100%)	0	100	100
21	P	134/134 (100%)	134 (100%)	0	100	100
22	Q	164/164 (100%)	164 (100%)	0	100	100
23	R	159/159 (100%)	159 (100%)	0	100	100
24	S	157/157 (100%)	157 (100%)	0	100	100
25	T	139/139 (100%)	139 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	U	88/88 (100%)	88 (100%)	0	100	100
27	V	101/101 (100%)	101 (100%)	0	100	100
28	W	86/100 (86%)	86 (100%)	0	100	100
29	X	106/106 (100%)	106 (100%)	0	100	100
30	Y	124/124 (100%)	124 (100%)	0	100	100
31	Z	117/117 (100%)	117 (100%)	0	100	100
32	a	119/119 (100%)	119 (100%)	0	100	100
33	b	84/95 (88%)	84 (100%)	0	100	100
34	c	84/84 (100%)	84 (100%)	0	100	100
35	d	98/98 (100%)	98 (100%)	0	100	100
36	e	114/114 (100%)	114 (100%)	0	100	100
37	f	88/88 (100%)	88 (100%)	0	100	100
38	g	98/98 (100%)	98 (100%)	0	100	100
39	h	109/109 (100%)	109 (100%)	0	100	100
40	i	86/86 (100%)	86 (100%)	0	100	100
41	j	73/73 (100%)	73 (100%)	0	100	100
42	k	64/64 (100%)	64 (100%)	0	100	100
43	l	47/47 (100%)	47 (100%)	0	100	100
44	m	46/46 (100%)	46 (100%)	0	100	100
45	n	24/24 (100%)	24 (100%)	0	100	100
46	o	91/91 (100%)	91 (100%)	0	100	100
47	p	74/74 (100%)	74 (100%)	0	100	100
48	r	108/108 (100%)	108 (100%)	0	100	100
49	AA	180/181 (99%)	180 (100%)	0	100	100
50	BB	194/194 (100%)	194 (100%)	0	100	100
51	CC	187/187 (100%)	187 (100%)	0	100	100
52	DD	190/190 (100%)	190 (100%)	0	100	100
53	EE	224/224 (100%)	224 (100%)	0	100	100
54	FF	158/161 (98%)	158 (100%)	0	100	100
55	GG	207/207 (100%)	207 (100%)	0	100	100
56	HH	165/169 (98%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	II	177/178 (99%)	177 (100%)	0	100	100
58	JJ	161/161 (100%)	161 (100%)	0	100	100
59	KK	87/87 (100%)	87 (100%)	0	100	100
60	LL	130/136 (96%)	130 (100%)	0	100	100
61	NN	130/130 (100%)	130 (100%)	0	100	100
62	OO	106/106 (100%)	106 (100%)	0	100	100
63	PP	109/109 (100%)	109 (100%)	0	100	100
64	QQ	117/117 (100%)	117 (100%)	0	100	100
65	RR	119/119 (100%)	119 (100%)	0	100	100
66	SS	125/125 (100%)	125 (100%)	0	100	100
67	TT	111/111 (100%)	111 (100%)	0	100	100
68	UU	92/92 (100%)	92 (100%)	0	100	100
69	VV	67/67 (100%)	67 (100%)	0	100	100
70	WW	112/112 (100%)	112 (100%)	0	100	100
71	XX	113/113 (100%)	113 (100%)	0	100	100
72	YY	107/107 (100%)	107 (100%)	0	100	100
73	ZZ	66/66 (100%)	66 (100%)	0	100	100
74	Aa	88/88 (100%)	88 (100%)	0	100	100
75	Bb	75/75 (100%)	75 (100%)	0	100	100
76	Cc	55/55 (100%)	55 (100%)	0	100	100
77	Dd	48/48 (100%)	48 (100%)	0	100	100
78	Ee	46/46 (100%)	46 (100%)	0	100	100
79	Gg	272/272 (100%)	272 (100%)	0	100	100
All	All	9581/9664 (99%)	9581 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
7	A	162	ASN
8	B	184	GLN
8	B	258	HIS
8	B	302	ASN

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Mol	Chain	Res	Type
9	C	60	HIS
9	C	89	GLN
9	C	212	ASN
9	C	346	ASN
9	C	347	HIS
10	D	131	ASN
10	D	138	GLN
10	D	250	ASN
10	D	275	GLN
11	E	138	GLN
11	E	253	GLN
12	F	150	ASN
13	G	82	ASN
13	G	91	ASN
13	G	96	GLN
13	G	135	GLN
13	G	259	GLN
14	H	98	HIS
14	H	189	GLN
15	I	95	HIS
15	I	112	GLN
15	I	143	GLN
16	J	112	HIS
17	L	19	GLN
17	L	115	GLN
18	M	20	HIS
18	M	48	GLN
18	M	56	GLN
19	N	15	GLN
19	N	57	GLN
20	O	5	GLN
20	O	26	GLN
20	O	96	GLN
21	P	72	GLN
21	P	80	GLN
23	R	66	ASN
24	S	91	HIS
24	S	146	HIS
25	T	66	ASN
25	T	90	ASN
26	U	94	ASN
28	W	104	GLN

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Mol	Chain	Res	Type
29	X	108	GLN
30	Y	72	GLN
30	Y	127	GLN
31	Z	78	ASN
31	Z	79	HIS
31	Z	127	ASN
32	a	28	HIS
32	a	44	ASN
33	b	6	ASN
33	b	19	ASN
33	b	50	ASN
36	e	52	GLN
38	g	3	GLN
38	g	112	GLN
39	h	108	GLN
41	j	13	ASN
42	k	58	GLN
44	m	83	ASN
46	o	102	GLN
48	r	21	ASN
48	r	31	ASN
48	r	103	HIS
49	AA	9	GLN
49	AA	113	GLN
49	AA	132	GLN
50	BB	40	ASN
50	BB	149	GLN
50	BB	158	HIS
50	BB	202	GLN
52	DD	57	ASN
53	EE	67	GLN
54	FF	36	GLN
54	FF	79	HIS
55	GG	13	GLN
55	GG	163	ASN
56	HH	68	GLN
56	HH	76	GLN
56	HH	91	HIS
57	II	7	ASN
58	JJ	113	GLN
58	JJ	154	GLN
59	KK	44	HIS

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Mol	Chain	Res	Type
59	KK	66	HIS
59	KK	84	HIS
60	LL	83	GLN
61	NN	5	HIS
61	NN	36	GLN
61	NN	69	ASN
62	OO	113	GLN
63	PP	32	GLN
63	PP	103	ASN
63	PP	104	GLN
64	QQ	35	ASN
64	QQ	86	GLN
64	QQ	142	GLN
65	RR	62	GLN
65	RR	83	ASN
67	TT	51	ASN
68	UU	100	GLN
69	VV	2	GLN
71	XX	31	HIS
72	YY	94	HIS
75	Bb	9	HIS
76	Cc	29	GLN
76	Cc	45	ASN
77	Dd	5	GLN
78	Ee	88	GLN
79	Gg	104	HIS
79	Gg	117	ASN
79	Gg	187	ASN
79	Gg	226	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	68/76 (89%)	11 (16%)	0
2	1	5/6 (83%)	1 (20%)	0
3	5	3524/3546 (99%)	694 (19%)	55 (1%)
4	7	119/120 (99%)	10 (8%)	0
5	8	149/156 (95%)	29 (19%)	1 (0%)
6	9	1687/1698 (99%)	330 (19%)	18 (1%)
All	All	5552/5602 (99%)	1075 (19%)	74 (1%)

All (1075) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	10	G
1	2	11	G
1	2	13	G
1	2	14	C
1	2	19	G
1	2	42	A
1	2	46	G
1	2	58	A
1	2	72	U
1	2	75	C
1	2	76	A
2	1	46	A
3	5	8	U
3	5	13	U
3	5	15	A
3	5	25	A
3	5	39	A
3	5	42	A
3	5	48	G
3	5	49	U
3	5	56	A
3	5	58	G
3	5	59	A
3	5	64	A
3	5	65	A
3	5	66	A
3	5	71	C
3	5	72	C
3	5	73	A
3	5	76	A
3	5	91	G
3	5	104	G
3	5	108	A
3	5	109	G
3	5	119	G
3	5	120	A
3	5	122	U
3	5	126	C
3	5	134	G
3	5	135	G
3	5	142	G
3	5	144	G
3	5	146	G

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Mol	Chain	Res	Type
3	5	149	A
3	5	157	U
3	5	159	C
3	5	171	U
3	5	172	C
3	5	173	C
3	5	182	G
3	5	200	U
3	5	201	C
3	5	209	U
3	5	216	C
3	5	218	A
3	5	219	G
3	5	220	C
3	5	224	U
3	5	233	U
3	5	234	G
3	5	235	A
3	5	237	B9B
3	5	246	G
3	5	265	C
3	5	266	C
3	5	280	G
3	5	297	U
3	5	306	A
3	5	315	G
3	5	316	U
3	5	334	A
3	5	340	C
3	5	344	A
3	5	345	C
3	5	350	C
3	5	363	A
3	5	372	A
3	5	386	A
3	5	387	G
3	5	407	A
3	5	410	A
3	5	412	G
3	5	413	G
3	5	415	G
3	5	431	G

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Mol	Chain	Res	Type
3	5	432	U
3	5	440	U
3	5	449	C
3	5	450	G
3	5	452	A
3	5	453	G
3	5	464	G
3	5	467	U
3	5	468	U
3	5	483	G
3	5	486	C
3	5	492	U
3	5	493	G
3	5	496	G
3	5	497	G
3	5	498	C
3	5	499	G
3	5	505	G
3	5	510	U
3	5	523	C
3	5	666	G
3	5	667	A
3	5	669	C
3	5	670	G
3	5	672	C
3	5	685	C
3	5	686	A
3	5	691	C
3	5	696	C
3	5	697	G
3	5	704	C
3	5	705	G
3	5	708	G
3	5	719	C
3	5	731	G
3	5	738	C
3	5	738(A)	C
3	5	742	G
3	5	744	G
3	5	749	G
3	5	758	G
3	5	914	U

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Mol	Chain	Res	Type
3	5	915	A
3	5	916	C
3	5	917	A
3	5	918	G
3	5	921	C
3	5	923	C
3	5	925	C
3	5	926	G
3	5	929	A
3	5	931	C
3	5	932	A
3	5	933	G
3	5	934	C
3	5	935	A
3	5	935(A)	G
3	5	936	C
3	5	939	G
3	5	941	C
3	5	943	A
3	5	944	A
3	5	945	U
3	5	946	C
3	5	956	A
3	5	959	G
3	5	960	A
3	5	961	G
3	5	966	A
3	5	967	C
3	5	968	C
3	5	983	U
3	5	1078	A
3	5	1079	C
3	5	1080	C
3	5	1081	C
3	5	1082	C
3	5	1084	C
3	5	1175	A
3	5	1179	U
3	5	1180	C
3	5	1187	G
3	5	1193	C
3	5	1195	G

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Mol	Chain	Res	Type
3	5	1211	G
3	5	1212	G
3	5	1214	C
3	5	1215	C
3	5	1234	G
3	5	1235	C
3	5	1236	C
3	5	1237	A
3	5	1239	G
3	5	1244	G
3	5	1272	C
3	5	1273	G
3	5	1275	G
3	5	1276	C
3	5	1284	G
3	5	1287	G
3	5	1291	G
3	5	1292	C
3	5	1293	G
3	5	1295	U
3	5	1296	G
3	5	1301	C
3	5	1303	A
3	5	1304	C
3	5	1314	C
3	5	1326	A2M
3	5	1330	A
3	5	1337	A
3	5	1348	P4U
3	5	1354	A
3	5	1358	G
3	5	1359	G
3	5	1371	A
3	5	1372	A
3	5	1377	G
3	5	1378	C
3	5	1381	U
3	5	1387	A
3	5	1394	G
3	5	1397	A
3	5	1398	A
3	5	1403	G

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Mol	Chain	Res	Type
3	5	1414	C
3	5	1415	G
3	5	1416	G
3	5	1419	G
3	5	1421	G
3	5	1428	U
3	5	1436	C
3	5	1437	C
3	5	1438	U
3	5	1440	U
3	5	1441	C
3	5	1455	G
3	5	1456	B8Q
3	5	1457	G
3	5	1475	G
3	5	1477	C
3	5	1482	G
3	5	1483	C
3	5	1497	A
3	5	1498	G
3	5	1502	G
3	5	1514	U
3	5	1516	G
3	5	1523	A
3	5	1534	A2M
3	5	1547	A
3	5	1566	C
3	5	1568	C
3	5	1578	U
3	5	1586	G
3	5	1591	U
3	5	1596	U
3	5	1602	U
3	5	1624	G
3	5	1625	OMG
3	5	1626	G
3	5	1631	A
3	5	1633	G
3	5	1634	A
3	5	1638	A
3	5	1641	G
3	5	1654	G

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Mol	Chain	Res	Type
3	5	1661	C
3	5	1676	C
3	5	1677	PSU
3	5	1678	C
3	5	1691	G
3	5	1731	C
3	5	1741	G
3	5	1742	A
3	5	1750	G
3	5	1751	A
3	5	1752	G
3	5	1755	C
3	5	1756	U
3	5	1757	U
3	5	1764	G
3	5	1768	C
3	5	1772	C
3	5	1773	U
3	5	1774	C
3	5	1775	A
3	5	1776	A
3	5	1781	U
3	5	1787	A
3	5	1804	A
3	5	1805	A
3	5	1806	G
3	5	1807	C
3	5	1812	C
3	5	1815	G
3	5	1819	G
3	5	1821	G
3	5	1828	C
3	5	1834	U
3	5	1835	G
3	5	1836	G
3	5	1837	A
3	5	1842	G
3	5	1855	G
3	5	1860	B8H
3	5	1869	G
3	5	1893	C
3	5	1897	A

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Mol	Chain	Res	Type
3	5	1916	G
3	5	1918	U
3	5	1920	C
3	5	1921	C
3	5	1922	G
3	5	1930	U
3	5	1931	C
3	5	1932	A
3	5	1940	G
3	5	1945	G
3	5	1948	G
3	5	1957	U
3	5	1958	A
3	5	1960	A
3	5	1961	G
3	5	1962	A
3	5	1964	A
3	5	1969	G
3	5	1972	G
3	5	1974	U
3	5	1975	G
3	5	1976	G
3	5	1977	C
3	5	1980	U
3	5	1983	A
3	5	1984	A
3	5	1987	C
3	5	1991	A
3	5	1992	U
3	5	1997	U
3	5	2001	G
3	5	2002	A
3	5	2003	G
3	5	2004	U
3	5	2007	G
3	5	2008	U
3	5	2010	A
3	5	2011	C
3	5	2026	A
3	5	2031	C
3	5	2044	U
3	5	2046	G

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Mol	Chain	Res	Type
3	5	2047	A
3	5	2048	U
3	5	2052	G
3	5	2055	G
3	5	2056	G
3	5	2069	A
3	5	2084	U
3	5	2090	U
3	5	2092	G
3	5	2093	G
3	5	2094	C
3	5	2097	A
3	5	2098	G
3	5	2100	G
3	5	2101	A
3	5	2102	G
3	5	2106	G
3	5	2107	A
3	5	2108	G
3	5	2109	A
3	5	2110	G
3	5	2259	G
3	5	2260	C
3	5	2268	A
3	5	2275	G
3	5	2279	A
3	5	2289	C
3	5	2300	A
3	5	2301	G
3	5	2306	G
3	5	2313	A
3	5	2314	G
3	5	2332	A
3	5	2333	G
3	5	2348	G
3	5	2351	C
3	5	2360	A
3	5	2364	OMG
3	5	2369	U
3	5	2380	B8W
3	5	2383	C
3	5	2395	A

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Mol	Chain	Res	Type
3	5	2396	A
3	5	2398	U
3	5	2417	A
3	5	2422	OMC
3	5	2424	OMG
3	5	2425	U
3	5	2433	G
3	5	2441	C
3	5	2450	G
3	5	2453	A
3	5	2470	C
3	5	2471	G
3	5	2474	G
3	5	2475	G
3	5	2488	C
3	5	2489	C
3	5	2490	U
3	5	2491	C
3	5	2495	U
3	5	2503	G
3	5	2504	C
3	5	2505	C
3	5	2506	G
3	5	2511	A
3	5	2513	A
3	5	2529	A
3	5	2530	U
3	5	2537	A
3	5	2544	G
3	5	2546	G
3	5	2547	G
3	5	2554	U
3	5	2568	C
3	5	2570	U
3	5	2571	C
3	5	2575	U
3	5	2577	C
3	5	2583	C
3	5	2586	G
3	5	2587	A
3	5	2588	C
3	5	2589	C

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Mol	Chain	Res	Type
3	5	2601	A
3	5	2618	G
3	5	2620	G
3	5	2627	C
3	5	2638	G
3	5	2640	G
3	5	2653	C
3	5	2661	U
3	5	2662	G
3	5	2663	G
3	5	2669	C
3	5	2677	G
3	5	2679	G
3	5	2687	U
3	5	2694	G
3	5	2695	A
3	5	2696	A
3	5	2705	G
3	5	2707	U
3	5	2708	U
3	5	2709	C
3	5	2710	C
3	5	2711	G
3	5	2714	G
3	5	2715	G
3	5	2716	C
3	5	2725	A
3	5	2726	G
3	5	2740	U
3	5	2743	A
3	5	2744	A
3	5	2753	G
3	5	2754	B9B
3	5	2755	A
3	5	2763	U
3	5	2769	U
3	5	2772	C
3	5	2787	A
3	5	2788	U
3	5	2790	U
3	5	2798	A
3	5	2806	A

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Mol	Chain	Res	Type
3	5	2814	C
3	5	2815	A
3	5	2826	U
3	5	2827	G
3	5	2842	G
3	5	2855	G
3	5	2867	C
3	5	2875	C
3	5	2898	G
3	5	3603	G
3	5	3605	C
3	5	3606	U
3	5	3615	G
3	5	3618	C
3	5	3619	G
3	5	3625	G
3	5	3626	G
3	5	3635	A
3	5	3644	U
3	5	3648	A
3	5	3662	A
3	5	3664	G
3	5	3673	C
3	5	3674	G
3	5	3696	C
3	5	3698	G
3	5	3711	A
3	5	3712	A
3	5	3714	G
3	5	3729	PSU
3	5	3748	A
3	5	3753	G
3	5	3759	A
3	5	3760	A
3	5	3762	B8H
3	5	3773	U
3	5	3774	A
3	5	3776	G
3	5	3777	G
3	5	3783	A
3	5	3784	A
3	5	3786	U

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Mol	Chain	Res	Type
3	5	3792	OMG
3	5	3810	C
3	5	3811	G
3	5	3813	A
3	5	3814	U
3	5	3817	A
3	5	3819	G
3	5	3822	U
3	5	3824	A
3	5	3838	U
3	5	3840	U
3	5	3867	A2M
3	5	3876	A
3	5	3877	A
3	5	3878	C
3	5	3879	G
3	5	3880	P7G
3	5	3889	G
3	5	3892	U
3	5	3897	B8K
3	5	3898	G
3	5	3901	A
3	5	3905	A
3	5	3906	A
3	5	3907	G
3	5	3908	A
3	5	3915	U
3	5	3916	G
3	5	3917	A
3	5	3938	G
3	5	3939	G
3	5	3946	G
3	5	3947	A
3	5	3948	C
3	5	4061	G
3	5	4066	U
3	5	4076	G
3	5	4085	A
3	5	4086	G
3	5	4097	G
3	5	4100	C
3	5	4118	U

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Mol	Chain	Res	Type
3	5	4119	C
3	5	4120	U
3	5	4122	G
3	5	4125	C
3	5	4127	A
3	5	4158	C
3	5	4162	C
3	5	4163	U
3	5	4164	C
3	5	4170	A
3	5	4183	G
3	5	4184	G
3	5	4191	G
3	5	4203	A
3	5	4225	G
3	5	4229	U
3	5	4233	A
3	5	4234	A
3	5	4249	G
3	5	4251	A
3	5	4254	G
3	5	4255	A
3	5	4256	A
3	5	4266	G
3	5	4268	A
3	5	4271	A
3	5	4273	A
3	5	4281	A
3	5	4291	G
3	5	4296	B8H
3	5	4305	G
3	5	4306	OMU
3	5	4314	C
3	5	4329	G
3	5	4330	G
3	5	4332	C
3	5	4339	A
3	5	4349	C
3	5	4354	U
3	5	4371	MHG
3	5	4373	G
3	5	4374	U

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Mol	Chain	Res	Type
3	5	4377	G
3	5	4378	A
3	5	4381	A
3	5	4387	C
3	5	4391	G
3	5	4394	A
3	5	4395	U
3	5	4396	A
3	5	4398	C
3	5	4419	U
3	5	4422	A
3	5	4426	C
3	5	4436	U
3	5	4440	G
3	5	4444	C
3	5	4448	G
3	5	4449	A
3	5	4452	U
3	5	4453	C
3	5	4464	A
3	5	4475	G
3	5	4500	PSU
3	5	4510	A
3	5	4511	A
3	5	4512	U
3	5	4513	A
3	5	4519	C
3	5	4520	G
3	5	4522	G
3	5	4524	G
3	5	4530	UR3
3	5	4531	PSU
3	5	4548	A
3	5	4573	G
3	5	4575	G
3	5	4584	A
3	5	4586	G
3	5	4589	A
3	5	4590	A
3	5	4627	U
3	5	4636	PSU
3	5	4637	OMG

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Mol	Chain	Res	Type
3	5	4639	G
3	5	4652	G
3	5	4656	A
3	5	4670	C
3	5	4672	A
3	5	4677	U
3	5	4691	A
3	5	4695	C
3	5	4700	A
3	5	4707	A
3	5	4709	U
3	5	4720	C
3	5	4721	G
3	5	4736	C
3	5	4745	G
3	5	4751	G
3	5	4754	G
3	5	4757	C
3	5	4759	C
3	5	4761	G
3	5	4765	G
3	5	4771	C
3	5	4772	C
3	5	4867	G
3	5	4870	OMG
3	5	4873	G
3	5	4875	G
3	5	4877	G
3	5	4882	U
3	5	4883	C
3	5	4885	U
3	5	4895	C
3	5	4902	C
3	5	4906	C
3	5	4910	A
3	5	4912	G
3	5	4913	G
3	5	4914	G
3	5	4915	G
3	5	4921	C
3	5	4924	C
3	5	4925	U

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Mol	Chain	Res	Type
3	5	4926	C
3	5	4931	G
3	5	4934	A
3	5	4937	C
3	5	4940	C
3	5	4944	C
3	5	4948	C
3	5	4950	U
3	5	4951	G
3	5	4956	A
3	5	4959	U
3	5	4960	G
3	5	4963	G
3	5	4964	C
3	5	4965	U
3	5	4966	A
3	5	4967	A
3	5	4976	U
3	5	4988	U
3	5	4990	C
3	5	4993	G
3	5	5006	U
3	5	5014	A
3	5	5017	G
3	5	5040	U
3	5	5041	G
3	5	5047	C
3	5	5050	C
3	5	5052	C
3	5	5053	U
3	5	5054	C
3	5	5061	A
3	5	5062	G
4	7	33	U
4	7	53	U
4	7	54	A
4	7	64	G
4	7	97	G
4	7	100	A
4	7	102	U
4	7	110	G
4	7	111	C

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Mol	Chain	Res	Type
4	7	120	U
5	8	2	G
5	8	3	A
5	8	34	U
5	8	35	C
5	8	39	G
5	8	59	A
5	8	62	A
5	8	63	U
5	8	74	U
5	8	75	G
5	8	78	G
5	8	87	G
5	8	90	C
5	8	94	G
5	8	103	A
5	8	105	C
5	8	108	A
5	8	109	C
5	8	110	U
5	8	111	U
5	8	114	G
5	8	122	G
5	8	124	U
5	8	125	C
5	8	126	C
5	8	127	U
5	8	151	G
5	8	153	C
5	8	156	U
6	9	2	A
6	9	3	C
6	9	4	C
6	9	17	C
6	9	25	A
6	9	26	U
6	9	33	G
6	9	41	G
6	9	44	U
6	9	46	A
6	9	56	G
6	9	58	C

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Mol	Chain	Res	Type
6	9	64	A
6	9	65	C
6	9	67	C
6	9	68	A
6	9	71	G
6	9	73	C
6	9	74	G
6	9	75	G
6	9	77	A
6	9	79	A
6	9	103	A
6	9	111	A
6	9	113	G
6	9	114	G
6	9	115	U
6	9	116	OMU
6	9	124	U
6	9	126	G
6	9	129	C
6	9	130	G
6	9	141	A
6	9	143	U
6	9	147	A
6	9	155	G
6	9	158	A
6	9	162	C
6	9	163	U
6	9	166	A2M
6	9	168	C
6	9	178	C
6	9	180	G
6	9	182	C
6	9	183	G
6	9	184	G
6	9	188	C
6	9	189	U
6	9	190	G
6	9	192	C
6	9	206	G
6	9	215	G
6	9	292	A
6	9	308	G

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Mol	Chain	Res	Type
6	9	310	C
6	9	312	G
6	9	318	A
6	9	319	C
6	9	323	C
6	9	339	A
6	9	347	G
6	9	350	C
6	9	351	G
6	9	360	A
6	9	362	C
6	9	364	A
6	9	367	U
6	9	368	U
6	9	370	G
6	9	385	G
6	9	386	C
6	9	398	A
6	9	400	C
6	9	407	G
6	9	408	A
6	9	409	C
6	9	418	A
6	9	434	G
6	9	435	A
6	9	447	A
6	9	448	A
6	9	449	A
6	9	450	C
6	9	465	A
6	9	466	G
6	9	471	G
6	9	472	C
6	9	473	A
6	9	474	G
6	9	476	A
6	9	482	G
6	9	487	U
6	9	492	C
6	9	516	A
6	9	525	A
6	9	530	U

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Mol	Chain	Res	Type
6	9	532	C
6	9	533	A
6	9	534	G
6	9	535	G
6	9	536	A
6	9	537	C
6	9	541	U
6	9	546	G
6	9	547	G
6	9	548	C
6	9	549	C
6	9	550	C
6	9	551	U
6	9	554	A
6	9	555	A
6	9	556	U
6	9	559	G
6	9	563	G
6	9	564	A
6	9	568	MMX
6	9	576	A
6	9	583	A
6	9	587	A
6	9	588	G
6	9	589	G
6	9	590	A
6	9	591	U
6	9	595	U
6	9	598	G
6	9	606	G
6	9	607	U
6	9	608	C
6	9	614	C
6	9	617	G
6	9	621	C
6	9	627	U
6	9	628	A
6	9	629	A
6	9	631	U
6	9	643	A
6	9	655	A
6	9	660	C

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Mol	Chain	Res	Type
6	9	666	U
6	9	668	A2M
6	9	669	A
6	9	671	A
6	9	672	A
6	9	673	G
6	9	683	OMG
6	9	688	U
6	9	689	U
6	9	690	G
6	9	732	U
6	9	752	G
6	9	753	C
6	9	754	G
6	9	799	U
6	9	810	A
6	9	811	A
6	9	821	G
6	9	822	PSU
6	9	830	A
6	9	847	A
6	9	870	A
6	9	871	U
6	9	872	A
6	9	874	G
6	9	875	A
6	9	876	C
6	9	878	G
6	9	887	U
6	9	888	U
6	9	890	U
6	9	892	U
6	9	894	G
6	9	898	U
6	9	901	G
6	9	909	G
6	9	913	A
6	9	914	U
6	9	920	A
6	9	930	C
6	9	933	G
6	9	934	G

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Mol	Chain	Res	Type
6	9	943	U
6	9	958	G
6	9	959	G
6	9	971	G
6	9	990	A
6	9	992	A
6	9	999	G
6	9	1017	U
6	9	1023	A
6	9	1041	G
6	9	1060	A
6	9	1061	U
6	9	1062	A
6	9	1071	G
6	9	1078	C
6	9	1083	A
6	9	1085	C
6	9	1097	G
6	9	1109	C
6	9	1115	U
6	9	1116	C
6	9	1117	C
6	9	1118	C
6	9	1120	U
6	9	1121	G
6	9	1126	G
6	9	1130	G
6	9	1133	A
6	9	1138	C
6	9	1139	C
6	9	1148	A
6	9	1149	A
6	9	1153	C
6	9	1154	U
6	9	1166	G
6	9	1195	A
6	9	1207	G
6	9	1215	C
6	9	1224	G
6	9	1242	U
6	9	1243	PSU
6	9	1251	A

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Mol	Chain	Res	Type
6	9	1253	A
6	9	1256	G
6	9	1257	G
6	9	1259	A
6	9	1260	A
6	9	1265	A
6	9	1274	G
6	9	1275	G
6	9	1282	A
6	9	1284	A
6	9	1285	G
6	9	1286	G
6	9	1287	A
6	9	1293	A
6	9	1294	G
6	9	1301	A
6	9	1302	G
6	9	1307	U
6	9	1308	U
6	9	1309	C
6	9	1314	U
6	9	1342	U
6	9	1371	U
6	9	1372	U
6	9	1378	A
6	9	1395	C
6	9	1396	A
6	9	1397	U
6	9	1401	A
6	9	1402	A
6	9	1404	U
6	9	1409	A
6	9	1428	G
6	9	1442	U
6	9	1454	A
6	9	1462	U
6	9	1463	U
6	9	1464	C
6	9	1466	G
6	9	1477	U
6	9	1480	A
6	9	1487	A

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Mol	Chain	Res	Type
6	9	1489	A
6	9	1490	G
6	9	1497	G
6	9	1498	A
6	9	1505	U
6	9	1507	G
6	9	1508	A
6	9	1509	U
6	9	1521	C
6	9	1522	A
6	9	1533	A
6	9	1552	G
6	9	1553	C
6	9	1563	G
6	9	1570	G
6	9	1574	C
6	9	1575	G
6	9	1579	A
6	9	1580	A
6	9	1586	U
6	9	1587	G
6	9	1588	A
6	9	1589	A
6	9	1601	A
6	9	1602	U
6	9	1604	G
6	9	1606	G
6	9	1619	A
6	9	1621	U
6	9	1623	A
6	9	1637	A
6	9	1638	G
6	9	1648	G
6	9	1665	G
6	9	1671	G
6	9	1695	A
6	9	1698	C
6	9	1699	A
6	9	1721	U
6	9	1722	G
6	9	1726	G
6	9	1727	G

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Mol	Chain	Res	Type
6	9	1732	G
6	9	1744	G
6	9	1748	G
6	9	1756	C
6	9	1779	G
6	9	1783	C
6	9	1784	G
6	9	1785	C
6	9	1823	A
6	9	1824	A
6	9	1829	G
6	9	1831	A
6	9	1835	A
6	9	1836	G
6	9	1838	U
6	9	1849	G
6	9	1851	MA6
6	9	1859	A
6	9	1861	G
6	9	1862	G
6	9	1863	A
6	9	1864	U
6	9	1865	C
6	9	1869	A

All (74) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	5	12	A
3	5	47	A
3	5	48	G
3	5	125	C
3	5	134	G
3	5	217	C
3	5	245	C
3	5	265	C
3	5	385	A
3	5	406	C
3	5	449	C
3	5	485	C
3	5	492	U
3	5	504	G

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Mol	Chain	Res	Type
3	5	684	G
3	5	685	C
3	5	696	C
3	5	930	G
3	5	1174	G
3	5	1211	G
3	5	1236	C
3	5	1238	C
3	5	1291	G
3	5	1329	G
3	5	1370	G
3	5	1438	U
3	5	1440	U
3	5	1474	C
3	5	1633	G
3	5	1804	A
3	5	1818	G
3	5	1979	A
3	5	1983	A
3	5	2046	G
3	5	2089	G
3	5	2440	U
3	5	2474	G
3	5	2502	A
3	5	2639	U
3	5	2661	U
3	5	2695	A
3	5	3625	G
3	5	3697	U
3	5	3876	A
3	5	3888	G
3	5	4065	G
3	5	4119	C
3	5	4232	U
3	5	4254	G
3	5	4448	G
3	5	4699	U
3	5	4884	G
3	5	4925	U
3	5	4936	G
3	5	4947	U
5	8	124	U

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Mol	Chain	Res	Type
6	9	24	C
6	9	110	U
6	9	140	U
6	9	434	G
6	9	465	A
6	9	532	C
6	9	553	U
6	9	642	U
6	9	688	U
6	9	752	G
6	9	870	A
6	9	874	G
6	9	1137	U
6	9	1394	G
6	9	1395	C
6	9	1489	A
6	9	1520	G
6	9	1637	A

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

139 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
6	MA6	9	1851	6	23,26,27	1.64	5 (21%)	33,38,41	3.83	14 (42%)
3	B9B	5	1574	3,80	25,28,29	1.79	6 (24%)	35,40,43	5.26	14 (40%)
3	7MG	5	2522	3	23,26,27	3.47	10 (43%)	27,39,42	2.20	9 (33%)
3	OMU	5	4620	3	19,22,23	3.03	8 (42%)	25,31,34	1.78	4 (16%)
3	PSU	5	3729	3	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	5	4403	3	18,21,22	1.10	1 (5%)	21,30,33	1.81	5 (23%)
2	4AC	1	45	2	21,24,25	3.28	9 (42%)	28,34,37	1.15	4 (14%)
3	1MA	5	4415	3	21,25,26	3.11	6 (28%)	30,37,40	2.34	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	5	2363	3,80	22,25,26	3.22	10 (45%)	30,36,39	2.90	10 (33%)
3	OMC	5	2422	3,80	19,22,23	3.02	8 (42%)	25,31,34	0.75	0
6	OMC	9	174	6	19,22,23	3.01	8 (42%)	25,31,34	0.73	0
6	OMG	9	644	6	23,26,27	2.34	8 (34%)	32,38,41	1.91	9 (28%)
3	7MG	5	1605	3	23,26,27	3.48	10 (43%)	27,39,42	2.17	9 (33%)
3	A2M	5	3825	3	22,25,26	3.22	10 (45%)	30,36,39	2.90	10 (33%)
6	A2M	9	27	6,80	22,25,26	3.21	10 (45%)	30,36,39	2.91	11 (36%)
3	OMU	5	4306	3	19,22,23	3.00	8 (42%)	25,31,34	1.82	5 (20%)
3	OMG	5	4494	3	23,26,27	2.36	8 (34%)	32,38,41	1.93	8 (25%)
3	OMG	5	4370	3	23,26,27	2.36	9 (39%)	32,38,41	1.87	8 (25%)
3	OMG	5	4637	3	23,26,27	2.38	8 (34%)	32,38,41	1.92	9 (28%)
3	A2M	5	4571	3	22,25,26	3.22	10 (45%)	30,36,39	2.90	10 (33%)
3	OMG	5	2424	3	23,26,27	2.38	8 (34%)	32,38,41	1.88	7 (21%)
6	OMG	9	683	6	23,26,27	2.35	8 (34%)	32,38,41	1.93	8 (25%)
3	B8K	5	3897	3	24,28,29	3.18	11 (45%)	29,42,45	2.36	11 (37%)
6	M7A	9	1806	6	19,25,26	1.64	2 (10%)	25,37,40	4.09	8 (32%)
6	B8Q	9	1219	6,80	18,22,23	2.96	4 (22%)	21,32,35	2.32	7 (33%)
3	B8W	5	2380	3	23,26,27	2.81	5 (21%)	33,38,41	2.89	15 (45%)
3	PSU	5	4628	3	18,21,22	1.12	1 (5%)	21,30,33	1.96	5 (23%)
3	B8W	5	4129	3	23,26,27	2.87	5 (21%)	33,38,41	2.73	17 (51%)
3	A2M	5	1524	3	22,25,26	3.24	10 (45%)	30,36,39	2.94	12 (40%)
3	UR3	5	4530	3	19,22,23	2.85	7 (36%)	26,32,35	1.63	3 (11%)
6	OMU	9	116	6	19,22,23	3.06	8 (42%)	25,31,34	1.81	6 (24%)
3	B8W	5	4529	3,80	23,26,27	2.87	5 (21%)	33,38,41	2.80	15 (45%)
6	PSU	9	119	6	18,21,22	1.02	1 (5%)	21,30,33	1.76	4 (19%)
6	MMX	9	568	6	20,23,24	3.83	5 (25%)	21,33,36	2.90	5 (23%)
3	2MG	5	4872	3	23,26,27	2.80	9 (39%)	33,38,41	2.61	15 (45%)
3	PSU	5	1683	3	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
3	OMC	5	4536	3	19,22,23	2.98	8 (42%)	25,31,34	0.80	0
3	OMG	5	3792	3	23,26,27	2.36	8 (34%)	32,38,41	1.91	9 (28%)
3	2MG	5	1517	3	23,26,27	2.81	8 (34%)	33,38,41	2.37	11 (33%)
3	PSU	5	4450	3,80	18,21,22	1.09	2 (11%)	21,30,33	2.03	5 (23%)
3	P7G	5	3880	3	24,28,29	3.62	11 (45%)	25,41,44	1.34	2 (8%)
6	6MZ	9	1832	6,80	22,25,26	2.43	4 (18%)	29,36,39	3.39	11 (37%)
9	MLZ	C	333	9	8,9,10	0.84	0	4,9,11	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	5	1582	3	18,21,22	1.04	1 (5%)	21,30,33	1.69	4 (19%)
3	OMC	5	2804	3	19,22,23	2.96	8 (42%)	25,31,34	0.70	0
3	PSU	5	4531	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	5 (23%)
6	PSU	9	612	6	18,21,22	1.10	1 (5%)	21,30,33	1.97	6 (28%)
6	A2M	9	484	6	22,25,26	3.23	10 (45%)	30,36,39	2.98	11 (36%)
3	M7A	5	4564	3	19,25,26	1.60	2 (10%)	25,37,40	4.23	8 (32%)
3	B8W	5	4185	3	23,26,27	2.82	5 (21%)	33,38,41	2.78	16 (48%)
6	PSU	9	823	6	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
3	OMG	5	4623	3	23,26,27	2.34	8 (34%)	32,38,41	1.93	8 (25%)
6	PSU	9	822	6	18,21,22	1.12	1 (5%)	21,30,33	1.96	5 (23%)
3	E7G	5	2297	3	24,27,28	3.57	11 (45%)	28,40,43	2.30	9 (32%)
6	A2M	9	1031	6	22,25,26	3.23	9 (40%)	30,36,39	3.00	11 (36%)
3	PSU	5	4500	3	18,21,22	1.10	1 (5%)	21,30,33	1.92	6 (28%)
6	B8N	9	1248	6	25,29,30	3.38	7 (28%)	28,42,45	2.00	7 (25%)
3	PSU	5	1677	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	5 (23%)
3	OMG	5	373	3	23,26,27	2.34	8 (34%)	32,38,41	1.90	8 (25%)
6	MA6	9	1850	6	23,26,27	1.64	5 (21%)	33,38,41	3.70	13 (39%)
3	PSU	5	4293	3	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
6	4AC	9	1337	6	21,24,25	3.19	9 (42%)	28,34,37	1.11	4 (14%)
3	OMG	5	4196	3	23,26,27	2.35	8 (34%)	32,38,41	1.93	9 (28%)
3	OMG	5	1522	3	23,26,27	2.33	9 (39%)	32,38,41	1.84	8 (25%)
3	B8T	5	4671	3	19,22,23	3.61	8 (42%)	25,31,34	0.90	1 (4%)
3	1MA	5	1322	3,80	21,25,26	3.05	6 (28%)	30,37,40	2.20	7 (23%)
3	B8W	5	4472	3	23,26,27	2.85	5 (21%)	33,38,41	2.69	15 (45%)
3	P4U	5	1348	3	21,24,25	3.41	8 (38%)	28,33,36	1.57	2 (7%)
3	A2M	5	1871	3,80	22,25,26	3.22	10 (45%)	30,36,39	2.94	11 (36%)
3	2MG	5	729	3	23,26,27	2.88	8 (34%)	33,38,41	2.21	7 (21%)
3	B8Q	5	1456	3	18,22,23	2.89	6 (33%)	21,32,35	1.91	4 (19%)
3	A2M	5	3867	3	22,25,26	3.21	10 (45%)	30,36,39	2.93	11 (36%)
3	P7G	5	1909	3	24,28,29	3.70	11 (45%)	25,41,44	1.29	2 (8%)
44	MLZ	m	72	44	8,9,10	0.79	0	4,9,11	0.61	0
3	OMG	5	2364	3	23,26,27	2.32	9 (39%)	32,38,41	1.86	8 (25%)
3	OMC	5	3887	3	19,22,23	3.00	8 (42%)	25,31,34	0.77	0
3	6MZ	5	4220	3	22,25,26	2.47	4 (18%)	29,36,39	3.45	12 (41%)
3	OMC	5	2365	3	19,22,23	2.97	8 (42%)	25,31,34	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	B9H	5	2786	3	21,25,26	3.03	4 (19%)	22,35,38	1.47	3 (13%)
3	PSU	5	4442	3	18,21,22	1.07	1 (5%)	21,30,33	1.92	5 (23%)
6	5MU	9	814	6	19,22,23	4.97	7 (36%)	27,32,35	3.55	10 (37%)
3	5MC	5	4335	3	19,22,23	3.87	8 (42%)	26,32,35	1.08	2 (7%)
1	T6A	2	37	1	31,34,35	1.75	8 (25%)	43,49,52	2.01	10 (23%)
3	A2M	5	2401	3,80	22,25,26	3.24	10 (45%)	30,36,39	2.97	11 (36%)
3	B8H	5	3762	3	19,22,23	6.83	6 (31%)	21,32,35	2.51	5 (23%)
3	E6G	5	4355	3	24,27,28	2.06	4 (16%)	34,39,42	3.02	16 (47%)
6	A2M	9	1678	6	22,25,26	3.17	9 (40%)	30,36,39	2.97	10 (33%)
6	OMU	9	121	6	19,22,23	3.05	8 (42%)	25,31,34	1.84	4 (16%)
6	4AC	9	1842	6	21,24,25	3.17	10 (47%)	28,34,37	1.05	4 (14%)
3	I4U	5	4194	3	20,24,25	3.40	8 (40%)	27,34,37	2.16	2 (7%)
3	OMG	5	1883	3	23,26,27	2.35	9 (39%)	32,38,41	1.93	8 (25%)
6	OMC	9	1710	6	19,22,23	3.02	8 (42%)	25,31,34	0.76	0
6	PSU	9	1081	6	18,21,22	1.04	1 (5%)	21,30,33	1.82	5 (23%)
3	OMC	5	3909	3	19,22,23	3.00	8 (42%)	25,31,34	0.96	1 (4%)
6	OMC	9	517	6	19,22,23	3.02	8 (42%)	25,31,34	0.77	0
3	PSU	5	4636	3	18,21,22	1.12	1 (5%)	21,30,33	2.03	6 (28%)
6	A2M	9	159	6	22,25,26	3.23	10 (45%)	30,36,39	2.97	11 (36%)
6	UR3	9	1830	6	19,22,23	2.92	7 (36%)	26,32,35	1.72	4 (15%)
3	OMC	5	3869	3	19,22,23	3.01	8 (42%)	25,31,34	0.75	0
3	OMG	5	4870	3	23,26,27	2.37	9 (39%)	32,38,41	1.86	8 (25%)
3	OMG	5	2773	3	23,26,27	2.37	9 (39%)	32,38,41	1.86	8 (25%)
3	A2M	5	398	3	22,25,26	3.23	9 (40%)	30,36,39	2.91	10 (33%)
3	B9B	5	2754	3,80	25,28,29	1.79	6 (24%)	35,40,43	5.49	13 (37%)
3	OMC	5	3701	3,80	19,22,23	2.99	8 (42%)	25,31,34	0.72	0
3	BGH	5	3899	3,80	25,29,30	4.50	18 (72%)	30,43,46	2.48	13 (43%)
3	A2M	5	1326	3	22,25,26	3.21	10 (45%)	30,36,39	2.90	10 (33%)
3	PSU	5	2508	3	18,21,22	1.07	1 (5%)	21,30,33	1.89	5 (23%)
3	UR3	5	4597	3	19,22,23	2.90	6 (31%)	26,32,35	1.53	3 (11%)
3	OMG	5	2050	3	23,26,27	2.35	9 (39%)	32,38,41	1.86	8 (25%)
3	B8H	5	4296	3	19,22,23	6.85	6 (31%)	21,32,35	2.51	5 (23%)
3	I4U	5	1659	3	20,24,25	3.43	8 (40%)	27,34,37	2.00	2 (7%)
3	B8K	5	4690	3	24,28,29	3.27	11 (45%)	29,42,45	2.45	11 (37%)
3	5MC	5	4447	3	19,22,23	3.76	8 (42%)	26,32,35	1.08	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PSU	9	1243	6	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
3	A2M	5	3718	3	22,25,26	3.24	10 (45%)	30,36,39	2.86	11 (36%)
3	A2M	5	3723	3	22,25,26	3.21	10 (45%)	30,36,39	2.91	10 (33%)
3	OMG	5	1316	3	23,26,27	2.33	9 (39%)	32,38,41	1.88	8 (25%)
3	A2M	5	1534	3,80	22,25,26	3.23	10 (45%)	30,36,39	2.96	11 (36%)
3	5MC	5	3782	3	19,22,23	3.79	8 (42%)	26,32,35	1.04	2 (7%)
3	UR3	5	1866	3	19,22,23	2.86	6 (31%)	26,32,35	1.57	3 (11%)
3	5MU	5	4083	3	19,22,23	4.97	7 (36%)	27,32,35	3.61	10 (37%)
3	PSU	5	3715	3	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
3	OMC	5	2861	3	19,22,23	3.00	8 (42%)	25,31,34	0.75	0
6	A2M	9	668	6,80	22,25,26	3.25	10 (45%)	30,36,39	2.99	11 (36%)
3	MHG	5	4371	3	29,32,33	3.55	11 (37%)	34,46,49	2.45	11 (32%)
3	E7G	5	1797	3	24,27,28	3.60	11 (45%)	28,40,43	2.33	9 (32%)
6	OMG	9	509	6,80	23,26,27	2.34	8 (34%)	32,38,41	1.88	8 (25%)
6	5MC	9	1374	6	19,22,23	3.80	8 (42%)	26,32,35	1.02	2 (7%)
3	7MG	5	4550	3	23,26,27	3.46	10 (43%)	27,39,42	2.11	9 (33%)
6	OMC	9	1703	6	19,22,23	3.01	8 (42%)	25,31,34	0.75	0
6	A2M	9	166	6	22,25,26	3.24	10 (45%)	30,36,39	2.93	13 (43%)
3	A2M	5	3785	3	22,25,26	3.23	10 (45%)	30,36,39	3.06	14 (46%)
3	B9B	5	237	3	25,28,29	1.80	6 (24%)	35,40,43	5.23	12 (34%)
3	B8T	5	4483	3	19,22,23	3.60	8 (42%)	25,31,34	0.91	1 (4%)
5	OMU	8	14	5,3	19,22,23	3.07	8 (42%)	25,31,34	1.81	5 (20%)
3	PSU	5	3764	3	18,21,22	1.12	1 (5%)	21,30,33	1.84	4 (19%)
3	A2M	5	4523	3,80	22,25,26	3.22	10 (45%)	30,36,39	2.97	11 (36%)
3	B8H	5	1860	3	19,22,23	6.84	6 (31%)	21,32,35	2.48	5 (23%)
3	OMG	5	1625	3,80	23,26,27	2.37	8 (34%)	32,38,41	1.94	9 (28%)

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
6	MA6	9	1851	6	-	2/11/29/30	0/3/3/3
3	B9B	5	1574	3,80	-	3/11/29/30	0/3/3/3
3	7MG	5	2522	3	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	5	4620	3	-	0/9/27/28	0/2/2/2
3	PSU	5	3729	3	-	2/7/25/26	0/2/2/2
3	PSU	5	4403	3	-	3/7/25/26	0/2/2/2
2	4AC	1	45	2	-	0/11/29/30	0/2/2/2
3	1MA	5	4415	3	-	1/7/25/26	0/3/3/3
3	A2M	5	2363	3,80	-	1/9/27/28	0/3/3/3
3	OMC	5	2422	3,80	-	1/9/27/28	0/2/2/2
6	OMC	9	174	6	-	1/9/27/28	0/2/2/2
6	OMG	9	644	6	-	2/9/27/28	0/3/3/3
3	7MG	5	1605	3	-	0/7/37/38	0/3/3/3
3	A2M	5	3825	3	-	0/9/27/28	0/3/3/3
6	A2M	9	27	6,80	-	1/9/27/28	0/3/3/3
3	OMU	5	4306	3	-	1/9/27/28	0/2/2/2
3	OMG	5	4494	3	-	1/9/27/28	0/3/3/3
3	OMG	5	4370	3	-	1/9/27/28	0/3/3/3
3	OMG	5	4637	3	-	2/9/27/28	0/3/3/3
3	A2M	5	4571	3	-	0/9/27/28	0/3/3/3
3	OMG	5	2424	3	-	2/9/27/28	0/3/3/3
6	OMG	9	683	6	-	2/9/27/28	0/3/3/3
3	B8K	5	3897	3	-	3/11/41/42	0/3/3/3
6	M7A	9	1806	6	-	0/7/37/38	0/3/3/3
6	B8Q	9	1219	6,80	-	2/7/42/43	0/2/2/2
3	B8W	5	2380	3	-	4/9/27/28	0/3/3/3
3	PSU	5	4628	3	-	0/7/25/26	0/2/2/2
3	B8W	5	4129	3	-	2/9/27/28	0/3/3/3
3	A2M	5	1524	3	-	2/9/27/28	0/3/3/3
3	UR3	5	4530	3	-	2/7/25/26	0/2/2/2
6	OMU	9	116	6	-	3/9/27/28	0/2/2/2
3	B8W	5	4529	3,80	-	2/9/27/28	0/3/3/3
6	PSU	9	119	6	-	0/7/25/26	0/2/2/2
6	MMX	9	568	6	-	4/9/44/45	0/2/2/2
3	2MG	5	4872	3	-	1/9/27/28	0/3/3/3
3	PSU	5	1683	3	-	0/7/25/26	0/2/2/2
3	OMC	5	4536	3	-	0/9/27/28	0/2/2/2
3	OMG	5	3792	3	-	2/9/27/28	0/3/3/3
3	2MG	5	1517	3	-	0/9/27/28	0/3/3/3
3	PSU	5	4450	3,80	-	1/7/25/26	0/2/2/2
3	P7G	5	3880	3	-	4/10/40/41	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	6MZ	9	1832	6,80	-	2/9/27/28	0/3/3/3
9	MLZ	C	333	9	-	1/7/8/10	-
3	PSU	5	1582	3	-	1/7/25/26	0/2/2/2
3	OMC	5	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	5	4531	3	-	2/7/25/26	0/2/2/2
6	PSU	9	612	6	-	0/7/25/26	0/2/2/2
6	A2M	9	484	6	-	0/9/27/28	0/3/3/3
3	M7A	5	4564	3	-	0/7/37/38	0/3/3/3
3	B8W	5	4185	3	-	2/9/27/28	0/3/3/3
6	PSU	9	823	6	-	0/7/25/26	0/2/2/2
3	OMG	5	4623	3	-	0/9/27/28	0/3/3/3
6	PSU	9	822	6	-	0/7/25/26	0/2/2/2
3	E7G	5	2297	3	-	1/9/39/40	0/3/3/3
6	A2M	9	1031	6	-	1/9/27/28	0/3/3/3
3	PSU	5	4500	3	-	3/7/25/26	0/2/2/2
6	B8N	9	1248	6	-	1/16/34/35	0/2/2/2
3	PSU	5	1677	3	-	3/7/25/26	0/2/2/2
3	OMG	5	373	3	-	1/9/27/28	0/3/3/3
6	MA6	9	1850	6	-	0/11/29/30	0/3/3/3
3	PSU	5	4293	3	-	0/7/25/26	0/2/2/2
6	4AC	9	1337	6	-	1/11/29/30	0/2/2/2
3	OMG	5	4196	3	-	1/9/27/28	0/3/3/3
3	OMG	5	1522	3	-	0/9/27/28	0/3/3/3
3	B8T	5	4671	3	-	1/7/27/28	0/2/2/2
3	1MA	5	1322	3,80	-	0/7/25/26	0/3/3/3
3	B8W	5	4472	3	-	2/9/27/28	0/3/3/3
3	P4U	5	1348	3	-	4/10/29/30	0/2/2/2
3	A2M	5	1871	3,80	-	0/9/27/28	0/3/3/3
3	2MG	5	729	3	-	0/9/27/28	0/3/3/3
3	B8Q	5	1456	3	-	0/7/42/43	0/2/2/2
3	A2M	5	3867	3	-	3/9/27/28	0/3/3/3
3	P7G	5	1909	3	-	2/10/40/41	0/3/3/3
44	MLZ	m	72	44	-	4/7/8/10	-
3	OMG	5	2364	3	-	2/9/27/28	0/3/3/3
3	OMC	5	3887	3	-	1/9/27/28	0/2/2/2
3	6MZ	5	4220	3	-	1/9/27/28	0/3/3/3
3	OMC	5	2365	3	-	0/9/27/28	0/2/2/2
3	B9H	5	2786	3	-	2/12/47/48	0/2/2/2
3	PSU	5	4442	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5MU	9	814	6	-	1/7/25/26	0/2/2/2
3	5MC	5	4335	3	-	0/7/25/26	0/2/2/2
1	T6A	2	37	1	-	2/23/41/42	0/3/3/3
3	A2M	5	2401	3,80	-	0/9/27/28	0/3/3/3
3	B8H	5	3762	3	-	2/7/25/26	0/2/2/2
3	E6G	5	4355	3	-	4/10/28/29	0/3/3/3
6	A2M	9	1678	6	-	2/9/27/28	0/3/3/3
6	OMU	9	121	6	-	1/9/27/28	0/2/2/2
6	4AC	9	1842	6	-	0/11/29/30	0/2/2/2
3	I4U	5	4194	3	-	1/9/29/30	0/2/2/2
3	OMG	5	1883	3	-	1/9/27/28	0/3/3/3
6	OMC	9	1710	6	-	0/9/27/28	0/2/2/2
6	PSU	9	1081	6	-	1/7/25/26	0/2/2/2
3	OMC	5	3909	3	-	2/9/27/28	0/2/2/2
6	OMC	9	517	6	-	1/9/27/28	0/2/2/2
3	PSU	5	4636	3	-	4/7/25/26	0/2/2/2
6	A2M	9	159	6	-	2/9/27/28	0/3/3/3
6	UR3	9	1830	6	-	2/7/25/26	0/2/2/2
3	OMC	5	3869	3	-	0/9/27/28	0/2/2/2
3	OMG	5	4870	3	-	3/9/27/28	0/3/3/3
3	OMG	5	2773	3	-	0/9/27/28	0/3/3/3
3	A2M	5	398	3	-	2/9/27/28	0/3/3/3
3	B9B	5	2754	3,80	-	4/11/29/30	0/3/3/3
3	OMC	5	3701	3,80	-	4/9/27/28	0/2/2/2
3	BGH	5	3899	3,80	-	0/13/43/44	0/3/3/3
3	A2M	5	1326	3	-	2/9/27/28	0/3/3/3
3	PSU	5	2508	3	-	0/7/25/26	0/2/2/2
3	UR3	5	4597	3	-	0/7/25/26	0/2/2/2
3	OMG	5	2050	3	-	0/9/27/28	0/3/3/3
3	B8H	5	4296	3	-	2/7/25/26	0/2/2/2
3	I4U	5	1659	3	-	0/9/29/30	0/2/2/2
3	B8K	5	4690	3	-	0/11/41/42	0/3/3/3
3	5MC	5	4447	3	-	0/7/25/26	0/2/2/2
6	PSU	9	1243	6	-	2/7/25/26	0/2/2/2
3	A2M	5	3718	3	-	1/9/27/28	0/3/3/3
3	A2M	5	3723	3	-	1/9/27/28	0/3/3/3
3	OMG	5	1316	3	-	1/9/27/28	0/3/3/3
3	A2M	5	1534	3,80	-	1/9/27/28	0/3/3/3
3	5MC	5	3782	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UR3	5	1866	3	-	0/7/25/26	0/2/2/2
3	5MU	5	4083	3	-	0/7/25/26	0/2/2/2
3	PSU	5	3715	3	-	0/7/25/26	0/2/2/2
3	OMC	5	2861	3	-	1/9/27/28	0/2/2/2
6	A2M	9	668	6,80	-	3/9/27/28	0/3/3/3
3	MHG	5	4371	3	-	6/16/46/47	0/3/3/3
3	E7G	5	1797	3	-	2/9/39/40	0/3/3/3
6	OMG	9	509	6,80	-	0/9/27/28	0/3/3/3
6	5MC	9	1374	6	-	0/7/25/26	0/2/2/2
3	7MG	5	4550	3	-	0/7/37/38	0/3/3/3
6	OMC	9	1703	6	-	2/9/27/28	0/2/2/2
6	A2M	9	166	6	-	2/9/27/28	0/3/3/3
3	A2M	5	3785	3	-	4/9/27/28	0/3/3/3
3	B9B	5	237	3	-	5/11/29/30	0/3/3/3
3	B8T	5	4483	3	-	0/7/27/28	0/2/2/2
5	OMU	8	14	5,3	-	1/9/27/28	0/2/2/2
3	PSU	5	3764	3	-	2/7/25/26	0/2/2/2
3	A2M	5	4523	3,80	-	0/9/27/28	0/3/3/3
3	B8H	5	1860	3	-	2/7/25/26	0/2/2/2
3	OMG	5	1625	3,80	-	1/9/27/28	0/3/3/3

All (956) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	4296	B8H	C6-C5	-16.57	1.11	1.35
3	5	1860	B8H	C6-C5	-16.55	1.11	1.35
3	5	3762	B8H	C6-C5	-16.37	1.11	1.35
3	5	4296	B8H	C4-N3	-15.63	1.09	1.38
3	5	1860	B8H	C4-N3	-15.60	1.09	1.38
3	5	3762	B8H	C4-N3	-15.55	1.09	1.38
3	5	3762	B8H	C4-C5	13.62	1.82	1.44
3	5	4296	B8H	C4-C5	13.54	1.81	1.44
3	5	1860	B8H	C4-C5	13.49	1.81	1.44
3	5	3762	B8H	C6-N1	12.64	1.67	1.36
3	5	4296	B8H	C6-N1	12.57	1.66	1.36
3	5	1860	B8H	C6-N1	12.55	1.66	1.36
3	5	3899	BGH	C3'-C2'	-12.21	1.26	1.53
6	9	814	5MU	C2-N1	11.87	1.57	1.38
3	5	4083	5MU	C2-N1	11.50	1.56	1.38
3	5	4083	5MU	C6-N1	10.93	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	814	5MU	C6-N1	10.78	1.56	1.38
3	5	1659	I4U	C4-N3	10.36	1.44	1.31
3	5	1348	P4U	C4-N3	10.32	1.44	1.31
6	9	568	MMX	C4-N3	10.26	1.54	1.45
3	5	4194	I4U	C4-N3	10.23	1.44	1.31
3	5	4083	5MU	C4-C5	10.07	1.61	1.44
3	5	4220	6MZ	C6-N6	9.92	1.45	1.34
6	9	1832	6MZ	C6-N6	9.74	1.45	1.34
6	9	814	5MU	C4-C5	9.73	1.60	1.44
3	5	4529	B8W	O6-C6	9.62	1.49	1.35
3	5	4415	1MA	C2-N3	9.59	1.48	1.30
3	5	4129	B8W	O6-C6	9.58	1.49	1.35
6	9	568	MMX	C2-N1	9.38	1.49	1.37
3	5	1322	1MA	C2-N3	9.29	1.47	1.30
3	5	4447	5MC	C6-C5	9.27	1.49	1.34
3	5	4472	B8W	O6-C6	9.26	1.49	1.35
3	5	1456	B8Q	C6-C5	9.19	1.52	1.33
3	5	4335	5MC	C6-C5	9.18	1.49	1.34
3	5	1524	A2M	C3'-C4'	-9.15	1.29	1.53
6	9	1374	5MC	C6-C5	9.09	1.49	1.34
3	5	4185	B8W	O6-C6	9.04	1.48	1.35
3	5	3782	5MC	C6-C5	9.02	1.49	1.34
6	9	1219	B8Q	C6-C5	9.01	1.52	1.33
6	9	668	A2M	C3'-C4'	-8.99	1.30	1.53
6	9	159	A2M	C3'-C4'	-8.96	1.30	1.53
6	9	166	A2M	C3'-C4'	-8.96	1.30	1.53
3	5	1871	A2M	C3'-C4'	-8.95	1.30	1.53
3	5	3867	A2M	C3'-C4'	-8.94	1.30	1.53
3	5	4523	A2M	C3'-C4'	-8.93	1.30	1.53
3	5	4571	A2M	C3'-C4'	-8.93	1.30	1.53
3	5	398	A2M	C3'-C4'	-8.93	1.30	1.53
3	5	2786	B9H	C2-N3	8.92	1.48	1.37
3	5	3825	A2M	C3'-C4'	-8.91	1.30	1.53
3	5	2363	A2M	C3'-C4'	-8.91	1.30	1.53
3	5	2401	A2M	C3'-C4'	-8.91	1.30	1.53
6	9	27	A2M	C3'-C4'	-8.87	1.30	1.53
3	5	2380	B8W	O6-C6	8.86	1.48	1.35
3	5	1326	A2M	C3'-C4'	-8.86	1.30	1.53
3	5	3723	A2M	C3'-C4'	-8.85	1.30	1.53
3	5	3718	A2M	C3'-C4'	-8.83	1.30	1.53
6	9	1678	A2M	C3'-C4'	-8.82	1.30	1.53
6	9	1031	A2M	C3'-C4'	-8.78	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	1534	A2M	C3'-C4'	-8.75	1.30	1.53
6	9	484	A2M	C3'-C4'	-8.74	1.30	1.53
3	5	4690	B8K	C8-N9	8.66	1.51	1.45
3	5	4371	MHG	C8-N9	8.64	1.51	1.45
3	5	3785	A2M	C3'-C4'	-8.46	1.31	1.53
3	5	2297	E7G	C8-N9	8.46	1.51	1.45
6	9	568	MMX	C2-N3	8.40	1.48	1.37
3	5	1909	P7G	C8-N9	8.31	1.51	1.45
3	5	1797	E7G	C8-N9	8.20	1.51	1.45
3	5	4550	7MG	C8-N9	8.15	1.51	1.45
3	5	3897	B8K	C8-N9	8.08	1.51	1.45
3	5	4129	B8W	C2-N2	8.04	1.49	1.33
6	9	1248	B8N	C4-N3	-8.04	1.26	1.40
3	5	4371	MHG	C2-N3	8.04	1.47	1.32
3	5	2522	7MG	C8-N9	8.03	1.51	1.45
3	5	4472	B8W	C2-N2	8.02	1.49	1.33
3	5	2380	B8W	C2-N2	8.00	1.49	1.33
3	5	4529	B8W	C2-N2	7.99	1.49	1.33
6	9	1248	B8N	C6-N1	7.99	1.55	1.36
3	5	4185	B8W	C2-N2	7.95	1.49	1.33
3	5	1605	7MG	C8-N9	7.94	1.51	1.45
3	5	1909	P7G	C5-N7	7.90	1.45	1.35
3	5	3785	A2M	O4'-C4'	7.86	1.62	1.45
3	5	3880	P7G	C8-N9	7.82	1.50	1.45
3	5	3718	A2M	O4'-C4'	7.80	1.62	1.45
3	5	398	A2M	O4'-C4'	7.80	1.62	1.45
6	9	166	A2M	O4'-C4'	7.76	1.62	1.45
3	5	729	2MG	C2-N3	7.73	1.46	1.32
6	9	159	A2M	O4'-C4'	7.73	1.62	1.45
3	5	2401	A2M	O4'-C4'	7.70	1.62	1.45
6	9	1031	A2M	O4'-C4'	7.69	1.62	1.45
3	5	1534	A2M	O4'-C4'	7.68	1.62	1.45
3	5	1797	E7G	C5-N7	7.67	1.45	1.35
3	5	2786	B9H	C6-C5	7.67	1.49	1.33
3	5	3825	A2M	O4'-C4'	7.64	1.62	1.45
3	5	3723	A2M	O4'-C4'	7.61	1.61	1.45
6	9	1248	B8N	C4-C5	7.60	1.64	1.47
3	5	1871	A2M	O4'-C4'	7.59	1.61	1.45
3	5	4523	A2M	O4'-C4'	7.57	1.61	1.45
3	5	4571	A2M	O4'-C4'	7.56	1.61	1.45
6	9	484	A2M	O4'-C4'	7.55	1.61	1.45
3	5	1326	A2M	O4'-C4'	7.52	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	2297	E7G	C5-N7	7.50	1.45	1.35
6	9	27	A2M	O4'-C4'	7.48	1.61	1.45
3	5	3880	P7G	C5-N7	7.47	1.45	1.35
3	5	2363	A2M	O4'-C4'	7.47	1.61	1.45
6	9	814	5MU	C4-N3	-7.44	1.24	1.38
3	5	4083	5MU	C4-N3	-7.43	1.24	1.38
2	1	45	4AC	C4-N3	7.40	1.45	1.32
3	5	3867	A2M	O4'-C4'	7.39	1.61	1.45
3	5	4671	B8T	C2-N3	7.38	1.51	1.36
6	9	1678	A2M	O4'-C4'	7.37	1.61	1.45
3	5	1524	A2M	O4'-C4'	7.35	1.61	1.45
3	5	4483	B8T	C2-N3	7.35	1.50	1.36
6	9	668	A2M	O4'-C4'	7.34	1.61	1.45
6	9	1830	UR3	C2-N1	7.32	1.48	1.38
5	8	14	OMU	C2-N1	7.31	1.49	1.38
3	5	4671	B8T	C4-N3	7.29	1.45	1.32
3	5	1517	2MG	C2-N3	7.27	1.45	1.32
3	5	4483	B8T	C4-N3	7.22	1.44	1.32
6	9	121	OMU	C2-N1	7.22	1.49	1.38
6	9	116	OMU	C2-N1	7.19	1.49	1.38
3	5	4371	MHG	C5-N7	7.14	1.44	1.35
3	5	4620	OMU	C2-N1	7.13	1.49	1.38
3	5	4597	UR3	C2-N1	7.12	1.48	1.38
6	9	1842	4AC	C4-N3	7.11	1.44	1.32
3	5	4872	2MG	C2-N3	7.11	1.45	1.32
6	9	1337	4AC	C4-N3	7.10	1.44	1.32
3	5	4415	1MA	C4-N3	7.06	1.50	1.35
3	5	4306	OMU	C2-N1	7.06	1.49	1.38
3	5	1866	UR3	C2-N1	6.97	1.48	1.38
6	9	116	OMU	C2-N3	6.96	1.50	1.38
3	5	1605	7MG	C5-N7	6.93	1.44	1.35
3	5	4483	B8T	C6-C5	6.90	1.51	1.35
3	5	4335	5MC	C5-C4	6.88	1.49	1.44
3	5	4550	7MG	C5-N7	6.86	1.44	1.35
5	8	14	OMU	C2-N3	6.85	1.49	1.38
3	5	1322	1MA	C4-N3	6.84	1.49	1.35
3	5	729	2MG	C4-N3	6.83	1.49	1.34
3	5	4530	UR3	C2-N1	6.83	1.48	1.38
3	5	4671	B8T	C6-C5	6.83	1.50	1.35
3	5	3782	5MC	C4-N3	6.82	1.45	1.34
3	5	2522	7MG	C5-N7	6.79	1.44	1.35
6	9	121	OMU	C2-N3	6.76	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	4620	OMU	C2-N3	6.76	1.49	1.38
3	5	4335	5MC	C4-N3	6.76	1.45	1.34
3	5	4597	UR3	C6-C5	6.74	1.50	1.35
3	5	4530	UR3	C6-C5	6.73	1.50	1.35
6	9	1830	UR3	C6-C5	6.72	1.50	1.35
3	5	1866	UR3	C6-C5	6.71	1.50	1.35
6	9	1374	5MC	C4-N3	6.68	1.44	1.34
3	5	4690	B8K	C2-N3	6.66	1.49	1.33
3	5	4306	OMU	C2-N3	6.65	1.49	1.38
3	5	3899	BGH	C8-N9	6.63	1.50	1.45
3	5	3897	B8K	C2-N3	6.60	1.49	1.33
3	5	4083	5MU	C6-C5	6.58	1.45	1.34
6	9	1374	5MC	C5-C4	6.56	1.49	1.44
6	9	814	5MU	C6-C5	6.54	1.45	1.34
3	5	1517	2MG	C4-N3	6.54	1.49	1.34
3	5	3880	P7G	C4-N3	6.53	1.48	1.37
3	5	3869	OMC	C2-N3	6.51	1.49	1.36
3	5	2786	B9H	C2-N1	6.51	1.47	1.38
3	5	3782	5MC	C5-C4	6.49	1.49	1.44
3	5	2422	OMC	C2-N3	6.48	1.49	1.36
6	9	1710	OMC	C2-N3	6.47	1.49	1.36
6	9	174	OMC	C2-N3	6.46	1.49	1.36
3	5	4637	OMG	C4-N3	6.44	1.49	1.34
6	9	1703	OMC	C2-N3	6.43	1.49	1.36
3	5	2861	OMC	C2-N3	6.43	1.49	1.36
3	5	1625	OMG	C4-N3	6.43	1.49	1.34
3	5	4447	5MC	C4-N3	6.42	1.44	1.34
6	9	517	OMC	C2-N3	6.41	1.49	1.36
3	5	3792	OMG	C4-N3	6.40	1.48	1.34
3	5	3701	OMC	C2-N3	6.40	1.49	1.36
3	5	1909	P7G	C4-N3	6.40	1.48	1.37
3	5	3887	OMC	C2-N3	6.39	1.49	1.36
3	5	2424	OMG	C4-N3	6.39	1.48	1.34
3	5	4870	OMG	C4-N3	6.39	1.48	1.34
3	5	4370	OMG	C4-N3	6.39	1.48	1.34
6	9	1219	B8Q	C2-N3	6.39	1.47	1.35
3	5	2773	OMG	C4-N3	6.38	1.48	1.34
6	9	509	OMG	C4-N3	6.37	1.48	1.34
3	5	4196	OMG	C4-N3	6.37	1.48	1.34
3	5	3909	OMC	C2-N3	6.37	1.49	1.36
6	9	683	OMG	C4-N3	6.37	1.48	1.34
3	5	4494	OMG	C4-N3	6.37	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	4194	I4U	C6-C5	6.36	1.49	1.35
6	9	644	OMG	C4-N3	6.36	1.48	1.34
3	5	2365	OMC	C2-N3	6.36	1.49	1.36
3	5	1883	OMG	C4-N3	6.35	1.48	1.34
2	1	45	4AC	C6-C5	6.34	1.49	1.35
3	5	2804	OMC	C2-N3	6.34	1.48	1.36
2	1	45	4AC	C2-N3	6.33	1.48	1.36
3	5	4623	OMG	C4-N3	6.32	1.48	1.34
6	9	1337	4AC	C6-C5	6.32	1.49	1.35
3	5	2050	OMG	C4-N3	6.32	1.48	1.34
3	5	4536	OMC	C2-N3	6.31	1.48	1.36
3	5	373	OMG	C4-N3	6.31	1.48	1.34
3	5	1522	OMG	C4-N3	6.29	1.48	1.34
3	5	1659	I4U	C6-C5	6.28	1.49	1.35
3	5	4371	MHG	C2-N1	6.27	1.46	1.36
3	5	2364	OMG	C4-N3	6.26	1.48	1.34
3	5	1316	OMG	C4-N3	6.24	1.48	1.34
6	9	1842	4AC	C6-C5	6.24	1.49	1.35
3	5	4671	B8T	C4-N4	6.21	1.48	1.36
3	5	4447	5MC	C5-C4	6.20	1.48	1.44
3	5	4483	B8T	C4-N4	6.18	1.48	1.36
3	5	3782	5MC	C2-N3	6.14	1.48	1.36
3	5	1348	P4U	C6-C5	6.13	1.49	1.35
3	5	4335	5MC	C2-N3	6.13	1.48	1.36
3	5	4872	2MG	C4-N3	6.12	1.48	1.34
6	9	1374	5MC	C2-N3	6.11	1.48	1.36
3	5	1348	P4U	C2-N3	6.10	1.48	1.36
6	9	1337	4AC	C2-N3	6.08	1.48	1.36
6	9	1842	4AC	C2-N3	6.08	1.48	1.36
3	5	3701	OMC	C6-C5	6.07	1.49	1.35
3	5	2422	OMC	C6-C5	6.06	1.49	1.35
3	5	1659	I4U	C2-N3	6.03	1.48	1.36
3	5	4355	E6G	C2-N2	6.03	1.45	1.33
3	5	2365	OMC	C6-C5	6.02	1.49	1.35
6	9	517	OMC	C6-C5	6.02	1.49	1.35
3	5	3880	P7G	C2-N2	6.01	1.48	1.34
3	5	4536	OMC	C6-C5	6.01	1.49	1.35
3	5	1909	P7G	C2-N2	6.01	1.48	1.34
3	5	3909	OMC	C6-C5	6.00	1.49	1.35
6	9	1703	OMC	C6-C5	6.00	1.49	1.35
6	9	174	OMC	C6-C5	6.00	1.49	1.35
6	9	1710	OMC	C6-C5	6.00	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	3887	OMC	C6-C5	5.97	1.48	1.35
3	5	2861	OMC	C6-C5	5.96	1.48	1.35
3	5	1797	E7G	C4-N3	5.96	1.47	1.34
3	5	3869	OMC	C6-C5	5.96	1.48	1.35
3	5	4447	5MC	C2-N3	5.93	1.48	1.36
3	5	3880	P7G	C4-N9	5.93	1.44	1.35
3	5	4355	E6G	O6-C6	5.93	1.43	1.34
3	5	2804	OMC	C6-C5	5.90	1.48	1.35
6	9	1248	B8N	C2-N1	5.89	1.56	1.39
3	5	1909	P7G	C4-N9	5.87	1.44	1.35
3	5	1456	B8Q	C2-N3	5.85	1.46	1.35
3	5	4371	MHG	C2-N2	5.84	1.45	1.33
3	5	4194	I4U	C2-N3	5.84	1.47	1.36
3	5	1797	E7G	C2-N3	5.84	1.47	1.33
3	5	2297	E7G	C4-N3	5.83	1.47	1.34
3	5	2522	7MG	C2-N3	5.82	1.47	1.33
3	5	1605	7MG	C2-N3	5.78	1.47	1.33
3	5	1605	7MG	C4-N3	5.76	1.47	1.34
3	5	729	2MG	C2-N2	5.75	1.45	1.33
3	5	4550	7MG	C2-N3	5.72	1.47	1.33
3	5	2297	E7G	C2-N3	5.69	1.47	1.33
3	5	2522	7MG	C4-N3	5.69	1.47	1.34
3	5	2754	B9B	C2-N2	5.69	1.45	1.33
3	5	3899	BGH	C4-N3	5.68	1.47	1.34
3	5	237	B9B	C2-N2	5.67	1.45	1.33
3	5	4550	7MG	C4-N3	5.66	1.47	1.34
3	5	4597	UR3	C2-N3	5.62	1.50	1.39
6	9	683	OMG	C2-N3	5.61	1.46	1.33
6	9	121	OMU	C6-C5	5.61	1.48	1.35
5	8	14	OMU	C6-C5	5.60	1.48	1.35
3	5	4371	MHG	C4-N3	5.60	1.47	1.34
3	5	1517	2MG	C2-N2	5.59	1.45	1.33
3	5	1625	OMG	C2-N3	5.59	1.46	1.33
3	5	4620	OMU	C6-C5	5.59	1.48	1.35
3	5	1574	B9B	C2-N2	5.58	1.45	1.33
6	9	1830	UR3	C2-N3	5.57	1.50	1.39
3	5	4196	OMG	C2-N3	5.55	1.46	1.33
3	5	4872	2MG	C2-N2	5.55	1.45	1.33
3	5	4494	OMG	C2-N3	5.55	1.46	1.33
6	9	116	OMU	C6-C5	5.55	1.47	1.35
3	5	2424	OMG	C2-N3	5.54	1.46	1.33
3	5	4637	OMG	C2-N3	5.53	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	3792	OMG	C2-N3	5.52	1.46	1.33
3	5	2773	OMG	C2-N3	5.52	1.46	1.33
3	5	4306	OMU	C6-C5	5.51	1.47	1.35
3	5	4870	OMG	C2-N3	5.48	1.46	1.33
6	9	644	OMG	C2-N3	5.47	1.46	1.33
3	5	1866	UR3	C2-N3	5.47	1.49	1.39
6	9	509	OMG	C2-N3	5.46	1.46	1.33
3	5	4370	OMG	C2-N3	5.44	1.46	1.33
3	5	4623	OMG	C2-N3	5.44	1.46	1.33
3	5	373	OMG	C2-N3	5.43	1.46	1.33
3	5	2050	OMG	C2-N3	5.43	1.46	1.33
3	5	4530	UR3	C2-N3	5.42	1.49	1.39
3	5	1797	E7G	C4-N9	5.41	1.44	1.37
3	5	3899	BGH	O4'-C1'	-5.39	1.29	1.42
3	5	1316	OMG	C2-N3	5.38	1.46	1.33
3	5	1883	OMG	C2-N3	5.37	1.46	1.33
3	5	2364	OMG	C2-N3	5.33	1.46	1.33
3	5	1909	P7G	C2-N1	5.30	1.46	1.33
3	5	3880	P7G	C2-N1	5.26	1.45	1.33
3	5	1522	OMG	C2-N3	5.26	1.45	1.33
6	9	1248	B8N	C6-C5	5.23	1.42	1.35
3	5	3899	BGH	C2-N3	5.23	1.45	1.33
3	5	1797	E7G	C2-N2	5.23	1.46	1.34
3	5	3869	OMC	C4-N3	5.20	1.44	1.34
3	5	2297	E7G	C2-N2	5.19	1.46	1.34
3	5	2861	OMC	C4-N3	5.18	1.44	1.34
6	9	1703	OMC	C4-N3	5.17	1.44	1.34
6	9	1710	OMC	C4-N3	5.16	1.44	1.34
3	5	3899	BGH	C2'-C1'	5.16	1.65	1.53
6	9	174	OMC	C4-N3	5.15	1.44	1.34
3	5	4690	B8K	C4-N9	5.15	1.44	1.37
3	5	3899	BGH	C4-N9	5.14	1.44	1.37
3	5	1605	7MG	C4-N9	5.13	1.44	1.37
3	5	3887	OMC	C4-N3	5.12	1.44	1.34
3	5	2422	OMC	C4-N3	5.12	1.44	1.34
6	9	517	OMC	C4-N3	5.11	1.44	1.34
3	5	3701	OMC	C4-N3	5.11	1.44	1.34
1	2	37	T6A	C10-N6	5.09	1.48	1.37
3	5	2297	E7G	C4-N9	5.08	1.44	1.37
6	9	668	A2M	O4'-C1'	-5.07	1.30	1.42
3	5	2804	OMC	C4-N3	5.06	1.44	1.34
3	5	4536	OMC	C4-N3	5.06	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	3785	A2M	O4'-C1'	-5.06	1.30	1.42
3	5	2365	OMC	C4-N3	5.03	1.44	1.34
3	5	2522	7MG	C4-N9	5.02	1.44	1.37
1	2	37	T6A	C10-N11	4.99	1.49	1.35
3	5	3899	BGH	O4'-C4'	4.98	1.56	1.45
3	5	4371	MHG	C4-N9	4.96	1.43	1.37
3	5	3909	OMC	C4-N3	4.95	1.44	1.34
3	5	1605	7MG	C2-N2	4.89	1.45	1.34
3	5	2522	7MG	C2-N2	4.88	1.45	1.34
3	5	3899	BGH	C2-N2	4.88	1.45	1.34
3	5	1534	A2M	O4'-C1'	-4.88	1.30	1.42
3	5	4550	7MG	C2-N2	4.88	1.45	1.34
3	5	4415	1MA	C2-N1	4.88	1.45	1.35
6	9	484	A2M	O4'-C1'	-4.87	1.30	1.42
3	5	4872	2MG	C2-N1	4.86	1.44	1.36
3	5	3897	B8K	C4-N9	4.86	1.43	1.37
3	5	3867	A2M	O4'-C1'	-4.84	1.30	1.42
3	5	1326	A2M	O4'-C1'	-4.84	1.30	1.42
3	5	2363	A2M	O4'-C1'	-4.80	1.30	1.42
6	9	27	A2M	O4'-C1'	-4.80	1.30	1.42
3	5	1524	A2M	O4'-C1'	-4.80	1.30	1.42
6	9	1710	OMC	C4-N4	4.77	1.45	1.33
6	9	1703	OMC	C4-N4	4.76	1.45	1.33
3	5	2861	OMC	C4-N4	4.76	1.45	1.33
3	5	3899	BGH	C5'-C4'	-4.76	1.37	1.51
3	5	3887	OMC	C4-N4	4.75	1.45	1.33
6	9	174	OMC	C4-N4	4.75	1.45	1.33
3	5	3869	OMC	C4-N4	4.75	1.45	1.33
3	5	4571	A2M	O4'-C1'	-4.75	1.31	1.42
3	5	2365	OMC	C4-N4	4.75	1.45	1.33
6	9	517	OMC	C4-N4	4.74	1.45	1.33
3	5	3701	OMC	C4-N4	4.73	1.45	1.33
6	9	1219	B8Q	C2-N1	4.73	1.45	1.38
3	5	2422	OMC	C4-N4	4.73	1.45	1.33
3	5	3825	A2M	O4'-C1'	-4.73	1.31	1.42
3	5	3909	OMC	C4-N4	4.72	1.45	1.33
6	9	1678	A2M	O4'-C1'	-4.72	1.31	1.42
3	5	2804	OMC	C4-N4	4.72	1.45	1.33
3	5	4550	7MG	C4-N9	4.72	1.43	1.37
3	5	4536	OMC	C4-N4	4.72	1.45	1.33
3	5	4671	B8T	C2-N1	4.71	1.50	1.40
6	9	1031	A2M	O4'-C1'	-4.71	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	3723	A2M	O4'-C1'	-4.69	1.31	1.42
6	9	517	OMC	C2-N1	4.69	1.49	1.40
3	5	4523	A2M	O4'-C1'	-4.66	1.31	1.42
3	5	3909	OMC	C2-N1	4.66	1.49	1.40
6	9	166	A2M	O4'-C1'	-4.66	1.31	1.42
3	5	1871	A2M	O4'-C1'	-4.66	1.31	1.42
3	5	3718	A2M	O4'-C1'	-4.65	1.31	1.42
3	5	2401	A2M	O4'-C1'	-4.65	1.31	1.42
6	9	1703	OMC	C2-N1	4.65	1.49	1.40
6	9	159	A2M	O4'-C1'	-4.65	1.31	1.42
3	5	4690	B8K	C4-N3	4.63	1.44	1.34
6	9	1710	OMC	C2-N1	4.62	1.49	1.40
3	5	4483	B8T	C2-N1	4.62	1.49	1.40
3	5	1322	1MA	C2-N1	4.62	1.45	1.35
3	5	1517	2MG	C2-N1	4.61	1.44	1.36
3	5	2422	OMC	C2-N1	4.60	1.49	1.40
3	5	398	A2M	O4'-C1'	-4.59	1.31	1.42
3	5	3897	B8K	C4-N3	4.57	1.44	1.34
3	5	3869	OMC	C2-N1	4.56	1.49	1.40
3	5	3762	B8H	C2-N3	4.56	1.45	1.38
3	5	729	2MG	C2-N1	4.52	1.43	1.36
6	9	174	OMC	C2-N1	4.52	1.49	1.40
3	5	4536	OMC	C2-N1	4.51	1.49	1.40
3	5	3887	OMC	C2-N1	4.50	1.49	1.40
3	5	4447	5MC	C6-N1	4.48	1.45	1.38
3	5	4335	5MC	C4-N4	4.46	1.45	1.34
3	5	2861	OMC	C2-N1	4.45	1.49	1.40
3	5	4335	5MC	C6-N1	4.45	1.45	1.38
6	9	1374	5MC	C6-N1	4.44	1.45	1.38
3	5	2804	OMC	C2-N1	4.44	1.49	1.40
6	9	116	OMU	C4-N3	4.44	1.46	1.38
3	5	1524	A2M	C6-N6	4.43	1.45	1.34
6	9	159	A2M	C6-N6	4.42	1.45	1.34
3	5	3723	A2M	C6-N6	4.41	1.45	1.34
3	5	3718	A2M	C6-N6	4.41	1.45	1.34
3	5	4571	A2M	C6-N6	4.41	1.45	1.34
6	9	1678	A2M	C6-N6	4.40	1.45	1.34
6	9	1031	A2M	C6-N6	4.39	1.45	1.34
6	9	166	A2M	C6-N6	4.39	1.45	1.34
3	5	1860	B8H	C2-N3	4.38	1.45	1.38
3	5	3782	5MC	C6-N1	4.38	1.45	1.38
6	9	484	A2M	C6-N6	4.38	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	3782	5MC	C4-N4	4.37	1.45	1.34
3	5	398	A2M	C6-N6	4.37	1.45	1.34
3	5	2401	A2M	C6-N6	4.37	1.45	1.34
3	5	3701	OMC	C2-N1	4.37	1.49	1.40
6	9	1374	5MC	C4-N4	4.36	1.45	1.34
6	9	568	MMX	C5-C4	-4.36	1.48	1.52
3	5	3867	A2M	C6-N6	4.36	1.45	1.34
3	5	4335	5MC	C2-N1	4.36	1.49	1.40
3	5	2365	OMC	C2-N1	4.36	1.49	1.40
3	5	4296	B8H	C2-N3	4.36	1.45	1.38
6	9	1806	M7A	C5-N7	4.36	1.49	1.39
6	9	27	A2M	C6-N6	4.35	1.45	1.34
3	5	4447	5MC	C4-N4	4.34	1.45	1.34
3	5	4523	A2M	C6-N6	4.34	1.45	1.34
3	5	1534	A2M	C6-N6	4.34	1.45	1.34
3	5	1348	P4U	O4-C4	4.34	1.40	1.35
3	5	3825	A2M	C6-N6	4.32	1.45	1.34
3	5	3782	5MC	C2-N1	4.32	1.49	1.40
2	1	45	4AC	C7-N4	4.31	1.45	1.37
6	9	668	A2M	C6-N6	4.31	1.45	1.34
3	5	2363	A2M	C6-N6	4.30	1.45	1.34
3	5	1871	A2M	C6-N6	4.30	1.45	1.34
6	9	1850	MA6	C6-N6	4.26	1.48	1.36
6	9	121	OMU	C4-N3	4.26	1.45	1.38
6	9	1806	M7A	C6-N6	4.26	1.45	1.34
3	5	1326	A2M	C6-N6	4.25	1.45	1.34
3	5	3785	A2M	C6-N6	4.25	1.45	1.34
6	9	1374	5MC	C2-N1	4.25	1.49	1.40
3	5	4306	OMU	C4-N3	4.25	1.45	1.38
5	8	14	OMU	C4-N3	4.24	1.45	1.38
2	1	45	4AC	C2-N1	4.23	1.48	1.40
3	5	1348	P4U	C2-N1	4.23	1.48	1.40
3	5	4620	OMU	C4-N3	4.23	1.45	1.38
6	9	1851	MA6	C6-N6	4.22	1.48	1.36
2	1	45	4AC	C4-N4	4.19	1.46	1.39
3	5	4564	M7A	C5-N7	4.16	1.49	1.39
6	9	1337	4AC	C2-N1	4.13	1.48	1.40
3	5	4447	5MC	C2-N1	4.12	1.48	1.40
3	5	4564	M7A	C6-N6	4.12	1.44	1.34
3	5	2424	OMG	C2-N2	4.11	1.43	1.34
6	9	1337	4AC	C7-N4	4.10	1.45	1.37
3	5	2773	OMG	C2-N2	4.08	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	2050	OMG	C2-N2	4.07	1.43	1.34
3	5	4370	OMG	C2-N2	4.07	1.43	1.34
3	5	3792	OMG	C2-N2	4.07	1.43	1.34
3	5	3897	B8K	C5-C6	4.07	1.53	1.43
3	5	4870	OMG	C2-N2	4.06	1.43	1.34
3	5	4494	OMG	C2-N2	4.06	1.43	1.34
3	5	1625	OMG	C2-N2	4.06	1.43	1.34
3	5	1659	I4U	C2-N1	4.06	1.48	1.40
3	5	4196	OMG	C2-N2	4.06	1.43	1.34
6	9	1842	4AC	C7-N4	4.05	1.45	1.37
6	9	644	OMG	C2-N2	4.05	1.43	1.34
3	5	1456	B8Q	C2-N1	4.04	1.44	1.38
3	5	4690	B8K	C5-C6	4.04	1.53	1.43
3	5	4637	OMG	C2-N2	4.04	1.43	1.34
3	5	1883	OMG	C2-N2	4.03	1.43	1.34
3	5	4623	OMG	C2-N2	4.01	1.43	1.34
3	5	1522	OMG	C2-N2	3.99	1.43	1.34
3	5	2364	OMG	C2-N2	3.98	1.43	1.34
3	5	1316	OMG	C2-N2	3.97	1.43	1.34
6	9	1337	4AC	C4-N4	3.96	1.45	1.39
3	5	373	OMG	C2-N2	3.95	1.43	1.34
6	9	1842	4AC	C2-N1	3.95	1.48	1.40
6	9	1842	4AC	C4-N4	3.94	1.45	1.39
6	9	683	OMG	C2-N2	3.94	1.43	1.34
3	5	3880	P7G	C2-N3	3.94	1.47	1.37
6	9	509	OMG	C2-N2	3.93	1.43	1.34
3	5	4194	I4U	C2-N1	3.93	1.48	1.40
2	1	45	4AC	C5-C4	3.89	1.49	1.41
3	5	1322	1MA	C5-C6	3.88	1.54	1.43
3	5	3899	BGH	C5-C6	3.86	1.53	1.43
3	5	1909	P7G	C2-N3	3.86	1.47	1.37
3	5	4415	1MA	C5-C6	3.85	1.53	1.43
6	9	1248	B8N	C1'-C5	3.82	1.58	1.50
3	5	3899	BGH	C2-N1	3.81	1.46	1.37
6	9	1337	4AC	C5-C4	3.80	1.49	1.41
3	5	1605	7MG	C2-N1	3.78	1.46	1.37
3	5	2297	E7G	C2-N1	3.76	1.46	1.37
3	5	4550	7MG	C2-N1	3.76	1.46	1.37
3	5	2754	B9B	O6-C6	3.76	1.40	1.34
3	5	1797	E7G	C2-N1	3.75	1.46	1.37
3	5	1909	P7G	C6-N1	3.73	1.44	1.38
3	5	2522	7MG	C2-N1	3.73	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	1842	4AC	C5-C4	3.72	1.49	1.41
3	5	3880	P7G	C6-N1	3.67	1.44	1.38
3	5	4671	B8T	C5-C4	3.67	1.49	1.41
3	5	3764	PSU	C6-C5	3.65	1.39	1.35
3	5	237	B9B	O6-C6	3.64	1.40	1.34
3	5	4403	PSU	C6-C5	3.59	1.39	1.35
3	5	4483	B8T	C5-C4	3.59	1.48	1.41
3	5	4690	B8K	C2-N2	3.58	1.42	1.34
3	5	4628	PSU	C6-C5	3.57	1.39	1.35
6	9	1243	PSU	C6-C5	3.56	1.39	1.35
3	5	1574	B9B	O6-C6	3.56	1.40	1.34
3	5	3897	B8K	C6-N1	3.56	1.45	1.38
3	5	3729	PSU	C6-C5	3.56	1.39	1.35
3	5	3897	B8K	C2-N2	3.55	1.42	1.34
3	5	4636	PSU	C6-C5	3.55	1.39	1.35
3	5	3715	PSU	C6-C5	3.55	1.39	1.35
6	9	823	PSU	C6-C5	3.54	1.39	1.35
3	5	4293	PSU	C6-C5	3.54	1.39	1.35
3	5	4531	PSU	C6-C5	3.53	1.39	1.35
3	5	4371	MHG	C5-C6	3.53	1.52	1.43
3	5	4355	E6G	C5-C4	-3.53	1.32	1.39
3	5	3897	B8K	C2-N1	3.51	1.46	1.37
6	9	822	PSU	C6-C5	3.51	1.39	1.35
3	5	4550	7MG	C5-C6	3.51	1.52	1.43
3	5	4690	B8K	C6-N1	3.51	1.45	1.38
3	5	4500	PSU	C6-C5	3.50	1.39	1.35
3	5	1797	E7G	C5-C6	3.49	1.52	1.43
3	5	2522	7MG	C5-C6	3.48	1.52	1.43
3	5	4371	MHG	C8-N7	3.47	1.52	1.45
3	5	4690	B8K	C2-N1	3.46	1.46	1.37
3	5	2508	PSU	C6-C5	3.45	1.39	1.35
3	5	2297	E7G	C5-C6	3.42	1.52	1.43
3	5	1582	PSU	C6-C5	3.42	1.39	1.35
3	5	1683	PSU	C6-C5	3.41	1.39	1.35
3	5	4442	PSU	C6-C5	3.40	1.39	1.35
3	5	4194	I4U	O4-C41	-3.38	1.39	1.47
3	5	4597	UR3	C6-N1	3.38	1.46	1.38
3	5	1605	7MG	C5-C6	3.38	1.52	1.43
6	9	612	PSU	C6-C5	3.38	1.39	1.35
6	9	119	PSU	C6-C5	3.37	1.39	1.35
3	5	3899	BGH	C5-N7	3.37	1.46	1.39
3	5	2297	E7G	C6-N1	3.34	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	1866	UR3	C6-N1	3.34	1.46	1.38
6	9	1031	A2M	C5-C4	-3.34	1.33	1.39
6	9	1830	UR3	C6-N1	3.33	1.46	1.38
3	5	4450	PSU	C6-C5	3.32	1.39	1.35
6	9	1081	PSU	C6-C5	3.32	1.39	1.35
3	5	1677	PSU	C6-C5	3.31	1.39	1.35
3	5	3899	BGH	C71-N7	3.31	1.47	1.39
3	5	3899	BGH	C6-N1	3.30	1.45	1.38
3	5	4690	B8K	C71-N7	3.27	1.46	1.39
6	9	1851	MA6	C9-N6	3.26	1.52	1.45
3	5	1574	B9B	C5-C4	-3.25	1.33	1.39
3	5	4483	B8T	C6-N1	3.25	1.45	1.38
3	5	2297	E7G	C8-N7	3.24	1.51	1.45
3	5	1797	E7G	C6-N1	3.23	1.44	1.38
6	9	1710	OMC	C6-N1	3.22	1.45	1.38
3	5	3785	A2M	C5-C4	-3.22	1.33	1.39
3	5	4194	I4U	C6-N1	3.21	1.45	1.38
3	5	2422	OMC	C6-N1	3.21	1.45	1.38
3	5	3887	OMC	C6-N1	3.21	1.45	1.38
3	5	1659	I4U	O4-C41	-3.20	1.40	1.47
3	5	4530	UR3	C6-N1	3.20	1.45	1.38
3	5	2401	A2M	C5-C4	-3.20	1.33	1.39
6	9	517	OMC	C6-N1	3.19	1.45	1.38
3	5	1659	I4U	C6-N1	3.19	1.45	1.38
3	5	3899	BGH	O3'-C3'	3.18	1.50	1.43
3	5	3869	OMC	C6-N1	3.18	1.45	1.38
6	9	174	OMC	C6-N1	3.18	1.45	1.38
3	5	4536	OMC	C6-N1	3.17	1.45	1.38
3	5	4185	B8W	C5-C4	-3.17	1.33	1.39
3	5	1871	A2M	C5-C4	-3.16	1.33	1.39
6	9	1703	OMC	C6-N1	3.15	1.45	1.38
6	9	484	A2M	C5-C4	-3.15	1.33	1.39
3	5	729	2MG	C5-N7	-3.15	1.32	1.39
3	5	3897	B8K	C71-N7	3.15	1.46	1.39
3	5	4671	B8T	C6-N1	3.15	1.45	1.38
3	5	1909	P7G	C8-N7	3.14	1.51	1.45
6	9	668	A2M	C5-C4	-3.14	1.33	1.39
3	5	4690	B8K	C5-N7	3.14	1.45	1.39
3	5	1797	E7G	C8-N7	3.14	1.51	1.45
2	1	45	4AC	C6-N1	3.14	1.45	1.38
3	5	3897	B8K	C5-N7	3.14	1.45	1.39
6	9	1850	MA6	C9-N6	3.14	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	2804	OMC	C6-N1	3.13	1.45	1.38
3	5	1322	1MA	C5-N7	-3.13	1.32	1.39
3	5	2861	OMC	C6-N1	3.12	1.45	1.38
3	5	3701	OMC	C6-N1	3.12	1.45	1.38
3	5	3909	OMC	C6-N1	3.12	1.45	1.38
3	5	4371	MHG	C6-N1	3.12	1.44	1.38
3	5	4523	A2M	C5-C4	-3.12	1.33	1.39
6	9	27	A2M	C5-C4	-3.12	1.33	1.39
3	5	2365	OMC	C6-N1	3.12	1.45	1.38
3	5	4415	1MA	C5-N7	-3.11	1.32	1.39
3	5	1534	A2M	C5-C4	-3.11	1.33	1.39
6	9	1842	4AC	C6-N1	3.11	1.45	1.38
6	9	1337	4AC	C6-N1	3.10	1.45	1.38
3	5	237	B9B	C5-C4	-3.10	1.33	1.39
3	5	1605	7MG	C6-N1	3.10	1.44	1.38
3	5	2380	B8W	C5-C4	-3.09	1.33	1.39
3	5	1326	A2M	C5-C4	-3.09	1.33	1.39
3	5	1348	P4U	C6-N1	3.09	1.45	1.38
3	5	1517	2MG	C5-N7	-3.09	1.32	1.39
3	5	2522	7MG	C6-N1	3.07	1.44	1.38
3	5	1524	A2M	C5-C4	-3.06	1.33	1.39
3	5	2363	A2M	C5-C4	-3.06	1.33	1.39
3	5	4637	OMG	C5-N7	-3.05	1.32	1.39
3	5	2754	B9B	C5-C4	-3.04	1.33	1.39
3	5	4447	5MC	O2-C2	-3.04	1.18	1.23
6	9	121	OMU	O4-C4	-3.04	1.18	1.24
3	5	4220	6MZ	C5-C4	-3.04	1.33	1.39
3	5	3909	OMC	O2-C2	-3.04	1.18	1.23
3	5	2380	B8W	C5-N7	-3.04	1.33	1.39
3	5	3825	A2M	C5-C4	-3.01	1.33	1.39
3	5	4550	7MG	C6-N1	3.01	1.44	1.38
3	5	4571	A2M	C5-C4	-3.01	1.33	1.39
5	8	14	OMU	O4-C4	-3.01	1.18	1.24
3	5	3785	A2M	O3'-C3'	3.00	1.50	1.43
3	5	3897	B8K	C5-C4	3.00	1.46	1.37
6	9	1851	MA6	C5-C4	-2.99	1.33	1.39
3	5	4690	B8K	C5-C4	2.99	1.46	1.37
3	5	4306	OMU	O4-C4	-2.97	1.18	1.24
3	5	1625	OMG	C5-N7	-2.97	1.33	1.39
6	9	1832	6MZ	C5-N7	-2.96	1.33	1.39
3	5	4083	5MU	O4-C4	-2.96	1.17	1.23
6	9	159	A2M	C5-C4	-2.96	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	4620	OMU	O4-C4	-2.96	1.18	1.24
3	5	3867	A2M	C5-C4	-2.96	1.33	1.39
3	5	1883	OMG	O6-C6	-2.95	1.18	1.23
3	5	398	A2M	C5-C4	-2.95	1.33	1.39
6	9	814	5MU	O4-C4	-2.95	1.18	1.23
3	5	3723	A2M	C5-C4	-2.94	1.33	1.39
6	9	1678	A2M	C5-C4	-2.94	1.33	1.39
6	9	166	A2M	C5-C4	-2.94	1.33	1.39
6	9	509	OMG	O6-C6	-2.94	1.18	1.23
3	5	4472	B8W	C5-C4	-2.93	1.33	1.39
6	9	1850	MA6	C5-C4	-2.93	1.33	1.39
3	5	3718	A2M	C5-C4	-2.93	1.33	1.39
6	9	484	A2M	O3'-C3'	2.92	1.50	1.43
6	9	116	OMU	O4-C4	-2.92	1.18	1.24
6	9	644	OMG	C5-N7	-2.92	1.33	1.39
3	5	3880	P7G	C8-N7	2.91	1.51	1.45
3	5	3899	BGH	C1'-N9	-2.91	1.41	1.46
3	5	2424	OMG	C5-N7	-2.90	1.33	1.39
3	5	4196	OMG	C5-N7	-2.90	1.33	1.39
6	9	1832	6MZ	C5-C4	-2.89	1.33	1.39
3	5	1316	OMG	O6-C6	-2.89	1.18	1.23
6	9	668	A2M	O3'-C3'	2.89	1.50	1.43
3	5	3792	OMG	C5-N7	-2.89	1.33	1.39
3	5	1534	A2M	O2'-C2'	-2.88	1.35	1.42
3	5	2364	OMG	O6-C6	-2.88	1.18	1.23
3	5	4637	OMG	O6-C6	-2.88	1.18	1.23
3	5	1316	OMG	C5-N7	-2.88	1.33	1.39
3	5	1522	OMG	C5-N7	-2.87	1.33	1.39
3	5	4623	OMG	C5-N7	-2.87	1.33	1.39
3	5	237	B9B	C5-N7	-2.87	1.33	1.39
3	5	4185	B8W	C5-N7	-2.87	1.33	1.39
3	5	1574	B9B	C5-N7	-2.87	1.33	1.39
3	5	1883	OMG	C5-N7	-2.86	1.33	1.39
3	5	4220	6MZ	C5-N7	-2.86	1.33	1.39
3	5	2050	OMG	C5-N7	-2.86	1.33	1.39
3	5	4872	2MG	C5-N7	-2.86	1.33	1.39
6	9	509	OMG	C5-N7	-2.86	1.33	1.39
3	5	4335	5MC	O2-C2	-2.85	1.18	1.23
3	5	2050	OMG	O6-C6	-2.85	1.18	1.23
3	5	373	OMG	C5-N7	-2.85	1.33	1.39
3	5	1625	OMG	O6-C6	-2.85	1.18	1.23
3	5	373	OMG	O6-C6	-2.85	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	644	OMG	O6-C6	-2.85	1.18	1.23
3	5	1522	OMG	O6-C6	-2.85	1.18	1.23
3	5	4494	OMG	C5-N7	-2.84	1.33	1.39
3	5	4870	OMG	O6-C6	-2.83	1.18	1.23
3	5	1348	P4U	O2-C2	-2.83	1.18	1.23
3	5	2861	OMC	O2-C2	-2.83	1.18	1.23
3	5	4196	OMG	O6-C6	-2.83	1.18	1.23
3	5	4370	OMG	O6-C6	-2.83	1.18	1.23
3	5	4494	OMG	O6-C6	-2.83	1.18	1.23
3	5	4623	OMG	O6-C6	-2.83	1.18	1.23
3	5	2401	A2M	O2'-C2'	-2.83	1.35	1.42
6	9	166	A2M	O2'-C2'	-2.82	1.35	1.42
3	5	2424	OMG	O6-C6	-2.82	1.18	1.23
5	8	14	OMU	C6-N1	2.82	1.44	1.38
3	5	1909	P7G	O6-C6	-2.82	1.18	1.23
3	5	3867	A2M	O2'-C2'	-2.81	1.35	1.42
6	9	1374	5MC	O2-C2	-2.81	1.18	1.23
3	5	4370	OMG	C5-N7	-2.81	1.33	1.39
6	9	121	OMU	C6-N1	2.81	1.44	1.38
3	5	3785	A2M	O2'-C2'	-2.80	1.35	1.42
3	5	1659	I4U	O2-C2	-2.80	1.18	1.23
3	5	2754	B9B	C5-N7	-2.79	1.34	1.39
3	5	4523	A2M	C8-N9	-2.79	1.32	1.37
3	5	4671	B8T	O2-C2	-2.79	1.18	1.23
3	5	2773	OMG	O6-C6	-2.79	1.18	1.23
3	5	3792	OMG	O6-C6	-2.79	1.18	1.23
3	5	1524	A2M	O2'-C2'	-2.79	1.35	1.42
3	5	398	A2M	O3'-C3'	2.79	1.49	1.43
3	5	3825	A2M	O2'-C2'	-2.78	1.35	1.42
3	5	4194	I4U	O2-C2	-2.78	1.18	1.23
3	5	2364	OMG	C5-N7	-2.78	1.33	1.39
3	5	4523	A2M	O2'-C2'	-2.78	1.35	1.42
3	5	4529	B8W	C5-N7	-2.78	1.34	1.39
3	5	4571	A2M	O2'-C2'	-2.78	1.35	1.42
3	5	3880	P7G	O6-C6	-2.78	1.18	1.23
3	5	1534	A2M	C8-N9	-2.77	1.32	1.37
6	9	1031	A2M	O3'-C3'	2.77	1.49	1.43
3	5	3718	A2M	O3'-C3'	2.77	1.49	1.43
3	5	2365	OMC	O2-C2	-2.77	1.18	1.23
3	5	4472	B8W	C5-N7	-2.77	1.34	1.39
3	5	4483	B8T	O2-C2	-2.77	1.18	1.23
3	5	3723	A2M	O3'-C3'	2.76	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	3899	BGH	O6-C6	-2.76	1.18	1.23
3	5	2401	A2M	O3'-C3'	2.76	1.49	1.43
3	5	2773	OMG	C5-N7	-2.76	1.33	1.39
3	5	3718	A2M	C8-N9	-2.76	1.32	1.37
3	5	1534	A2M	O3'-C3'	2.76	1.49	1.43
6	9	668	A2M	O2'-C2'	-2.75	1.35	1.42
3	5	3718	A2M	O2'-C2'	-2.75	1.35	1.42
6	9	1031	A2M	O2'-C2'	-2.75	1.35	1.42
6	9	27	A2M	O2'-C2'	-2.75	1.35	1.42
3	5	2363	A2M	O2'-C2'	-2.75	1.35	1.42
3	5	4536	OMC	O2-C2	-2.75	1.18	1.23
3	5	4523	A2M	O3'-C3'	2.74	1.49	1.43
6	9	159	A2M	O2'-C2'	-2.74	1.35	1.42
3	5	2422	OMC	O2-C2	-2.74	1.18	1.23
6	9	1842	4AC	O2-C2	-2.74	1.18	1.23
3	5	3887	OMC	O2-C2	-2.74	1.18	1.23
6	9	517	OMC	O2-C2	-2.73	1.18	1.23
3	5	1871	A2M	O2'-C2'	-2.73	1.35	1.42
3	5	4620	OMU	C6-N1	2.73	1.44	1.38
3	5	3869	OMC	O2-C2	-2.73	1.18	1.23
6	9	484	A2M	O2'-C2'	-2.73	1.35	1.42
3	5	1326	A2M	O2'-C2'	-2.73	1.35	1.42
3	5	3782	5MC	O2-C2	-2.72	1.18	1.23
3	5	3867	A2M	O3'-C3'	2.72	1.49	1.43
6	9	683	OMG	C5-N7	-2.71	1.33	1.39
6	9	668	A2M	C8-N9	-2.71	1.32	1.37
3	5	4571	A2M	O3'-C3'	2.71	1.49	1.43
3	5	1871	A2M	C8-N9	-2.71	1.32	1.37
3	5	2804	OMC	O2-C2	-2.70	1.18	1.23
3	5	4306	OMU	C6-N1	2.70	1.44	1.38
3	5	4129	B8W	C5-C4	-2.70	1.34	1.39
3	5	398	A2M	O2'-C2'	-2.70	1.36	1.42
3	5	1326	A2M	C8-N9	-2.70	1.33	1.37
6	9	484	A2M	C8-N9	-2.69	1.33	1.37
3	5	1524	A2M	C8-N9	-2.69	1.33	1.37
6	9	1337	4AC	O2-C2	-2.69	1.18	1.23
6	9	1031	A2M	C8-N9	-2.69	1.33	1.37
3	5	1909	P7G	C5-C4	2.69	1.43	1.36
3	5	2363	A2M	C8-N9	-2.69	1.33	1.37
6	9	174	OMC	O2-C2	-2.69	1.18	1.23
6	9	1678	A2M	O2'-C2'	-2.68	1.36	1.42
6	9	1703	OMC	O2-C2	-2.68	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	4550	7MG	O6-C6	-2.68	1.18	1.23
3	5	3701	OMC	O2-C2	-2.68	1.18	1.23
6	9	27	A2M	C8-N9	-2.68	1.33	1.37
6	9	1710	OMC	O2-C2	-2.67	1.18	1.23
3	5	1326	A2M	O3'-C3'	2.67	1.49	1.43
6	9	683	OMG	O6-C6	-2.67	1.18	1.23
6	9	116	OMU	C6-N1	2.66	1.44	1.38
3	5	3723	A2M	O2'-C2'	-2.66	1.36	1.42
3	5	4870	OMG	C5-N7	-2.65	1.33	1.39
3	5	3825	A2M	O3'-C3'	2.65	1.49	1.43
3	5	2401	A2M	C8-N9	-2.65	1.33	1.37
3	5	3723	A2M	C8-N9	-2.64	1.33	1.37
3	5	1524	A2M	O3'-C3'	2.64	1.49	1.43
6	9	1678	A2M	O3'-C3'	2.64	1.49	1.43
6	9	166	A2M	C8-N9	-2.63	1.33	1.37
3	5	3880	P7G	C5-C4	2.63	1.43	1.36
3	5	1871	A2M	O3'-C3'	2.63	1.49	1.43
3	5	4083	5MU	O2-C2	-2.63	1.18	1.23
6	9	814	5MU	O2-C2	-2.63	1.18	1.23
3	5	4129	B8W	C5-N7	-2.63	1.34	1.39
3	5	4529	B8W	C5-C4	-2.62	1.34	1.39
3	5	2363	A2M	O3'-C3'	2.61	1.49	1.43
3	5	1605	7MG	O6-C6	-2.61	1.18	1.23
6	9	1678	A2M	C8-N9	-2.61	1.33	1.37
3	5	1517	2MG	O6-C6	-2.61	1.18	1.23
6	9	27	A2M	O3'-C3'	2.61	1.49	1.43
3	5	4872	2MG	O6-C6	-2.59	1.18	1.23
6	9	159	A2M	O3'-C3'	2.59	1.49	1.43
3	5	4872	2MG	C6-N1	2.59	1.43	1.38
2	1	45	4AC	O2-C2	-2.59	1.18	1.23
3	5	3825	A2M	C8-N9	-2.58	1.33	1.37
3	5	3785	A2M	C8-N9	-2.58	1.33	1.37
3	5	1866	UR3	C4-N3	2.58	1.45	1.40
3	5	2522	7MG	O6-C6	-2.57	1.18	1.23
3	5	4571	A2M	C8-N9	-2.57	1.33	1.37
3	5	3867	A2M	C8-N9	-2.56	1.33	1.37
3	5	4529	B8W	C8-N9	-2.55	1.33	1.37
3	5	4306	OMU	O2-C2	-2.55	1.18	1.23
3	5	2773	OMG	C2-N1	2.55	1.43	1.37
6	9	159	A2M	C8-N9	-2.54	1.33	1.37
6	9	166	A2M	O3'-C3'	2.54	1.49	1.43
3	5	4870	OMG	C6-N1	2.54	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	2424	OMG	C2-N1	2.54	1.43	1.37
3	5	398	A2M	C8-N9	-2.54	1.33	1.37
3	5	4870	OMG	C2-N1	2.53	1.43	1.37
3	5	729	2MG	O6-C6	-2.53	1.18	1.23
3	5	4472	B8W	C8-N9	-2.53	1.33	1.37
3	5	1322	1MA	CM1-N1	-2.53	1.41	1.46
3	5	4597	UR3	C4-N3	2.53	1.45	1.40
3	5	4530	UR3	C4-N3	2.52	1.45	1.40
3	5	4872	2MG	C5-C6	2.52	1.53	1.44
3	5	2363	A2M	C5-N7	-2.51	1.34	1.39
3	5	4129	B8W	C8-N9	-2.50	1.33	1.37
3	5	1797	E7G	O6-C6	-2.50	1.18	1.23
3	5	3792	OMG	C2-N1	2.50	1.43	1.37
6	9	1830	UR3	C4-N3	2.49	1.45	1.40
3	5	4370	OMG	C2-N1	2.49	1.43	1.37
3	5	1883	OMG	C2-N1	2.49	1.43	1.37
6	9	1031	A2M	C5-N7	-2.49	1.34	1.39
6	9	484	A2M	C5-N7	-2.49	1.34	1.39
6	9	683	OMG	C2-N1	2.48	1.43	1.37
6	9	683	OMG	C5-C6	2.48	1.53	1.44
3	5	3718	A2M	C5-N7	-2.48	1.34	1.39
3	5	2424	OMG	C6-N1	2.48	1.43	1.38
3	5	2297	E7G	O6-C6	-2.48	1.18	1.23
3	5	2050	OMG	C2-N1	2.47	1.43	1.37
3	5	4623	OMG	C2-N1	2.47	1.43	1.37
3	5	2773	OMG	C6-N1	2.46	1.43	1.38
6	9	517	OMC	C5-C4	2.46	1.48	1.42
3	5	4620	OMU	O2-C2	-2.46	1.18	1.23
3	5	1625	OMG	C2-N1	2.45	1.43	1.37
3	5	1326	A2M	C5-N7	-2.45	1.34	1.39
3	5	1316	OMG	C2-N1	2.45	1.43	1.37
6	9	683	OMG	C6-N1	2.45	1.43	1.38
6	9	1710	OMC	C5-C4	2.45	1.48	1.42
6	9	121	OMU	O2-C2	-2.45	1.18	1.23
3	5	4494	OMG	C2-N1	2.45	1.43	1.37
5	8	14	OMU	O2-C2	-2.44	1.18	1.23
3	5	3701	OMC	C5-C4	2.44	1.48	1.42
3	5	2364	OMG	C2-N1	2.44	1.43	1.37
3	5	2773	OMG	C5-C6	2.43	1.53	1.44
3	5	2380	B8W	C8-N9	-2.42	1.33	1.37
3	5	4185	B8W	C8-N9	-2.42	1.33	1.37
6	9	174	OMC	C5-C4	2.42	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	2422	OMC	C5-C4	2.42	1.48	1.42
3	5	4637	OMG	C2-N1	2.42	1.43	1.37
3	5	4371	MHG	O6-C6	-2.42	1.19	1.23
6	9	509	OMG	C2-N1	2.42	1.43	1.37
3	5	1517	2MG	C5-C6	2.41	1.53	1.44
3	5	3792	OMG	C6-N1	2.41	1.43	1.38
3	5	3867	A2M	C5-N7	-2.41	1.34	1.39
3	5	729	2MG	C5-C6	2.41	1.53	1.44
6	9	1703	OMC	C5-C4	2.41	1.48	1.42
3	5	4872	2MG	C4-N9	-2.41	1.31	1.38
3	5	4494	OMG	C6-N1	2.41	1.43	1.38
3	5	1883	OMG	C6-N1	2.41	1.43	1.38
3	5	2364	OMG	C6-N1	2.41	1.43	1.38
3	5	4870	OMG	C5-C6	2.40	1.53	1.44
3	5	4523	A2M	C5-N7	-2.40	1.34	1.39
6	9	166	A2M	C5-N7	-2.40	1.34	1.39
3	5	2401	A2M	C5-N7	-2.40	1.34	1.39
3	5	2050	OMG	C6-N1	2.40	1.43	1.38
3	5	3887	OMC	C5-C4	2.40	1.48	1.42
3	5	2365	OMC	C5-C4	2.40	1.48	1.42
3	5	4196	OMG	C2-N1	2.39	1.43	1.37
3	5	373	OMG	C2-N1	2.39	1.43	1.37
6	9	644	OMG	C2-N1	2.39	1.43	1.37
1	2	37	T6A	ODA-C13	2.39	1.29	1.22
3	5	3909	OMC	C5-C4	2.39	1.48	1.42
6	9	1850	MA6	C5-N7	-2.39	1.34	1.39
3	5	237	B9B	C5-C6	-2.38	1.37	1.41
3	5	4370	OMG	C6-N1	2.38	1.43	1.38
3	5	4637	OMG	C6-N1	2.38	1.43	1.38
6	9	116	OMU	O2-C2	-2.37	1.18	1.23
6	9	1678	A2M	C5-N7	-2.37	1.34	1.39
3	5	1522	OMG	C2-N1	2.37	1.43	1.37
3	5	2861	OMC	C5-C4	2.37	1.48	1.42
3	5	1534	A2M	C5-N7	-2.37	1.34	1.39
3	5	1871	A2M	C5-N7	-2.37	1.34	1.39
3	5	3825	A2M	C5-N7	-2.37	1.34	1.39
3	5	4536	OMC	C5-C4	2.36	1.48	1.42
3	5	2364	OMG	C5-C6	2.36	1.53	1.44
6	9	668	A2M	C5-N7	-2.36	1.34	1.39
3	5	3723	A2M	C5-N7	-2.36	1.34	1.39
3	5	4370	OMG	C5-C6	2.36	1.53	1.44
3	5	3869	OMC	C5-C4	2.36	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	4494	OMG	C5-C6	2.35	1.53	1.44
3	5	373	OMG	C5-C6	2.35	1.53	1.44
3	5	4571	A2M	C5-N7	-2.35	1.34	1.39
6	9	27	A2M	C5-N7	-2.34	1.34	1.39
6	9	121	OMU	C5-C4	2.34	1.48	1.43
3	5	4623	OMG	C5-C6	2.33	1.53	1.44
3	5	1522	OMG	C5-C6	2.33	1.53	1.44
3	5	4196	OMG	C5-C6	2.33	1.53	1.44
3	5	4194	I4U	C5-C4	2.33	1.49	1.43
3	5	3792	OMG	C5-C6	2.33	1.53	1.44
3	5	1625	OMG	C6-N1	2.33	1.43	1.38
6	9	1832	6MZ	C8-N9	-2.33	1.33	1.37
3	5	4623	OMG	C6-N1	2.33	1.43	1.38
6	9	159	A2M	C5-N7	-2.33	1.34	1.39
6	9	509	OMG	C5-C6	2.33	1.53	1.44
3	5	1625	OMG	C5-C6	2.33	1.53	1.44
3	5	1524	A2M	C5-N7	-2.33	1.34	1.39
3	5	1522	OMG	C6-N1	2.32	1.43	1.38
3	5	398	A2M	C5-N7	-2.32	1.34	1.39
3	5	2050	OMG	C5-C6	2.32	1.53	1.44
3	5	4530	UR3	O2-C2	-2.31	1.18	1.22
3	5	4355	E6G	C8-N9	-2.31	1.33	1.37
1	2	37	T6A	C2-N1	2.31	1.38	1.33
3	5	1316	OMG	C5-C6	2.31	1.53	1.44
5	8	14	OMU	C5-C4	2.31	1.48	1.43
3	5	1574	B9B	C8-N9	-2.30	1.33	1.37
3	5	4637	OMG	C5-C6	2.30	1.53	1.44
3	5	373	OMG	C6-N1	2.30	1.43	1.38
3	5	2804	OMC	C5-C4	2.30	1.48	1.42
3	5	3785	A2M	C5-N7	-2.30	1.34	1.39
6	9	1851	MA6	C5-N7	-2.30	1.34	1.39
6	9	644	OMG	C5-C6	2.29	1.53	1.44
3	5	4306	OMU	C5-C4	2.29	1.48	1.43
3	5	1574	B9B	C5-C6	-2.29	1.37	1.41
3	5	4620	OMU	C5-C4	2.28	1.48	1.43
3	5	2424	OMG	C5-C6	2.28	1.52	1.44
3	5	4220	6MZ	C8-N9	-2.28	1.33	1.37
6	9	644	OMG	C6-N1	2.27	1.43	1.38
3	5	1517	2MG	C6-N1	2.25	1.43	1.38
3	5	4196	OMG	C6-N1	2.25	1.43	1.38
6	9	1830	UR3	C5-C4	2.25	1.49	1.43
3	5	1524	A2M	C4-N9	-2.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	2754	B9B	C8-N9	-2.24	1.33	1.37
3	5	1883	OMG	C5-C6	2.24	1.52	1.44
3	5	1659	I4U	C5-C4	2.24	1.49	1.43
6	9	116	OMU	C5-C4	2.24	1.48	1.43
3	5	2363	A2M	C4-N9	-2.23	1.33	1.37
3	5	1316	OMG	C6-N1	2.23	1.43	1.38
3	5	4597	UR3	C5-C4	2.23	1.49	1.43
6	9	509	OMG	C6-N1	2.22	1.43	1.38
3	5	4530	UR3	C5-C4	2.22	1.49	1.43
3	5	237	B9B	C8-N9	-2.22	1.33	1.37
1	2	37	T6A	O10-C10	-2.21	1.18	1.23
3	5	2401	A2M	C4-N9	-2.21	1.33	1.37
3	5	1866	UR3	C5-C4	2.20	1.49	1.43
3	5	1456	B8Q	O2-C2	-2.20	1.18	1.22
1	2	37	T6A	C5-N7	-2.18	1.35	1.39
3	5	4415	1MA	CM1-N1	-2.17	1.42	1.46
3	5	1871	A2M	C4-N9	-2.17	1.33	1.37
3	5	1456	B8Q	C4-C5	2.17	1.54	1.49
3	5	2786	B9H	C31-N3	-2.16	1.43	1.46
3	5	4296	B8H	O4-C4	-2.16	1.19	1.23
6	9	668	A2M	C4-N9	-2.14	1.33	1.37
3	5	1326	A2M	C4-N9	-2.14	1.33	1.37
6	9	27	A2M	C4-N9	-2.13	1.33	1.37
3	5	4870	OMG	C4-N9	-2.13	1.32	1.38
3	5	3785	A2M	C4-N9	-2.12	1.33	1.37
3	5	4571	A2M	C4-N9	-2.12	1.33	1.37
3	5	3825	A2M	C4-N9	-2.12	1.33	1.37
6	9	1219	B8Q	O2-C2	-2.12	1.18	1.22
6	9	1248	B8N	O4-C4	-2.11	1.18	1.23
3	5	1860	B8H	O4-C4	-2.11	1.19	1.23
3	5	1534	A2M	C4-N9	-2.10	1.33	1.37
3	5	4523	A2M	C4-N9	-2.10	1.33	1.37
6	9	1830	UR3	O2-C2	-2.10	1.18	1.22
3	5	2754	B9B	C5-C6	-2.10	1.37	1.41
3	5	3762	B8H	O4-C4	-2.09	1.19	1.23
3	5	1456	B8Q	C6-N1	2.08	1.43	1.38
6	9	1851	MA6	C8-N9	-2.08	1.34	1.37
3	5	1348	P4U	C5-C4	2.08	1.48	1.43
3	5	1883	OMG	C4-N9	-2.08	1.32	1.38
6	9	166	A2M	C4-N9	-2.07	1.33	1.37
3	5	1522	OMG	C4-N9	-2.07	1.32	1.38
3	5	2050	OMG	C4-N9	-2.06	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	1842	4AC	O7-C7	-2.05	1.18	1.23
3	5	3718	A2M	C4-N9	-2.05	1.33	1.37
6	9	484	A2M	C4-N9	-2.05	1.33	1.37
6	9	1850	MA6	C8-N9	-2.04	1.34	1.37
3	5	2364	OMG	C4-N9	-2.04	1.32	1.38
6	9	568	MMX	O2-C2	-2.03	1.18	1.22
3	5	3867	A2M	C4-N9	-2.02	1.33	1.37
1	2	37	T6A	C6-N6	2.02	1.43	1.39
1	2	37	T6A	C5-C4	-2.02	1.35	1.39
3	5	3723	A2M	C4-N9	-2.02	1.33	1.37
3	5	729	2MG	C6-N1	2.02	1.42	1.38
3	5	1316	OMG	C4-N9	-2.01	1.32	1.38
3	5	4370	OMG	C4-N9	-2.01	1.32	1.38
3	5	4450	PSU	C4-C5	-2.01	1.38	1.44
6	9	159	A2M	C4-N9	-2.01	1.33	1.37
3	5	2773	OMG	C4-N9	-2.00	1.33	1.38

All (967) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	2754	B9B	O6-C6-C5	21.64	145.31	116.73
3	5	1574	B9B	O6-C6-C5	20.67	144.03	116.73
3	5	237	B9B	O6-C6-C5	20.33	143.58	116.73
3	5	2754	B9B	O6-C6-N1	-20.10	93.18	120.02
3	5	1574	B9B	O6-C6-N1	-19.23	94.34	120.02
3	5	237	B9B	O6-C6-N1	-18.79	94.93	120.02
3	5	4564	M7A	C5-C6-N6	14.20	147.88	123.75
6	9	1851	MA6	N1-C6-N6	-14.06	99.72	116.86
6	9	1806	M7A	C5-C6-N6	13.75	147.12	123.75
6	9	1850	MA6	N1-C6-N6	-13.41	100.52	116.86
3	5	4083	5MU	C5-C4-N3	11.79	125.57	115.32
3	5	4564	M7A	N6-C6-N1	-11.61	92.52	118.38
6	9	814	5MU	C5-C4-N3	11.60	125.40	115.32
6	9	1806	M7A	N6-C6-N1	-11.39	93.00	118.38
3	5	4220	6MZ	C4-N9-C1'	-10.03	103.17	126.63
3	5	4194	I4U	O4-C4-C5	9.91	122.49	115.45
3	5	4220	6MZ	C1'-N9-C8	9.79	148.83	127.09
3	5	4083	5MU	C5-C6-N1	-9.54	112.95	123.31
6	9	814	5MU	C5-C6-N1	-9.49	113.00	123.31
6	9	1851	MA6	C5-C6-N6	9.40	140.21	125.33
6	9	1832	6MZ	C4-N9-C1'	-9.36	104.74	126.63
6	9	1832	6MZ	C1'-N9-C8	9.23	147.57	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	1659	I4U	O4-C4-C5	9.20	121.98	115.45
6	9	1850	MA6	C5-C6-N6	9.05	139.66	125.33
6	9	568	MMX	N3-C2-N1	8.28	122.27	116.83
6	9	568	MMX	C4-N3-C2	-8.25	113.90	121.62
3	5	4355	E6G	N2-C2-N3	7.31	128.18	117.22
3	5	2380	B8W	C5-C4-N3	-7.23	119.57	127.18
3	5	1517	2MG	C2-N3-C4	7.16	120.96	112.00
3	5	2754	B9B	C5-C4-N3	-7.15	119.65	127.18
3	5	4529	B8W	C5-C4-N3	-7.08	119.72	127.18
3	5	237	B9B	C5-C4-N3	-7.08	119.72	127.18
3	5	1534	A2M	N6-C6-N1	-6.95	102.89	118.38
3	5	1574	B9B	C5-C4-N3	-6.95	119.86	127.18
3	5	4355	E6G	C5-C4-N3	-6.94	119.87	127.18
3	5	2380	B8W	N2-C2-N3	6.90	127.56	117.22
3	5	4185	B8W	C5-C4-N3	-6.88	119.94	127.18
3	5	4472	B8W	C5-C4-N3	-6.83	119.99	127.18
3	5	4185	B8W	N2-C2-N3	6.81	127.44	117.22
3	5	4296	B8H	C4-N3-C2	-6.81	118.42	127.34
3	5	729	2MG	C2-N3-C4	6.79	120.49	112.00
3	5	4472	B8W	N2-C2-N3	6.76	127.35	117.22
3	5	3762	B8H	C4-N3-C2	-6.75	118.48	127.34
3	5	3785	A2M	N6-C6-N1	-6.75	103.34	118.38
3	5	2401	A2M	N6-C6-N1	-6.75	103.34	118.38
3	5	4129	B8W	N2-C2-N3	6.74	127.33	117.22
6	9	484	A2M	N6-C6-N1	-6.73	103.39	118.38
3	5	4529	B8W	N2-C2-N3	6.70	127.27	117.22
6	9	668	A2M	N6-C6-N1	-6.70	103.45	118.38
3	5	1871	A2M	N6-C6-N1	-6.67	103.52	118.38
6	9	159	A2M	N6-C6-N1	-6.66	103.53	118.38
3	5	1326	A2M	N6-C6-N1	-6.65	103.57	118.38
3	5	2363	A2M	N6-C6-N1	-6.65	103.57	118.38
3	5	1860	B8H	C4-N3-C2	-6.63	118.64	127.34
3	5	3867	A2M	N6-C6-N1	-6.62	103.62	118.38
6	9	27	A2M	N6-C6-N1	-6.61	103.66	118.38
3	5	1524	A2M	N6-C6-N1	-6.60	103.67	118.38
3	5	3718	A2M	N6-C6-N1	-6.59	103.69	118.38
6	9	1678	A2M	N6-C6-N1	-6.58	103.72	118.38
3	5	398	A2M	N6-C6-N1	-6.57	103.73	118.38
3	5	4872	2MG	C2-N3-C4	6.56	120.21	112.00
3	5	3825	A2M	N6-C6-N1	-6.56	103.76	118.38
3	5	3723	A2M	N6-C6-N1	-6.56	103.77	118.38
3	5	4355	E6G	O6-C6-N1	6.55	128.77	120.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	9	166	A2M	N6-C6-N1	-6.54	103.81	118.38
3	5	4523	A2M	N6-C6-N1	-6.54	103.81	118.38
3	5	4571	A2M	N6-C6-N1	-6.54	103.82	118.38
3	5	4872	2MG	N1-C2-N2	6.52	123.22	116.56
6	9	1031	A2M	N6-C6-N1	-6.52	103.85	118.38
3	5	4564	M7A	N3-C4-N9	6.51	135.02	126.88
3	5	3762	B8H	N3-C2-N1	6.49	121.49	115.22
3	5	4129	B8W	C5-C4-N3	-6.47	120.36	127.18
3	5	4415	1MA	C1'-N9-C8	-6.47	108.35	126.73
3	5	4371	MHG	C2-N3-C4	6.46	120.08	112.00
3	5	1860	B8H	N3-C2-N1	6.33	121.34	115.22
3	5	1348	P4U	O4-C4-C5	6.31	119.93	115.45
3	5	4296	B8H	N3-C2-N1	6.31	121.32	115.22
3	5	2297	E7G	C4-C5-N7	6.24	110.00	104.94
6	9	668	A2M	N9-C8-N7	-6.17	105.18	113.94
3	5	1797	E7G	C4-C5-N7	6.15	109.93	104.94
6	9	1031	A2M	N9-C8-N7	-6.12	105.25	113.94
3	5	729	2MG	C5-C4-N3	-6.11	118.67	128.39
3	5	4371	MHG	C4-C5-N7	6.10	109.89	104.94
3	5	2401	A2M	N9-C8-N7	-6.08	105.31	113.94
3	5	4523	A2M	N9-C8-N7	-6.01	105.41	113.94
3	5	3785	A2M	N9-C8-N7	-6.01	105.41	113.94
3	5	1524	A2M	N9-C8-N7	-6.00	105.42	113.94
6	9	1678	A2M	N9-C8-N7	-5.99	105.43	113.94
6	9	27	A2M	N9-C8-N7	-5.98	105.46	113.94
6	9	159	A2M	N9-C8-N7	-5.96	105.47	113.94
3	5	1871	A2M	N9-C8-N7	-5.96	105.48	113.94
6	9	484	A2M	N9-C8-N7	-5.94	105.50	113.94
3	5	1534	A2M	N9-C8-N7	-5.91	105.55	113.94
3	5	1326	A2M	N9-C8-N7	-5.91	105.56	113.94
3	5	3785	A2M	N3-C2-N1	-5.89	119.66	128.58
3	5	4571	A2M	N9-C8-N7	-5.89	105.58	113.94
6	9	1031	A2M	N3-C2-N1	-5.88	119.68	128.58
3	5	3867	A2M	N9-C8-N7	-5.83	105.66	113.94
6	9	121	OMU	C4-N3-C2	-5.81	119.40	126.61
6	9	1832	6MZ	C5-C4-N3	-5.80	118.73	126.72
3	5	3825	A2M	N9-C8-N7	-5.79	105.73	113.94
3	5	3723	A2M	N9-C8-N7	-5.78	105.73	113.94
3	5	1517	2MG	C5-C4-N3	-5.78	119.19	128.39
3	5	2363	A2M	N9-C8-N7	-5.76	105.76	113.94
3	5	398	A2M	N9-C8-N7	-5.76	105.77	113.94
3	5	3899	BGH	C5-C6-N1	5.76	121.07	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	1326	A2M	N3-C2-N1	-5.75	119.87	128.58
3	5	1524	A2M	N3-C2-N1	-5.75	119.88	128.58
3	5	2401	A2M	N3-C2-N1	-5.73	119.91	128.58
3	5	1871	A2M	N3-C2-N1	-5.72	119.93	128.58
6	9	1851	MA6	N1-C2-N3	-5.70	119.95	128.58
3	5	4306	OMU	C4-N3-C2	-5.70	119.54	126.61
3	5	4523	A2M	N3-C2-N1	-5.69	119.97	128.58
6	9	668	A2M	C4-N9-C8	5.69	111.71	105.74
6	9	668	A2M	N3-C2-N1	-5.68	119.99	128.58
3	5	1534	A2M	N3-C2-N1	-5.66	120.01	128.58
6	9	484	A2M	N3-C2-N1	-5.65	120.03	128.58
6	9	166	A2M	N9-C8-N7	-5.64	105.93	113.94
3	5	4571	A2M	N3-C2-N1	-5.64	120.05	128.58
6	9	1806	M7A	N3-C2-N1	-5.64	120.05	128.58
6	9	1678	A2M	N3-C2-N1	-5.62	120.07	128.58
3	5	1322	1MA	N1-C2-N3	-5.60	119.34	126.00
6	9	1850	MA6	N1-C2-N3	-5.60	120.10	128.58
6	9	159	A2M	N3-C2-N1	-5.59	120.11	128.58
3	5	3723	A2M	N3-C2-N1	-5.59	120.12	128.58
6	9	1832	6MZ	N1-C2-N3	-5.58	120.13	128.58
6	9	27	A2M	N3-C2-N1	-5.58	120.14	128.58
3	5	4523	A2M	C4-N9-C8	5.58	111.59	105.74
6	9	166	A2M	N3-C2-N1	-5.57	120.14	128.58
3	5	2363	A2M	N3-C2-N1	-5.57	120.15	128.58
6	9	1031	A2M	C4-N9-C8	5.56	111.58	105.74
3	5	4564	M7A	N3-C2-N1	-5.56	120.17	128.58
3	5	3867	A2M	N3-C2-N1	-5.56	120.17	128.58
3	5	3825	A2M	N3-C2-N1	-5.55	120.19	128.58
3	5	398	A2M	N3-C2-N1	-5.54	120.19	128.58
5	8	14	OMU	C4-N3-C2	-5.53	119.74	126.61
6	9	1806	M7A	N3-C4-N9	5.52	133.78	126.88
6	9	27	A2M	C4-N9-C8	5.52	111.53	105.74
3	5	3785	A2M	C4-N9-C8	5.52	111.53	105.74
3	5	4530	UR3	C4-N3-C2	-5.51	120.14	124.58
3	5	2401	A2M	C4-N9-C8	5.50	111.52	105.74
3	5	1524	A2M	C4-N9-C8	5.50	111.51	105.74
3	5	4690	B8K	C5-C6-N1	5.50	120.62	110.94
6	9	1678	A2M	C4-N9-C8	5.50	111.51	105.74
3	5	1534	A2M	C5-C6-N6	5.48	136.86	123.29
1	2	37	T6A	N3-C2-N1	-5.48	120.29	128.58
6	9	116	OMU	C4-N3-C2	-5.47	119.82	126.61
3	5	1871	A2M	C4-N9-C8	5.46	111.47	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4220	6MZ	N1-C2-N3	-5.45	120.33	128.58
3	5	1625	OMG	C5-C4-N3	-5.45	119.72	128.39
3	5	4571	A2M	C4-N9-C8	5.43	111.44	105.74
3	5	4415	1MA	C1'-N9-C4	5.42	142.51	126.49
3	5	2401	A2M	C5-C6-N6	5.42	136.70	123.29
3	5	1322	1MA	C1'-N9-C8	-5.41	111.35	126.73
3	5	3899	BGH	C4-C5-N7	5.41	109.30	104.93
3	5	4620	OMU	C4-N3-C2	-5.40	119.91	126.61
3	5	3718	A2M	N9-C8-N7	-5.39	106.28	113.94
6	9	159	A2M	C4-N9-C8	5.39	111.40	105.74
3	5	3897	B8K	C5-C6-N1	5.38	120.42	110.94
3	5	4637	OMG	C5-C4-N3	-5.38	119.82	128.39
3	5	3718	A2M	N3-C2-N1	-5.38	120.43	128.58
3	5	4196	OMG	C5-C4-N3	-5.38	119.83	128.39
3	5	1326	A2M	C4-N9-C8	5.38	111.39	105.74
3	5	1524	A2M	C5-C6-N6	5.38	136.60	123.29
6	9	484	A2M	C4-N9-C8	5.37	111.38	105.74
3	5	3825	A2M	C4-N9-C8	5.37	111.37	105.74
6	9	159	A2M	C5-C6-N6	5.37	136.57	123.29
3	5	2363	A2M	C5-C6-N6	5.36	136.56	123.29
6	9	668	A2M	C5-C6-N6	5.36	136.56	123.29
3	5	4220	6MZ	C5-C4-N3	-5.36	119.34	126.72
3	5	3867	A2M	C4-N9-C8	5.34	111.35	105.74
3	5	3718	A2M	C5-C6-N6	5.34	136.51	123.29
3	5	1866	UR3	C4-N3-C2	-5.34	120.28	124.58
3	5	4690	B8K	C4-C5-N7	5.34	109.25	104.93
3	5	1871	A2M	C5-C6-N6	5.33	136.48	123.29
6	9	484	A2M	C5-C6-N6	5.32	136.46	123.29
3	5	1326	A2M	C5-C6-N6	5.29	136.39	123.29
3	5	1534	A2M	C4-N9-C8	5.29	111.29	105.74
3	5	3723	A2M	C5-C6-N6	5.28	136.35	123.29
3	5	2363	A2M	C4-N9-C8	5.27	111.28	105.74
3	5	3723	A2M	C4-N9-C8	5.27	111.27	105.74
6	9	644	OMG	C5-C4-N3	-5.27	120.01	128.39
6	9	166	A2M	C5-C6-N6	5.26	136.31	123.29
3	5	3867	A2M	C5-C6-N6	5.26	136.30	123.29
3	5	3785	A2M	C5-C6-N6	5.25	136.28	123.29
3	5	3792	OMG	C5-C4-N3	-5.25	120.04	128.39
6	9	1678	A2M	C5-C6-N6	5.25	136.28	123.29
3	5	4494	OMG	C5-C4-N3	-5.24	120.05	128.39
6	9	1219	B8Q	C1'-N1-C2	5.24	125.62	117.04
3	5	4623	OMG	C5-C4-N3	-5.24	120.05	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	9	27	A2M	C5-C6-N6	5.24	136.26	123.29
3	5	4415	1MA	N1-C2-N3	-5.23	119.78	126.00
3	5	4571	A2M	C5-C6-N6	5.23	136.23	123.29
3	5	4523	A2M	C5-C6-N6	5.23	136.23	123.29
6	9	1830	UR3	C4-N3-C2	-5.21	120.39	124.58
3	5	3825	A2M	C5-C6-N6	5.21	136.18	123.29
3	5	398	A2M	C5-C6-N6	5.20	136.16	123.29
3	5	398	A2M	C4-N9-C8	5.19	111.19	105.74
3	5	373	OMG	C5-C4-N3	-5.18	120.14	128.39
6	9	166	A2M	C4-N9-C8	5.17	111.17	105.74
3	5	4597	UR3	C4-N3-C2	-5.17	120.42	124.58
6	9	1031	A2M	C5-C6-N6	5.17	136.08	123.29
3	5	2754	B9B	N2-C2-N3	5.13	124.92	117.22
6	9	509	OMG	C5-C4-N3	-5.13	120.23	128.39
6	9	683	OMG	C5-C4-N3	-5.11	120.26	128.39
6	9	814	5MU	O4-C4-C5	-5.11	119.08	124.92
3	5	4371	MHG	C5-C6-N1	5.09	119.91	110.94
3	5	2424	OMG	C5-C4-N3	-5.09	120.28	128.39
1	2	37	T6A	N6-C10-N11	5.08	120.76	113.77
3	5	2380	B8W	C4-C5-C6	5.06	120.19	115.22
3	5	1316	OMG	C5-C4-N3	-5.06	120.33	128.39
6	9	1248	B8N	C5-C4-N3	5.05	125.32	116.15
3	5	1797	E7G	C5-C6-N1	5.04	119.81	110.94
3	5	1883	OMG	C5-C4-N3	-5.03	120.38	128.39
3	5	4355	E6G	C4-C5-C6	5.03	120.16	115.22
3	5	237	B9B	N2-C2-N3	5.02	124.75	117.22
3	5	4450	PSU	C4-N3-C2	-5.02	119.46	126.37
3	5	4636	PSU	C4-N3-C2	-5.02	119.46	126.37
3	5	1456	B8Q	N3-C2-N1	5.02	124.15	117.16
3	5	4450	PSU	N1-C2-N3	5.00	120.44	115.17
3	5	1683	PSU	N1-C2-N3	5.00	120.44	115.17
3	5	2297	E7G	C5-C6-N1	5.00	119.73	110.94
3	5	3897	B8K	C4-C5-N7	5.00	108.97	104.93
3	5	2050	OMG	C5-C4-N3	-4.98	120.46	128.39
3	5	1605	7MG	C5-C6-N1	4.98	119.71	110.94
6	9	1851	MA6	C5-C4-N3	-4.98	119.86	126.72
3	5	2773	OMG	C5-C4-N3	-4.97	120.48	128.39
3	5	4636	PSU	N1-C2-N3	4.97	120.41	115.17
3	5	4293	PSU	N1-C2-N3	4.97	120.41	115.17
3	5	4370	OMG	C5-C4-N3	-4.96	120.49	128.39
6	9	1851	MA6	N9-C8-N7	-4.96	106.90	113.94
3	5	2522	7MG	C5-C6-N1	4.96	119.66	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4529	B8W	C4-C5-C6	4.94	120.07	115.22
3	5	2364	OMG	C5-C4-N3	-4.94	120.53	128.39
3	5	4531	PSU	C4-N3-C2	-4.93	119.58	126.37
3	5	4628	PSU	C4-N3-C2	-4.93	119.58	126.37
3	5	3880	P7G	C4-C5-N7	4.91	110.02	106.71
6	9	822	PSU	N1-C2-N3	4.91	120.34	115.17
3	5	1677	PSU	C4-N3-C2	-4.90	119.62	126.37
3	5	4628	PSU	N1-C2-N3	4.89	120.33	115.17
3	5	4293	PSU	C4-N3-C2	-4.88	119.65	126.37
3	5	4083	5MU	O4-C4-C5	-4.88	119.34	124.92
3	5	4550	7MG	C5-C6-N1	4.87	119.51	110.94
3	5	1683	PSU	C4-N3-C2	-4.87	119.67	126.37
6	9	1850	MA6	C5-C4-N3	-4.86	120.02	126.72
3	5	1522	OMG	C5-C4-N3	-4.86	120.66	128.39
6	9	823	PSU	C4-N3-C2	-4.86	119.68	126.37
3	5	1677	PSU	N1-C2-N3	4.85	120.28	115.17
3	5	4442	PSU	N1-C2-N3	4.85	120.28	115.17
3	5	2508	PSU	C4-N3-C2	-4.85	119.69	126.37
3	5	4083	5MU	C4-N3-C2	-4.83	121.01	127.34
1	2	37	T6A	C5-C4-N3	-4.82	120.08	126.72
3	5	4531	PSU	N1-C2-N3	4.82	120.25	115.17
3	5	3729	PSU	C4-N3-C2	-4.82	119.73	126.37
3	5	3718	A2M	C4-N9-C8	4.82	110.80	105.74
6	9	823	PSU	N1-C2-N3	4.82	120.25	115.17
6	9	612	PSU	N1-C2-N3	4.81	120.25	115.17
3	5	3899	BGH	C2-N3-C4	4.81	120.58	112.30
3	5	3729	PSU	N1-C2-N3	4.81	120.24	115.17
3	5	4442	PSU	C4-N3-C2	-4.80	119.76	126.37
6	9	612	PSU	C4-N3-C2	-4.79	119.77	126.37
6	9	1243	PSU	C4-N3-C2	-4.79	119.77	126.37
3	5	4872	2MG	C5-C4-N3	-4.79	120.77	128.39
3	5	4500	PSU	C4-N3-C2	-4.79	119.78	126.37
6	9	1850	MA6	N9-C8-N7	-4.77	107.17	113.94
3	5	4690	B8K	C2-N3-C4	4.77	120.51	112.30
6	9	822	PSU	C4-N3-C2	-4.77	119.81	126.37
3	5	3715	PSU	N1-C2-N3	4.76	120.18	115.17
3	5	4870	OMG	C5-C4-N3	-4.74	120.84	128.39
3	5	4500	PSU	N1-C2-N3	4.73	120.16	115.17
3	5	3715	PSU	C4-N3-C2	-4.72	119.86	126.37
3	5	2508	PSU	N1-C2-N3	4.72	120.15	115.17
3	5	4083	5MU	N3-C2-N1	4.72	121.03	114.89
6	9	814	5MU	C4-N3-C2	-4.72	121.16	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4185	B8W	C4-C5-C6	4.70	119.83	115.22
3	5	3897	B8K	C2-N3-C4	4.68	120.36	112.30
6	9	1243	PSU	N1-C2-N3	4.67	120.10	115.17
3	5	4403	PSU	C4-N3-C2	-4.65	119.97	126.37
3	5	3764	PSU	N1-C2-N3	4.64	120.06	115.17
3	5	2380	B8W	N3-C4-N9	4.64	132.88	126.99
6	9	1219	B8Q	O2-C2-N3	-4.64	116.44	122.95
6	9	814	5MU	N3-C2-N1	4.64	120.93	114.89
6	9	1081	PSU	C4-N3-C2	-4.64	119.98	126.37
3	5	398	A2M	C5-C4-N3	-4.63	120.35	126.72
3	5	237	B9B	N3-C4-N9	4.62	132.85	126.99
3	5	1909	P7G	C4-C5-N7	4.61	109.82	106.71
3	5	4472	B8W	C4-C5-C6	4.60	119.73	115.22
3	5	4415	1MA	C5-C4-N3	-4.59	120.51	127.27
6	9	1031	A2M	C5-C4-N3	-4.59	120.40	126.72
6	9	683	OMG	C2-N3-C4	4.57	120.18	112.30
3	5	1625	OMG	C2-N3-C4	4.57	120.18	112.30
3	5	4494	OMG	C2-N3-C4	4.57	120.17	112.30
3	5	4196	OMG	C2-N3-C4	4.56	120.16	112.30
3	5	2522	7MG	C2-N3-C4	4.56	120.16	112.30
3	5	4872	2MG	C2-N1-C6	-4.55	119.05	124.55
3	5	3718	A2M	C5-C4-N3	-4.55	120.45	126.72
3	5	4637	OMG	C2-N3-C4	4.54	120.12	112.30
3	5	2364	OMG	C2-N3-C4	4.54	120.11	112.30
6	9	1081	PSU	N1-C2-N3	4.53	119.95	115.17
3	5	1534	A2M	C5-C4-N3	-4.53	120.48	126.72
3	5	4403	PSU	N1-C2-N3	4.53	119.94	115.17
3	5	3764	PSU	C4-N3-C2	-4.53	120.13	126.37
3	5	1456	B8Q	C31-N3-C4	4.52	122.58	114.76
3	5	1797	E7G	C2-N3-C4	4.52	120.08	112.30
3	5	1883	OMG	C2-N3-C4	4.52	120.08	112.30
6	9	119	PSU	N1-C2-N3	4.52	119.93	115.17
3	5	3792	OMG	C2-N3-C4	4.51	120.06	112.30
3	5	4623	OMG	C2-N3-C4	4.50	120.06	112.30
3	5	2050	OMG	C2-N3-C4	4.50	120.05	112.30
6	9	484	A2M	C5-C4-N3	-4.50	120.52	126.72
3	5	3723	A2M	C5-C4-N3	-4.48	120.54	126.72
3	5	2424	OMG	C2-N3-C4	4.48	120.01	112.30
6	9	644	OMG	C2-N3-C4	4.48	120.01	112.30
3	5	4870	OMG	C2-N3-C4	4.47	120.00	112.30
3	5	1605	7MG	C2-N3-C4	4.46	119.99	112.30
6	9	1678	A2M	C5-C4-N3	-4.46	120.58	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4370	OMG	C2-N3-C4	4.46	119.98	112.30
3	5	2363	A2M	C5-C4-N3	-4.45	120.58	126.72
6	9	119	PSU	C4-N3-C2	-4.45	120.24	126.37
3	5	2297	E7G	C2-N3-C4	4.45	119.96	112.30
3	5	2773	OMG	C2-N3-C4	4.45	119.96	112.30
3	5	1522	OMG	C2-N3-C4	4.45	119.96	112.30
3	5	3867	A2M	C5-C4-N3	-4.44	120.60	126.72
3	5	1517	2MG	C2-N1-C6	-4.44	119.18	124.55
6	9	159	A2M	C5-C4-N3	-4.44	120.61	126.72
6	9	1219	B8Q	N3-C2-N1	4.43	123.34	117.16
3	5	373	OMG	C2-N3-C4	4.43	119.94	112.30
3	5	3825	A2M	C5-C4-N3	-4.43	120.61	126.72
6	9	166	A2M	C5-C4-N3	-4.43	120.62	126.72
6	9	1851	MA6	C4-N9-C1'	-4.43	116.28	126.63
3	5	3867	A2M	C1'-N9-C8	-4.42	117.28	127.09
3	5	1316	OMG	C2-N3-C4	4.42	119.91	112.30
6	9	1850	MA6	C4-N9-C1'	-4.41	116.33	126.63
3	5	4523	A2M	C5-C4-N3	-4.39	120.67	126.72
3	5	4129	B8W	N9-C8-N7	-4.39	107.71	113.94
3	5	4185	B8W	N9-C8-N7	-4.38	107.72	113.94
3	5	4550	7MG	C2-N3-C4	4.37	119.83	112.30
3	5	237	B9B	C4-C5-C6	4.36	119.50	115.22
6	9	509	OMG	C2-N3-C4	4.36	119.81	112.30
3	5	4690	B8K	C72-C71-N7	4.35	125.22	118.80
6	9	1248	B8N	C4-N3-C2	-4.35	120.27	125.62
3	5	1322	1MA	C1'-N9-C4	4.34	139.32	126.49
3	5	1582	PSU	N1-C2-N3	4.33	119.73	115.17
3	5	4129	B8W	C4-C5-C6	4.32	119.47	115.22
6	9	27	A2M	C5-C4-N3	-4.32	120.77	126.72
3	5	1326	A2M	C5-C4-N3	-4.32	120.77	126.72
6	9	1678	A2M	C1'-N9-C8	-4.31	117.52	127.09
3	5	2754	B9B	N3-C4-N9	4.31	132.46	126.99
3	5	2401	A2M	C5-C4-N3	-4.31	120.78	126.72
6	9	668	A2M	C5-C4-N3	-4.30	120.79	126.72
3	5	4355	E6G	N9-C8-N7	-4.30	107.83	113.94
3	5	1871	A2M	C5-C4-N3	-4.30	120.80	126.72
3	5	2786	B9H	C31-N3-C2	4.30	122.57	117.29
3	5	1582	PSU	C4-N3-C2	-4.29	120.47	126.37
3	5	729	2MG	C2-N1-C6	-4.28	119.37	124.55
3	5	2380	B8W	N9-C8-N7	-4.28	107.86	113.94
3	5	3785	A2M	C5-C4-N3	-4.28	120.82	126.72
3	5	2522	7MG	C5-C4-N3	-4.27	120.11	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4571	A2M	C5-C4-N3	-4.27	120.84	126.72
3	5	1574	B9B	N2-C2-N3	4.25	123.60	117.22
3	5	4472	B8W	N9-C8-N7	-4.24	107.92	113.94
3	5	2363	A2M	C1'-N9-C8	-4.24	117.69	127.09
6	9	1248	B8N	C1'-C5-C4	4.23	124.03	117.61
3	5	4529	B8W	N9-C8-N7	-4.20	107.98	113.94
3	5	1605	7MG	C5-C4-N3	-4.18	120.28	128.13
3	5	1797	E7G	C5-C4-N3	-4.18	120.28	128.13
3	5	1574	B9B	N9-C8-N7	-4.18	108.01	113.94
3	5	4185	B8W	N3-C4-N9	4.16	132.27	126.99
3	5	4355	E6G	N3-C4-N9	4.15	132.26	126.99
3	5	2754	B9B	C4-C5-C6	4.15	119.30	115.22
3	5	729	2MG	N9-C4-N3	4.14	134.23	125.95
3	5	3723	A2M	C1'-N9-C8	-4.12	117.95	127.09
6	9	1850	MA6	C4-C5-C6	4.12	120.17	115.91
3	5	4355	E6G	O6-C6-C5	-4.11	111.30	116.73
3	5	3718	A2M	C1'-N9-C8	-4.11	117.97	127.09
3	5	2380	B8W	O6-C6-N1	4.10	124.41	118.96
3	5	4371	MHG	C5-C4-N3	-4.10	120.44	128.13
6	9	1031	A2M	C1'-N9-C8	-4.08	118.03	127.09
3	5	1524	A2M	C5-C4-N3	-4.08	121.09	126.72
3	5	4220	6MZ	C4-C5-C6	4.08	120.17	116.78
6	9	484	A2M	C1'-N9-C8	-4.08	118.05	127.09
3	5	1517	2MG	N1-C2-N2	4.07	120.71	116.56
3	5	237	B9B	N9-C8-N7	-4.06	108.17	113.94
3	5	1574	B9B	N3-C4-N9	4.05	132.13	126.99
3	5	398	A2M	C1'-N9-C8	-4.04	118.12	127.09
3	5	1322	1MA	C5-C4-N3	-4.04	121.32	127.27
3	5	4472	B8W	N3-C4-N9	4.03	132.11	126.99
3	5	2754	B9B	N9-C8-N7	-4.03	108.22	113.94
3	5	1574	B9B	C4-C5-C6	4.02	119.17	115.22
3	5	3825	A2M	C1'-N9-C8	-4.02	118.18	127.09
6	9	159	A2M	C1'-N9-C8	-4.01	118.19	127.09
3	5	4529	B8W	N3-C4-N9	4.00	132.07	126.99
6	9	1031	A2M	N3-C4-N9	4.00	133.97	127.17
3	5	4571	A2M	C1'-N9-C8	-4.00	118.22	127.09
3	5	3897	B8K	C72-C71-N7	4.00	124.70	118.80
3	5	2297	E7G	C5-C4-N3	-3.99	120.64	128.13
3	5	4550	7MG	C5-C4-N3	-3.98	120.65	128.13
6	9	166	A2M	C1'-N9-C8	-3.95	118.34	127.09
3	5	1605	7MG	C4-C5-N7	3.94	110.03	105.38
3	5	4523	A2M	C1'-N9-C8	-3.93	118.37	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	1456	B8Q	O2-C2-N3	-3.93	117.44	122.95
6	9	1832	6MZ	C4-C5-C6	3.93	120.04	116.78
3	5	2522	7MG	C4-C5-N7	3.92	110.01	105.38
3	5	4220	6MZ	N9-C8-N7	-3.92	108.37	113.94
3	5	1326	A2M	C1'-N9-C8	-3.88	118.47	127.09
3	5	398	A2M	N3-C4-N9	3.88	133.77	127.17
3	5	4083	5MU	C5M-C5-C6	-3.87	117.61	122.85
3	5	4371	MHG	C2-N1-C6	-3.87	119.88	124.55
3	5	2401	A2M	C1'-N9-C8	-3.86	118.52	127.09
6	9	1832	6MZ	N3-C4-N9	3.86	133.73	127.17
6	9	121	OMU	N3-C2-N1	3.85	119.90	114.89
6	9	1851	MA6	C4-C5-C6	3.84	119.88	115.91
6	9	1678	A2M	N3-C4-N9	3.84	133.69	127.17
6	9	27	A2M	C1'-N9-C8	-3.83	118.60	127.09
3	5	3867	A2M	N3-C4-N9	3.83	133.68	127.17
6	9	121	OMU	C5-C4-N3	3.82	120.15	114.80
3	5	4529	B8W	C61-O6-C6	3.82	120.77	117.20
3	5	1871	A2M	C1'-N9-C8	-3.81	118.63	127.09
3	5	3825	A2M	N3-C4-N9	3.81	133.65	127.17
3	5	4371	MHG	N1-C2-N2	3.80	120.44	116.56
6	9	1219	B8Q	C31-N3-C4	3.80	121.34	114.76
6	9	484	A2M	N3-C4-N9	3.79	133.62	127.17
3	5	4355	E6G	N2-C2-N1	-3.79	111.54	117.22
3	5	4306	OMU	N3-C2-N1	3.78	119.81	114.89
5	8	14	OMU	C5-C4-N3	3.77	120.08	114.80
3	5	4523	A2M	N3-C4-N9	3.76	133.57	127.17
3	5	2363	A2M	N3-C4-N9	3.76	133.56	127.17
3	5	4415	1MA	C2-N3-C4	3.76	119.90	112.53
3	5	3723	A2M	N3-C4-N9	3.76	133.56	127.17
6	9	116	OMU	N3-C2-N1	3.76	119.78	114.89
3	5	1524	A2M	C1'-N9-C8	-3.75	118.76	127.09
6	9	1832	6MZ	N9-C8-N7	-3.75	108.61	113.94
3	5	4550	7MG	C4-C5-N7	3.75	109.81	105.38
6	9	166	A2M	N3-C4-N9	3.75	133.54	127.17
3	5	4185	B8W	O6-C6-N1	3.74	123.93	118.96
3	5	4620	OMU	N3-C2-N1	3.74	119.76	114.89
6	9	668	A2M	C1'-N9-C8	-3.74	118.80	127.09
3	5	1534	A2M	C1'-N9-C8	-3.73	118.81	127.09
3	5	1322	1MA	C2-N3-C4	3.73	119.84	112.53
3	5	4690	B8K	C5-C4-N9	3.73	111.11	106.33
3	5	4296	B8H	C5-C4-N3	3.71	124.72	116.55
3	5	3718	A2M	N3-C4-N9	3.71	133.47	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	9	159	A2M	N3-C4-N9	3.71	133.47	127.17
6	9	1832	6MZ	C2-N3-C4	3.70	120.87	111.83
6	9	1851	MA6	C4-N9-C8	3.70	109.62	105.74
6	9	1219	B8Q	C6-N1-C2	-3.70	118.78	121.80
3	5	2380	B8W	C61-O6-C6	-3.69	113.75	117.20
3	5	4083	5MU	C5M-C5-C4	3.69	122.72	118.78
3	5	2786	B9H	C4-N3-C2	-3.68	115.37	122.00
3	5	4306	OMU	C5-C4-N3	3.68	119.95	114.80
5	8	14	OMU	N3-C2-N1	3.67	119.67	114.89
3	5	4597	UR3	C5-C4-N3	3.67	119.87	115.04
6	9	27	A2M	N3-C4-N9	3.66	133.40	127.17
3	5	3897	B8K	C5-C4-N9	3.65	111.01	106.33
3	5	1534	A2M	N3-C4-N9	3.65	133.38	127.17
3	5	3785	A2M	C1'-N9-C8	-3.65	119.00	127.09
6	9	668	A2M	N3-C4-N9	3.64	133.36	127.17
3	5	4129	B8W	N1-C2-N3	-3.64	119.90	125.48
3	5	3785	A2M	N3-C4-N9	3.64	133.36	127.17
3	5	1860	B8H	C5-C4-N3	3.64	124.56	116.55
3	5	4447	5MC	C5-C6-N1	-3.64	119.36	123.31
3	5	4571	A2M	N3-C4-N9	3.64	133.35	127.17
3	5	1326	A2M	N3-C4-N9	3.63	133.34	127.17
3	5	1860	B8H	O2-C2-N1	-3.63	119.11	122.78
3	5	1322	1MA	N9-C8-N7	-3.63	106.68	113.40
3	5	1866	UR3	C5-C4-N3	3.63	119.81	115.04
6	9	568	MMX	O2-C2-N3	-3.61	117.48	122.10
3	5	4872	2MG	CM2-N2-C2	-3.61	115.89	123.65
3	5	4129	B8W	C2-N1-C6	3.60	120.96	115.96
3	5	3762	B8H	C5-C4-N3	3.60	124.47	116.55
3	5	1871	A2M	N3-C4-N9	3.59	133.28	127.17
6	9	1851	MA6	N3-C4-N9	3.58	133.26	127.17
1	2	37	T6A	C4-C5-C6	3.58	119.75	116.78
3	5	2401	A2M	N3-C4-N9	3.56	133.23	127.17
3	5	4220	6MZ	N3-C4-N9	3.56	133.22	127.17
3	5	4472	B8W	N1-C2-N3	-3.55	120.04	125.48
3	5	4194	I4U	C5-C4-N3	-3.54	119.66	124.86
6	9	1850	MA6	N3-C4-N9	3.54	133.19	127.17
3	5	3762	B8H	O2-C2-N1	-3.53	119.20	122.78
3	5	4185	B8W	N1-C2-N3	-3.53	120.06	125.48
6	9	1031	A2M	C5-N7-C8	3.53	109.00	103.45
3	5	1517	2MG	N9-C4-N3	3.53	133.01	125.95
3	5	4620	OMU	C5-C4-N3	3.53	119.74	114.80
6	9	668	A2M	C5-N7-C8	3.52	108.98	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	9	1248	B8N	N3-C2-N1	3.51	121.01	116.72
6	9	1830	UR3	C5-C4-N3	3.51	119.66	115.04
1	2	37	T6A	N9-C8-N7	-3.50	108.97	113.94
6	9	1850	MA6	C4-N9-C8	3.50	109.41	105.74
3	5	4529	B8W	C5-N7-C8	3.49	108.94	103.45
6	9	1830	UR3	C1'-N1-C2	3.48	122.73	117.04
3	5	1659	I4U	C5-C4-N3	-3.48	119.76	124.86
6	9	1851	MA6	C2-N3-C4	3.48	120.32	111.83
6	9	1678	A2M	C5-N7-C8	3.47	108.91	103.45
3	5	4530	UR3	C5-C4-N3	3.47	119.61	115.04
3	5	4690	B8K	C5-C4-N3	-3.47	121.62	128.13
6	9	116	OMU	C5-C4-N3	3.47	119.66	114.80
3	5	4129	B8W	N3-C4-N9	3.46	131.38	126.99
6	9	159	A2M	C5-N7-C8	3.46	108.88	103.45
3	5	4523	A2M	C5-N7-C8	3.45	108.87	103.45
3	5	4220	6MZ	C2-N3-C4	3.45	120.25	111.83
3	5	3899	BGH	C72-C71-N7	3.45	123.88	118.80
3	5	4296	B8H	O2-C2-N1	-3.44	119.30	122.78
3	5	1348	P4U	C5-C4-N3	-3.44	119.81	124.86
3	5	2401	A2M	C5-N7-C8	3.44	108.85	103.45
3	5	1534	A2M	C5-N7-C8	3.43	108.84	103.45
3	5	4872	2MG	C1'-N9-C4	-3.42	116.37	126.49
3	5	3899	BGH	C5-C4-N9	3.42	110.72	106.33
3	5	4129	B8W	C5-N7-C8	3.41	108.81	103.45
3	5	2380	B8W	N2-C2-N1	-3.41	112.11	117.22
3	5	4415	1MA	N9-C8-N7	-3.40	107.09	113.40
3	5	4355	E6G	N3-C2-N1	-3.40	120.28	125.48
3	5	1524	A2M	C5-N7-C8	3.39	108.77	103.45
3	5	1625	OMG	N9-C4-N3	3.38	132.71	125.95
6	9	1374	5MC	C5-C6-N1	-3.38	119.65	123.31
3	5	3899	BGH	C5-C4-N3	-3.37	121.80	128.13
3	5	3899	BGH	N9-C8-N7	3.37	107.75	103.31
6	9	484	A2M	C5-N7-C8	3.37	108.74	103.45
3	5	4529	B8W	N1-C2-N3	-3.36	120.32	125.48
3	5	1326	A2M	C5-N7-C8	3.36	108.74	103.45
3	5	2380	B8W	N1-C2-N3	-3.36	120.33	125.48
3	5	1871	A2M	C5-N7-C8	3.36	108.73	103.45
6	9	27	A2M	C5-N7-C8	3.36	108.73	103.45
3	5	4355	E6G	C61-O6-C6	-3.36	114.24	117.57
6	9	1850	MA6	C2-N1-C6	3.36	120.03	111.83
3	5	1524	A2M	N3-C4-N9	3.35	132.86	127.17
3	5	4196	OMG	N9-C4-N3	3.34	132.64	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4870	OMG	N9-C8-N7	-3.34	107.20	113.40
3	5	3785	A2M	C5-N7-C8	3.34	108.69	103.45
3	5	3723	A2M	C5-N7-C8	3.34	108.69	103.45
3	5	3867	A2M	C5-N7-C8	3.33	108.69	103.45
3	5	398	A2M	C5-N7-C8	3.33	108.69	103.45
6	9	683	OMG	N9-C8-N7	-3.31	107.25	113.40
3	5	4335	5MC	C5-C6-N1	-3.31	119.71	123.31
6	9	1851	MA6	C2-N1-C6	3.31	119.92	111.83
3	5	3897	B8K	C5-C4-N3	-3.31	121.92	128.13
3	5	4637	OMG	N9-C4-N3	3.30	132.56	125.95
6	9	1031	A2M	C2-N3-C4	3.30	119.89	111.83
3	5	4571	A2M	C5-N7-C8	3.30	108.63	103.45
3	5	2754	B9B	N3-C2-N1	-3.29	120.44	125.48
3	5	4371	MHG	C5-C4-N9	3.29	110.55	106.33
6	9	1850	MA6	C2-N3-C4	3.29	119.86	111.83
3	5	1534	A2M	C2-N3-C4	3.29	119.86	111.83
3	5	2363	A2M	C5-N7-C8	3.27	108.59	103.45
3	5	3792	OMG	N9-C4-N3	3.27	132.49	125.95
6	9	644	OMG	N9-C4-N3	3.27	132.49	125.95
1	2	37	T6A	C2-N3-C4	3.26	119.79	111.83
3	5	3785	A2M	C2-N3-C4	3.25	119.78	111.83
6	9	814	5MU	C5M-C5-C6	-3.25	118.45	122.85
3	5	4690	B8K	N9-C8-N7	3.25	107.59	103.31
3	5	237	B9B	N3-C2-N1	-3.24	120.52	125.48
3	5	4529	B8W	C2-N1-C6	3.24	120.46	115.96
6	9	1850	MA6	C1'-N9-C8	3.22	134.25	127.09
3	5	3825	A2M	C5-N7-C8	3.22	108.51	103.45
3	5	1574	B9B	N3-C2-N1	-3.22	120.54	125.48
3	5	398	A2M	C2-N3-C4	3.22	119.70	111.83
6	9	484	A2M	C2-N3-C4	3.21	119.68	111.83
3	5	4529	B8W	N2-C2-N1	-3.21	112.41	117.22
3	5	4550	7MG	C5-C4-N9	3.21	110.45	106.33
3	5	4523	A2M	C2-N3-C4	3.21	119.67	111.83
6	9	166	A2M	C5-N7-C8	3.21	108.49	103.45
3	5	4494	OMG	N9-C4-N3	3.20	132.35	125.95
3	5	4623	OMG	N9-C4-N3	3.18	132.32	125.95
6	9	1678	A2M	C2-N3-C4	3.18	119.60	111.83
3	5	1522	OMG	N9-C8-N7	-3.18	107.50	113.40
3	5	1883	OMG	N9-C8-N7	-3.18	107.50	113.40
3	5	2401	A2M	C2-N3-C4	3.18	119.59	111.83
3	5	4872	2MG	C1'-N9-C8	3.17	135.74	126.73
3	5	4872	2MG	N2-C2-N3	-3.17	116.47	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	1326	A2M	C2-N3-C4	3.16	119.56	111.83
3	5	4637	OMG	C2-N1-C6	-3.16	119.38	125.11
3	5	4623	OMG	C2-N1-C6	-3.16	119.38	125.11
6	9	1851	MA6	C5-N7-C8	3.16	108.41	103.45
3	5	2364	OMG	N9-C8-N7	-3.16	107.55	113.40
3	5	1871	A2M	C2-N3-C4	3.16	119.54	111.83
3	5	3723	A2M	C2-N3-C4	3.16	119.54	111.83
6	9	159	A2M	C2-N3-C4	3.15	119.53	111.83
3	5	4370	OMG	N9-C8-N7	-3.15	107.56	113.40
3	5	3867	A2M	C2-N3-C4	3.15	119.53	111.83
6	9	1851	MA6	C1'-N9-C8	3.15	134.09	127.09
3	5	4185	B8W	N2-C2-N1	-3.15	112.50	117.22
3	5	1883	OMG	N9-C4-N3	3.15	132.25	125.95
6	9	509	OMG	C2-N1-C6	-3.15	119.40	125.11
3	5	3825	A2M	C2-N3-C4	3.15	119.52	111.83
6	9	668	A2M	C2-N3-C4	3.14	119.51	111.83
3	5	4623	OMG	N9-C8-N7	-3.14	107.59	113.40
3	5	373	OMG	N9-C4-N3	3.13	132.22	125.95
3	5	3782	5MC	C5-C6-N1	-3.13	119.91	123.31
3	5	2424	OMG	N9-C4-N3	3.13	132.22	125.95
3	5	3718	A2M	C5-N7-C8	3.13	108.37	103.45
6	9	27	A2M	C2-N3-C4	3.13	119.47	111.83
3	5	4571	A2M	C2-N3-C4	3.12	119.46	111.83
6	9	166	A2M	C2-N3-C4	3.12	119.46	111.83
3	5	4494	OMG	N9-C8-N7	-3.12	107.61	113.40
3	5	4450	PSU	C6-C5-C4	3.12	120.28	118.17
3	5	1316	OMG	N9-C8-N7	-3.12	107.62	113.40
3	5	1625	OMG	C2-N1-C6	-3.12	119.46	125.11
3	5	2363	A2M	C2-N3-C4	3.11	119.43	111.83
3	5	4530	UR3	C6-N1-C2	-3.11	119.26	121.80
3	5	2773	OMG	N9-C8-N7	-3.11	107.64	113.40
3	5	1524	A2M	C2-N3-C4	3.11	119.42	111.83
3	5	373	OMG	N9-C8-N7	-3.11	107.64	113.40
6	9	644	OMG	N9-C8-N7	-3.10	107.64	113.40
3	5	373	OMG	C2-N1-C6	-3.10	119.48	125.11
3	5	3897	B8K	N9-C8-N7	3.09	107.39	103.31
3	5	2522	7MG	C5-C4-N9	3.09	110.30	106.33
3	5	2297	E7G	C5-C4-N9	3.09	110.29	106.33
6	9	644	OMG	C2-N1-C6	-3.09	119.51	125.11
6	9	116	OMU	O4-C4-C5	-3.09	119.83	125.16
3	5	4129	B8W	C5-C6-N1	-3.09	119.36	123.49
3	5	4472	B8W	C2-N1-C6	3.09	120.25	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4529	B8W	C4-C5-N7	-3.09	107.05	110.58
3	5	3718	A2M	C2-N3-C4	3.09	119.37	111.83
3	5	4196	OMG	C2-N1-C6	-3.08	119.52	125.11
3	5	2050	OMG	N9-C8-N7	-3.08	107.69	113.40
3	5	4472	B8W	N2-C2-N1	-3.08	112.61	117.22
3	5	4494	OMG	C2-N1-C6	-3.08	119.53	125.11
3	5	4129	B8W	C61-O6-C6	3.08	120.08	117.20
3	5	4472	B8W	C5-N7-C8	3.08	108.28	103.45
3	5	2424	OMG	C2-N1-C6	-3.08	119.53	125.11
6	9	1806	M7A	C2-N3-C4	3.07	119.33	111.83
3	5	1883	OMG	C2-N1-C6	-3.07	119.55	125.11
3	5	4129	B8W	C4-C5-N7	-3.06	107.08	110.58
6	9	509	OMG	N9-C4-N3	3.06	132.07	125.95
3	5	4872	2MG	N9-C8-N7	-3.06	107.73	113.40
6	9	1832	6MZ	C9-N6-C6	-3.05	120.02	122.85
3	5	4529	B8W	C5-C6-N1	-3.05	119.41	123.49
6	9	683	OMG	N9-C4-N3	3.05	132.04	125.95
6	9	509	OMG	N9-C8-N7	-3.04	107.76	113.40
3	5	3899	BGH	C6-C5-C4	-3.04	117.05	122.40
3	5	4196	OMG	N9-C8-N7	-3.03	107.77	113.40
6	9	1850	MA6	C5-N7-C8	3.02	108.19	103.45
3	5	3792	OMG	N9-C8-N7	-3.02	107.81	113.40
5	8	14	OMU	O4-C4-C5	-3.01	119.97	125.16
6	9	683	OMG	C2-N1-C6	-3.01	119.65	125.11
3	5	3792	OMG	C2-N1-C6	-3.01	119.65	125.11
3	5	2050	OMG	C2-N1-C6	-3.01	119.66	125.11
6	9	568	MMX	C31-N3-C2	3.01	121.26	117.49
3	5	1316	OMG	N9-C4-N3	3.00	131.94	125.95
3	5	4185	B8W	C5-N7-C8	2.99	108.15	103.45
3	5	3897	B8K	C6-C5-C4	-2.98	117.15	122.40
3	5	4450	PSU	O2-C2-N1	-2.98	119.71	122.79
3	5	4564	M7A	C2-N3-C4	2.98	119.11	111.83
3	5	2380	B8W	C5-N7-C8	2.97	108.12	103.45
3	5	4129	B8W	N2-C2-N1	-2.97	112.77	117.22
3	5	2364	OMG	C2-N1-C6	-2.96	119.74	125.11
3	5	1797	E7G	C5-C4-N9	2.95	110.12	106.33
3	5	4370	OMG	N9-C4-N3	2.95	131.86	125.95
3	5	4870	OMG	C2-N1-C6	-2.95	119.75	125.11
3	5	4370	OMG	C2-N1-C6	-2.95	119.76	125.11
3	5	1625	OMG	N9-C8-N7	-2.95	107.93	113.40
3	5	2297	E7G	O6-C6-C5	-2.95	120.39	127.62
3	5	2424	OMG	N9-C8-N7	-2.94	107.95	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4306	OMU	O4-C4-C5	-2.94	120.10	125.16
3	5	1316	OMG	C2-N1-C6	-2.94	119.79	125.11
3	5	2364	OMG	N9-C4-N3	2.93	131.82	125.95
3	5	4690	B8K	C6-C5-C4	-2.93	117.25	122.40
3	5	4371	MHG	O6-C6-C5	-2.93	120.43	127.62
3	5	2050	OMG	N9-C4-N3	2.93	131.81	125.95
3	5	4185	B8W	C2-N1-C6	2.93	120.03	115.96
3	5	4637	OMG	N9-C8-N7	-2.92	107.98	113.40
3	5	2773	OMG	C2-N1-C6	-2.92	119.82	125.11
6	9	121	OMU	O4-C4-C5	-2.91	120.14	125.16
3	5	1605	7MG	C5-C4-N9	2.91	110.06	106.33
3	5	4185	B8W	C4-N9-C1'	-2.91	119.83	126.63
3	5	4355	E6G	C5-N7-C8	2.91	108.02	103.45
3	5	3899	BGH	C2-N1-C6	-2.91	119.84	125.11
6	9	1830	UR3	C6-N1-C2	-2.91	119.42	121.80
2	1	45	4AC	C6-C5-C4	2.90	120.50	117.00
3	5	4472	B8W	O6-C6-N1	2.90	122.82	118.96
6	9	1243	PSU	O2-C2-N1	-2.89	119.81	122.79
3	5	2773	OMG	N9-C4-N3	2.89	131.73	125.95
6	9	823	PSU	O2-C2-N1	-2.89	119.81	122.79
3	5	1797	E7G	O6-C6-C5	-2.88	120.55	127.62
3	5	1522	OMG	C2-N1-C6	-2.87	119.91	125.11
3	5	4620	OMU	O4-C4-C5	-2.87	120.22	125.16
3	5	1605	7MG	N9-C4-N3	2.86	129.65	125.46
1	2	37	T6A	N3-C4-N9	2.86	132.02	127.17
6	9	612	PSU	O2-C2-N1	-2.85	119.85	122.79
3	5	1909	P7G	N9-C8-N7	2.83	107.38	103.37
3	5	1797	E7G	N9-C4-N3	2.83	129.60	125.46
3	5	1605	7MG	O6-C6-C5	-2.82	120.69	127.62
3	5	2522	7MG	O6-C6-C5	-2.82	120.69	127.62
3	5	2522	7MG	N9-C4-N3	2.82	129.59	125.46
3	5	2522	7MG	C2-N1-C6	-2.80	120.03	125.11
3	5	2297	E7G	C2-N1-C6	-2.80	120.03	125.11
3	5	1683	PSU	O2-C2-N1	-2.80	119.90	122.79
3	5	1797	E7G	C2-N1-C6	-2.80	120.04	125.11
3	5	1605	7MG	C2-N1-C6	-2.79	120.04	125.11
6	9	1832	6MZ	C5-N7-C8	2.79	107.83	103.45
3	5	1517	2MG	C5-C6-N1	2.79	120.35	113.25
3	5	4355	E6G	C2-N1-C6	2.77	119.82	115.96
3	5	1574	B9B	C5-N7-C8	2.76	107.79	103.45
3	5	1522	OMG	N9-C4-N3	2.76	131.48	125.95
6	9	1806	M7A	C71-N7-C5	-2.76	111.93	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	2754	B9B	C5-N7-C8	2.76	107.78	103.45
3	5	4564	M7A	N9-C8-N7	-2.75	99.47	103.37
3	5	4628	PSU	O2-C2-N1	-2.74	119.97	122.79
3	5	1517	2MG	N9-C8-N7	-2.74	108.33	113.40
3	5	3785	A2M	O4'-C1'-N9	2.73	113.34	108.09
6	9	1248	B8N	O4-C4-N3	-2.73	115.56	119.99
3	5	3764	PSU	O2-C2-N1	-2.73	119.97	122.79
3	5	1883	OMG	O6-C6-C5	-2.73	119.34	126.53
3	5	3715	PSU	O2-C2-N1	-2.72	119.98	122.79
3	5	4872	2MG	C5-C6-N1	2.72	120.17	113.25
3	5	4671	B8T	C6-C5-C4	2.72	120.27	117.00
3	5	4500	PSU	O2-C2-N1	-2.71	119.99	122.79
3	5	1883	OMG	C5-C6-N1	2.71	120.15	113.25
3	5	4293	PSU	O2-C2-N1	-2.71	120.00	122.79
3	5	4870	OMG	C5-C6-N1	2.71	120.14	113.25
3	5	3729	PSU	O2-C2-N1	-2.70	120.00	122.79
6	9	509	OMG	C5-C6-N1	2.70	120.13	113.25
3	5	3764	PSU	C6-N1-C2	-2.70	120.18	122.69
3	5	4442	PSU	O2-C2-N1	-2.70	120.00	122.79
3	5	4870	OMG	N9-C4-N3	2.69	131.33	125.95
3	5	1683	PSU	C6-N1-C2	-2.69	120.20	122.69
3	5	2424	OMG	C5-C6-N1	2.68	120.09	113.25
3	5	4637	OMG	C5-C6-N1	2.68	120.08	113.25
3	5	729	2MG	C5-C6-N1	2.68	120.07	113.25
3	5	2050	OMG	C5-C6-N1	2.68	120.07	113.25
3	5	4550	7MG	O6-C6-C5	-2.67	121.06	127.62
3	5	4494	OMG	C5-C6-N1	2.67	120.05	113.25
3	5	4083	5MU	O4-C4-N3	-2.67	115.09	120.11
3	5	4636	PSU	O2-C2-N1	-2.67	120.04	122.79
3	5	4296	B8H	O4-C4-N3	-2.67	115.10	120.11
3	5	4550	7MG	C2-N1-C6	-2.67	120.28	125.11
3	5	4472	B8W	C5-C6-N1	-2.66	119.92	123.49
3	5	4623	OMG	C5-C6-N1	2.66	120.03	113.25
6	9	822	PSU	C6-N1-C2	-2.66	120.22	122.69
3	5	4220	6MZ	C5-N7-C8	2.66	107.63	103.45
3	5	4196	OMG	C5-C6-N1	2.66	120.03	113.25
6	9	644	OMG	C5-C6-N1	2.66	120.02	113.25
3	5	4355	E6G	C5-C6-N1	-2.66	119.93	123.49
3	5	3762	B8H	O4-C4-N3	-2.65	115.12	120.11
6	9	1081	PSU	O2-C2-N1	-2.65	120.05	122.79
3	5	237	B9B	C61-O6-C6	-2.65	113.04	117.66
3	5	2364	OMG	C5-C6-N1	2.65	120.00	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	1625	OMG	C5-C6-N1	2.65	120.00	113.25
6	9	1337	4AC	C6-C5-C4	2.65	120.19	117.00
3	5	4370	OMG	C5-C6-N1	2.65	119.99	113.25
6	9	683	OMG	C5-C6-N1	2.64	119.98	113.25
3	5	4472	B8W	C4-N9-C1'	-2.64	120.47	126.63
3	5	237	B9B	C5-N7-C8	2.63	107.59	103.45
3	5	4531	PSU	O2-C2-N1	-2.63	120.08	122.79
3	5	373	OMG	C5-C6-N1	2.62	119.93	113.25
3	5	2380	B8W	C2-N1-C6	2.62	119.61	115.96
6	9	822	PSU	O2-C2-N1	-2.61	120.09	122.79
3	5	4636	PSU	C6-C5-C4	2.61	119.94	118.17
6	9	1832	6MZ	C5-C6-N1	2.61	120.96	118.15
6	9	814	5MU	C5M-C5-C4	2.61	121.57	118.78
3	5	2424	OMG	O6-C6-C5	-2.61	119.65	126.53
3	5	1677	PSU	C6-C5-C4	2.61	119.93	118.17
3	5	1860	B8H	O4-C4-N3	-2.60	115.22	120.11
3	5	3792	OMG	C5-C6-N1	2.60	119.88	113.25
3	5	1677	PSU	O2-C2-N1	-2.60	120.11	122.79
3	5	1522	OMG	C5-C6-N1	2.60	119.86	113.25
3	5	4690	B8K	C2-N1-C6	-2.59	120.41	125.11
3	5	4872	2MG	O6-C6-C5	-2.59	119.69	126.53
1	2	37	T6A	O10-C10-N6	-2.59	119.04	123.64
3	5	2773	OMG	C5-C6-N1	2.59	119.84	113.25
3	5	1517	2MG	O6-C6-C5	-2.58	119.72	126.53
6	9	1248	B8N	C31-N3-C4	2.58	120.83	117.18
3	5	3909	OMC	O2-C2-N3	-2.57	118.28	122.33
3	5	4564	M7A	C71-N7-C5	-2.56	112.75	123.44
3	5	1574	B9B	C2-N3-C4	2.56	120.37	113.51
3	5	3899	BGH	C2'-C1'-N9	-2.55	108.95	114.14
3	5	1316	OMG	C5-C6-N1	2.55	119.73	113.25
3	5	4129	B8W	C4-N9-C1'	-2.55	120.68	126.63
3	5	3785	A2M	C2'-C1'-N9	-2.54	109.57	113.75
3	5	2754	B9B	C2-N3-C4	2.54	120.31	113.51
3	5	729	2MG	N9-C8-N7	-2.53	108.70	113.40
6	9	1219	B8Q	C31-N3-C2	2.53	121.68	117.70
3	5	4637	OMG	O6-C6-C5	-2.53	119.85	126.53
1	2	37	T6A	C5-N7-C8	2.52	107.41	103.45
3	5	4531	PSU	C6-C5-C4	2.52	119.87	118.17
3	5	2522	7MG	N9-C8-N7	2.51	106.92	103.37
3	5	2050	OMG	O6-C6-C5	-2.50	119.92	126.53
6	9	568	MMX	C5-C6-N1	2.50	114.52	110.64
3	5	3897	B8K	C2-N1-C6	-2.50	120.58	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	1625	OMG	O6-C6-C5	-2.50	119.94	126.53
3	5	4494	OMG	O6-C6-C5	-2.50	119.94	126.53
3	5	4483	B8T	C6-C5-C4	2.50	120.01	117.00
3	5	2786	B9H	O2-C2-N1	-2.50	117.21	122.78
3	5	2380	B8W	C4-N9-C1'	-2.50	120.79	126.63
3	5	4185	B8W	C5-C6-N1	-2.49	120.15	123.49
6	9	683	OMG	C8-N7-C5	2.48	108.69	104.26
6	9	1842	4AC	C6-C5-C4	2.48	119.99	117.00
3	5	4623	OMG	O6-C6-C5	-2.48	119.99	126.53
6	9	644	OMG	O6-C6-C5	-2.47	120.00	126.53
3	5	4472	B8W	C4-C5-N7	-2.47	107.75	110.58
6	9	612	PSU	C6-N1-C2	-2.47	120.40	122.69
3	5	3715	PSU	C6-N1-C2	-2.47	120.40	122.69
3	5	3792	OMG	O6-C6-C5	-2.47	120.02	126.53
3	5	2401	A2M	C2'-C1'-N9	-2.47	109.69	113.75
6	9	119	PSU	C6-N1-C2	-2.47	120.40	122.69
3	5	2297	E7G	N9-C4-N3	2.46	129.07	125.46
3	5	237	B9B	C2-N3-C4	2.46	120.10	113.51
3	5	1605	7MG	N9-C8-N7	2.46	106.85	103.37
6	9	119	PSU	O2-C2-N1	-2.46	120.25	122.79
3	5	2364	OMG	O6-C6-C5	-2.46	120.05	126.53
2	1	45	4AC	N4-C4-N3	2.46	117.86	113.87
3	5	729	2MG	O6-C6-C5	-2.46	120.05	126.53
3	5	3880	P7G	N9-C8-N7	2.45	106.85	103.37
3	5	4870	OMG	O6-C6-C5	-2.45	120.07	126.53
3	5	4564	M7A	C5-C4-N3	-2.45	120.90	126.56
6	9	814	5MU	O4-C4-N3	-2.45	115.52	120.11
3	5	4472	B8W	C2-N3-C4	2.44	120.05	113.51
3	5	4293	PSU	C6-N1-C2	-2.44	120.43	122.69
3	5	3729	PSU	C6-N1-C2	-2.44	120.43	122.69
3	5	4370	OMG	O6-C6-C5	-2.44	120.10	126.53
3	5	4442	PSU	C6-N1-C2	-2.44	120.43	122.69
3	5	4529	B8W	C2-N3-C4	2.43	120.02	113.51
3	5	373	OMG	O6-C6-C5	-2.43	120.13	126.53
6	9	1219	B8Q	C1'-N1-C6	-2.42	115.60	120.78
3	5	4371	MHG	N9-C4-N3	2.42	129.01	125.46
6	9	612	PSU	O4'-C1'-C2'	2.42	108.50	105.15
6	9	484	A2M	C2'-C1'-N9	-2.41	109.78	113.75
3	5	4196	OMG	O6-C6-C5	-2.41	120.17	126.53
3	5	4185	B8W	C2-N3-C4	2.41	119.97	113.51
3	5	4523	A2M	C2'-C1'-N9	-2.40	109.79	113.75
6	9	1806	M7A	C5-C4-N3	-2.40	121.00	126.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4129	B8W	C2-N3-C4	2.40	119.95	113.51
6	9	823	PSU	C6-N1-C2	-2.40	120.46	122.69
3	5	4355	E6G	C2-N3-C4	2.40	119.94	113.51
3	5	4628	PSU	C6-N1-C2	-2.40	120.47	122.69
3	5	2380	B8W	C2-N3-C4	2.40	119.93	113.51
3	5	4185	B8W	C4-N9-C8	2.39	108.25	105.74
3	5	1582	PSU	C6-N1-C2	-2.39	120.47	122.69
3	5	4415	1MA	N9-C4-N3	2.39	132.34	126.90
3	5	4220	6MZ	C5-C6-N1	2.39	120.71	118.15
6	9	822	PSU	O4'-C1'-C2'	2.38	108.45	105.15
3	5	2773	OMG	O6-C6-C5	-2.38	120.25	126.53
3	5	4355	E6G	C4-N9-C8	2.38	108.23	105.74
3	5	4450	PSU	C6-N1-C2	-2.38	120.49	122.69
3	5	4083	5MU	O2-C2-N1	-2.37	119.70	122.80
6	9	814	5MU	C6-C5-C4	2.37	119.97	118.02
3	5	1871	A2M	C2'-C1'-N9	-2.37	109.85	113.75
3	5	3729	PSU	C6-C5-C4	2.37	119.77	118.17
6	9	509	OMG	O6-C6-C5	-2.37	120.28	126.53
3	5	1322	1MA	C8-N7-C5	2.37	108.47	104.26
6	9	159	A2M	C2'-C1'-N9	-2.36	109.86	113.75
3	5	4500	PSU	C6-N1-C2	-2.35	120.51	122.69
3	5	1316	OMG	O6-C6-C5	-2.35	120.34	126.53
3	5	4550	7MG	N9-C4-N3	2.35	128.90	125.46
3	5	4196	OMG	C1'-N9-C8	-2.34	120.08	126.73
6	9	166	A2M	C5'-C4'-C3'	-2.34	106.79	115.21
3	5	2508	PSU	O2-C2-N1	-2.34	120.38	122.79
3	5	3899	BGH	O6-C6-C5	-2.34	121.88	127.62
2	1	45	4AC	CM7-C7-N4	2.33	119.03	115.27
6	9	1806	M7A	C4-N9-C1'	-2.33	121.20	126.63
3	5	2380	B8W	C5-C6-N1	-2.33	120.38	123.49
6	9	166	A2M	C2'-C1'-N9	-2.33	109.92	113.75
6	9	1337	4AC	C5-C4-N3	-2.32	118.97	122.60
2	1	45	4AC	C5-C4-N3	-2.31	118.98	122.60
6	9	1031	A2M	C2'-C1'-N9	-2.31	109.94	113.75
3	5	237	B9B	C4-N9-C8	2.31	108.17	105.74
3	5	1522	OMG	O6-C6-C5	-2.30	120.46	126.53
3	5	2380	B8W	C4-N9-C8	2.30	108.15	105.74
6	9	1243	PSU	C6-N1-C2	-2.30	120.56	122.69
6	9	1842	4AC	N4-C4-N3	2.29	117.59	113.87
3	5	4636	PSU	C6-N1-C2	-2.29	120.56	122.69
3	5	4472	B8W	C4-N9-C8	2.29	108.14	105.74
3	5	1574	B9B	C61-O6-C6	-2.29	113.67	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4129	B8W	C4-N9-C8	2.29	108.14	105.74
3	5	4403	PSU	O2-C2-N1	-2.29	120.43	122.79
3	5	4403	PSU	O4'-C1'-C2'	2.28	108.31	105.15
3	5	1677	PSU	C6-N1-C2	-2.28	120.57	122.69
3	5	4371	MHG	N9-C8-N7	2.28	106.60	103.37
3	5	1582	PSU	O2-C2-N1	-2.28	120.44	122.79
6	9	1842	4AC	C5-C4-N3	-2.27	119.04	122.60
3	5	4403	PSU	C6-N1-C2	-2.27	120.58	122.69
3	5	3785	A2M	O4'-C1'-C2'	-2.27	102.68	106.59
3	5	1797	E7G	N9-C8-N7	2.27	106.59	103.37
3	5	1524	A2M	C2'-C1'-N9	-2.27	110.02	113.75
3	5	4415	1MA	C8-N7-C5	2.27	108.30	104.26
3	5	4129	B8W	O6-C6-C5	2.26	119.90	117.17
3	5	4220	6MZ	C9-N6-C6	-2.26	120.75	122.85
3	5	4529	B8W	O6-C6-C5	2.26	119.90	117.17
6	9	683	OMG	O6-C6-C5	-2.25	120.59	126.53
3	5	1522	OMG	C8-N7-C5	2.24	108.26	104.26
3	5	4870	OMG	C8-N7-C5	2.24	108.26	104.26
3	5	1316	OMG	C8-N7-C5	2.24	108.25	104.26
3	5	4129	B8W	C5-C4-N9	2.24	108.25	105.81
6	9	116	OMU	C1'-N1-C2	2.24	121.61	117.59
3	5	4597	UR3	C6-N1-C2	-2.23	119.97	121.80
3	5	4623	OMG	C8-N7-C5	2.23	108.23	104.26
3	5	3792	OMG	C1'-N9-C8	-2.23	120.40	126.73
3	5	4355	E6G	C4-C5-N7	-2.22	108.05	110.58
3	5	4690	B8K	O6-C6-C5	-2.21	122.19	127.62
3	5	4550	7MG	N9-C8-N7	2.21	106.50	103.37
6	9	1081	PSU	C6-N1-C2	-2.21	120.64	122.69
3	5	2297	E7G	N9-C8-N7	2.21	106.50	103.37
3	5	4500	PSU	O4'-C1'-C2'	2.20	108.20	105.15
3	5	1517	2MG	CM2-N2-C2	-2.20	118.92	123.65
3	5	4636	PSU	O4'-C1'-C2'	2.20	108.19	105.15
3	5	4529	B8W	C5-C4-N9	2.20	108.21	105.81
6	9	1248	B8N	O4'-C1'-C2'	2.20	108.19	105.15
6	9	644	OMG	C1'-N9-C8	-2.20	120.48	126.73
3	5	1625	OMG	C1'-N9-C8	-2.20	120.49	126.73
6	9	612	PSU	C6-C5-C4	2.20	119.66	118.17
3	5	4531	PSU	C6-N1-C2	-2.20	120.65	122.69
3	5	4494	OMG	C8-N7-C5	2.19	108.16	104.26
3	5	3897	B8K	O6-C6-C5	-2.19	122.25	127.62
3	5	4370	OMG	C8-N7-C5	2.18	108.15	104.26
3	5	4185	B8W	C4-C5-N7	-2.18	108.08	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	1517	2MG	N1-C2-N3	-2.18	120.00	123.68
3	5	1574	B9B	C4-N9-C8	2.18	108.03	105.74
3	5	4185	B8W	C1'-N9-C8	2.17	131.92	127.09
3	5	4442	PSU	O4'-C1'-C2'	2.17	108.15	105.15
6	9	644	OMG	C8-N7-C5	2.17	108.12	104.26
3	5	2773	OMG	C8-N7-C5	2.17	108.12	104.26
6	9	1337	4AC	CM7-C7-N4	2.16	118.76	115.27
3	5	2508	PSU	C6-N1-C2	-2.16	120.69	122.69
3	5	4220	6MZ	C4-N9-C8	2.15	108.00	105.74
3	5	4872	2MG	N9-C4-N3	2.15	130.26	125.95
3	5	373	OMG	C8-N7-C5	2.15	108.09	104.26
5	8	14	OMU	C1'-N1-C2	2.15	121.45	117.59
3	5	4371	MHG	C21-N2-C2	-2.15	119.03	123.65
3	5	4196	OMG	C8-N7-C5	2.15	108.08	104.26
3	5	4306	OMU	O2-C2-N1	-2.15	120.00	122.80
6	9	509	OMG	C8-N7-C5	2.14	108.07	104.26
3	5	2364	OMG	C8-N7-C5	2.14	108.07	104.26
3	5	4872	2MG	C8-N7-C5	2.14	108.06	104.26
3	5	1866	UR3	C6-N1-C2	-2.13	120.06	121.80
3	5	3792	OMG	C8-N7-C5	2.12	108.04	104.26
3	5	2508	PSU	C6-C5-C4	2.12	119.61	118.17
3	5	1574	B9B	C4-C5-N7	-2.12	108.16	110.58
3	5	1534	A2M	C4-C5-N7	-2.12	108.16	110.58
3	5	4637	OMG	C8-N7-C5	2.11	108.02	104.26
6	9	1081	PSU	O4'-C1'-C2'	2.11	108.07	105.15
6	9	814	5MU	C1'-N1-C2	2.11	121.38	117.59
3	5	1625	OMG	C8-N7-C5	2.11	108.01	104.26
3	5	4500	PSU	C6-C5-C4	2.11	119.59	118.17
3	5	3899	BGH	O4'-C4'-C3'	-2.10	100.98	105.15
3	5	3782	5MC	CM5-C5-C6	-2.10	120.01	122.85
3	5	4872	2MG	C4-C5-N7	-2.10	107.34	110.67
3	5	1683	PSU	C6-C5-C4	2.10	119.59	118.17
3	5	2050	OMG	C8-N7-C5	2.09	107.98	104.26
6	9	1842	4AC	CM7-C7-N4	2.09	118.64	115.27
3	5	4293	PSU	C6-C5-C4	2.09	119.58	118.17
6	9	1851	MA6	C4-C5-N7	-2.09	108.19	110.58
6	9	823	PSU	O4'-C1'-C2'	2.08	108.03	105.15
3	5	1883	OMG	C8-N7-C5	2.08	107.97	104.26
3	5	3785	A2M	C4'-O4'-C1'	-2.08	104.87	109.47
3	5	2754	B9B	C4-C5-N7	-2.08	108.20	110.58
3	5	4637	OMG	C1'-N9-C8	-2.07	120.84	126.73
3	5	1456	B8Q	C31-N3-C2	2.07	120.95	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4628	PSU	C6-C5-C4	2.07	119.57	118.17
6	9	1337	4AC	N4-C4-N3	2.07	117.22	113.87
3	5	3718	A2M	C2'-C1'-N9	-2.07	110.35	113.75
3	5	2754	B9B	C4-N9-C8	2.06	107.90	105.74
6	9	27	A2M	C2'-C1'-N9	-2.06	110.37	113.75
6	9	116	OMU	O2-C2-N1	-2.05	120.13	122.80
3	5	2754	B9B	C2-N1-C6	2.05	118.81	115.96
3	5	1524	A2M	C4-C5-N7	-2.05	108.24	110.58
1	2	37	T6A	C4-C5-N7	-2.05	108.24	110.58
3	5	3897	B8K	N1-C2-N3	-2.04	119.58	123.32
3	5	4690	B8K	N1-C2-N3	-2.03	119.60	123.32
6	9	1374	5MC	CM5-C5-C6	-2.02	120.11	122.85
3	5	1517	2MG	C8-N7-C5	2.02	107.86	104.26
6	9	166	A2M	C2'-C3'-C4'	2.02	106.33	101.99
3	5	3867	A2M	C4-N9-C1'	2.01	131.34	126.63
3	5	1574	B9B	C5-C4-N9	2.01	108.00	105.81
6	9	668	A2M	C4-C5-N7	-2.01	108.28	110.58
3	5	4335	5MC	CM5-C5-C6	-2.01	120.13	122.85
3	5	3899	BGH	N1-C2-N3	-2.01	119.65	123.32
3	5	4083	5MU	C6-C5-C4	2.01	119.67	118.02
3	5	4872	2MG	N1-C2-N3	-2.00	120.31	123.68

There are no chirality outliers.

All (180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	333	MLZ	CD-CE-NZ-CM
3	5	237	B9B	C5-C6-O6-C61
3	5	237	B9B	N1-C6-O6-C61
3	5	237	B9B	C3'-C4'-C5'-O5'
3	5	237	B9B	O4'-C4'-C5'-O5'
3	5	398	A2M	C1'-C2'-O2'-CM'
3	5	1316	OMG	C1'-C2'-O2'-CM2
3	5	1326	A2M	C1'-C2'-O2'-CM'
3	5	1348	P4U	O4'-C4'-C5'-O5'
3	5	1574	B9B	C5-C6-O6-C61
3	5	1574	B9B	N1-C6-O6-C61
3	5	1582	PSU	C2'-C1'-C5-C4
3	5	1860	B8H	O4'-C4'-C5'-O5'
3	5	2380	B8W	C5-C6-O6-C61
3	5	2380	B8W	O4'-C4'-C5'-O5'
3	5	2424	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	5	2754	B9B	C5-C6-O6-C61
3	5	2754	B9B	N1-C6-O6-C61
3	5	2861	OMC	C1'-C2'-O2'-CM2
3	5	3723	A2M	C1'-C2'-O2'-CM'
3	5	3762	B8H	C3'-C4'-C5'-O5'
3	5	3762	B8H	O4'-C4'-C5'-O5'
3	5	3792	OMG	O4'-C4'-C5'-O5'
3	5	3867	A2M	O4'-C4'-C5'-O5'
3	5	3867	A2M	C3'-C4'-C5'-O5'
3	5	3867	A2M	C1'-C2'-O2'-CM'
3	5	3880	P7G	O4'-C4'-C5'-O5'
3	5	3897	B8K	O4'-C4'-C5'-O5'
3	5	4129	B8W	C5-C6-O6-C61
3	5	4129	B8W	N1-C6-O6-C61
3	5	4185	B8W	C5-C6-O6-C61
3	5	4185	B8W	N1-C6-O6-C61
3	5	4196	OMG	C1'-C2'-O2'-CM2
3	5	4306	OMU	C1'-C2'-O2'-CM2
3	5	4355	E6G	C5-C6-O6-C61
3	5	4355	E6G	N1-C6-O6-C61
3	5	4371	MHG	C2'-C1'-N9-C8
3	5	4371	MHG	C71-C72-C73-C75
3	5	4403	PSU	C2'-C1'-C5-C4
3	5	4403	PSU	O4'-C1'-C5-C4
3	5	4403	PSU	O4'-C1'-C5-C6
3	5	4472	B8W	C5-C6-O6-C61
3	5	4472	B8W	N1-C6-O6-C61
3	5	4500	PSU	O4'-C4'-C5'-O5'
3	5	4529	B8W	C5-C6-O6-C61
3	5	4529	B8W	N1-C6-O6-C61
3	5	4530	UR3	O4'-C4'-C5'-O5'
3	5	4530	UR3	C3'-C4'-C5'-O5'
3	5	4870	OMG	O4'-C4'-C5'-O5'
5	8	14	OMU	C1'-C2'-O2'-CM2
6	9	27	A2M	C1'-C2'-O2'-CM'
6	9	116	OMU	C1'-C2'-O2'-CM2
6	9	116	OMU	O4'-C4'-C5'-O5'
6	9	121	OMU	C1'-C2'-O2'-CM2
6	9	166	A2M	O4'-C4'-C5'-O5'
6	9	174	OMC	C1'-C2'-O2'-CM2
6	9	568	MMX	O4'-C1'-N1-C2
6	9	568	MMX	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
6	9	644	OMG	C1'-C2'-O2'-CM2
6	9	683	OMG	O4'-C4'-C5'-O5'
6	9	1678	A2M	C1'-C2'-O2'-CM'
6	9	1830	UR3	O4'-C1'-N1-C6
6	9	1830	UR3	O4'-C1'-N1-C2
6	9	1832	6MZ	N1-C6-N6-C9
6	9	1851	MA6	O4'-C4'-C5'-O5'
44	m	72	MLZ	N-CA-CB-CG
44	m	72	MLZ	C-CA-CB-CG
44	m	72	MLZ	CD-CE-NZ-CM
3	5	1348	P4U	C3'-C4'-C5'-O5'
3	5	2364	OMG	O4'-C4'-C5'-O5'
3	5	2380	B8W	C3'-C4'-C5'-O5'
3	5	2424	OMG	C3'-C4'-C5'-O5'
3	5	3764	PSU	C3'-C4'-C5'-O5'
3	5	3764	PSU	O4'-C4'-C5'-O5'
3	5	3792	OMG	C3'-C4'-C5'-O5'
3	5	4500	PSU	C3'-C4'-C5'-O5'
3	5	4637	OMG	C3'-C4'-C5'-O5'
3	5	4870	OMG	C3'-C4'-C5'-O5'
6	9	116	OMU	C3'-C4'-C5'-O5'
6	9	166	A2M	C3'-C4'-C5'-O5'
6	9	568	MMX	C3'-C4'-C5'-O5'
6	9	668	A2M	C3'-C4'-C5'-O5'
6	9	683	OMG	C3'-C4'-C5'-O5'
3	5	2380	B8W	N1-C6-O6-C61
3	5	1677	PSU	C3'-C4'-C5'-O5'
3	5	1677	PSU	O4'-C4'-C5'-O5'
3	5	1797	E7G	O4'-C4'-C5'-O5'
3	5	3880	P7G	C3'-C4'-C5'-O5'
3	5	4296	B8H	C3'-C4'-C5'-O5'
3	5	4296	B8H	O4'-C4'-C5'-O5'
6	9	568	MMX	O4'-C4'-C5'-O5'
6	9	1703	OMC	O4'-C4'-C5'-O5'
3	5	4355	E6G	C62-C61-O6-C6
3	5	3701	OMC	C2'-C1'-N1-C6
3	5	1860	B8H	C3'-C4'-C5'-O5'
3	5	3729	PSU	O4'-C4'-C5'-O5'
3	5	3785	A2M	O4'-C4'-C5'-O5'
3	5	3785	A2M	C3'-C4'-C5'-O5'
6	9	1851	MA6	C3'-C4'-C5'-O5'
3	5	3897	B8K	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	5	4371	MHG	O4'-C4'-C5'-O5'
3	5	4531	PSU	O4'-C4'-C5'-O5'
6	9	159	A2M	C3'-C4'-C5'-O5'
6	9	1243	PSU	O4'-C4'-C5'-O5'
6	9	668	A2M	O4'-C4'-C5'-O5'
3	5	2297	E7G	C72-C71-N7-C8
3	5	237	B9B	O6-C61-C62-C63
3	5	2364	OMG	C3'-C4'-C5'-O5'
3	5	2422	OMC	O4'-C4'-C5'-O5'
3	5	2786	B9H	C32-C31-N3-C2
3	5	1348	P4U	O4-C41-C42-C43
44	m	72	MLZ	CE-CD-CG-CB
3	5	1909	P7G	C72-C71-N7-C8
3	5	398	A2M	O4'-C4'-C5'-O5'
3	5	1797	E7G	C3'-C4'-C5'-O5'
6	9	1703	OMC	C3'-C4'-C5'-O5'
3	5	1348	P4U	N3-C4-O4-C41
3	5	3701	OMC	C2'-C1'-N1-C2
3	5	4637	OMG	O4'-C4'-C5'-O5'
3	5	3718	A2M	C1'-C2'-O2'-CM'
3	5	4415	1MA	C3'-C4'-C5'-O5'
3	5	4531	PSU	C3'-C4'-C5'-O5'
3	5	3701	OMC	O4'-C1'-N1-C6
6	9	1832	6MZ	C5-C6-N6-C9
3	5	4872	2MG	O4'-C4'-C5'-O5'
6	9	159	A2M	O4'-C4'-C5'-O5'
6	9	517	OMC	O4'-C4'-C5'-O5'
3	5	4870	OMG	C4'-C5'-O5'-P
3	5	2754	B9B	C62-C61-O6-C6
3	5	3785	A2M	C3'-C2'-O2'-CM'
3	5	2754	B9B	C4'-C5'-O5'-P
3	5	3897	B8K	C4'-C5'-O5'-P
6	9	644	OMG	C4'-C5'-O5'-P
1	2	37	T6A	C13-C12-C14-C15
3	5	1677	PSU	O4'-C1'-C5-C4
3	5	4450	PSU	O4'-C1'-C5-C4
6	9	1248	B8N	O4'-C1'-C5-C4
3	5	3701	OMC	O4'-C1'-N1-C2
3	5	4371	MHG	C3'-C4'-C5'-O5'
3	5	373	OMG	C4'-C5'-O5'-P
6	9	1337	4AC	O4'-C4'-C5'-O5'
3	5	3729	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	5	1524	A2M	C3'-C2'-O2'-CM'
3	5	2363	A2M	C3'-C2'-O2'-CM'
3	5	4370	OMG	C3'-C2'-O2'-CM2
3	5	3880	P7G	N7-C71-C72-C73
3	5	1534	A2M	C4'-C5'-O5'-P
3	5	4194	I4U	O4'-C4'-C5'-O5'
3	5	4355	E6G	O4'-C4'-C5'-O5'
3	5	1326	A2M	C4'-C5'-O5'-P
3	5	1625	OMG	C4'-C5'-O5'-P
3	5	3887	OMC	C4'-C5'-O5'-P
3	5	4636	PSU	C4'-C5'-O5'-P
1	2	37	T6A	O4'-C4'-C5'-O5'
3	5	1883	OMG	C3'-C4'-C5'-O5'
3	5	1909	P7G	C72-C71-N7-C5
3	5	3785	A2M	C1'-C2'-O2'-CM'
6	9	1031	A2M	C1'-C2'-O2'-CM'
3	5	4500	PSU	C4'-C5'-O5'-P
6	9	1243	PSU	C3'-C4'-C5'-O5'
3	5	4636	PSU	O4'-C1'-C5-C6
3	5	3880	P7G	C72-C71-N7-C8
3	5	3909	OMC	C2'-C1'-N1-C6
6	9	1219	B8Q	C2'-C1'-N1-C6
3	5	1574	B9B	C62-C61-O6-C6
6	9	1678	A2M	O4'-C4'-C5'-O5'
6	9	668	A2M	C2'-C1'-N9-C8
3	5	4371	MHG	C72-C73-C74-C76
3	5	4371	MHG	C75-C73-C74-C76
3	5	4636	PSU	C2'-C1'-C5-C6
3	5	1524	A2M	O4'-C1'-N9-C8
6	9	1219	B8Q	C2'-C1'-N1-C2
3	5	4494	OMG	C3'-C2'-O2'-CM2
3	5	4220	6MZ	N1-C6-N6-C9
3	5	3909	OMC	C2'-C1'-N1-C2
6	9	814	5MU	C2'-C1'-N1-C2
3	5	4671	B8T	C4'-C5'-O5'-P
6	9	1081	PSU	C4'-C5'-O5'-P
3	5	2786	B9H	C32-C31-N3-C4
3	5	4636	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

62 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	9	1851	MA6	1	0
3	5	1574	B9B	1	0
3	5	2522	7MG	1	0
3	5	4620	OMU	2	0
3	5	4415	1MA	1	0
3	5	2363	A2M	1	0
6	9	174	OMC	1	0
6	9	644	OMG	1	0
3	5	1605	7MG	1	0
3	5	3825	A2M	1	0
6	9	27	A2M	1	0
3	5	4306	OMU	1	0
3	5	4637	OMG	2	0
3	5	2424	OMG	1	0
6	9	683	OMG	1	0
3	5	3897	B8K	2	0
3	5	1524	A2M	1	0
6	9	116	OMU	2	0
6	9	568	MMX	1	0
3	5	4872	2MG	1	0
3	5	1683	PSU	3	0
3	5	4536	OMC	1	0
3	5	4450	PSU	1	0
9	C	333	MLZ	1	0
6	9	612	PSU	1	0
6	9	484	A2M	1	0
3	5	4564	M7A	1	0
6	9	1031	A2M	1	0
3	5	4500	PSU	1	0
3	5	4472	B8W	2	0
3	5	1871	A2M	1	0
3	5	729	2MG	2	0
3	5	1456	B8Q	1	0
3	5	3867	A2M	2	0
3	5	4220	6MZ	1	0
6	9	814	5MU	1	0
1	2	37	T6A	3	0
3	5	3762	B8H	1	0
6	9	1678	A2M	2	0
6	9	121	OMU	2	0
3	5	3909	OMC	1	0
3	5	4636	PSU	1	0
6	9	1830	UR3	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	5	4870	OMG	1	0
3	5	2773	OMG	1	0
3	5	398	A2M	1	0
3	5	2754	B9B	1	0
3	5	1326	A2M	2	0
3	5	4296	B8H	1	0
3	5	3718	A2M	3	0
3	5	3723	A2M	4	0
3	5	1316	OMG	1	0
3	5	1534	A2M	1	0
3	5	1866	UR3	1	0
3	5	4083	5MU	1	0
6	9	509	OMG	1	0
3	5	4550	7MG	1	0
6	9	166	A2M	1	0
3	5	3785	A2M	2	0
5	8	14	OMU	2	0
3	5	4523	A2M	1	0
3	5	1860	B8H	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 304 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
81	MQ6	5	5294	-	40,42,42	1.27	5 (12%)	40,65,65	2.64	9 (22%)

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	MQ6	5	5294	-	-	14/26/73/73	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	5	5294	MQ6	O37-C06	-3.48	1.36	1.43
81	5	5294	MQ6	O14-C12	2.40	1.38	1.34
81	5	5294	MQ6	C30-C31	2.16	1.35	1.32
81	5	5294	MQ6	C17-C16	2.11	1.54	1.51
81	5	5294	MQ6	C24-C23	-2.05	1.49	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	5	5294	MQ6	O37-C06-C05	-12.42	89.01	108.88
81	5	5294	MQ6	O37-C06-C07	6.16	123.42	109.38
81	5	5294	MQ6	O14-C12-C06	4.87	120.18	111.24
81	5	5294	MQ6	C23-C22-C21	-3.49	111.78	119.35
81	5	5294	MQ6	C28-C29-N25	2.58	107.64	103.94
81	5	5294	MQ6	C15-O14-C12	2.50	121.17	117.24
81	5	5294	MQ6	C20-C21-C22	-2.36	117.55	121.10
81	5	5294	MQ6	O14-C12-O13	-2.26	119.95	123.95
81	5	5294	MQ6	C21-C22-C17	2.04	122.06	119.49

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	5	5294	MQ6	C31-C15-O14-C12
81	5	5294	MQ6	C07-C06-C12-O13
81	5	5294	MQ6	C07-C06-C12-O14
81	5	5294	MQ6	C06-C12-O14-C15
81	5	5294	MQ6	C30-C31-O32-C33
81	5	5294	MQ6	O13-C12-O14-C15
81	5	5294	MQ6	C07-C08-O10-C11
81	5	5294	MQ6	O09-C08-O10-C11
81	5	5294	MQ6	O37-C06-C07-C08
81	5	5294	MQ6	C05-C06-C12-O13
81	5	5294	MQ6	C05-C06-C12-O14

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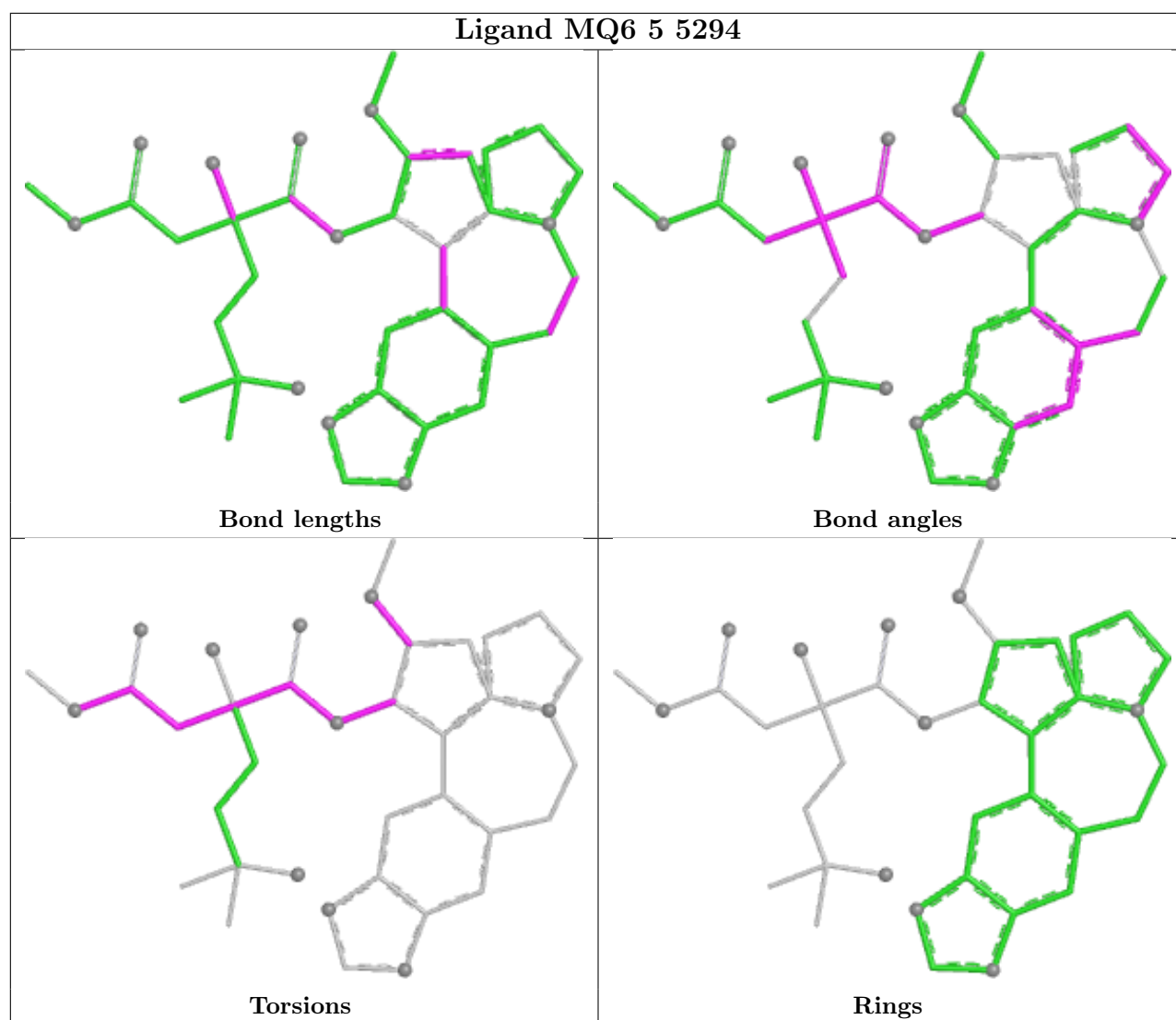
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Mol	Chain	Res	Type	Atoms
81	5	5294	MQ6	O37-C06-C12-O14
81	5	5294	MQ6	C06-C07-C08-O10
81	5	5294	MQ6	C06-C07-C08-O09

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	5	24
6	9	11

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.43
1	5	1252:C	O3'	1271:G	P	35.31
1	5	1219:G	O3'	1233:G	P	20.31
1	5	4101:C	O3'	4107:G	P	17.50
1	5	1407:G	O3'	1410:C	P	17.49
1	9	697:G	O3'	729:C	P	17.38
1	9	834:C	O3'	841:G	P	17.21
1	5	523:C	O3'	638:G	P	17.20
1	9	756:C	O3'	788:G	P	17.09
1	9	1417:C	O3'	1423:C	P	16.92
1	5	3949:A	O3'	4060:U	P	16.50
1	5	990:U	O3'	1064:G	P	16.15
1	9	323:C	O3'	329:G	P	16.11
1	9	1761:U	O3'	1771:G	P	15.92
1	5	4138:C	O3'	4146:G	P	15.81
1	5	1696:C	O3'	1720:C	P	15.03
1	5	760:G	O3'	904:C	P	14.80
1	5	4777:C	O3'	4859:C	P	14.59
1	9	130:G	O3'	140:U	P	14.50
1	5	5022:U	O3'	5028:G	P	13.85
1	5	1364:U	O3'	1368:A	P	13.70
1	5	2901:G	O3'	3597:G	P	13.31
1	5	182:G	O3'	189:G	P	10.59
1	5	1180:C	O3'	1183:C	P	9.14
1	5	4729:A	O3'	4735:G	P	9.10
1	9	225:G	O3'	287:U	P	7.51
1	9	745:C	O3'	749:U	P	6.75
1	9	736:C	O3'	743:U	P	6.58
1	5	512:U	O3'	515:C	P	6.30
1	5	500:G	O3'	504:G	P	5.97
1	9	1432:U	O3'	1438:A	P	4.94
1	5	4740:G	O3'	4743:G	P	3.98
1	5	1100:U	O3'	1168:G	P	3.65
1	5	1239:G	O3'	1244:G	P	3.12
1	5	4899:G	O3'	4902:C	P	3.12

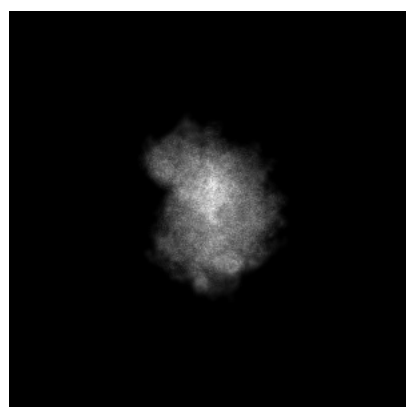
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26445. These allow visual inspection of the internal detail of the map and identification of artifacts.

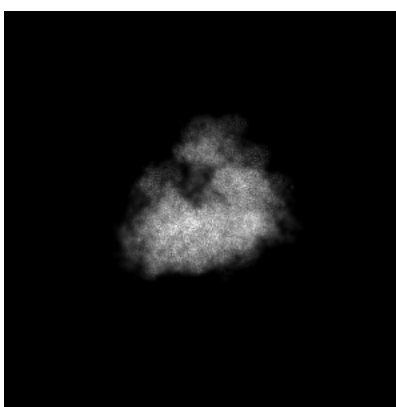
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

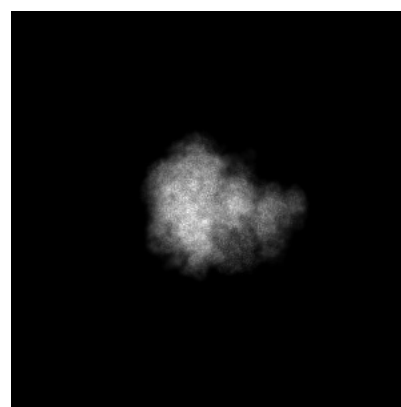
6.1.1 Primary map



X



Y

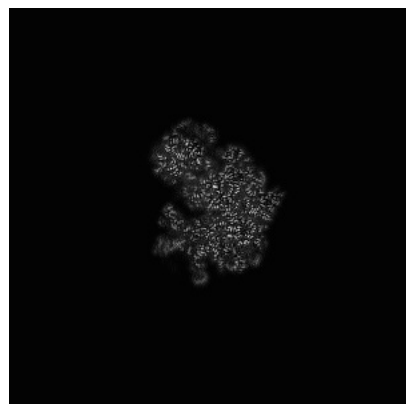


Z

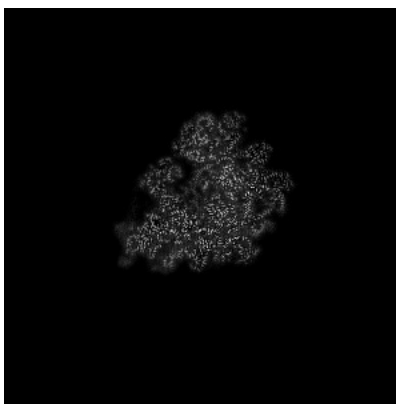
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

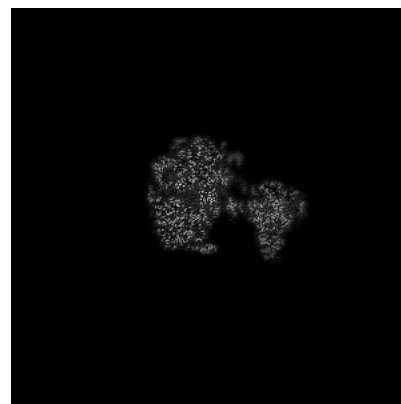
6.2.1 Primary map



X Index: 240



Y Index: 240

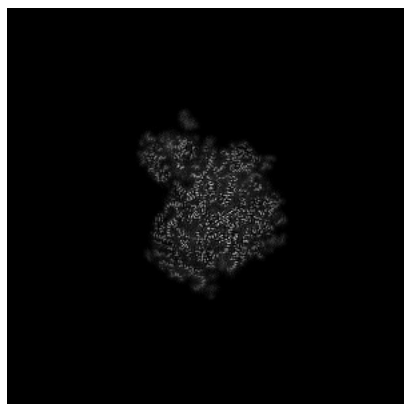


Z Index: 240

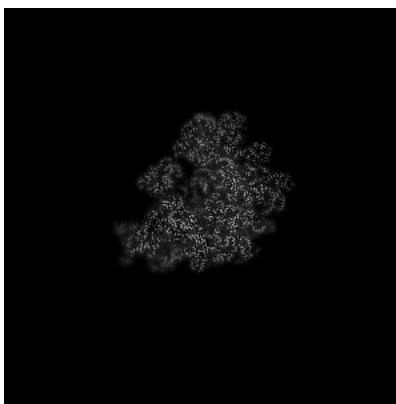
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

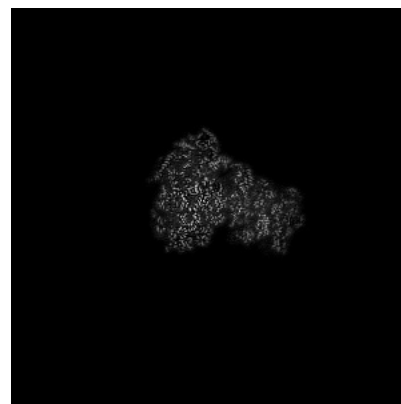
6.3.1 Primary map



X Index: 221



Y Index: 242

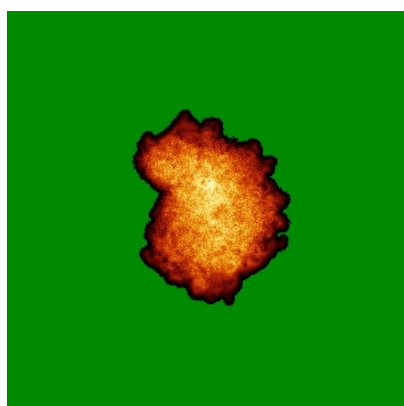


Z Index: 255

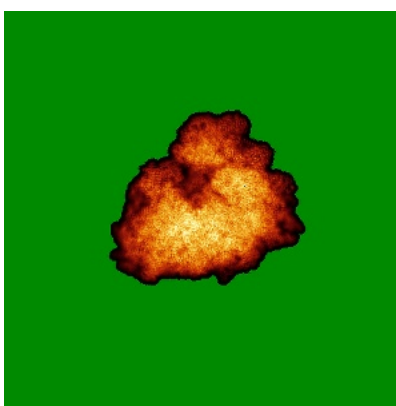
The images above show the largest variance slices of the map in three orthogonal directions.

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

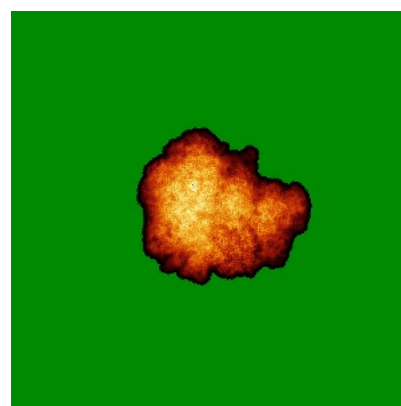
6.4.1 Primary map



X



Y

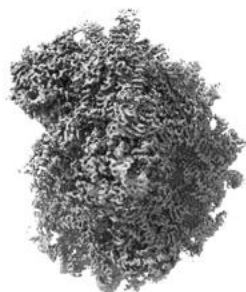


Z

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](#)

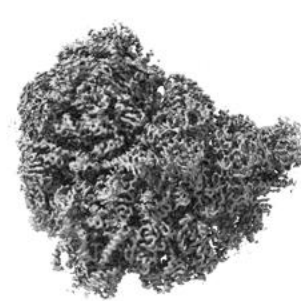
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

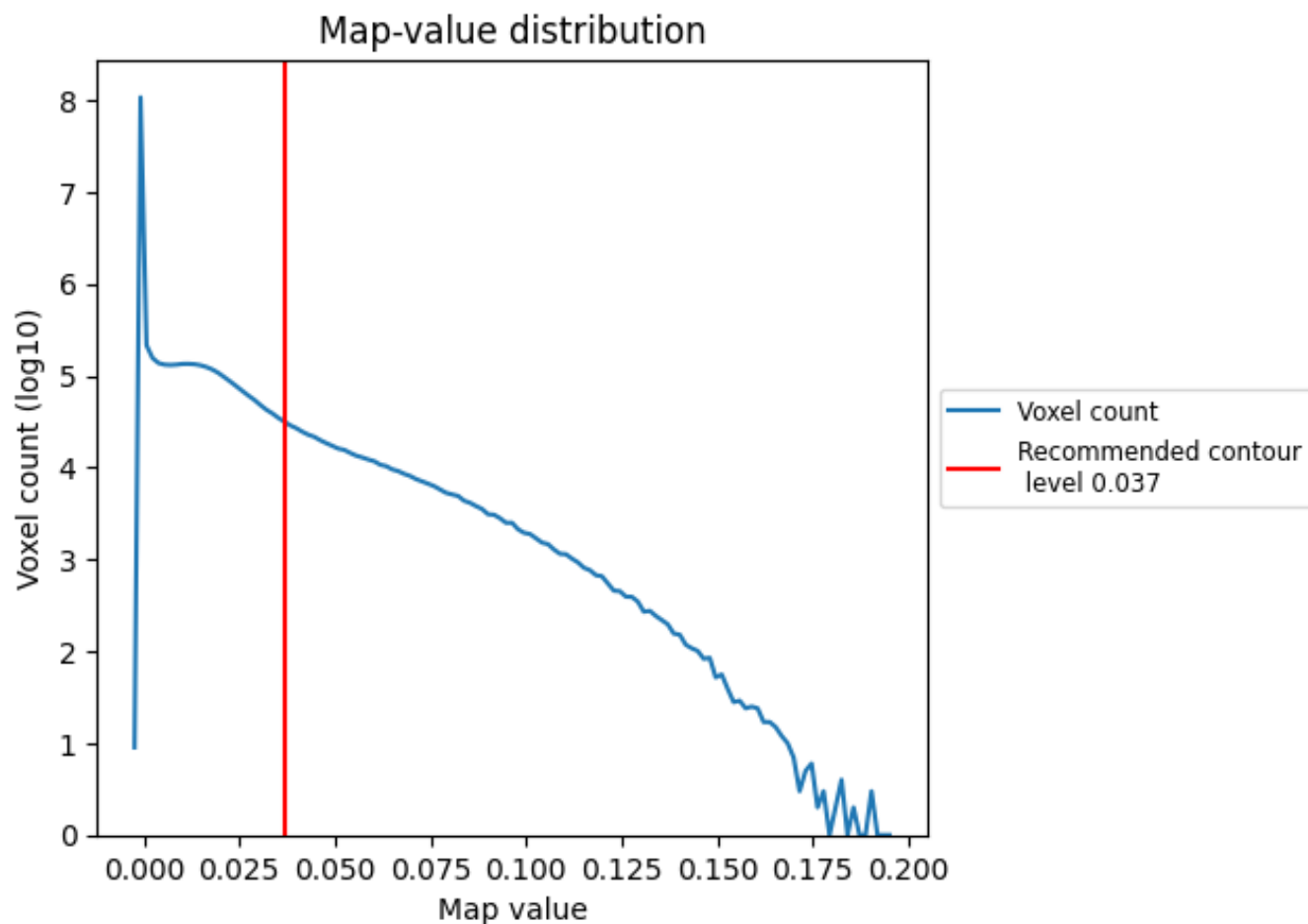
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

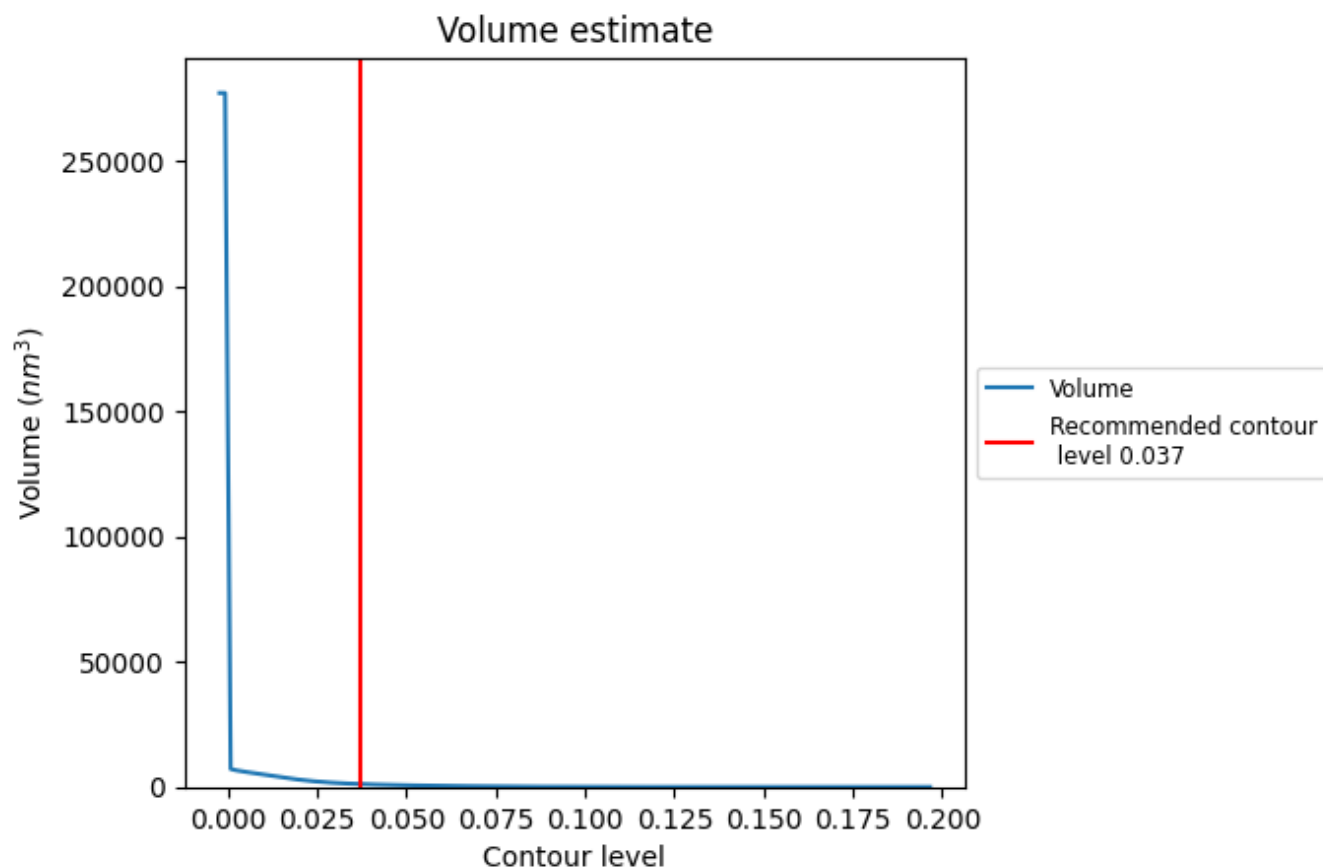
This section contains the results of statistical analysis of the map.

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.

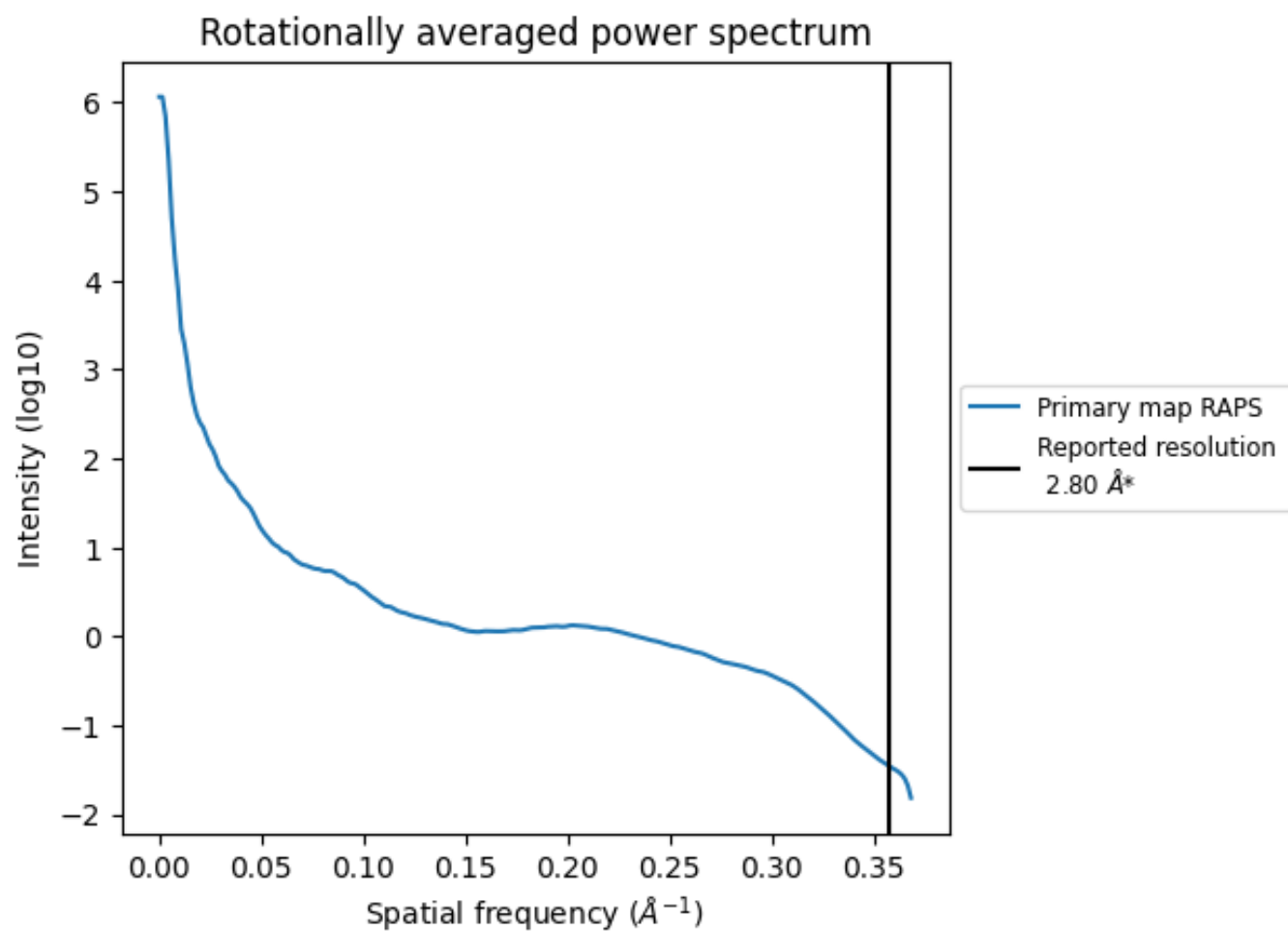
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1162 nm^3 ; this corresponds to an approximate mass of 1050 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 0.357 Å⁻¹

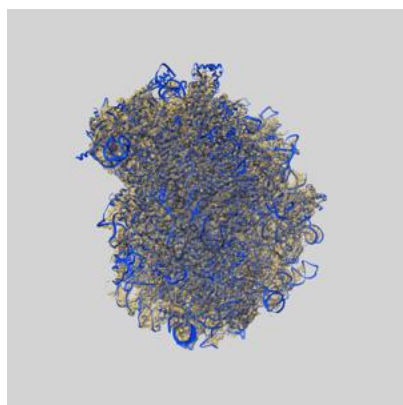
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

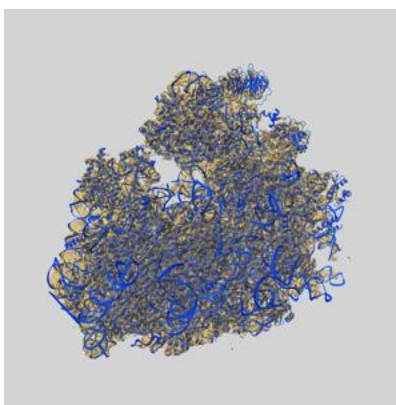
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26445 and PDB model 7UCK. Per-residue inclusion information can be found in section [3](#) on page [22](#).

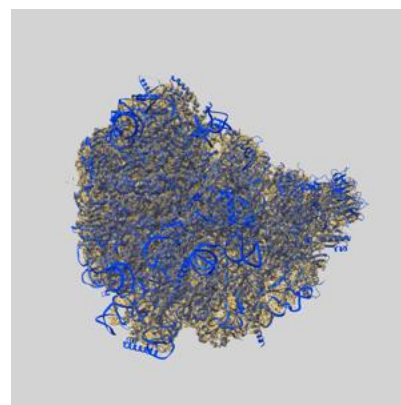
9.1 Map-model overlay [i](#)



X



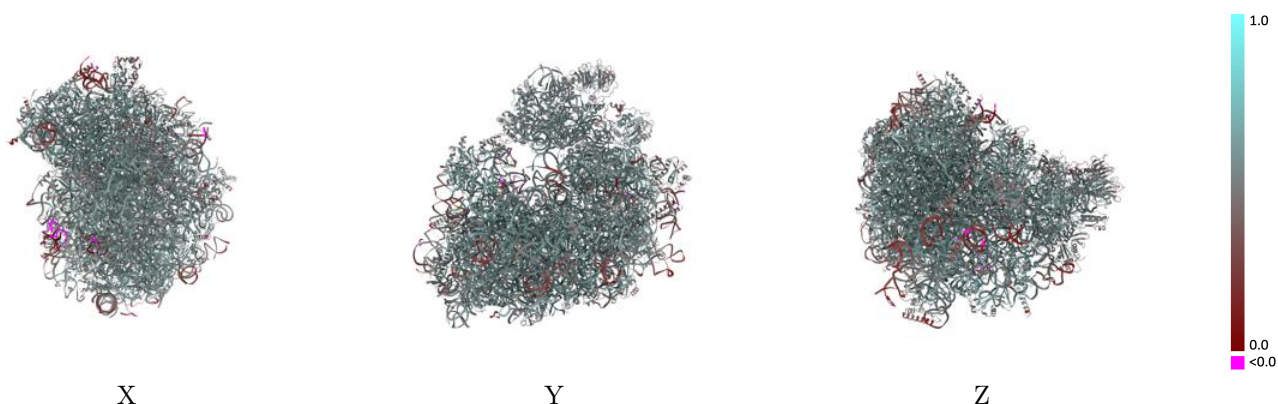
Y



Z

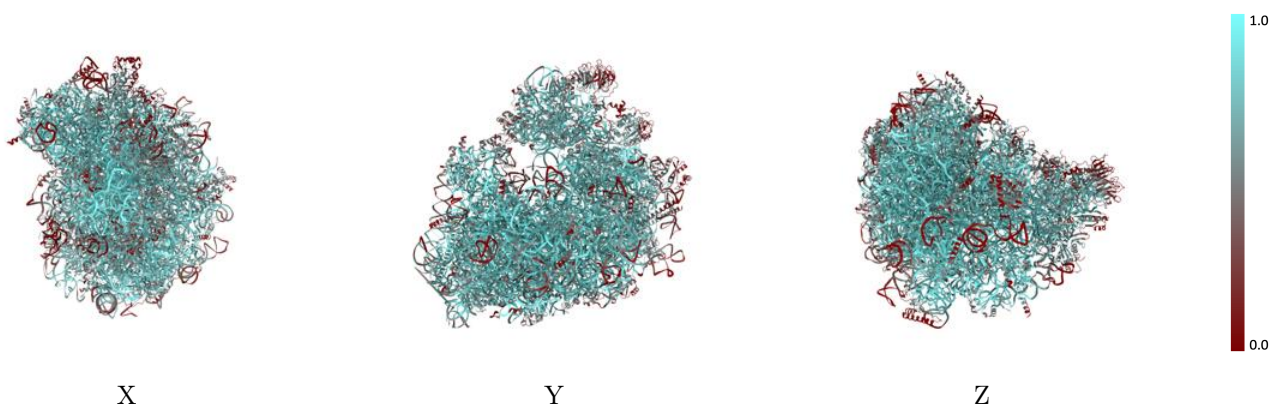
The images above show the 3D surface view of the map at the recommended contour level 0.037 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



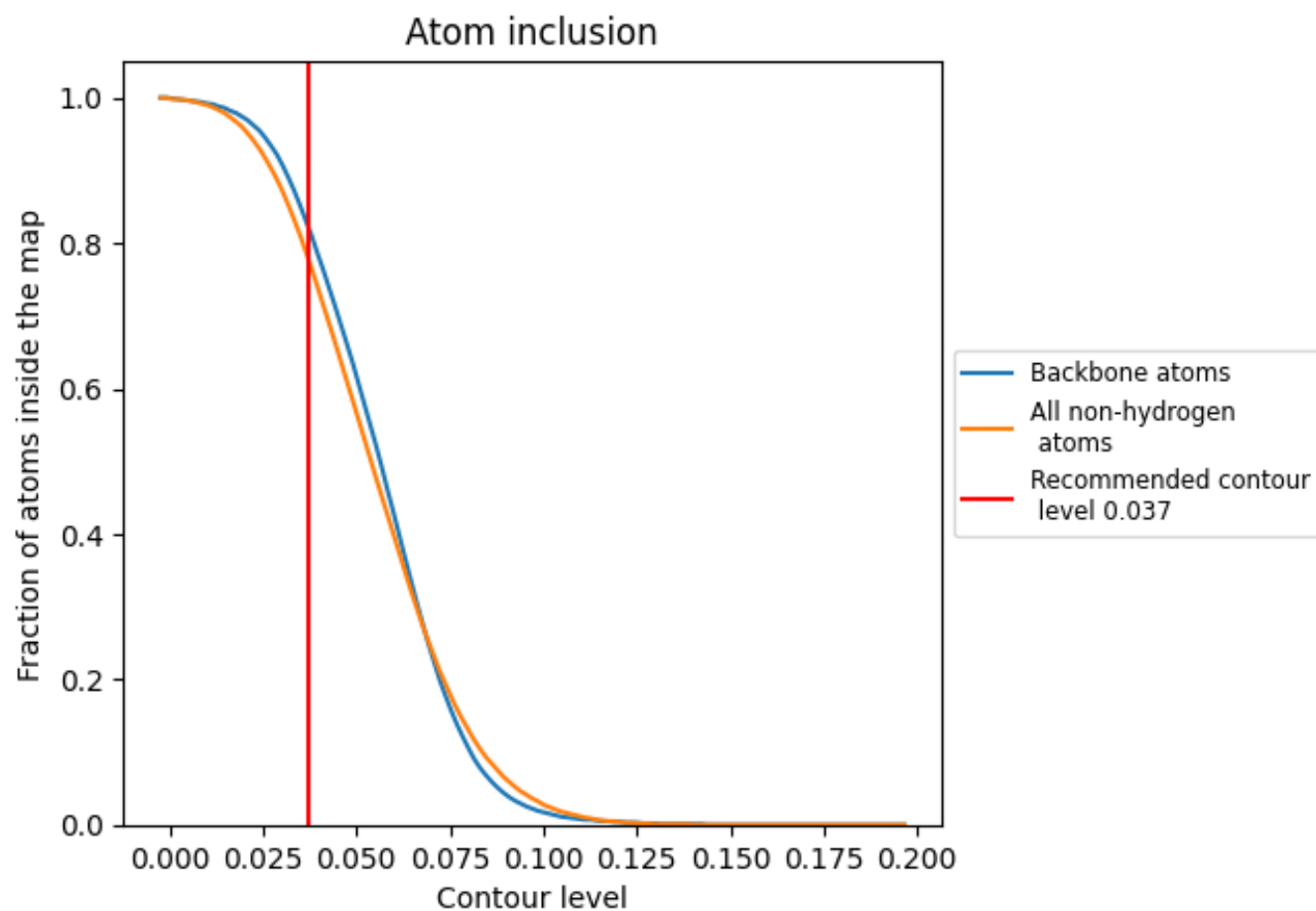
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.037).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7810	 0.5480
1	 0.9170	 0.5710
2	 0.4110	 0.5020
5	 0.8450	 0.5480
7	 0.9200	 0.5820
8	 0.8760	 0.5650
9	 0.8550	 0.5460
A	 0.8750	 0.5890
AA	 0.5810	 0.5490
Aa	 0.7760	 0.5540
B	 0.7290	 0.5740
BB	 0.6570	 0.5410
Bb	 0.5670	 0.5220
C	 0.8220	 0.5720
CC	 0.7270	 0.5640
Cc	 0.5130	 0.4950
D	 0.6320	 0.5460
DD	 0.5910	 0.5160
Dd	 0.8390	 0.5710
E	 0.7140	 0.5420
EE	 0.7840	 0.5690
Ee	 0.5750	 0.5190
F	 0.8690	 0.5750
FF	 0.6510	 0.5330
G	 0.5690	 0.5200
GG	 0.5460	 0.4980
Gg	 0.3380	 0.4730
H	 0.6070	 0.5480
HH	 0.3700	 0.4780
I	 0.6420	 0.5480
II	 0.7610	 0.5540
J	 0.5230	 0.5080
JJ	 0.7540	 0.5570
KK	 0.5340	 0.4910
L	 0.6920	 0.5400



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Chain	Atom inclusion	Q-score
LL	 0.8160	 0.5770
M	 0.7560	 0.5510
N	 0.9090	 0.5940
NN	 0.7920	 0.5700
O	 0.8140	 0.5680
OO	 0.7130	 0.5460
P	 0.7850	 0.5790
PP	 0.5230	 0.5030
Q	 0.8700	 0.5930
QQ	 0.7080	 0.5370
R	 0.7610	 0.5420
RR	 0.4210	 0.5000
S	 0.8200	 0.5780
SS	 0.5770	 0.5160
T	 0.7650	 0.5560
TT	 0.6660	 0.5380
U	 0.5400	 0.5040
UU	 0.5030	 0.4950
V	 0.7220	 0.5730
VV	 0.5920	 0.5590
W	 0.5160	 0.4740
WW	 0.8260	 0.5840
X	 0.6660	 0.5450
XX	 0.7820	 0.5750
Y	 0.6420	 0.5410
YY	 0.6530	 0.5350
Z	 0.6530	 0.5460
ZZ	 0.4490	 0.5020
a	 0.8650	 0.6000
b	 0.6970	 0.5320
c	 0.6910	 0.5390
d	 0.6980	 0.5630
e	 0.8580	 0.5920
f	 0.8930	 0.5900
g	 0.8020	 0.5640
h	 0.6180	 0.5280
i	 0.6680	 0.5350
j	 0.9140	 0.5980
k	 0.4520	 0.5000
l	 0.8270	 0.5740
m	 0.7100	 0.5630
n	 0.9130	 0.5840

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Chain	Atom inclusion	Q-score
o	 0.7530	 0.5730
p	 0.8010	 0.5630
r	 0.8140	 0.5810