



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 04:40 AM EDT

PDB ID : 6MTD / pdb_00006mtd
EMDB ID : EMD-9240
Title : Rabbit 80S ribosome with eEF2 and SERBP1 (unrotated state with 40S head swivel)
Authors : Brown, A.; Baird, M.R.; Yip, M.C.J.; Murray, J.; Shao, S.
Deposited on : 2018-10-19
Resolution : 3.30 Å(reported)
Based on initial model : 5LZV

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

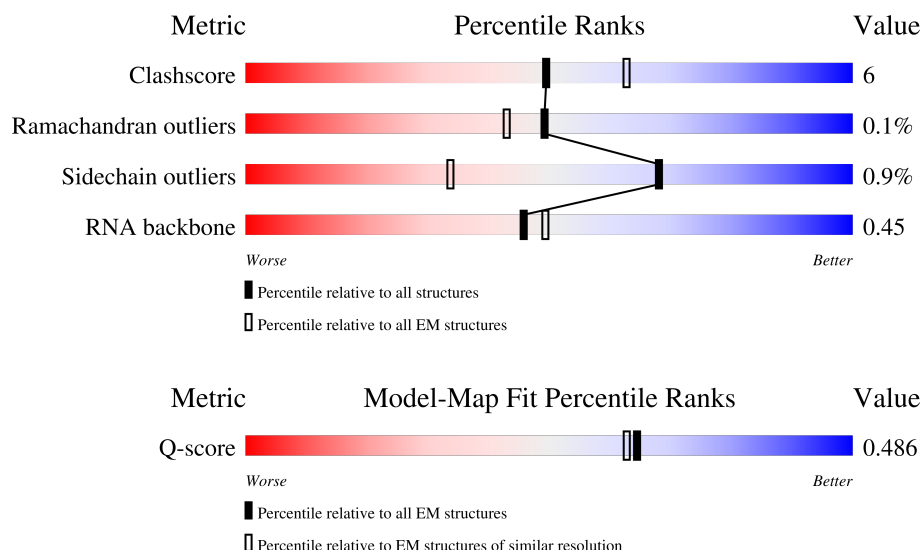
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	5	3597	
2	7	120	
3	8	151	

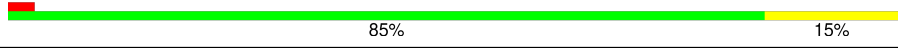
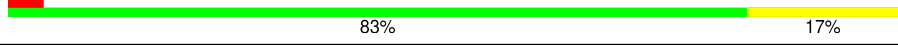
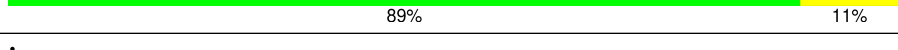
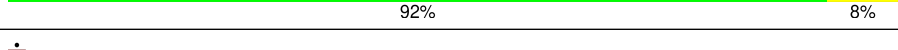
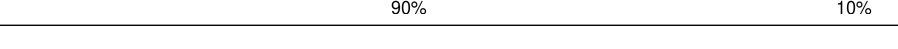
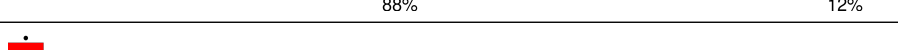
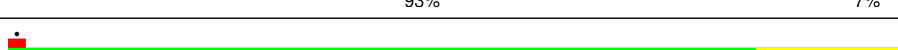
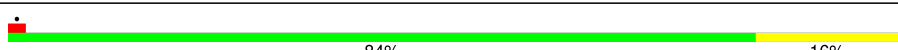
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Mol	Chain	Length	Quality of chain
4	A	248	
5	B	394	
6	C	362	
7	D	293	
8	E	291	
9	F	225	
10	G	319	
11	H	190	
12	I	214	
13	J	170	
14	L	210	
15	M	138	
16	N	203	
17	O	199	
18	P	153	
19	Q	187	
20	R	180	
21	S	176	
22	T	159	
23	U	99	
24	V	131	
25	W	157	
26	X	118	
27	Y	134	
28	Z	135	

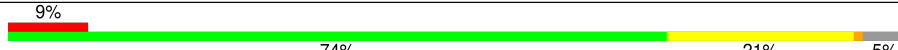
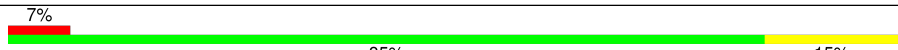
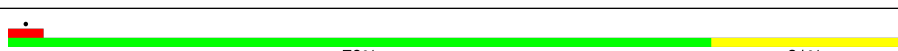
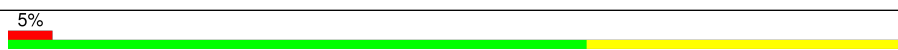
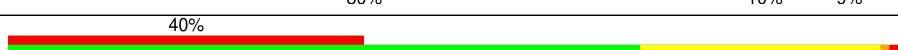
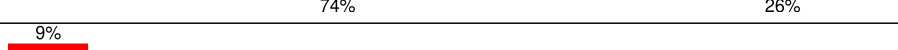
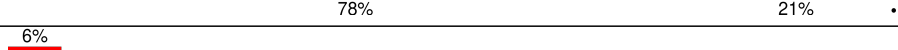
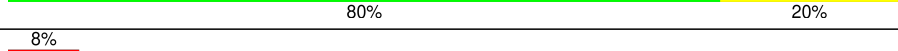
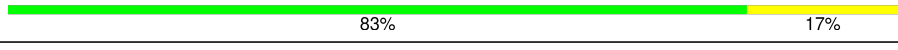
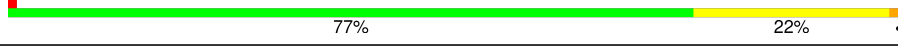
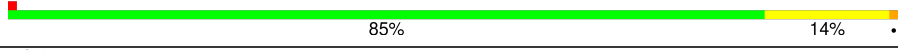
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Mol	Chain	Length	Quality of chain
29	a	147	
30	b	245	
31	c	98	
32	d	107	
33	e	128	
34	f	109	
35	g	114	
36	h	122	
37	i	102	
38	j	86	
39	k	69	
40	l	50	
41	m	52	
42	n	25	
43	o	103	
44	p	91	
45	r	124	
46	s	196	
47	t	153	
48	u	206	
49	v	839	
50	w	26	
51	9	1698	
52	AA	217	
53	BB	213	

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Mol	Chain	Length	Quality of chain
54	CC	221	
55	DD	228	
56	EE	262	
57	FF	204	
58	GG	237	
59	HH	194	
60	II	206	
61	JJ	185	
62	KK	96	
63	LL	158	
64	MM	117	
65	NN	149	
66	OO	136	
67	PP	120	
68	QQ	142	
69	RR	132	
70	SS	144	
71	TT	141	
72	UU	100	
73	VV	83	
74	WW	129	
75	XX	141	
76	YY	124	
77	ZZ	75	
78	aa	101	

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Mol	Chain	Length	Quality of chain
79	bb	83	
80	cc	62	
81	dd	55	
82	ee	55	
83	ff	68	
84	gg	313	

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 222072 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 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3597	Total	C	N	O	P	0	0
			77254	34469	14127	25061	3597		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	151	Total	C	N	O	P	0	0
			3209	1433	564	1062	150		

- Molecule 4 is a protein called uL2.

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

- Molecule 5 is a protein called uL3.

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

- Molecule 6 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	362	Total	C	N	O	S	0	0
			2884	1813	577	480	14		

- Molecule 7 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 8 is a protein called eL6.

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

- Molecule 9 is a protein called uL30.

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

- Molecule 10 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

- Molecule 11 is a protein called uL6.

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

- Molecule 12 is a protein called uL16.

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

- Molecule 13 is a protein called uL5.

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

- Molecule 14 is a protein called eL13.

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

- Molecule 15 is a protein called eL14.

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

- Molecule 16 is a protein called eL15.

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

- Molecule 17 is a protein called uL13.

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

- Molecule 18 is a protein called uL22.

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

- Molecule 19 is a protein called eL18.

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

- Molecule 20 is a protein called eL19.

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

- Molecule 21 is a protein called eL20.

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

- Molecule 22 is a protein called eL21.

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

- Molecule 23 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 24 is a protein called uL14.

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

- Molecule 25 is a protein called eL24.

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

- Molecule 26 is a protein called uL23.

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

- Molecule 27 is a protein called uL24.

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

- Molecule 28 is a protein called eL27.

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

- Molecule 29 is a protein called uL15.

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

- Molecule 30 is a protein called eL29.

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

- Molecule 31 is a protein called eL30.

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

- Molecule 32 is a protein called eL31.

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

- Molecule 33 is a protein called eL32.

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

- Molecule 34 is a protein called eL33.

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

- Molecule 35 is a protein called eL34.

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

- Molecule 36 is a protein called uL29.

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

- Molecule 37 is a protein called eL36.

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

- Molecule 38 is a protein called eL37.

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

- Molecule 39 is a protein called eL38.

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

- Molecule 40 is a protein called eL39.

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

- Molecule 41 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 42 is a protein called eL41.

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

- Molecule 43 is a protein called eL42.

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

- Molecule 44 is a protein called eL43.

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

- Molecule 45 is a protein called eL28.

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

- Molecule 46 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 47 is a protein called eL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 48 is a protein called uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	206	Total	C	N	O	S	0	0
			1654	1058	297	291	8		

- Molecule 49 is a protein called eEF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	839	Total	C	N	O	S	0	0
			6544	4162	1122	1216	44		

- Molecule 50 is a protein called SERBP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	w	26	Total	C	N	O	0	0
			216	129	43	44		

- Molecule 51 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1698	Total	C	N	O	P	0	0
			36263	16190	6509	11867	1697		

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	II	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	MM	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	ff	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	5	198	Total	Mg	0
			198	198	
85	7	7	Total	Mg	0
			7	7	
85	8	6	Total	Mg	0
			6	6	
85	A	1	Total	Mg	0
			1	1	
85	B	1	Total	Mg	0
			1	1	
85	P	1	Total	Mg	0
			1	1	
85	V	1	Total	Mg	0
			1	1	
85	a	1	Total	Mg	0
			1	1	
85	g	1	Total	Mg	0
			1	1	
85	j	1	Total	Mg	0
			1	1	
85	v	1	Total	Mg	0
			1	1	
85	9	74	Total	Mg	0
			74	74	
85	SS	2	Total	Mg	0
			2	2	
85	TT	1	Total	Mg	0
			1	1	
85	dd	1	Total	Mg	0
			1	1	

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

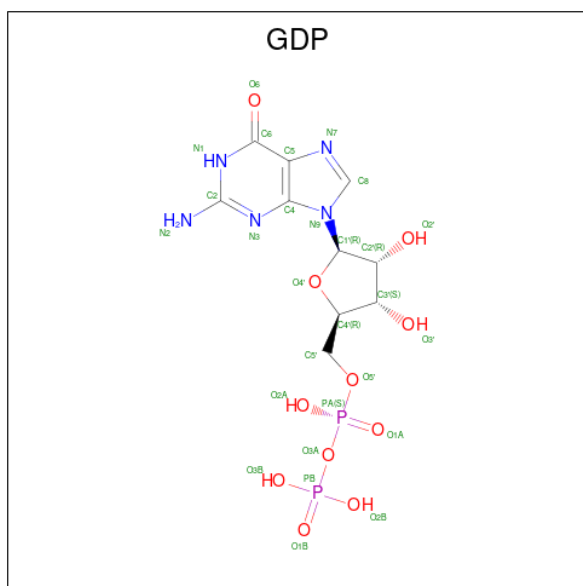
Mol	Chain	Residues	Atoms		AltConf
86	g	1	Total	Zn	0
			1	1	
86	j	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
86	m	1	Total	Zn	0
			1	1	
86	o	1	Total	Zn	0
			1	1	
86	p	1	Total	Zn	0
			1	1	
86	aa	1	Total	Zn	0
			1	1	
86	dd	1	Total	Zn	0
			1	1	
86	ff	1	Total	Zn	0
			1	1	

- Molecule 87 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

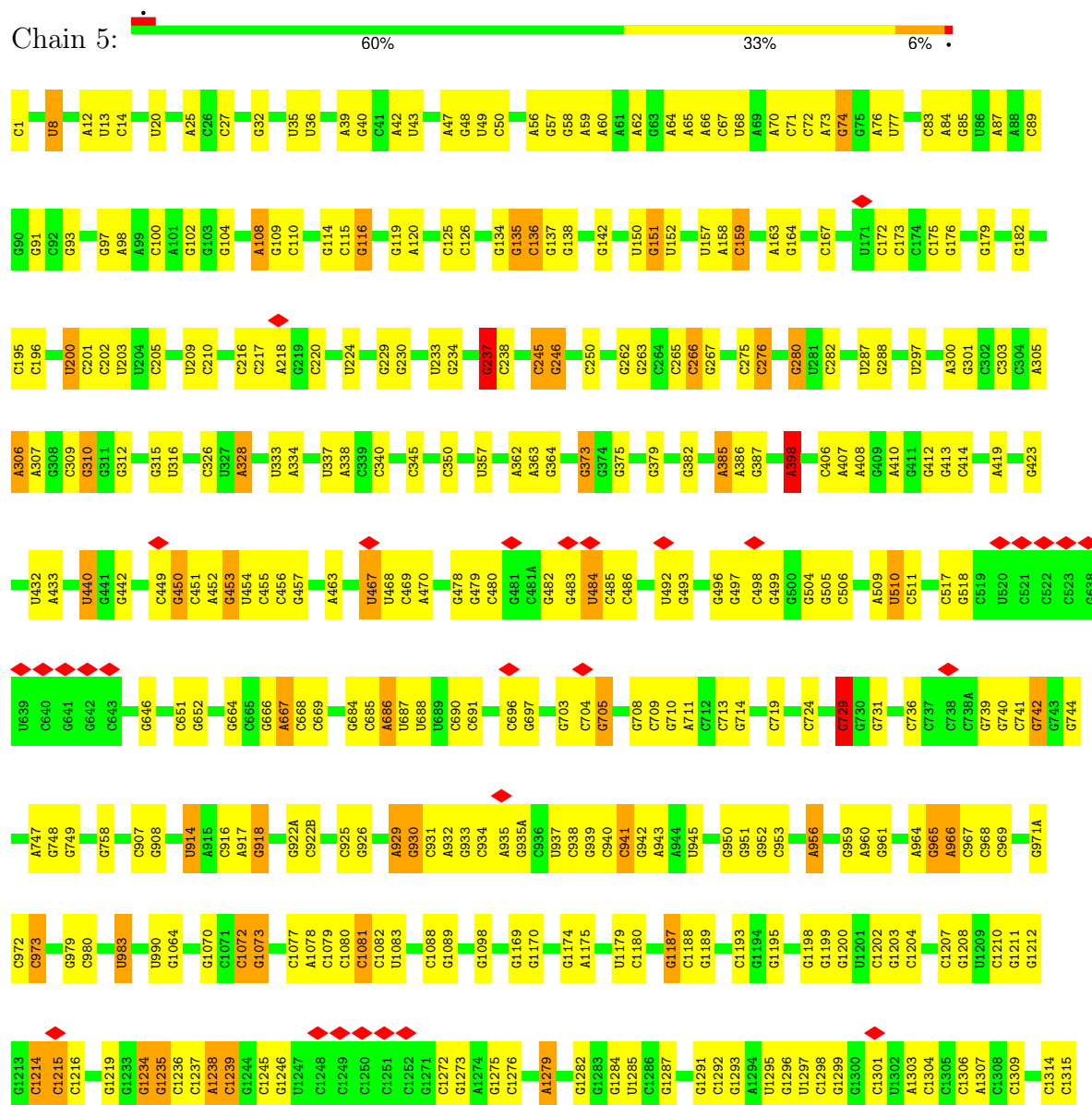


Mol	Chain	Residues	Atoms					AltConf
87	v	1	Total	C	N	O	P	0
			28	10	5	11	2	

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: 28S rRNA

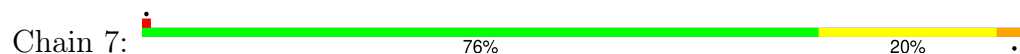




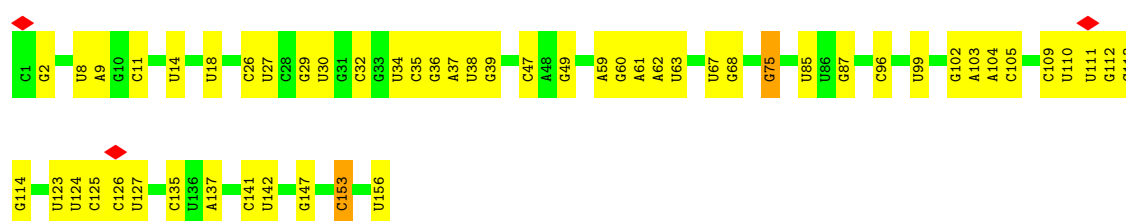




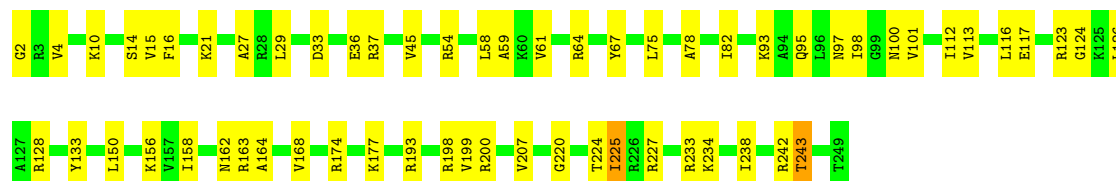
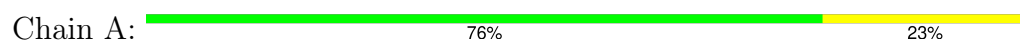
• Molecule 2: 5S rRNA



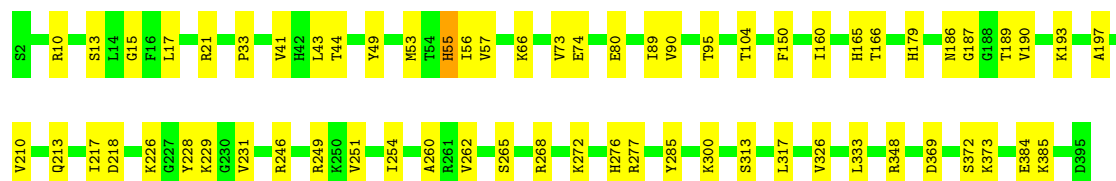
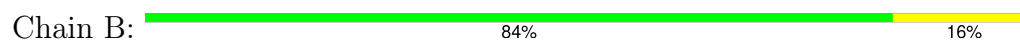
• Molecule 3: 5.8S rRNA



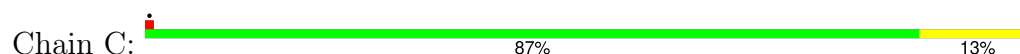
• Molecule 4: uL2



• Molecule 5: uL3

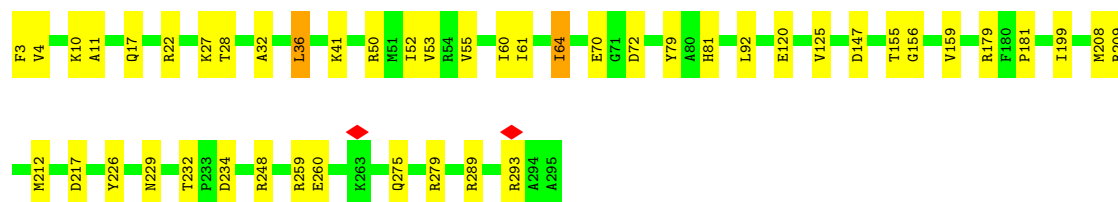
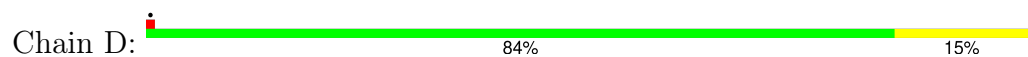


• Molecule 6: uL4

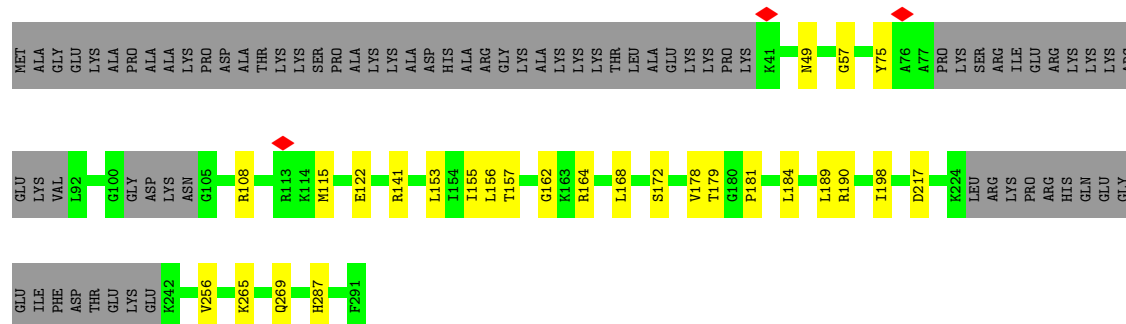




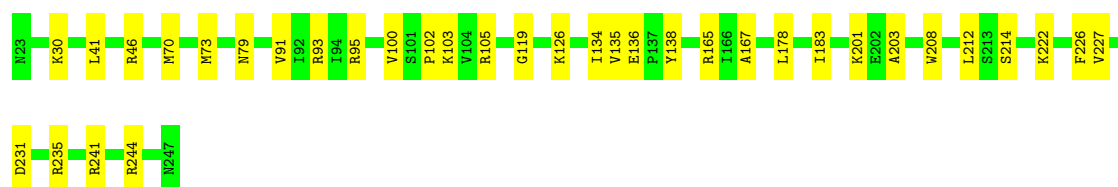
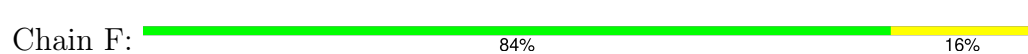
• Molecule 7: uL18



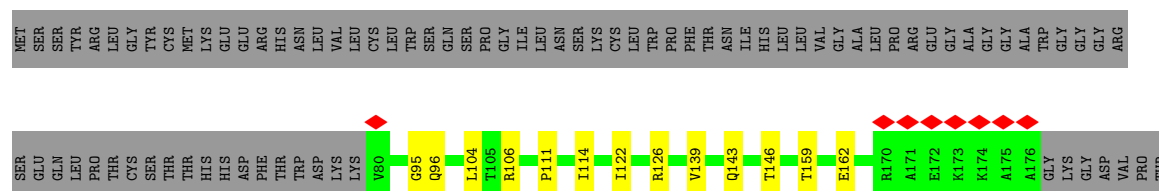
• Molecule 8: eL6



• Molecule 9: uL30

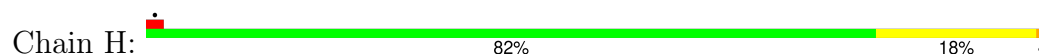


• Molecule 10: eL8

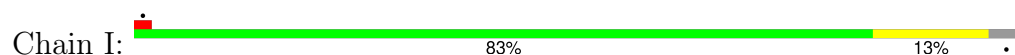




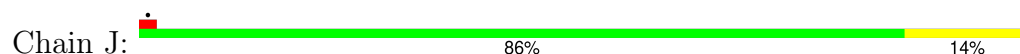
• Molecule 11: uL6



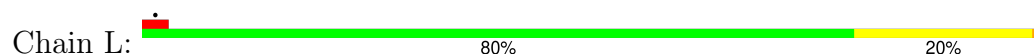
• Molecule 12: uL16



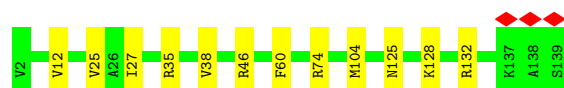
• Molecule 13: uL5



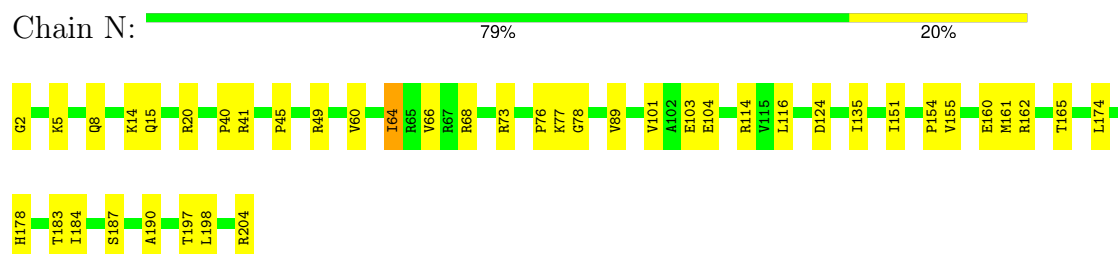
• Molecule 14: eL13



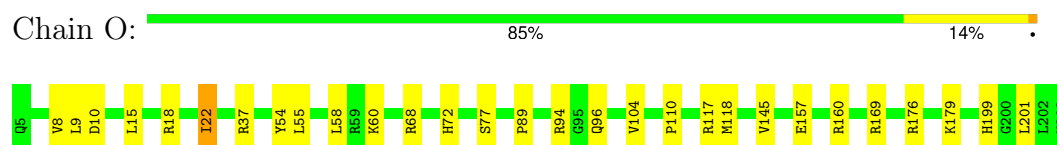
• Molecule 15: eL14



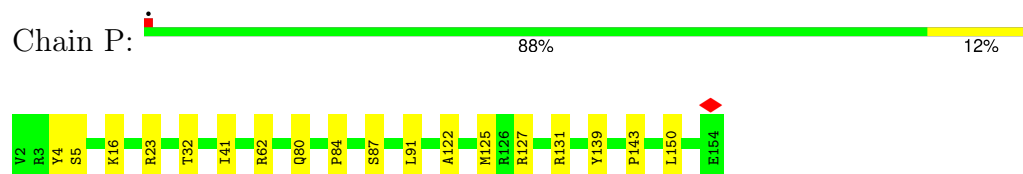
● Molecule 16: eL15



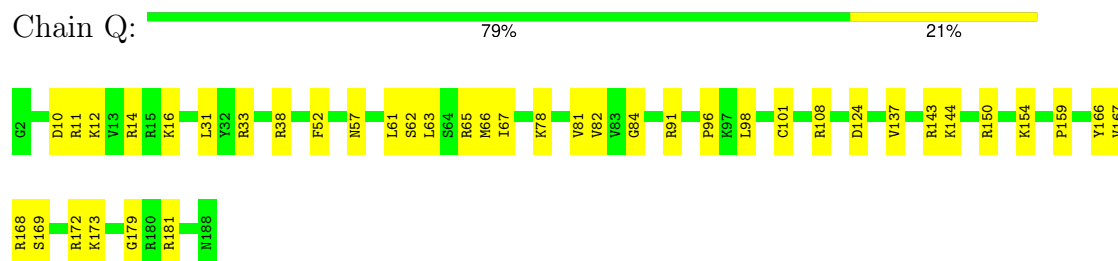
● Molecule 17: uL13



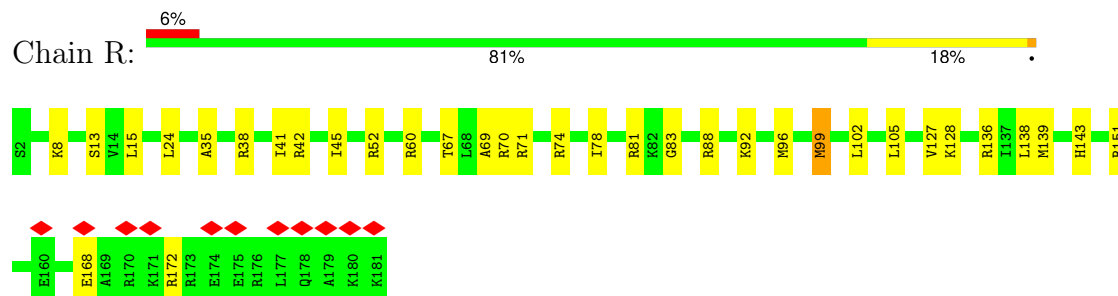
● Molecule 18: uL22



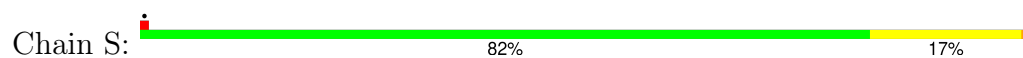
● Molecule 19: eL18

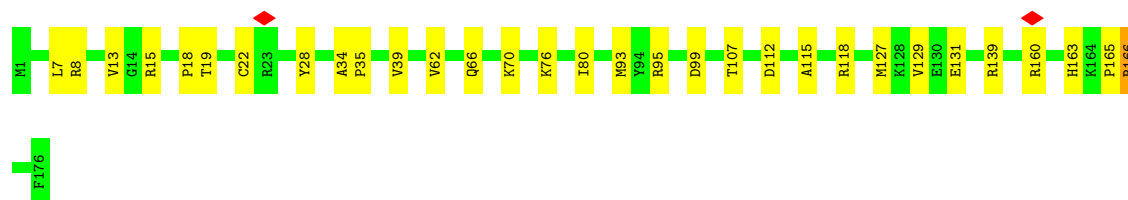


● Molecule 20: eL19

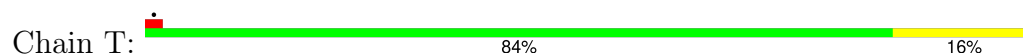


● Molecule 21: eL20

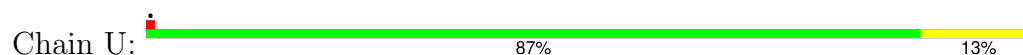




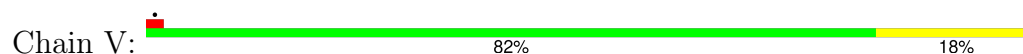
- Molecule 22: eL21



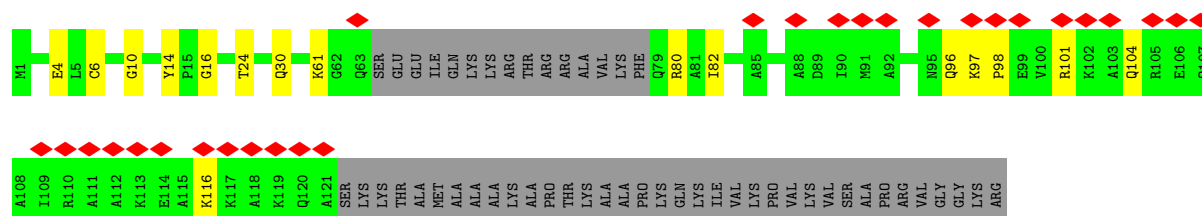
- Molecule 23: eL22



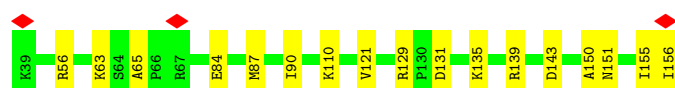
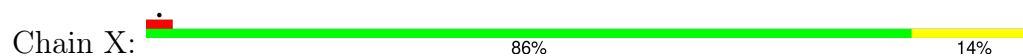
- Molecule 24: uL14



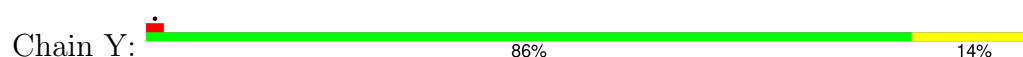
- Molecule 25: eL24

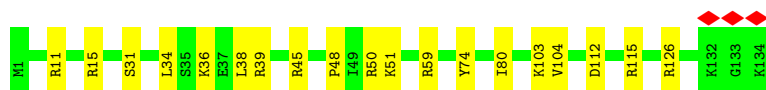


- Molecule 26: uL23

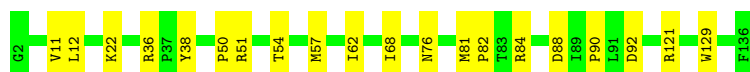
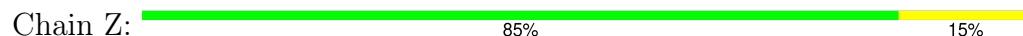


- Molecule 27: uL24

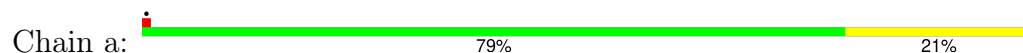




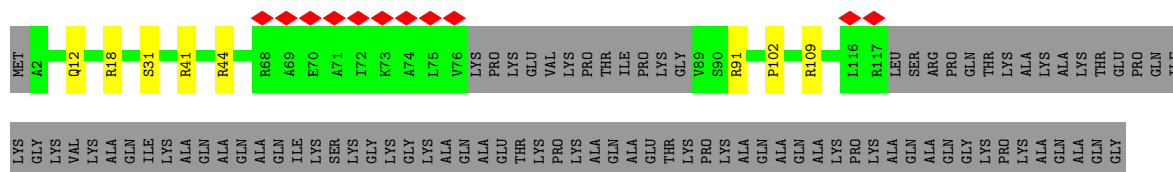
• Molecule 28: eL27



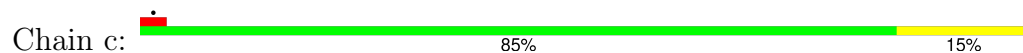
• Molecule 29: uL15



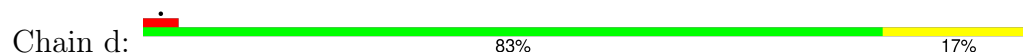
• Molecule 30: eL29



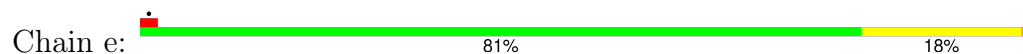
• Molecule 31: eL30



• Molecule 32: eL31

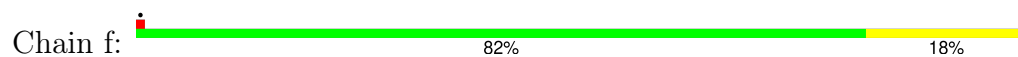


• Molecule 33: eL32

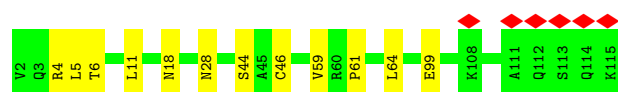
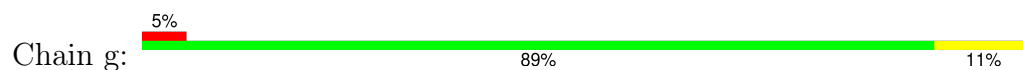




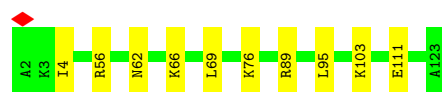
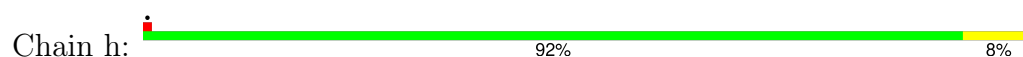
• Molecule 34: eL33



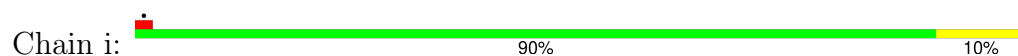
• Molecule 35: eL34



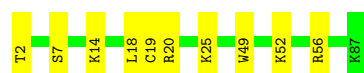
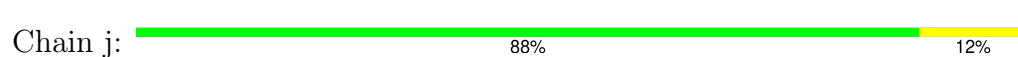
• Molecule 36: uL29



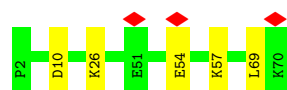
• Molecule 37: eL36



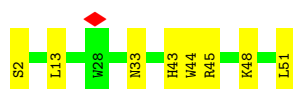
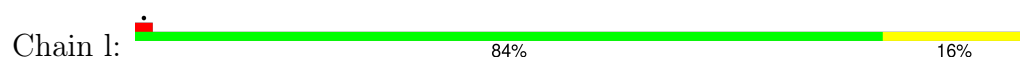
• Molecule 38: eL37



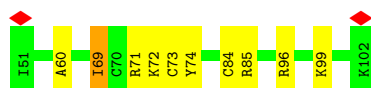
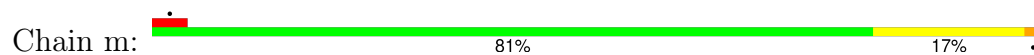
• Molecule 39: eL38



• Molecule 40: eL39



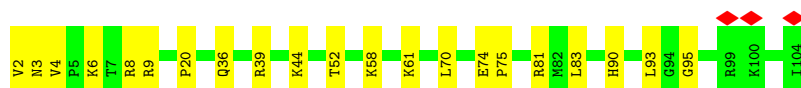
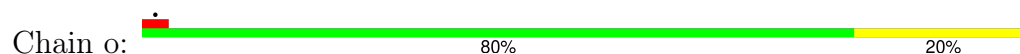
- Molecule 41: eL40



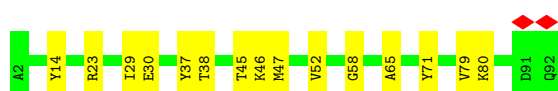
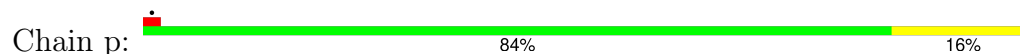
- Molecule 42: eL41



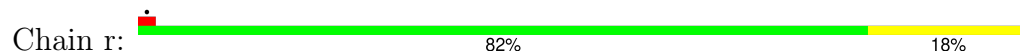
- Molecule 43: eL42



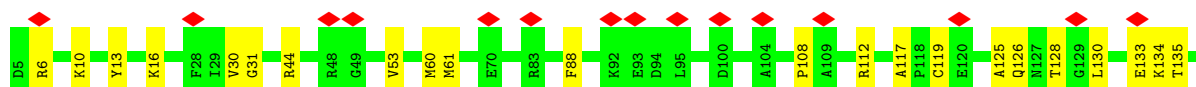
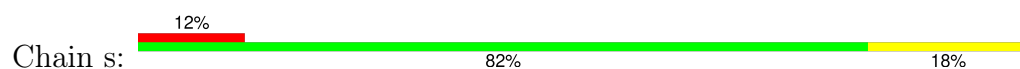
- Molecule 44: eL43

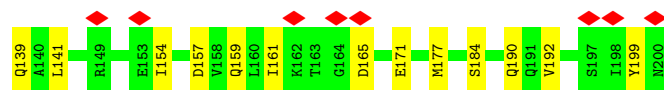


- Molecule 45: eL28

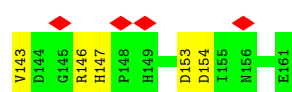
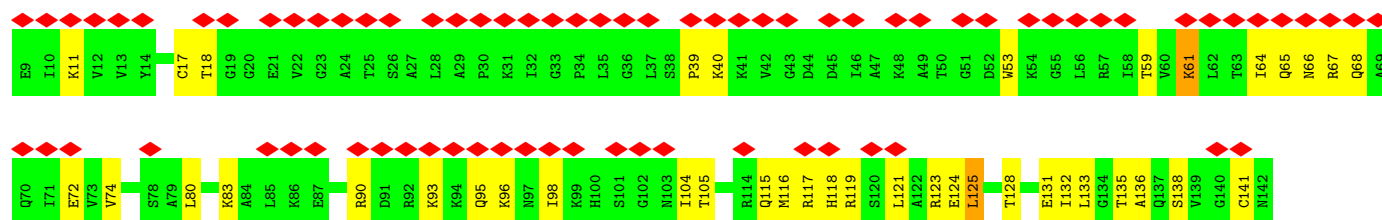


- Molecule 46: uL10

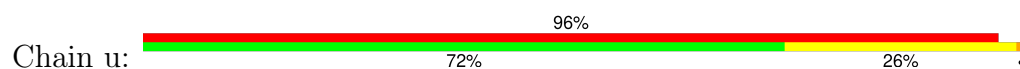




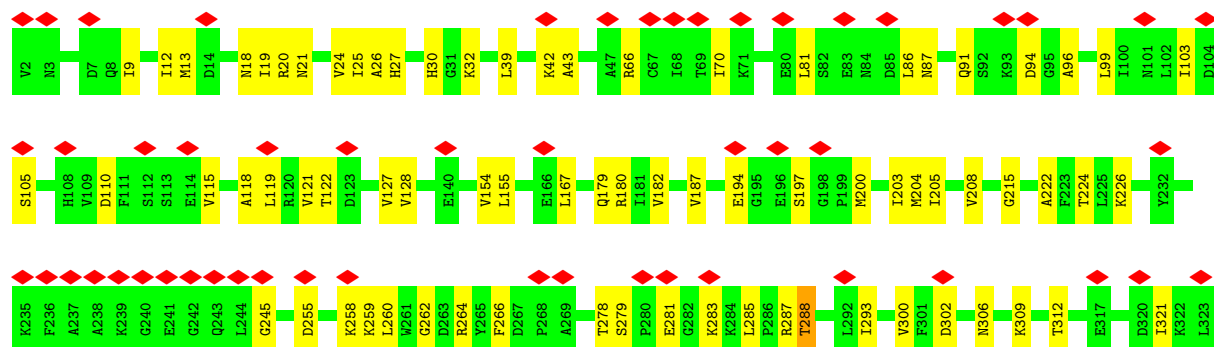
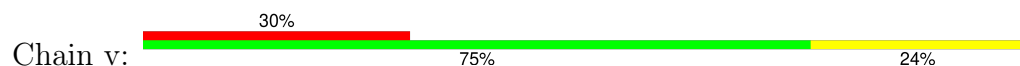
• Molecule 47: eL11

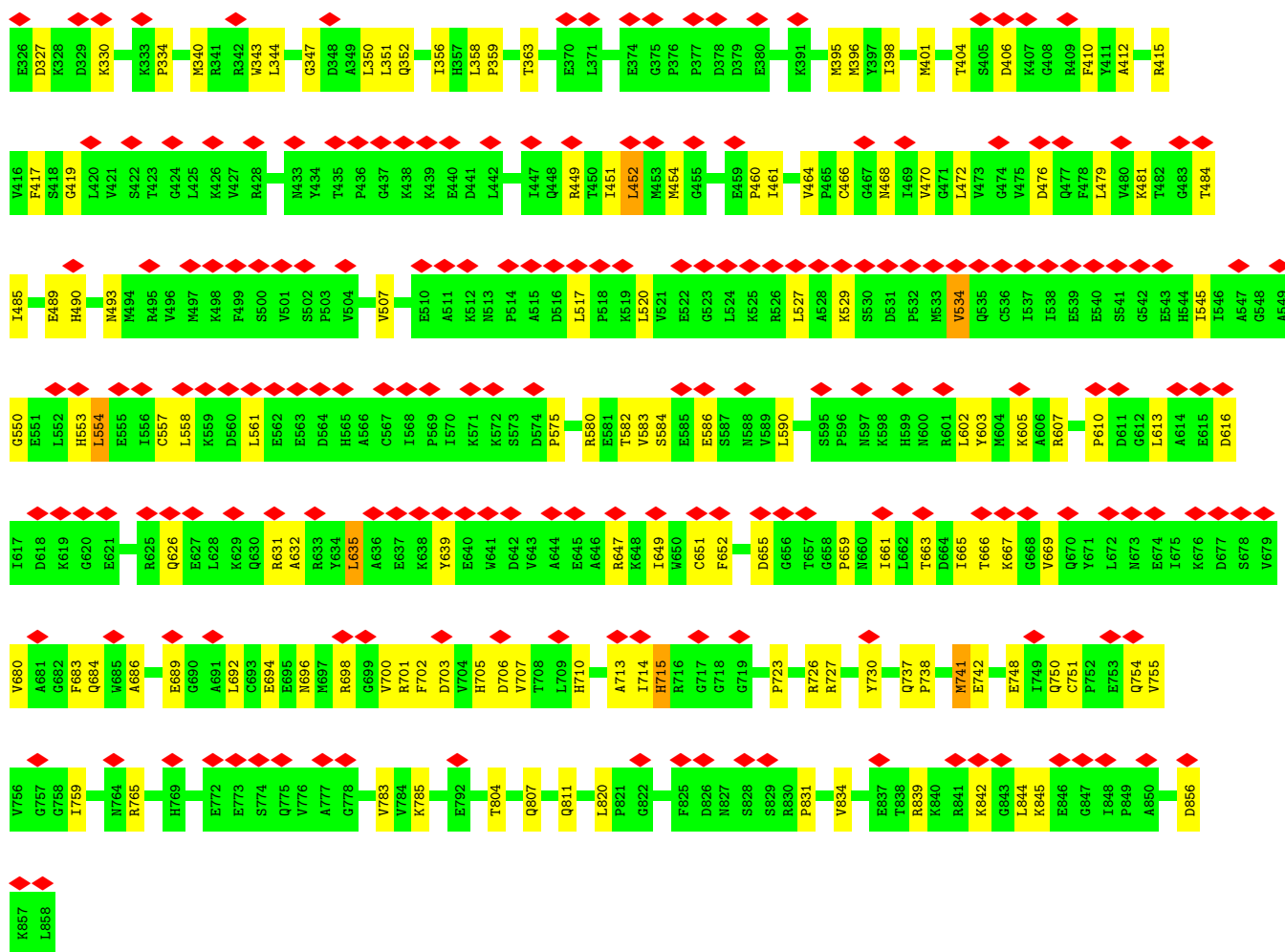


• Molecule 48: uL1



• Molecule 49: eEF2

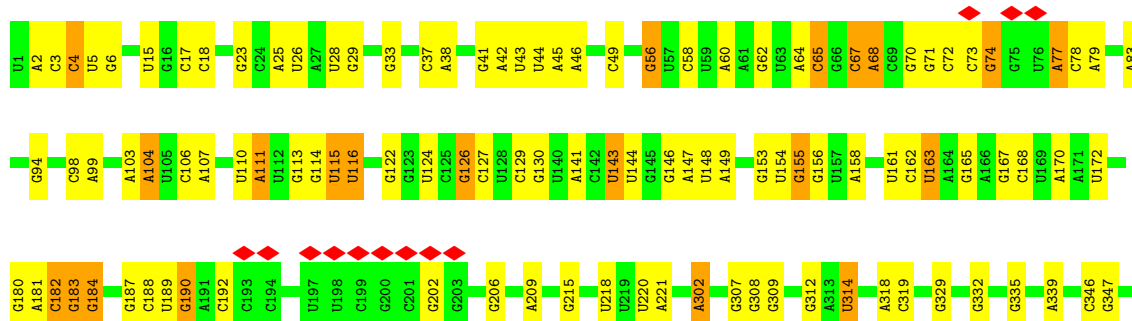


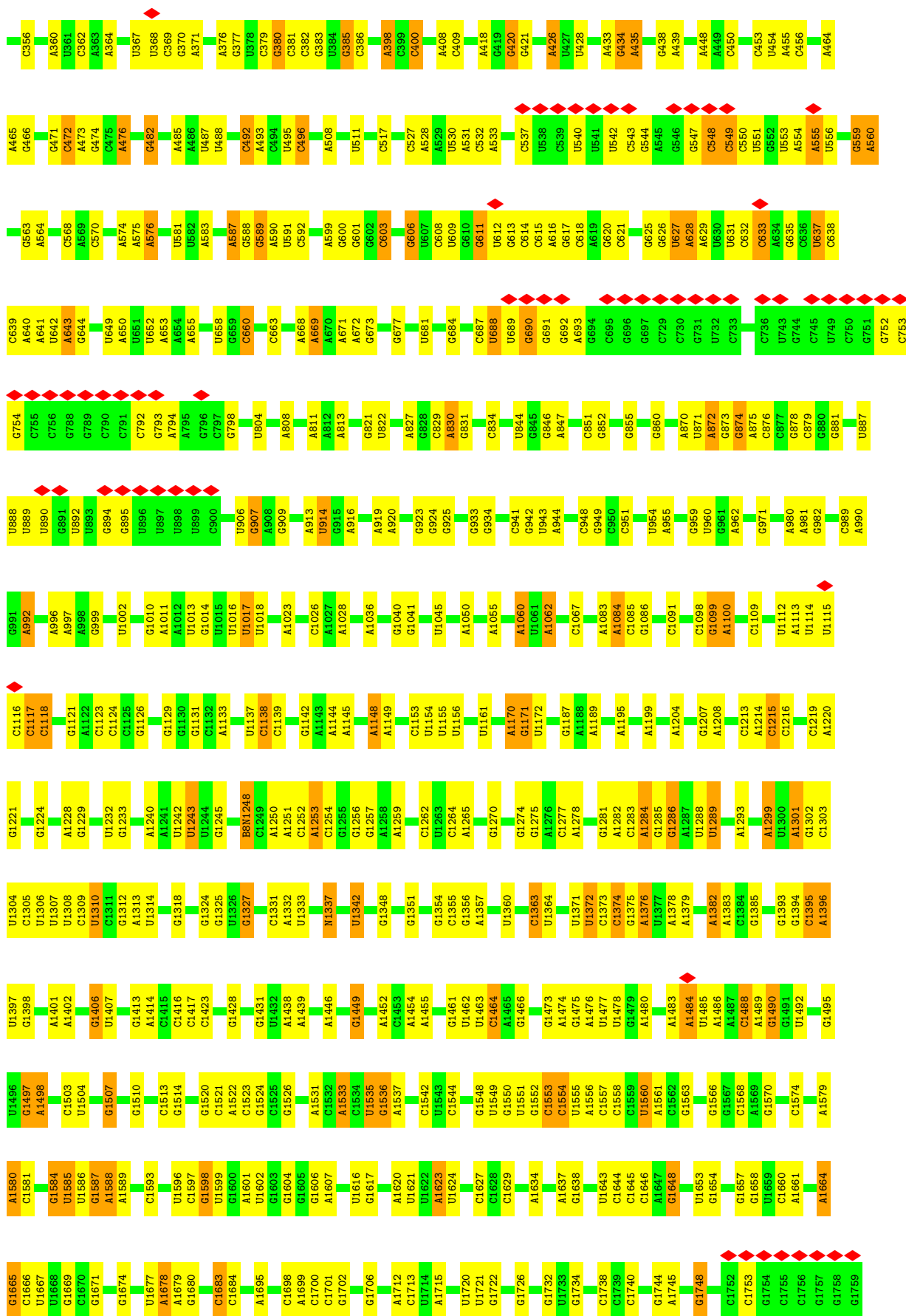


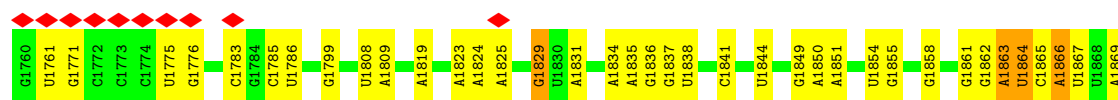
- Molecule 50: SERBP1



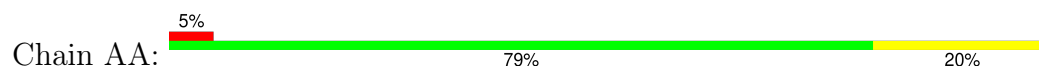
- Molecule 51: 18S rRNA



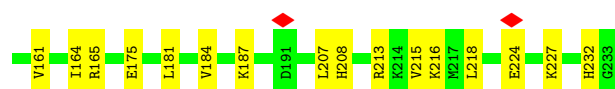
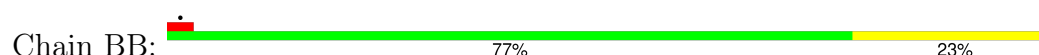




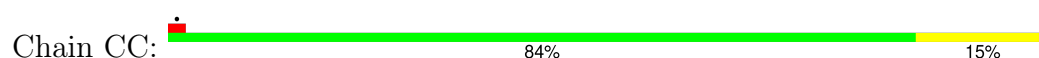
• Molecule 52: uS2



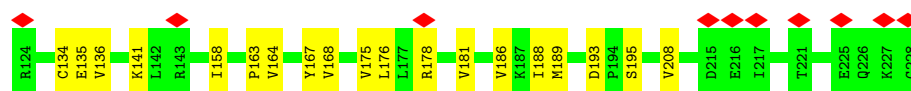
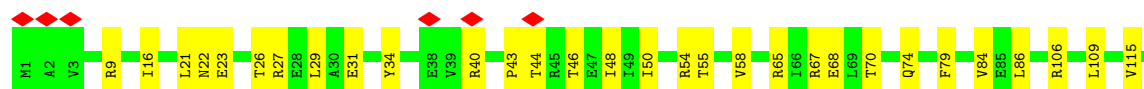
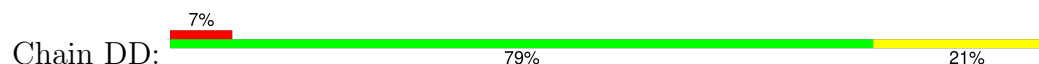
• Molecule 53: eS1



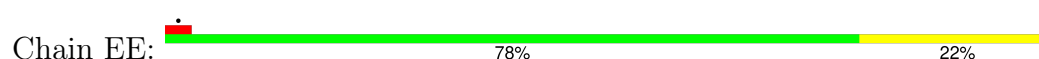
• Molecule 54: uS5

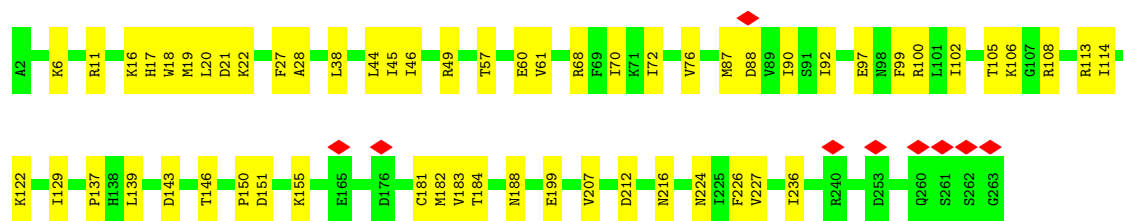


• Molecule 55: uS3

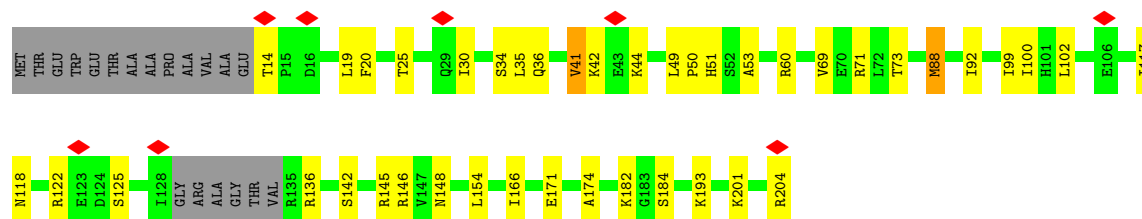


• Molecule 56: eS4

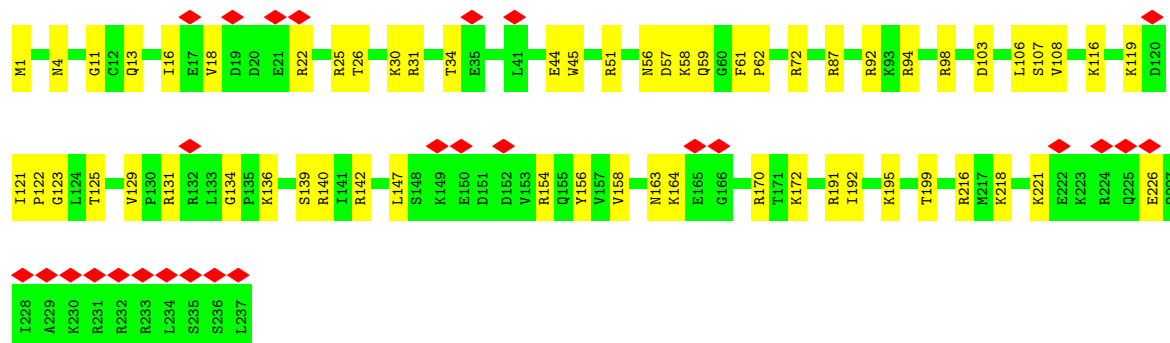
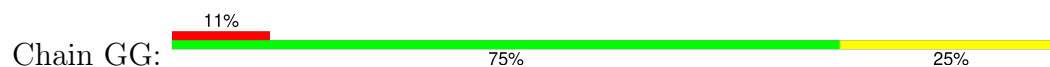




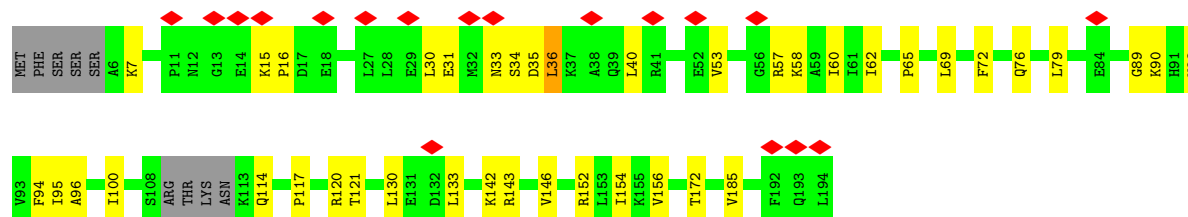
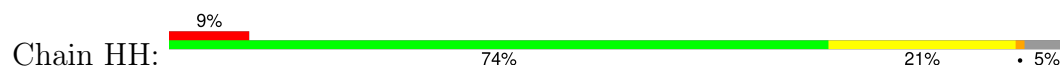
• Molecule 57: uS7



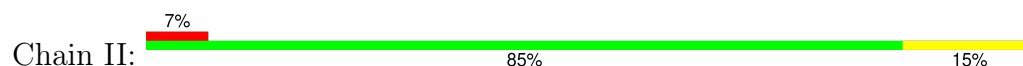
• Molecule 58: eS6

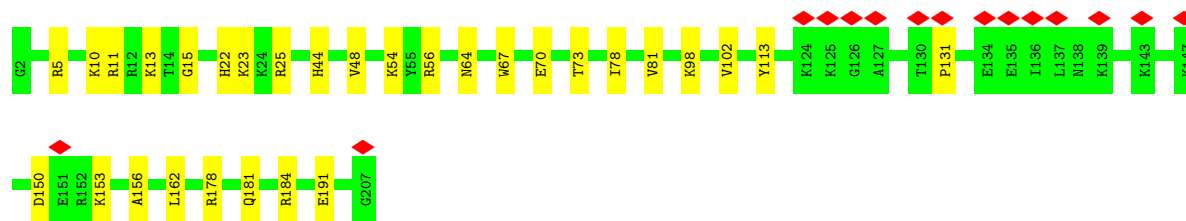


• Molecule 59: eS7

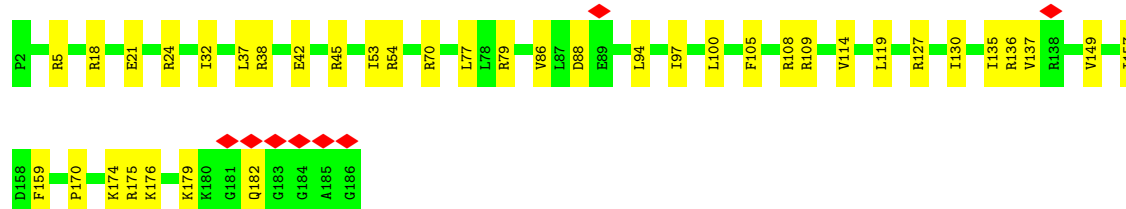
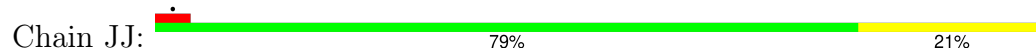


• Molecule 60: eS8





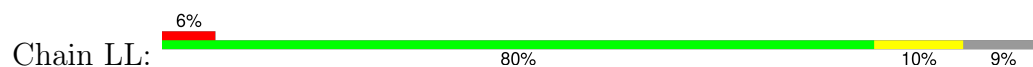
• Molecule 61: uS4



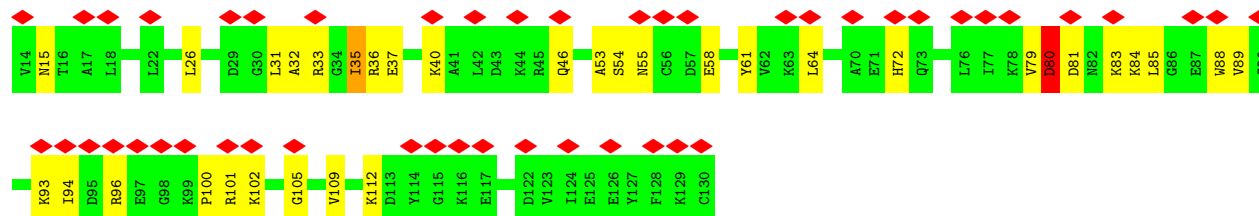
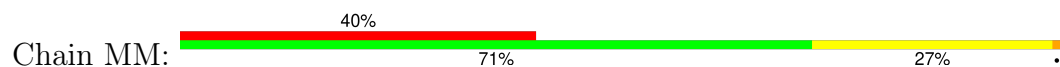
• Molecule 62: eS10



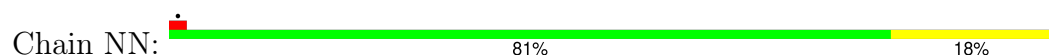
• Molecule 63: uS17



• Molecule 64: eS12

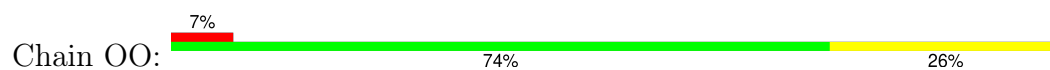


• Molecule 65: uS15

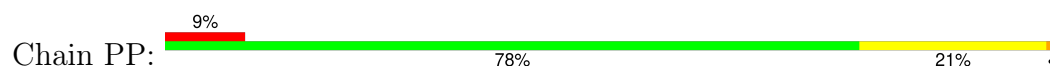




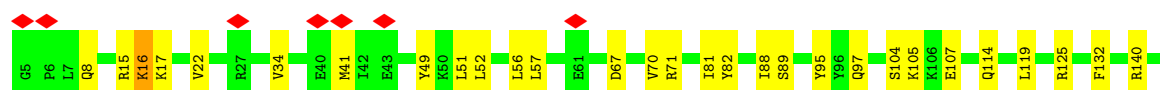
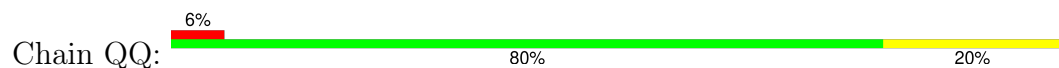
• Molecule 66: uS11



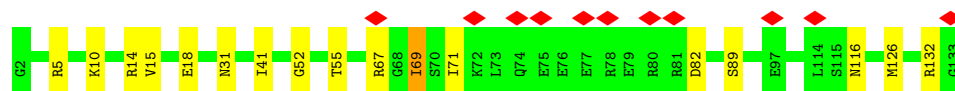
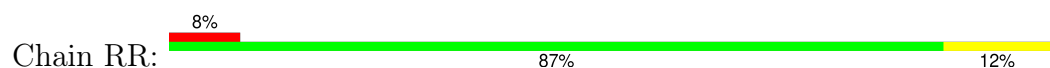
• Molecule 67: uS19



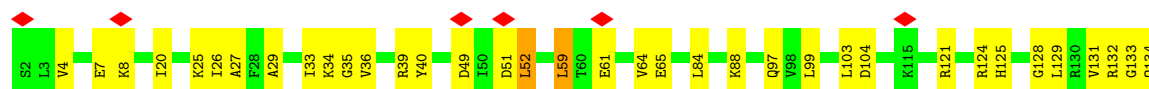
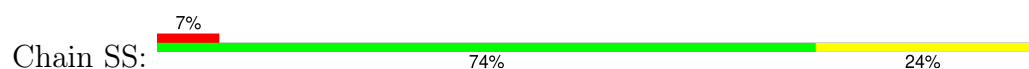
• Molecule 68: uS9

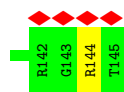


• Molecule 69: eS17

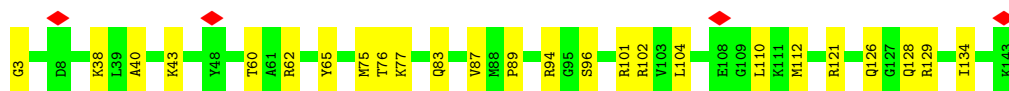
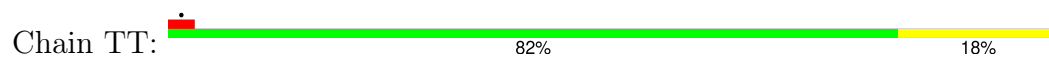


• Molecule 70: uS13

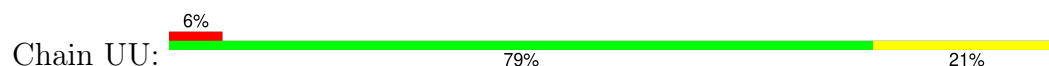




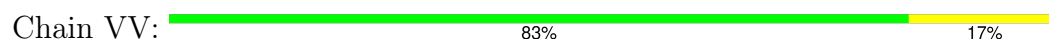
• Molecule 71: eS19



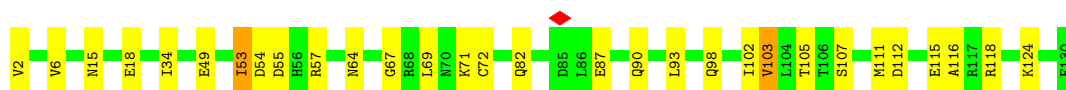
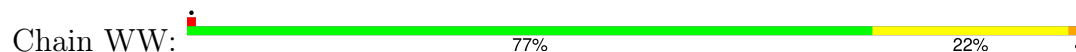
• Molecule 72: uS10



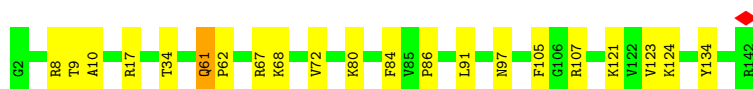
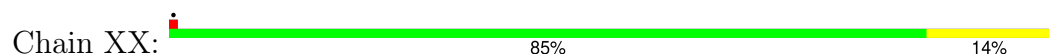
• Molecule 73: eS21



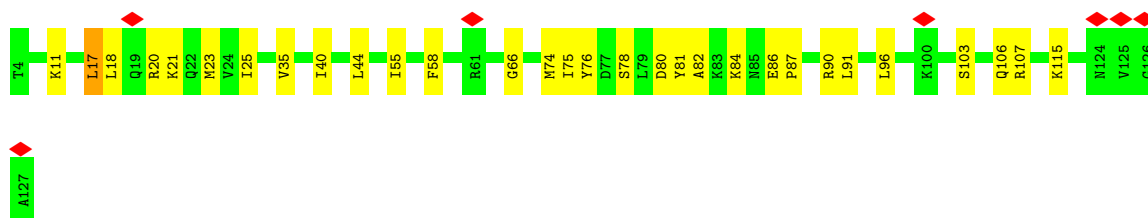
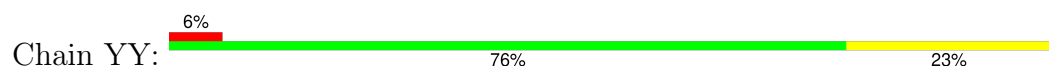
• Molecule 74: uS8



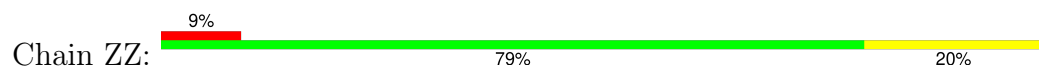
• Molecule 75: uS12



• Molecule 76: eS24



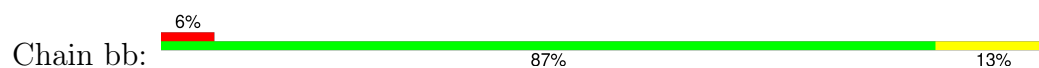
- Molecule 77: eS25



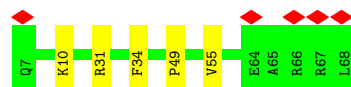
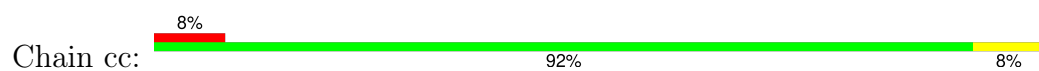
- Molecule 78: eS26



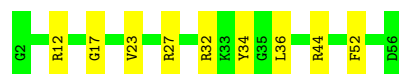
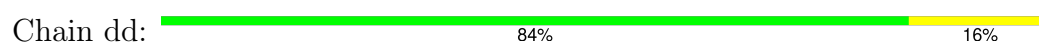
- Molecule 79: eS27



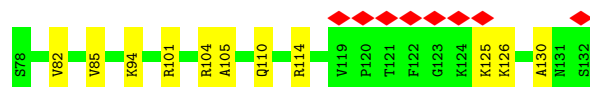
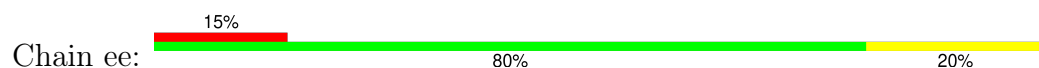
- Molecule 80: eS28



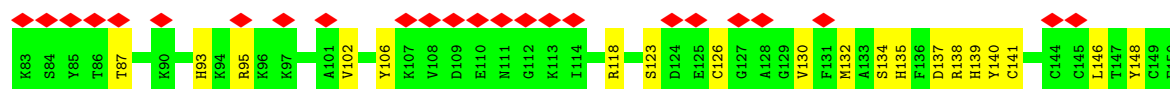
- Molecule 81: uS14



- Molecule 82: eS30

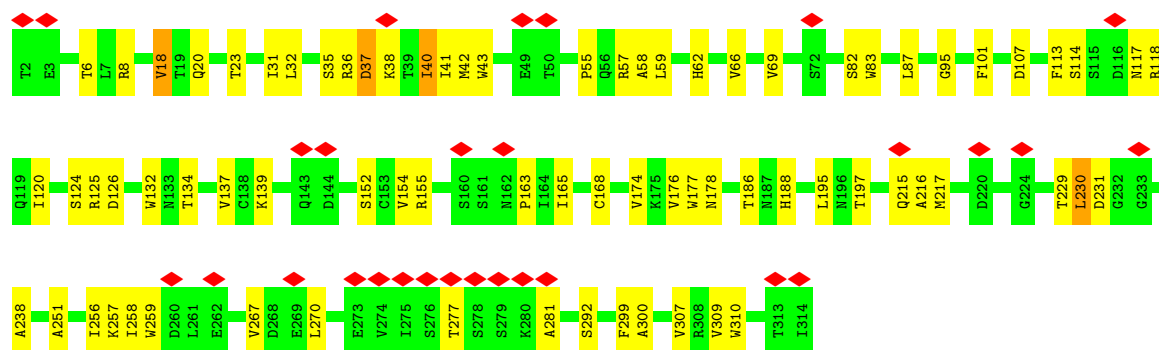


- Molecule 83: eS31



● Molecule 84: RACK1

Chain gg: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146801	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.732	Depositor
Minimum map value	-0.379	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	5	0.38	3/83821 (0.0%)	0.45	13/130598 (0.0%)
2	7	0.36	0/2858	0.37	0/4455
3	8	0.37	0/3559	0.41	0/5543
4	A	0.43	0/1936	0.70	1/2596 (0.0%)
5	B	0.46	0/3240	0.68	0/4339
6	C	0.41	0/2927	0.61	0/3932
7	D	0.34	0/2437	0.61	2/3264 (0.1%)
8	E	0.33	0/1762	0.61	0/2362
9	F	0.42	0/1911	0.69	1/2549 (0.0%)
10	G	0.36	0/1910	0.68	0/2569
11	H	0.41	0/1535	0.72	0/2063
12	I	0.39	0/1702	0.60	0/2272
13	J	0.35	0/1385	0.70	0/1852
14	L	0.39	0/1733	0.63	0/2316
15	M	0.41	0/1158	0.67	0/1547
16	N	0.46	0/1746	0.68	0/2338
17	O	0.43	0/1662	0.66	1/2222 (0.0%)
18	P	0.41	0/1268	0.66	0/1700
19	Q	0.43	0/1539	0.71	0/2054
20	R	0.40	0/1524	0.73	3/2013 (0.1%)
21	S	0.43	0/1501	0.66	0/2012
22	T	0.38	0/1326	0.61	0/1770
23	U	0.33	0/823	0.73	0/1104
24	V	0.42	0/993	0.66	0/1332
25	W	0.39	0/873	0.69	0/1158
26	X	0.35	0/984	0.62	0/1323
27	Y	0.36	0/1132	0.65	0/1504
28	Z	0.36	0/1130	0.61	0/1507
29	a	0.43	0/1191	0.63	0/1590
30	b	0.30	0/861	0.59	0/1138

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	c	0.37	0/771	0.62	0/1034
32	d	0.40	0/903	0.73	0/1216
33	e	0.41	0/1071	0.62	0/1429
34	f	0.42	0/895	0.63	0/1198
35	g	0.38	0/916	0.62	0/1220
36	h	0.34	0/1021	0.65	0/1348
37	i	0.33	0/841	0.61	0/1112
38	j	0.40	0/720	0.72	0/952
39	k	0.33	0/575	0.64	0/761
40	l	0.39	0/459	0.63	0/608
41	m	0.43	0/425	0.78	0/561
42	n	0.32	0/240	0.70	0/305
43	o	0.35	0/855	0.59	0/1128
44	p	0.39	0/718	0.64	0/953
45	r	0.42	0/1010	0.69	0/1354
46	s	0.25	0/1530	0.69	0/2064
47	t	0.30	0/1174	0.80	0/1582
48	u	0.29	0/1680	0.83	0/2255
49	v	0.30	0/6651	0.78	6/8982 (0.1%)
50	w	0.44	0/218	0.96	2/287 (0.7%)
51	9	0.35	8/40385 (0.0%)	0.53	18/62909 (0.0%)
52	AA	0.41	1/1747 (0.1%)	0.89	2/2374 (0.1%)
53	BB	0.31	0/1756	0.69	0/2350
54	CC	0.36	0/1753	0.67	0/2369
55	DD	0.35	0/1796	0.73	2/2417 (0.1%)
56	EE	0.31	0/2118	0.66	0/2849
57	FF	0.33	0/1492	0.72	1/2005 (0.0%)
58	GG	0.28	0/1946	0.67	0/2590
59	HH	0.33	1/1510 (0.1%)	0.76	4/2022 (0.2%)
60	II	0.35	0/1715	0.72	2/2287 (0.1%)
61	JJ	0.29	0/1550	0.62	0/2069
62	KK	0.39	0/834	0.85	4/1125 (0.4%)
63	LL	0.35	0/1195	0.63	0/1597
64	MM	0.27	0/918	0.75	1/1233 (0.1%)
65	NN	0.33	0/1226	0.63	0/1649
66	OO	0.35	0/1029	0.70	0/1380
67	PP	0.32	0/1017	0.76	0/1358
68	QQ	0.32	0/1146	0.71	2/1534 (0.1%)
69	RR	0.30	0/1082	0.70	0/1452
70	SS	0.31	0/1208	0.70	0/1618
71	TT	0.30	0/1115	0.65	0/1493
72	UU	0.33	0/805	0.72	0/1081
73	VV	0.36	0/643	0.68	0/860

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	WW	0.37	0/1051	0.73	2/1406 (0.1%)
75	XX	0.33	0/1116	0.67	0/1490
76	YY	0.26	0/1028	0.63	0/1366
77	ZZ	0.24	0/604	0.60	0/810
78	aa	0.37	0/828	0.71	0/1109
79	bb	0.29	0/665	0.64	0/891
80	cc	0.29	0/490	0.74	0/656
81	dd	0.34	0/470	0.73	1/623 (0.2%)
82	ee	0.30	0/447	0.70	0/587
83	ff	0.25	0/567	0.63	0/753
84	gg	0.29	0/2493	0.72	0/3394
All	All	0.37	13/234845 (0.0%)	0.57	68/343077 (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
5	B	0	1
10	G	0	1
11	H	0	2
14	L	0	2
16	N	0	3
21	S	0	1
32	d	0	1
46	s	0	1
47	t	0	2
48	u	0	2
49	v	0	3
52	AA	0	1
56	EE	0	1
57	FF	0	2
62	KK	0	1
64	MM	0	2
67	PP	0	2
70	SS	0	1
73	VV	0	1
74	WW	0	1
75	XX	0	1
77	ZZ	0	1
84	gg	0	1
All	All	0	34

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1286	G	N9-C4	12.74	1.63	1.38
51	9	1284	A	N9-C4	12.59	1.63	1.37
51	9	1286	G	N9-C8	-11.18	1.15	1.37
51	9	1284	A	N9-C8	-10.28	1.17	1.37
52	AA	197	VAL	C-N	-6.37	1.21	1.33
51	9	1286	G	N3-C4	6.27	1.48	1.35
59	HH	100	ILE	C-N	-6.03	1.24	1.33
51	9	1284	A	N3-C4	5.99	1.46	1.34
1	5	4523	A2M	O3'-P	5.38	1.61	1.56
51	9	1284	A	C8-N7	5.32	1.42	1.31
1	5	3785	A2M	O3'-P	5.31	1.61	1.56
1	5	1534	A2M	O3'-P	5.23	1.61	1.56
51	9	1286	G	C8-N7	5.02	1.41	1.30

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1284	A	N7-C8-N9	-24.47	40.38	113.80
51	9	1286	G	N7-C8-N9	-24.05	40.96	113.10
51	9	1284	A	C4-C5-N7	-23.06	41.51	110.70
51	9	1286	G	C4-C5-N7	-22.95	41.95	110.80
52	AA	197	VAL	CA-C-N	18.98	146.10	120.67
52	AA	197	VAL	C-N-CA	18.98	146.10	120.67
51	9	1286	G	C8-N9-C4	-17.60	53.60	106.40
51	9	1284	A	C8-N9-C4	-17.23	54.10	105.80
51	9	1284	A	C5-N7-C8	10.37	135.00	103.90
51	9	1286	G	C5-N7-C8	10.02	134.37	104.30
51	9	1286	G	C8-N9-C1'	-9.92	97.23	127.00
51	9	1284	A	C4-N9-C1'	9.48	154.75	126.30
51	9	1286	G	C6-C5-N7	9.46	158.76	130.40
1	5	4056	A	OP1-P-O3'	-9.20	80.41	108.00
51	9	1284	A	C8-N9-C1'	-9.02	100.64	127.70
51	9	1284	A	C6-C5-N7	8.49	157.78	132.30
51	9	1286	G	C4-N9-C1'	8.11	150.83	126.50
59	HH	65	PRO	CA-C-N	7.83	125.17	120.24
59	HH	65	PRO	C-N-CA	7.83	125.17	120.24
1	5	4056	A	OP2-P-O3'	-7.19	86.42	108.00
50	w	195	ARG	N-CA-C	6.61	118.48	111.28
20	R	99	MET	CA-CB-CG	-6.25	101.61	114.10
74	WW	53	ILE	CA-C-N	-6.22	114.33	123.05
74	WW	53	ILE	C-N-CA	-6.22	114.33	123.05
62	KK	63	ALA	CA-C-N	6.21	133.40	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	KK	63	ALA	C-N-CA	6.21	133.40	121.54
49	v	452	LEU	CA-CB-CG	6.16	137.84	116.30
49	v	741	MET	CA-C-N	6.16	138.85	120.69
49	v	741	MET	C-N-CA	6.16	138.85	120.69
64	MM	80	ASP	N-CA-C	6.15	117.86	111.03
55	DD	43	PRO	CA-C-N	5.99	132.98	121.54
55	DD	43	PRO	C-N-CA	5.99	132.98	121.54
4	A	15	VAL	N-CA-C	-5.83	107.07	113.43
59	HH	133	LEU	CA-C-N	-5.81	116.19	121.65
59	HH	133	LEU	C-N-CA	-5.81	116.19	121.65
9	F	135	VAL	N-CA-CB	-5.71	105.93	112.21
1	5	2661	U	C2'-C3'-O3'	5.71	118.06	109.50
1	5	1406(B)	C	C2'-C3'-O3'	5.71	118.06	109.50
1	5	3904	G	C2'-C3'-O3'	5.65	117.97	109.50
1	5	2046	G	P-O3'-C3'	5.49	128.43	120.20
68	QQ	16	LYS	CA-C-N	5.48	132.00	121.54
68	QQ	16	LYS	C-N-CA	5.48	132.00	121.54
51	9	1284	A	N3-C4-N9	5.44	143.72	127.40
62	KK	31	LYS	CA-C-N	5.41	128.01	120.65
62	KK	31	LYS	C-N-CA	5.41	128.01	120.65
17	O	110	PRO	N-CA-C	5.39	117.28	110.70
1	5	1406(B)	C	OP1-P-O3'	5.39	117.05	105.20
60	II	78	ILE	CA-C-N	-5.34	117.48	122.66
60	II	78	ILE	C-N-CA	-5.34	117.48	122.66
1	5	2661	U	P-O3'-C3'	5.34	128.21	120.20
1	5	2695	A	P-O3'-C3'	5.32	128.18	120.20
1	5	4925	U	P-O3'-C3'	5.31	128.17	120.20
49	v	287	ARG	CA-CB-CG	5.29	124.69	114.10
1	5	1406(B)	C	P-O3'-C3'	5.24	125.98	119.70
7	D	229	ASN	CA-C-N	5.23	131.53	121.54
7	D	229	ASN	C-N-CA	5.23	131.53	121.54
1	5	3888	G	C2'-C3'-O3'	5.23	121.54	113.70
51	9	1286	G	N3-C4-N9	5.22	141.66	126.00
81	dd	23	VAL	N-CA-C	-5.18	107.77	112.12
50	w	192	GLU	N-CA-C	5.17	116.92	111.28
49	v	554	LEU	CA-C-N	5.15	127.43	120.38
49	v	554	LEU	C-N-CA	5.15	127.43	120.38
51	9	688	U	P-O3'-C3'	5.11	127.87	120.20
1	5	3876	A	P-O3'-C3'	5.09	127.84	120.20
51	9	1363	C	C2'-C3'-O3'	5.07	117.10	109.50
57	FF	88	MET	CG-SD-CE	-5.02	89.86	100.90
20	R	35	ALA	CA-C-N	5.00	131.09	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R	35	ALA	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	AA	43	SER	Peptide
5	B	55	HIS	Peptide
56	EE	155	LYS	Peptide
57	FF	19	LEU	Peptide
57	FF	41	VAL	Peptide
10	G	215	ASP	Peptide
11	H	129	ARG	Peptide
11	H	50	LYS	Peptide
62	KK	38	LYS	Peptide
14	L	46	ILE	Peptide
14	L	62	PRO	Peptide
64	MM	100	PRO	Peptide
64	MM	72	HIS	Peptide
16	N	184	ILE	Peptide
16	N	76	PRO	Peptide
16	N	78	GLY	Peptide
67	PP	17	TYR	Peptide
67	PP	38	SER	Peptide
21	S	165	PRO	Peptide
70	SS	99	LEU	Peptide
73	VV	32	ILE	Peptide
74	WW	54	ASP	Peptide
75	XX	61	GLN	Peptide
77	ZZ	50	PHE	Peptide
32	d	95	ASP	Peptide
84	gg	37	ASP	Peptide
46	s	119	CYS	Peptide
47	t	53	TRP	Peptide
47	t	96	LYS	Peptide
48	u	38	LEU	Peptide
48	u	60	ARG	Peptide
49	v	410	PHE	Peptide
49	v	666	THR	Peptide
49	v	845	LYS	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	5	77254	0	38806	601	0
2	7	2558	0	1296	15	0
3	8	3209	0	1631	24	0
4	A	1898	0	1993	45	0
5	B	3172	0	3310	47	0
6	C	2884	0	3054	35	0
7	D	2391	0	2424	31	0
8	E	1729	0	1887	20	0
9	F	1875	0	1995	27	0
10	G	1879	0	2027	23	0
11	H	1516	0	1596	25	0
12	I	1664	0	1712	19	0
13	J	1362	0	1399	15	0
14	L	1702	0	1820	34	0
15	M	1137	0	1209	10	0
16	N	1701	0	1749	32	0
17	O	1630	0	1778	21	0
18	P	1242	0	1274	12	0
19	Q	1515	0	1634	34	0
20	R	1508	0	1664	22	0
21	S	1462	0	1508	22	0
22	T	1298	0	1366	21	0
23	U	809	0	833	7	0
24	V	979	0	1039	16	0
25	W	860	0	903	14	0
26	X	967	0	1040	13	0
27	Y	1115	0	1205	16	0
28	Z	1107	0	1182	13	0
29	a	1162	0	1209	28	0
30	b	848	0	920	8	0
31	c	761	0	794	8	0
32	d	888	0	930	12	0
33	e	1053	0	1147	19	0
34	f	876	0	912	14	0
35	g	906	0	998	7	0
36	h	1013	0	1147	8	0
37	i	830	0	916	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	j	705	0	737	7	0
39	k	569	0	637	4	0
40	l	447	0	480	6	0
41	m	430	0	466	8	0
42	n	239	0	289	6	0
43	o	842	0	912	13	0
44	p	708	0	756	12	0
45	r	994	0	1051	17	0
46	s	1507	0	1564	20	0
47	t	1160	0	1218	25	0
48	u	1654	0	1760	42	0
49	v	6544	0	6638	137	0
50	w	216	0	197	62	0
51	9	36263	0	18296	343	0
52	AA	1710	0	1707	26	0
53	BB	1729	0	1803	35	0
54	CC	1716	0	1806	25	0
55	DD	1768	0	1866	32	0
56	EE	2076	0	2177	34	0
57	FF	1471	0	1522	30	0
58	GG	1923	0	2089	44	0
59	HH	1488	0	1582	23	0
60	II	1686	0	1772	23	0
61	JJ	1525	0	1640	23	0
62	KK	810	0	836	52	0
63	LL	1175	0	1249	14	0
64	MM	908	0	939	23	0
65	NN	1202	0	1289	19	0
66	OO	1016	0	1039	22	0
67	PP	997	0	1045	19	0
68	QQ	1128	0	1195	20	0
69	RR	1068	0	1121	14	0
70	SS	1190	0	1248	22	0
71	TT	1097	0	1132	21	0
72	UU	795	0	862	14	0
73	VV	636	0	637	7	0
74	WW	1034	0	1080	21	0
75	XX	1098	0	1167	19	0
76	YY	1011	0	1083	19	0
77	ZZ	598	0	656	15	0
78	aa	814	0	864	10	0
79	bb	651	0	672	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	cc	488	0	514	5	0
81	dd	459	0	448	8	0
82	ee	443	0	492	10	0
83	ff	555	0	563	15	0
84	gg	2436	0	2393	43	0
85	5	198	0	0	0	0
85	7	7	0	0	0	0
85	8	6	0	0	0	0
85	9	74	0	0	0	0
85	A	1	0	0	0	0
85	B	1	0	0	0	0
85	P	1	0	0	0	0
85	SS	2	0	0	0	0
85	TT	1	0	0	0	0
85	V	1	0	0	0	0
85	a	1	0	0	0	0
85	dd	1	0	0	0	0
85	g	1	0	0	0	0
85	j	1	0	0	0	0
85	v	1	0	0	0	0
86	aa	1	0	0	0	0
86	dd	1	0	0	0	0
86	ff	1	0	0	0	0
86	g	1	0	0	0	0
86	j	1	0	0	0	0
86	m	1	0	0	0	0
86	o	1	0	0	0	0
86	p	1	0	0	0	0
87	v	28	0	12	1	0
All	All	222072	0	167808	2140	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 6.

All (2140) 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)
1:5:1860:B8H:C4	1:5:1860:B8H:C5	1.82	1.56
1:5:3762:B8H:C4	1:5:3762:B8H:C5	1.83	1.52
1:5:4296:B8H:N1	1:5:4296:B8H:C6	1.68	1.52
1:5:4296:B8H:C5	1:5:4296:B8H:C4	1.82	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1860:B8H:C6	1:5:1860:B8H:N1	1.68	1.50
1:5:3762:B8H:C6	1:5:3762:B8H:N1	1.69	1.49
1:5:398:A2M:C1'	1:5:398:A2M:O4'	1.63	1.29
1:5:3718:A2M:C1'	1:5:3718:A2M:O4'	1.63	1.25
50:w:282:THR:CG2	62:KK:95:ARG:CD	2.15	1.25
1:5:4523:A2M:C1'	1:5:4523:A2M:O4'	1.64	1.24
50:w:282:THR:CG2	62:KK:95:ARG:HD3	1.67	1.24
50:w:195:ARG:CB	51:9:1701:C:O2	1.87	1.23
1:5:1574:B9B:C1'	1:5:1574:B9B:O4'	1.64	1.22
50:w:286:TRP:CZ2	62:KK:86:PRO:HG2	1.74	1.22
1:5:2754:B9B:C1'	1:5:2754:B9B:O4'	1.64	1.21
1:5:1871:A2M:C1'	1:5:1871:A2M:O4'	1.63	1.20
1:5:4571:A2M:C1'	1:5:4571:A2M:O4'	1.63	1.19
50:w:282:THR:HG22	62:KK:95:ARG:CD	1.70	1.19
51:9:1351:G:O6	51:9:1360:U:O4	1.60	1.17
1:5:3723:A2M:C1'	1:5:3723:A2M:O4'	1.64	1.16
50:w:286:TRP:CZ2	62:KK:86:PRO:CG	2.28	1.15
51:9:1678:A2M:C1'	51:9:1678:A2M:O4'	1.64	1.14
50:w:195:ARG:HB3	51:9:1701:C:O2	1.50	1.11
1:5:237:B9B:C1'	1:5:237:B9B:O4'	1.65	1.11
1:5:3899:BGH:C4'	1:5:3899:BGH:O4'	1.66	1.10
50:w:282:THR:HG22	62:KK:95:ARG:HD2	1.30	1.10
51:9:1700:C:C2	51:9:1834:A:N6	2.24	1.06
50:w:286:TRP:CE2	62:KK:86:PRO:HG2	1.91	1.05
50:w:286:TRP:HB2	62:KK:89:ILE:HG21	1.08	1.04
50:w:286:TRP:CB	62:KK:89:ILE:HG21	1.90	1.00
50:w:191:ARG:HH11	50:w:191:ARG:HG2	1.25	1.00
1:5:3951:G:N1	1:5:4062:A:C2	2.31	0.98
1:5:3952:A:H2	1:5:4061:G:H1	1.08	0.96
49:v:714:ILE:HD11	50:w:198:GLY:HA2	1.46	0.96
50:w:195:ARG:HB2	51:9:1701:C:O2	1.66	0.94
1:5:3951:G:N1	1:5:4062:A:H2	1.62	0.93
6:C:218:VAL:O	6:C:222:ARG:HB2	1.68	0.92
50:w:282:THR:HG21	62:KK:95:ARG:HD3	1.48	0.91
51:9:1533:A:H62	51:9:1602:U:H3	1.18	0.91
50:w:282:THR:CG2	62:KK:95:ARG:HD2	1.93	0.91
51:9:1351:G:H1	51:9:1360:U:H3	0.95	0.90
1:5:4296:B8H:N1	1:5:4296:B8H:C5	2.36	0.88
1:5:3951:G:H1	1:5:4062:A:H2	0.89	0.87
50:w:286:TRP:HB2	62:KK:89:ILE:CG2	2.01	0.86
50:w:286:TRP:CE2	62:KK:86:PRO:CG	2.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:w:286:TRP:CH2	62:KK:86:PRO:HG2	2.13	0.84
50:w:195:ARG:HB2	51:9:1701:C:C2	2.13	0.82
49:v:714:ILE:HG23	50:w:200:ASP:N	1.94	0.82
49:v:714:ILE:CG2	50:w:200:ASP:N	2.42	0.82
64:MM:53:ALA:HA	64:MM:79:VAL:O	1.80	0.81
49:v:713:ALA:HB3	50:w:199:SER:HA	1.62	0.80
50:w:283:LEU:HD23	62:KK:17:LYS:HB3	1.63	0.80
51:9:1324:G:H1	51:9:1504:U:H3	1.24	0.80
1:5:3762:B8H:C5	1:5:3762:B8H:N1	2.37	0.79
52:AA:126:ASP:O	52:AA:130:ASP:HB2	1.83	0.78
49:v:714:ILE:HG23	50:w:199:SER:C	2.10	0.77
7:D:32:ALA:O	7:D:36:LEU:HB2	1.83	0.77
50:w:286:TRP:CZ2	62:KK:86:PRO:HG3	2.17	0.76
48:u:53:VAL:O	48:u:154:THR:HA	1.86	0.76
51:9:925:G:H1	51:9:1017:U:H3	1.34	0.75
50:w:282:THR:HG23	62:KK:95:ARG:CD	2.14	0.75
1:5:1860:B8H:C6	1:5:1860:B8H:C2	2.66	0.73
1:5:3692:A:H62	1:5:3823:G:H21	1.37	0.73
1:5:4296:B8H:C6	1:5:4296:B8H:C2	2.65	0.73
50:w:286:TRP:CE2	62:KK:86:PRO:CD	2.71	0.72
1:5:3952:A:H2	1:5:4061:G:N1	1.87	0.71
49:v:714:ILE:CG2	50:w:199:SER:C	2.63	0.71
49:v:347:GLY:O	49:v:351:LEU:HB2	1.90	0.71
12:I:6:ALA:O	12:I:10:ARG:HB2	1.90	0.70
66:OO:99:ALA:H	66:OO:133:THR:HG22	1.56	0.70
53:BB:224:GLU:HG3	53:BB:227:LYS:HE2	1.73	0.70
51:9:1396:A:O2'	51:9:1398:G:N7	2.25	0.69
50:w:191:ARG:HG2	50:w:191:ARG:NH1	1.95	0.69
1:5:3722:G:H2'	1:5:3723:A2M:H8	1.75	0.68
48:u:59:PRO:HB2	48:u:170:GLY:H	1.57	0.68
5:B:10:ARG:HH22	5:B:265:SER:HB2	1.57	0.68
1:5:4895:C:H1'	15:M:132:ARG:HH12	1.58	0.68
8:E:115:MET:O	45:r:87:ARG:NH1	2.27	0.68
1:5:1870:C:H2'	1:5:1871:A2M:H8	1.76	0.68
51:9:1533:A:N6	51:9:1602:U:H3	1.90	0.68
50:w:282:THR:HG22	62:KK:95:ARG:HD3	1.44	0.68
64:MM:33:ARG:HD3	64:MM:89:VAL:HG21	1.74	0.68
1:5:1661:C:OP1	33:e:36:ARG:NH2	2.27	0.67
49:v:19:ILE:HG22	49:v:99:LEU:HB3	1.76	0.67
51:9:1452:A:H61	51:9:1473:G:H21	1.42	0.67
1:5:4523:A2M:H5''	1:5:4524:G:H5'	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4162:C:H5	10:G:126:ARG:HH12	1.42	0.67
64:MM:32:ALA:HB1	64:MM:37:GLU:HB3	1.76	0.67
1:5:4419:U:O2	49:v:765:ARG:NH2	2.27	0.67
51:9:851:C:H5''	51:9:852:G:H5'	1.77	0.67
51:9:1542:C:H5''	71:TT:62:ARG:HH22	1.60	0.67
1:5:3762:B8H:C6	1:5:3762:B8H:C2	2.66	0.67
51:9:1677:U:H2'	51:9:1678:A2M:H8	1.77	0.67
1:5:2845:A:H61	1:5:3843:C:H42	1.43	0.66
51:9:379:C:H5''	60:II:56:ARG:HH12	1.60	0.66
59:HH:72:PHE:O	59:HH:76:GLN:HB2	1.95	0.66
50:w:286:TRP:NE1	62:KK:86:PRO:CD	2.58	0.66
1:5:1:C:H42	3:8:156:U:H3	1.42	0.66
84:gg:87:LEU:HB2	84:gg:101:PHE:HB2	1.78	0.66
84:gg:174:VAL:HG23	84:gg:188:HIS:HB2	1.78	0.66
51:9:122:G:H21	56:EE:146:THR:HG21	1.60	0.66
20:R:15:LEU:HD23	20:R:52:ARG:HB3	1.78	0.66
47:t:116:MET:O	47:t:119:ARG:NH1	2.29	0.66
52:AA:79:SER:HA	52:AA:101:GLY:HA2	1.77	0.66
20:R:42:ARG:HA	20:R:45:ILE:HD12	1.78	0.65
67:PP:93:MET:SD	67:PP:104:GLN:NE2	2.70	0.65
24:V:69:LYS:HE3	24:V:72:LEU:HD13	1.77	0.65
1:5:1459:A:OP1	19:Q:65:ARG:NH2	2.29	0.65
51:9:1498:A:OP2	55:DD:27:ARG:NH2	2.30	0.65
1:5:4296:B8H:C6	1:5:4296:B8H:CN1	2.74	0.65
1:5:4735:G:H1	1:5:4965:U:H3	1.44	0.65
51:9:1305:C:OP2	83:ff:93:HIS:ND1	2.30	0.65
27:Y:59:ARG:HB2	27:Y:103:LYS:HG2	1.78	0.64
51:9:1616:U:H3	51:9:1620:A:H2	1.46	0.64
14:L:8:MET:HG3	19:Q:166:TYR:HB3	1.79	0.64
4:A:97:ASN:OD1	4:A:100:ASN:ND2	2.30	0.64
1:5:3908:A:N7	1:5:4449:A:N6	2.45	0.64
49:v:507:VAL:HG21	49:v:558:LEU:HD21	1.79	0.64
51:9:639:C:H2'	51:9:640:A:H8	1.62	0.64
14:L:56:ARG:O	14:L:116:ARG:NH2	2.31	0.64
46:s:134:LYS:HE3	46:s:177:MET:HE3	1.80	0.64
49:v:603:TYR:HB2	49:v:706:ASP:O	1.98	0.64
25:W:96:GLN:NE2	58:GG:156:TYR:OH	2.31	0.64
1:5:3762:B8H:C6	1:5:3762:B8H:CN1	2.74	0.64
1:5:3951:G:O6	1:5:4062:A:N1	2.31	0.64
6:C:245:HIS:ND1	45:r:13:CYS:SG	2.71	0.64
49:v:91:GLN:HE22	49:v:359:PRO:HA	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4525:C:OP1	5:B:246:ARG:NH1	2.31	0.63
12:I:36:LEU:HD11	12:I:69:ARG:HH21	1.63	0.63
41:m:71:ARG:HE	41:m:96:ARG:HB3	1.63	0.63
64:MM:15:ASN:HB2	64:MM:88:TRP:HH2	1.63	0.63
48:u:90:LEU:O	48:u:94:ASN:HB2	1.98	0.63
56:EE:20:LEU:HD11	56:EE:46:ILE:HD12	1.79	0.63
60:II:178:ARG:HE	60:II:181:GLN:HG3	1.61	0.63
72:UU:78:ASP:OD2	81:dd:44:ARG:NH1	2.31	0.63
48:u:67:VAL:HG12	48:u:111:LEU:HB3	1.80	0.63
56:EE:90:ILE:HG23	56:EE:99:PHE:HB2	1.80	0.63
1:5:3952:A:C2	1:5:4061:G:N1	2.51	0.63
1:5:4494:OMG:HM21	24:V:22:VAL:HG21	1.80	0.63
49:v:590:LEU:HD21	49:v:603:TYR:HB3	1.81	0.63
9:F:231:ASP:OD1	9:F:235:ARG:NH2	2.31	0.63
49:v:714:ILE:HG22	50:w:200:ASP:HB3	1.80	0.63
1:5:2520:C:O2	1:5:2640:G:N2	2.32	0.62
72:UU:80:PHE:HB3	81:dd:52:PHE:HB3	1.80	0.62
1:5:4039:G:H21	1:5:4051:C:H1'	1.63	0.62
1:5:4621:C:OP1	24:V:48:ARG:NH2	2.33	0.62
49:v:714:ILE:CD1	50:w:198:GLY:HA2	2.04	0.62
24:V:82:ILE:HG22	24:V:83:ARG:HG3	1.81	0.62
51:9:1337:4AC:OP1	81:dd:44:ARG:NH2	2.33	0.62
56:EE:72:ILE:HD11	56:EE:88:ASP:HB3	1.82	0.62
74:WW:69:LEU:HD21	74:WW:72:CYS:HB2	1.82	0.62
1:5:2334:C:OP2	6:C:195:LYS:NZ	2.33	0.62
7:D:50:ARG:O	7:D:64:ILE:HA	2.00	0.62
7:D:259:ARG:NH2	7:D:260:GLU:O	2.33	0.62
50:w:286:TRP:NE1	62:KK:86:PRO:HD2	2.15	0.62
57:FF:71:ARG:NH1	57:FF:148:ASN:OD1	2.32	0.62
51:9:658:U:O2	75:XX:17:ARG:NH2	2.32	0.62
57:FF:118:ASN:O	57:FF:193:LYS:NZ	2.33	0.62
1:5:1552:G:O2'	1:5:1574:B9B:N2	2.32	0.62
1:5:1604:G:H2'	1:5:1605:7MG:H82	1.82	0.61
28:Z:54:THR:H	28:Z:57:MET:HE2	1.64	0.61
84:gg:18:VAL:HA	84:gg:35:SER:HA	1.81	0.61
27:Y:112:ASP:H	27:Y:115:ARG:HB3	1.65	0.61
51:9:380:G:N3	60:II:5:ARG:NH1	2.48	0.61
50:w:198:GLY:H	51:9:1331:C:H5	1.49	0.61
75:XX:84:PHE:H	75:XX:121:LYS:HA	1.65	0.61
52:AA:76:VAL:HG12	52:AA:123:VAL:HB	1.81	0.61
58:GG:98:ARG:NH2	58:GG:103:ASP:OD1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3641:U:OP2	1:5:3646:A:N6	2.34	0.61
48:u:26:ARG:HH21	48:u:210:MET:H	1.47	0.61
62:KK:14:LEU:HD22	62:KK:35:LEU:HB3	1.83	0.61
1:5:2305:U:HO2'	33:e:104:SER:HG	1.47	0.61
14:L:116:ARG:NH1	14:L:155:MET:O	2.33	0.61
49:v:649:ILE:HG22	49:v:663:THR:HG22	1.81	0.61
57:FF:204:ARG:O	66:OO:117:ARG:NH1	2.34	0.61
53:BB:30:TRP:NE1	66:OO:17:LEU:O	2.34	0.61
53:BB:72:ALA:HB3	66:OO:128:ARG:HH12	1.65	0.61
58:GG:121:ILE:HG13	58:GG:123:GLY:H	1.66	0.61
70:SS:26:ILE:HG21	70:SS:59:LEU:HD21	1.83	0.61
51:9:1858:G:OP2	66:OO:146:ARG:NH2	2.34	0.61
1:5:1860:B8H:C6	1:5:1860:B8H:CN1	2.75	0.61
1:5:2380:B8W:N2	1:5:2425:U:OP1	2.33	0.61
1:5:2528:G:H4'	1:5:2783:A:H4'	1.81	0.61
15:M:104:MET:HE2	17:O:199:HIS:HB3	1.82	0.61
1:5:1493:G:OP2	30:b:44:ARG:NH1	2.34	0.60
53:BB:136:ARG:HE	53:BB:218:LEU:HD21	1.66	0.60
51:9:1138:C:OP1	52:AA:155:ARG:NH1	2.33	0.60
84:gg:43:TRP:HA	84:gg:55:PRO:HA	1.83	0.60
1:5:2046:G:H5'	17:O:60:LYS:HE3	1.82	0.60
13:J:89:VAL:HG21	13:J:114:ASP:HB3	1.83	0.60
32:d:36:VAL:HG11	32:d:44:ARG:HD2	1.83	0.60
51:9:616:A:H62	51:9:625:G:N2	2.00	0.60
55:DD:163:PRO:O	55:DD:167:TYR:HB2	2.00	0.60
1:5:1759:G:H1	1:5:1773:U:H3	1.47	0.60
20:R:139:MET:O	20:R:143:HIS:ND1	2.34	0.60
49:v:260:LEU:HD13	49:v:293:ILE:HD11	1.83	0.60
49:v:750:GLN:HG3	49:v:783:VAL:HG12	1.82	0.60
1:5:4949:G:H4'	1:5:4950:U:H5'	1.82	0.60
4:A:36:GLU:OE1	4:A:163:ARG:NH1	2.35	0.60
11:H:23:ARG:HH21	11:H:39:ASN:HA	1.67	0.60
1:5:4939:C:OP1	8:E:190:ARG:NH1	2.33	0.60
4:A:117:GLU:HB3	4:A:162:ASN:HB2	1.83	0.60
1:5:67:C:OP2	1:5:312:G:N2	2.34	0.60
1:5:2793:G:H5'	1:5:2794:C:H5''	1.84	0.60
1:5:3952:A:N1	1:5:4061:G:O6	2.35	0.60
51:9:190:G:O2'	51:9:209:A:N6	2.34	0.60
51:9:1091:C:HO2'	74:WW:2:VAL:N	1.99	0.60
59:HH:117:PRO:HG2	59:HH:120:ARG:HD3	1.82	0.60
1:5:1073:G:H1	1:5:1238:A:H2	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4753:U:OP1	34:f:100:ARG:NH1	2.34	0.60
20:R:102:LEU:HD22	20:R:138:LEU:HD13	1.83	0.60
51:9:380:G:OP1	60:II:56:ARG:NH2	2.34	0.60
51:9:1664:A:O2'	51:9:1666:C:N4	2.35	0.60
83:ff:123:SER:OG	83:ff:126:CYS:SG	2.60	0.60
8:E:141:ARG:NH1	8:E:172:SER:O	2.35	0.60
20:R:78:ILE:HG22	20:R:81:ARG:HH21	1.66	0.60
49:v:754:GLN:HG2	49:v:755:VAL:HG13	1.83	0.60
51:9:1657:G:H1	51:9:1667:U:H3	1.49	0.60
7:D:50:ARG:NH2	7:D:147:ASP:OD2	2.35	0.60
51:9:1351:G:O6	51:9:1360:U:C4	2.49	0.60
1:5:2836:A:H4'	5:B:229:LYS:HA	1.82	0.59
49:v:661:ILE:O	49:v:702:PHE:HB2	2.02	0.59
1:5:4761:G:H2'	1:5:4762:A:H8	1.68	0.59
16:N:5:LYS:HG3	37:i:40:VAL:HG11	1.83	0.59
19:Q:154:LYS:NZ	19:Q:159:PRO:O	2.35	0.59
31:c:31:TYR:OH	31:c:59:GLU:OE2	2.20	0.59
51:9:616:A:H62	51:9:625:G:H21	1.48	0.59
64:MM:80:ASP:OD1	64:MM:80:ASP:N	2.34	0.59
1:5:3688:U:OP2	4:A:198:ARG:NH2	2.34	0.59
21:S:34:ALA:HB1	21:S:39:VAL:HG13	1.84	0.59
49:v:25:ILE:O	49:v:127:VAL:HA	2.01	0.59
51:9:496:C:OP1	56:EE:49:ARG:NH1	2.36	0.59
51:9:992:A:N7	78:aa:15:ARG:NH2	2.50	0.59
9:F:227:VAL:HG13	21:S:39:VAL:HG23	1.85	0.59
59:HH:154:ILE:HB	59:HH:185:VAL:HG22	1.85	0.59
1:5:40:G:N2	1:5:4380:A:N7	2.51	0.59
1:5:729:2MG:N2	21:S:66:GLN:O	2.32	0.59
1:5:2837:U:OP1	5:B:249:ARG:NH1	2.36	0.59
65:NN:4:MET:SD	65:NN:124:ARG:NH1	2.75	0.59
1:5:3651:A:OP2	4:A:200:ARG:NH1	2.36	0.59
3:8:75:G:OP2	27:Y:74:TYR:OH	2.19	0.59
47:t:39:PRO:HG2	47:t:40:LYS:HD2	1.85	0.59
49:v:652:PHE:O	49:v:684:GLN:NE2	2.36	0.59
51:9:111:A:O2'	63:LL:69:ARG:NH1	2.36	0.59
23:U:111:GLU:OE2	23:U:113:ARG:NH1	2.36	0.59
29:a:76:ASP:HB3	29:a:115:GLY:HA3	1.84	0.59
49:v:179:GLN:OE1	49:v:180:ARG:NH2	2.35	0.59
51:9:941:C:H5''	53:BB:136:ARG:HH22	1.68	0.59
51:9:1584:G:OP1	71:TT:77:LYS:NZ	2.36	0.59
58:GG:22:ARG:HA	58:GG:25:ARG:HE	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:116:LEU:HB3	4:A:126:LEU:HB2	1.84	0.58
51:9:1289:U:OP2	83:ff:95:ARG:NH2	2.34	0.58
51:9:1373:C:O2'	69:RR:10:LYS:NZ	2.36	0.58
54:CC:200:ARG:O	61:JJ:54:ARG:NH1	2.33	0.58
66:OO:53:ILE:HG23	66:OO:88:LEU:HD22	1.85	0.58
1:5:1492:G:O2'	30:b:41:ARG:NH1	2.36	0.58
1:5:1739:G:N3	1:5:1742:A:N6	2.51	0.58
1:5:3937:C:O2'	16:N:124:ASP:OD1	2.21	0.58
1:5:690:C:H4'	45:r:85:ASN:HD22	1.67	0.58
1:5:1970:A:OP2	46:s:112:ARG:NH2	2.34	0.58
48:u:48:ARG:NH2	48:u:159:MET:O	2.35	0.58
51:9:1617:G:O6	67:PP:43:ARG:NH1	2.36	0.58
54:CC:142:LYS:HD3	54:CC:153:GLY:HA3	1.84	0.58
1:5:230:G:OP1	27:Y:15:ARG:NH1	2.37	0.58
1:5:1895:G:OP1	9:F:95:ARG:NH2	2.37	0.58
1:5:3659:G:H4'	4:A:227:ARG:HH22	1.66	0.58
51:9:153:G:N3	58:GG:13:GLN:NE2	2.45	0.58
51:9:433:A:H5''	60:II:22:HIS:HB3	1.85	0.58
59:HH:146:VAL:HG22	59:HH:152:ARG:HG2	1.86	0.58
14:L:21:ARG:HB3	16:N:197:THR:HG22	1.86	0.58
51:9:1148:A:OP1	78:aa:6:ARG:NH2	2.36	0.58
1:5:973:C:O2	1:5:1282:G:N2	2.35	0.58
1:5:4930:C:H5'	8:E:269:GLN:HG2	1.86	0.58
12:I:96:VAL:HG12	12:I:125:THR:HG22	1.85	0.58
49:v:208:VAL:HB	49:v:258:LYS:HA	1.85	0.58
51:9:94:G:OP1	56:EE:6:LYS:NZ	2.36	0.58
51:9:346:C:H5''	56:EE:38:LEU:HB2	1.86	0.58
84:gg:6:THR:O	84:gg:310:TRP:HA	2.03	0.58
3:8:85:U:O4	27:Y:50:ARG:NH2	2.36	0.58
16:N:155:VAL:O	16:N:162:ARG:NH2	2.37	0.58
28:Z:84:ARG:NH1	35:g:99:GLU:OE1	2.37	0.58
1:5:2429:A:H5''	40:l:43:HIS:HE2	1.68	0.58
5:B:10:ARG:NH1	5:B:265:SER:O	2.37	0.58
11:H:107:GLU:HG3	11:H:110:SER:HB2	1.85	0.58
22:T:112:ASN:HA	22:T:115:LYS:HG2	1.85	0.58
22:T:112:ASN:HB2	22:T:128:LEU:HD22	1.86	0.58
62:KK:85:LEU:HB3	62:KK:89:ILE:HD11	1.86	0.58
64:MM:36:ARG:HH12	64:MM:40:LYS:HE3	1.67	0.58
1:5:4333:C:O2	22:T:8:ARG:NH1	2.37	0.58
21:S:13:VAL:HG23	21:S:62:VAL:HB	1.85	0.58
51:9:38:A:H5''	61:JJ:5:ARG:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DD:67:ARG:HH22	62:KK:96:ARG:HA	1.69	0.58
55:DD:168:VAL:HA	55:DD:188:ILE:O	2.04	0.58
1:5:364:G:O6	38:j:52:LYS:NZ	2.37	0.57
51:9:830:A:OP2	51:9:846:G:N2	2.36	0.57
51:9:1262:C:O2'	81:dd:12:ARG:NH1	2.37	0.57
56:EE:68:ARG:HG3	56:EE:76:VAL:HG11	1.86	0.57
70:SS:84:LEU:HD22	70:SS:97:GLN:HB2	1.86	0.57
1:5:1670:G:OP1	30:b:12:GLN:NE2	2.37	0.57
46:s:61:MET:HG2	46:s:88:PHE:HE2	1.69	0.57
46:s:135:THR:HG21	49:v:187:VAL:HG21	1.87	0.57
49:v:723:PRO:O	49:v:727:ARG:NE	2.36	0.57
51:9:919:A:OP2	65:NN:64:ARG:NH2	2.37	0.57
51:9:1252:C:OP1	72:UU:75:LYS:NZ	2.36	0.57
51:9:1417:C:N3	51:9:1423:C:N4	2.52	0.57
51:9:1627:C:OP1	71:TT:83:GLN:NE2	2.37	0.57
1:5:1840:G:OP2	9:F:201:LYS:NZ	2.36	0.57
1:5:4558:U:OP2	5:B:246:ARG:NH2	2.37	0.57
1:5:2521:G:H2'	1:5:2522:7MG:H82	1.86	0.57
1:5:2533:C:OP1	26:X:139:ARG:NH2	2.36	0.57
1:5:4146:G:H2'	1:5:4147:G:H8	1.70	0.57
41:m:84:CYS:SG	41:m:85:ARG:N	2.76	0.57
51:9:1036:A:N3	51:9:1844:U:O2'	2.38	0.57
64:MM:83:LYS:HA	64:MM:105:GLY:HA2	1.85	0.57
1:5:2422:OMC:OP1	18:P:127:ARG:NH2	2.38	0.57
1:5:4473:A:H5''	41:m:69:ILE:HG12	1.85	0.57
1:5:4910:A:H4'	5:B:95:THR:HG22	1.86	0.57
11:H:91:LYS:HG2	11:H:145:VAL:HG22	1.87	0.57
49:v:396:MET:HG3	49:v:485:ILE:HG23	1.87	0.57
60:II:162:LEU:HD11	60:II:191:GLU:HG2	1.86	0.57
1:5:200:U:O4	27:Y:103:LYS:NZ	2.37	0.57
1:5:4981:G:O6	5:B:21:ARG:NH2	2.38	0.57
6:C:78:ARG:HB3	6:C:88:GLY:HA2	1.87	0.57
49:v:86:LEU:HD21	49:v:96:ALA:HA	1.87	0.57
51:9:1551:U:OP1	55:DD:9:ARG:NH2	2.37	0.57
1:5:935:A:H5'	1:5:935(A):G:H4'	1.85	0.57
1:5:1214:C:O2	30:b:91:ARG:NH1	2.37	0.57
4:A:158:ILE:HG23	4:A:162:ASN:HD21	1.69	0.57
11:H:16:VAL:O	11:H:52:LYS:NZ	2.38	0.57
11:H:113:GLU:HG2	11:H:125:ARG:HG2	1.86	0.57
16:N:174:LEU:HA	16:N:183:THR:HG21	1.86	0.57
51:9:492:C:OP2	76:YY:107:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:874:G:N3	59:HH:114:GLN:NE2	2.49	0.57
51:9:1745:A:O3'	58:GG:31:ARG:NH1	2.37	0.57
53:BB:121:ILE:HG12	53:BB:161:VAL:HG13	1.87	0.57
25:W:116:LYS:NZ	51:9:329:G:N7	2.52	0.57
47:t:141:CYS:O	47:t:146:ARG:NH1	2.37	0.57
51:9:603:C:N4	51:9:620:G:O6	2.37	0.57
51:9:1533:A:N6	51:9:1602:U:C2	2.72	0.57
51:9:1700:C:O2	51:9:1834:A:N6	2.36	0.57
1:5:1315:C:OP1	33:e:44:ARG:NH2	2.36	0.57
1:5:1951:G:O2'	21:S:95:ARG:NH1	2.37	0.57
1:5:4052:C:O2'	48:u:210:MET:SD	2.62	0.57
13:J:18:ARG:HG3	13:J:135:GLY:HA3	1.87	0.57
19:Q:67:ILE:HD12	19:Q:96:PRO:HD2	1.87	0.57
56:EE:137:PRO:HB2	56:EE:150:PRO:HD2	1.87	0.57
68:QQ:97:GLN:HB2	68:QQ:105:LYS:HG3	1.87	0.57
1:5:2526:C:N4	26:X:84:GLU:OE2	2.37	0.57
7:D:55:VAL:HG12	7:D:60:ILE:HG12	1.87	0.57
19:Q:78:LYS:HG2	19:Q:137:VAL:HG23	1.86	0.57
49:v:87:ASN:ND2	49:v:245:GLY:O	2.36	0.57
51:9:64:A:H2	51:9:83:A:H62	1.52	0.57
74:WW:111:MET:HE3	74:WW:116:ALA:HA	1.87	0.57
1:5:303:C:OP2	16:N:68:ARG:NH2	2.38	0.56
1:5:2489:C:O2'	1:5:2491:C:N4	2.38	0.56
1:5:2872:C:H5''	42:n:25:LYS:HD3	1.87	0.56
51:9:1563:G:OP1	71:TT:121:ARG:NH2	2.38	0.56
51:9:1669:G:OP1	72:UU:79:ARG:NH2	2.38	0.56
55:DD:106:ARG:HG2	55:DD:175:VAL:HB	1.86	0.56
73:VV:15:ARG:HH11	73:VV:33:GLN:HG3	1.70	0.56
49:v:321:ILE:HD13	49:v:343:TRP:HB2	1.87	0.56
51:9:1599:U:OP1	77:ZZ:80:ARG:NH2	2.39	0.56
1:5:979:G:OP1	8:E:49:ASN:ND2	2.38	0.56
1:5:990:U:H3	1:5:1064:G:H1	1.52	0.56
1:5:1279:A:O2'	6:C:323:ARG:NH2	2.39	0.56
1:5:4115:G:OP1	4:A:93:LYS:NZ	2.39	0.56
20:R:151:ARG:HH12	63:LL:118:ARG:HB3	1.70	0.56
51:9:1629:C:OP1	70:SS:39:ARG:NH2	2.38	0.56
52:AA:89:LYS:NZ	69:RR:82:ASP:O	2.36	0.56
67:PP:61:ARG:NH2	67:PP:88:GLU:OE2	2.39	0.56
71:TT:104:LEU:HD22	71:TT:121:ARG:HG3	1.87	0.56
76:YY:103:SER:OG	76:YY:106:GLN:OE1	2.24	0.56
1:5:2444:U:O2'	3:8:112:G:O2'	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:217:ILE:HD11	5:B:333:LEU:HD21	1.87	0.56
48:u:118:LYS:O	48:u:122:ARG:NH1	2.39	0.56
52:AA:77:ILE:HB	52:AA:124:VAL:HG23	1.88	0.56
1:5:467:U:O2	1:5:686:A:N6	2.38	0.56
1:5:3967:G:N2	48:u:164:CYS:SG	2.74	0.56
11:H:94:SER:HB3	11:H:142:ASP:HB3	1.86	0.56
45:r:98:ARG:HH21	45:r:107:ARG:HH22	1.53	0.56
50:w:196:HIS:N	50:w:196:HIS:CD2	2.73	0.56
51:9:925:G:OP1	65:NN:121:ARG:NH2	2.39	0.56
51:9:1761:U:H3	51:9:1771:G:H22	1.54	0.56
55:DD:23:GLU:OE2	55:DD:27:ARG:NH2	2.38	0.56
1:5:1468:C:OP1	29:a:132:ARG:NH2	2.38	0.56
1:5:1895:G:O2'	1:5:1907:A:N3	2.35	0.56
2:7:27:G:OP1	13:J:146:ARG:NH1	2.38	0.56
5:B:41:VAL:HA	5:B:187:GLY:HA3	1.88	0.56
48:u:102:LYS:HG3	48:u:105:LYS:HD3	1.87	0.56
51:9:104:A:H62	51:9:356:C:H5	1.53	0.56
51:9:1617:G:N7	67:PP:47:ARG:NH1	2.49	0.56
64:MM:33:ARG:HG2	64:MM:109:VAL:HG22	1.87	0.56
79:bb:23:ARG:NH1	79:bb:27:SER:O	2.39	0.56
1:5:1654:G:N2	1:5:1678:C:OP1	2.38	0.56
51:9:1199:A:OP1	78:aa:2:THR:N	2.38	0.56
65:NN:45:LEU:HG	65:NN:49:GLN:HG3	1.87	0.56
51:9:1513:C:H2'	51:9:1514:G:H8	1.70	0.56
56:EE:11:ARG:NH2	56:EE:21:ASP:OD1	2.38	0.56
56:EE:122:LYS:NZ	56:EE:143:ASP:OD2	2.37	0.56
66:OO:57:THR:H	66:OO:60:MET:HE3	1.68	0.56
1:5:1802:A:O2'	1:5:1837:A:OP1	2.23	0.56
1:5:1969:G:OP2	46:s:112:ARG:NH1	2.39	0.56
45:r:63:VAL:HG22	45:r:79:ARG:HG2	1.87	0.56
51:9:1374:5MC:OP1	69:RR:14:ARG:NH2	2.36	0.56
53:BB:138:PHE:O	53:BB:213:ARG:N	2.36	0.56
68:QQ:132:PHE:O	68:QQ:140:ARG:NH2	2.39	0.56
71:TT:76:THR:HB	71:TT:94:ARG:HB3	1.88	0.56
1:5:1364:U:OP2	14:L:36:ARG:NH2	2.37	0.56
1:5:3919:C:OP1	4:A:2:GLY:N	2.39	0.56
19:Q:16:LYS:O	19:Q:33:ARG:NH2	2.38	0.56
49:v:631:ARG:HD2	49:v:649:ILE:HD11	1.88	0.56
51:9:439:A:OP2	60:II:23:LYS:NZ	2.38	0.56
65:NN:46:THR:HG22	65:NN:49:GLN:HG2	1.88	0.56
74:WW:103:VAL:HA	74:WW:112:ASP:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:XX:91:LEU:HB3	82:ee:82:VAL:HG21	1.88	0.56
1:5:3796:U:HO2'	51:9:1720:U:HO2'	1.53	0.55
26:X:129:ARG:NH2	26:X:131:ASP:OD2	2.39	0.55
51:9:555:A:N6	51:9:589:G:N3	2.54	0.55
51:9:1550:G:H3'	51:9:1579:A:H61	1.70	0.55
54:CC:264:SER:HB3	54:CC:267:GLN:HG3	1.88	0.55
1:5:66:A:H61	1:5:282:C:HO2'	1.55	0.55
1:5:4258:C:H5'	13:J:68:ILE:HD11	1.88	0.55
12:I:87:ILE:HG12	12:I:138:ILE:HG12	1.88	0.55
32:d:29:ILE:HD11	32:d:84:ILE:HG12	1.89	0.55
51:9:1617:G:N1	51:9:1620:A:OP2	2.39	0.55
22:T:119:ALA:HA	22:T:122:LYS:HB2	1.87	0.55
46:s:44:ARG:HE	46:s:53:VAL:HG13	1.71	0.55
47:t:59:THR:HG23	47:t:74:VAL:HB	1.88	0.55
51:9:4:C:O2'	61:JJ:18:ARG:NH1	2.40	0.55
51:9:643:A:OP2	61:JJ:38:ARG:NH2	2.29	0.55
51:9:1310:U:OP1	64:MM:36:ARG:NH1	2.39	0.55
51:9:1623:A:H5''	70:SS:133:GLY:HA3	1.88	0.55
1:5:87:A:OP2	19:Q:173:LYS:NZ	2.39	0.55
25:W:6:CYS:HB3	25:W:10:GLY:H	1.70	0.55
51:9:1497:G:N7	62:KK:25:LYS:NZ	2.43	0.55
57:FF:51:HIS:ND1	68:QQ:82:TYR:OH	2.31	0.55
64:MM:93:LYS:HE3	64:MM:96:ARG:HG2	1.89	0.55
1:5:89:C:OP1	29:a:59:ARG:NH1	2.40	0.55
1:5:262:G:H2'	1:5:263:G:H8	1.70	0.55
1:5:1326:A2M:OP2	1:5:4445:U:O2'	2.24	0.55
24:V:99:GLU:HB3	25:W:24:THR:HG23	1.87	0.55
53:BB:105:LEU:HD23	53:BB:213:ARG:HA	1.88	0.55
77:ZZ:73:VAL:HG21	77:ZZ:88:LEU:HD11	1.87	0.55
1:5:1391:A:OP1	19:Q:181:ARG:NH1	2.39	0.55
48:u:195:LYS:HE2	48:u:196:LYS:HE3	1.88	0.55
1:5:136:C:N4	36:h:76:LYS:O	2.40	0.55
1:5:2725:A:N6	20:R:88:ARG:O	2.39	0.55
1:5:2743:A:H1'	4:A:21:LYS:HE3	1.89	0.55
1:5:4522:G:O2'	1:5:4525:C:OP2	2.25	0.55
51:9:15:U:O2'	51:9:669:A:N6	2.39	0.55
51:9:94:G:HO2'	51:9:508:A:HO2'	1.50	0.55
1:5:2400:G:H21	35:g:6:THR:HG22	1.71	0.55
13:J:19:LYS:HG2	13:J:133:VAL:HG12	1.87	0.55
51:9:1100:A:O5'	69:RR:132:ARG:NH2	2.40	0.55
57:FF:44:LYS:NZ	68:QQ:114:GLN:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SS:4:VAL:HA	77:ZZ:50:PHE:HB2	1.89	0.55
84:gg:152:SER:OG	84:gg:168:CYS:SG	2.64	0.55
1:5:70:A:OP2	29:a:64:LYS:NZ	2.38	0.55
1:5:1355:G:OP1	19:Q:108:ARG:NH2	2.38	0.55
1:5:4296:B8H:C5	1:5:4296:B8H:C2	2.84	0.55
1:5:4358:U:H4'	14:L:197:LYS:HD2	1.87	0.55
24:V:104:VAL:HG21	24:V:132:ILE:HD11	1.88	0.55
26:X:87:MET:HA	26:X:90:ILE:HG12	1.89	0.55
34:f:50:VAL:HG22	34:f:69:VAL:HG12	1.89	0.55
51:9:1270:G:O2'	51:9:1301:A:N7	2.40	0.55
51:9:1616:U:OP2	67:PP:43:ARG:NH2	2.39	0.55
65:NN:130:LYS:NZ	65:NN:139:TRP:O	2.33	0.55
70:SS:34:LYS:HE3	70:SS:103:LEU:HD23	1.87	0.55
1:5:480:C:OP1	45:r:67:ARG:NH1	2.40	0.55
1:5:4212:A:N1	22:T:3:ASN:ND2	2.44	0.55
1:5:4280:A:N6	7:D:28:THR:O	2.38	0.55
8:E:189:LEU:HD21	8:E:256:VAL:HG11	1.89	0.55
51:9:170:A:OP2	58:GG:140:ARG:NH1	2.39	0.55
51:9:1156:U:O4	54:CC:194:ARG:NH1	2.40	0.55
51:9:1452:A:N6	51:9:1473:G:H21	2.04	0.55
62:KK:32:HIS:HE1	62:KK:34:GLU:HB3	1.71	0.55
1:5:419:A:N3	1:5:1332:C:O2'	2.39	0.54
15:M:27:ILE:HA	15:M:38:VAL:HG23	1.89	0.54
44:p:37:TYR:HB2	44:p:47:MET:HB2	1.89	0.54
52:AA:157:VAL:O	73:VV:65:SER:OG	2.23	0.54
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.89	0.54
57:FF:14:THR:OG1	68:QQ:56:LEU:O	2.25	0.54
76:YY:78:SER:OG	76:YY:80:ASP:OD1	2.25	0.54
1:5:83:C:O2'	1:5:100:C:N4	2.40	0.54
31:c:56:ARG:HA	31:c:59:GLU:HG2	1.89	0.54
48:u:112:ALA:HB1	48:u:116:LEU:HD21	1.88	0.54
49:v:583:VAL:HG22	49:v:700:VAL:HG12	1.89	0.54
49:v:659:PRO:HG2	49:v:698:ARG:HA	1.88	0.54
52:AA:36:GLN:O	52:AA:53:ARG:NH1	2.40	0.54
55:DD:16:ILE:HD11	81:dd:36:LEU:HD23	1.89	0.54
4:A:29:LEU:O	4:A:123:ARG:NH1	2.40	0.54
5:B:160:ILE:HD11	5:B:190:VAL:HG13	1.87	0.54
12:I:54:SER:HB2	12:I:135:ILE:HD11	1.88	0.54
47:t:61:LYS:HD3	47:t:72:GLU:HG2	1.89	0.54
49:v:464:VAL:HG11	49:v:470:VAL:HG21	1.89	0.54
53:BB:32:ASP:OD1	53:BB:46:LYS:NZ	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:II:113:TYR:OH	60:II:156:ALA:O	2.26	0.54
70:SS:27:ALA:HB2	70:SS:52:LEU:HD21	1.90	0.54
8:E:153:LEU:O	8:E:164:ARG:HA	2.07	0.54
21:S:115:ALA:O	21:S:118:ARG:NH2	2.41	0.54
52:AA:37:TYR:OH	52:AA:57:LYS:NZ	2.31	0.54
1:5:1316:OMG:OP1	33:e:43:ASN:ND2	2.40	0.54
1:5:2845:A:H61	1:5:3843:C:N4	2.05	0.54
1:5:4289:U:HO2'	1:5:4320:G:HO2'	1.46	0.54
1:5:4293:PSU:O2'	43:o:81:ARG:NH2	2.41	0.54
1:5:4735:G:N2	1:5:4965:U:O2	2.40	0.54
7:D:120:GLU:O	7:D:248:ARG:NH2	2.37	0.54
14:L:207:VAL:HA	14:L:210:LYS:HG2	1.90	0.54
26:X:110:LYS:NZ	26:X:121:VAL:O	2.40	0.54
45:r:17:LEU:HD11	45:r:19:LYS:HE3	1.88	0.54
51:9:1396:A:N7	51:9:1449:G:O6	2.41	0.54
61:JJ:38:ARG:HA	82:ee:104:ARG:HB3	1.89	0.54
69:RR:15:VAL:HA	69:RR:18:GLU:HG2	1.89	0.54
1:5:1187:G:H1'	7:D:275:GLN:HE21	1.73	0.54
1:5:2411:C:H2'	1:5:2412:A:H8	1.72	0.54
11:H:152:GLU:O	11:H:156:ASN:HB2	2.08	0.54
14:L:186:ARG:HH21	37:i:9:VAL:HG11	1.73	0.54
51:9:537:C:N3	51:9:547:G:N2	2.56	0.54
51:9:989:C:O2	78:aa:32:LYS:NZ	2.41	0.54
1:5:1628:C:OP1	4:A:14:SER:OG	2.25	0.54
1:5:1883:OMG:HM22	1:5:2070:U:H3	1.72	0.54
1:5:2580:U:O2	28:Z:76:ASN:ND2	2.41	0.54
11:H:107:GLU:OE2	11:H:127:ARG:NH2	2.37	0.54
12:I:150:GLU:OE2	12:I:153:ARG:NH1	2.41	0.54
20:R:168:GLU:OE1	20:R:172:ARG:NH1	2.40	0.54
44:p:38:THR:HA	44:p:45:THR:HA	1.90	0.54
49:v:451:ILE:HA	49:v:460:PRO:HA	1.90	0.54
57:FF:145:ARG:HB2	80:cc:49:PRO:HD2	1.89	0.54
1:5:1362:G:OP1	14:L:39:ARG:NH2	2.36	0.54
3:8:153:C:OP1	10:G:238:LYS:NZ	2.33	0.54
42:n:2:ARG:NH1	51:9:1841:C:OP2	2.41	0.54
51:9:1553:C:O2'	51:9:1554:C:O4'	2.26	0.54
51:9:1566:G:N7	71:TT:101:ARG:NH1	2.51	0.54
52:AA:94:THR:OG1	52:AA:186:ARG:NH2	2.40	0.54
53:BB:122:GLU:O	53:BB:165:ARG:NH2	2.40	0.54
1:5:300:A:H2'	1:5:301:G:H8	1.72	0.54
49:v:155:LEU:HD22	49:v:205:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:HH:53:VAL:HG21	59:HH:172:THR:HA	1.90	0.54
1:5:2089:G:H1	1:5:2099:C:H41	1.56	0.54
1:5:2607:C:H5''	20:R:96:MET:HE1	1.90	0.54
1:5:3685:C:OP1	4:A:193:ARG:NH1	2.39	0.54
1:5:4099:G:H1	1:5:4110:C:H42	1.53	0.54
1:5:4760:G:OP1	17:O:117:ARG:NH2	2.40	0.54
1:5:4894:A:H5''	1:5:4895:C:H2'	1.88	0.54
45:r:85:ASN:N	45:r:85:ASN:OD1	2.41	0.54
1:5:4473:A:O2'	41:m:96:ARG:NH2	2.42	0.53
5:B:57:VAL:HG22	5:B:73:VAL:HG12	1.89	0.53
10:G:111:PRO:HD2	10:G:114:ILE:HD12	1.90	0.53
27:Y:50:ARG:HB2	27:Y:115:ARG:HH22	1.73	0.53
51:9:1293:A:H61	51:9:1306:U:H3	1.56	0.53
51:9:1507:G:N2	83:f:87:THR:O	2.33	0.53
61:JJ:137:VAL:HG22	61:JJ:157:ILE:HG12	1.88	0.53
66:OO:65:ASP:HA	66:OO:68:GLU:HG3	1.90	0.53
51:9:640:A:OP2	82:ee:110:GLN:NE2	2.41	0.53
84:gg:38:LYS:NZ	84:gg:62:HIS:O	2.39	0.53
1:5:1516:G:O2'	14:L:18:TRP:NE1	2.36	0.53
1:5:1521:C:OP1	6:C:100:ARG:NH2	2.38	0.53
1:5:4769:G:H5'	17:O:176:ARG:HD3	1.90	0.53
49:v:613:LEU:HA	49:v:616:ASP:HB2	1.90	0.53
56:EE:45:ILE:HG13	56:EE:61:VAL:HG21	1.89	0.53
65:NN:47:PRO:HA	65:NN:50:ILE:HG12	1.90	0.53
49:v:401:MET:HG3	49:v:412:ALA:HA	1.90	0.53
49:v:651:CYS:SG	49:v:652:PHE:N	2.82	0.53
64:MM:46:GLN:HB3	64:MM:112:LYS:HD3	1.91	0.53
84:gg:107:ASP:HB2	84:gg:125:ARG:HD2	1.91	0.53
14:L:14:PHE:HE1	16:N:198:LEU:HD11	1.73	0.53
51:9:1748:G:H1	51:9:1786:U:H3	1.55	0.53
61:JJ:86:VAL:HG21	61:JJ:105:PHE:HE1	1.73	0.53
61:JJ:170:PRO:O	61:JJ:175:ARG:NH1	2.40	0.53
65:NN:99:ARG:NH2	65:NN:119:GLU:OE2	2.37	0.53
72:UU:20:ILE:HD12	72:UU:116:ILE:HA	1.91	0.53
3:8:30:U:OP1	14:L:34:ARG:NH2	2.42	0.53
14:L:116:ARG:HH22	14:L:157:ILE:HD11	1.73	0.53
25:W:80:ARG:NH1	58:GG:129:VAL:O	2.31	0.53
29:a:85:GLN:HA	29:a:88:VAL:HG22	1.90	0.53
48:u:104:ALA:HB2	48:u:133:LYS:HE2	1.91	0.53
49:v:330:LYS:HD3	49:v:334:PRO:HB2	1.90	0.53
49:v:710:HIS:CD2	49:v:715:DDE:HD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:482:G:N1	51:9:485:A:OP2	2.39	0.53
55:DD:50:ILE:HD11	55:DD:86:LEU:HD23	1.91	0.53
84:gg:154:VAL:O	84:gg:155:ARG:NH1	2.40	0.53
1:5:2322:G:OP1	33:e:36:ARG:NH1	2.41	0.53
1:5:3896:C:O2'	5:B:268:ARG:NH1	2.40	0.53
47:t:136:ALA:HB3	47:t:146:ARG:HH22	1.74	0.53
49:v:686:ALA:O	49:v:730:TYR:OH	2.26	0.53
49:v:755:VAL:HG21	49:v:807:GLN:HG3	1.91	0.53
62:KK:11:ILE:HD11	62:KK:45:VAL:HG22	1.90	0.53
1:5:942:G:OP1	9:F:244:ARG:NH1	2.42	0.53
1:5:1502:G:OP2	19:Q:62:SER:OG	2.26	0.53
1:5:4896:G:H2'	1:5:4897:G:H8	1.74	0.53
11:H:7:ASN:HB3	11:H:58:ASP:HB3	1.90	0.53
1:5:4862:G:H2'	1:5:4863:G:H8	1.74	0.53
51:9:1204:A:O2'	51:9:1700:C:OP2	2.26	0.53
51:9:1416:C:O2	71:TT:3:GLY:N	2.42	0.53
51:9:1568:C:OP1	71:TT:96:SER:OG	2.23	0.53
55:DD:109:LEU:HD11	55:DD:115:VAL:HG22	1.90	0.53
1:5:3680:U:OP1	4:A:54:ARG:NH2	2.37	0.53
1:5:4895:C:O2	15:M:132:ARG:NH2	2.32	0.53
18:P:23:ARG:NH1	18:P:125:MET:SD	2.82	0.53
48:u:93:LEU:HD11	48:u:99:LEU:HB2	1.91	0.53
51:9:1533:A:N6	51:9:1602:U:N3	2.45	0.53
74:WW:87:GLU:HA	74:WW:90:GLN:HG2	1.89	0.53
76:YY:17:LEU:HD12	76:YY:18:LEU:HD12	1.90	0.53
1:5:229:G:H5''	27:Y:11:ARG:HG3	1.91	0.52
1:5:5001:U:H4'	5:B:317:LEU:HB3	1.91	0.52
5:B:44:THR:HG21	5:B:186:ASN:HD22	1.75	0.52
7:D:22:ARG:HE	7:D:27:LYS:HB2	1.73	0.52
25:W:80:ARG:HH12	58:GG:11:GLY:HA3	1.73	0.52
51:9:77:A:H5''	58:GG:154:ARG:HB3	1.91	0.52
52:AA:94:THR:O	52:AA:186:ARG:NH2	2.41	0.52
1:5:4194:I4U:O2'	12:I:116:ARG:NH1	2.39	0.52
32:d:23:ARG:NH1	32:d:25:TYR:OH	2.39	0.52
46:s:117:ALA:HB3	46:s:165:ASP:H	1.75	0.52
49:v:694:GLU:O	49:v:842:LYS:NZ	2.42	0.52
50:w:286:TRP:CH2	62:KK:86:PRO:CG	2.83	0.52
51:9:1738:C:OP1	58:GG:92:ARG:NH1	2.40	0.52
58:GG:1:MET:HE2	58:GG:106:LEU:HB2	1.90	0.52
59:HH:130:LEU:HD21	59:HH:156:VAL:HG21	1.90	0.52
1:5:2016:C:H2'	1:5:2017:A:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4124:G:N2	10:G:96:GLN:O	2.43	0.52
13:J:9:GLU:OE2	13:J:13:ARG:NH1	2.43	0.52
23:U:24:ASP:OD1	23:U:24:ASP:N	2.38	0.52
49:v:632:ALA:HB2	49:v:647:ARG:HA	1.91	0.52
51:9:872:A:C6	51:9:914:U:O4	2.62	0.52
51:9:1124:C:H5''	53:BB:150:ILE:HG13	1.91	0.52
54:CC:191:VAL:HG11	54:CC:236:PHE:HA	1.92	0.52
1:5:4327:C:OP1	22:T:70:HIS:NE2	2.42	0.52
2:7:6:C:H4'	7:D:52:ILE:HD13	1.91	0.52
28:Z:12:LEU:HB2	28:Z:81:MET:HB3	1.91	0.52
53:BB:121:ILE:HD11	53:BB:161:VAL:HG22	1.90	0.52
84:gg:35:SER:H	84:gg:66:VAL:HG23	1.74	0.52
84:gg:258:ILE:HB	84:gg:267:VAL:HB	1.91	0.52
1:5:238:C:OP2	27:Y:45:ARG:NH2	2.43	0.52
1:5:1994:C:H2'	1:5:1995:G:H8	1.74	0.52
1:5:2394:G:O2'	1:5:2819:U:O4	2.25	0.52
1:5:2810:U:H5''	20:R:70:ARG:HH22	1.74	0.52
1:5:3717:A:OP2	1:5:3735:G:N2	2.39	0.52
1:5:3877:A:O2'	1:5:4400:G:N2	2.42	0.52
1:5:4586:G:OP1	17:O:72:HIS:N	2.42	0.52
50:w:191:ARG:HH11	50:w:191:ARG:CG	2.07	0.52
51:9:804:U:OP1	74:WW:82:GLN:NE2	2.42	0.52
51:9:1653:U:H3	51:9:1671:G:H1	1.57	0.52
55:DD:29:LEU:HD22	55:DD:58:VAL:HG23	1.91	0.52
1:5:1921:C:H1'	21:S:160:ARG:HB3	1.90	0.52
8:E:122:GLU:HG3	33:e:7:LEU:HD22	1.91	0.52
31:c:37:MET:SD	31:c:42:LYS:NZ	2.82	0.52
51:9:398:A:H5''	51:9:400:C:H5'	1.92	0.52
67:PP:17:TYR:O	67:PP:20:VAL:N	2.41	0.52
1:5:1867:A:OP1	12:I:13:LYS:NZ	2.43	0.52
1:5:2777:G:H5''	1:5:2778:G:H5'	1.91	0.52
1:5:2848:G:O2'	1:5:3838:U:O4	2.28	0.52
1:5:4688:C:O2'	11:H:155:SER:OG	2.26	0.52
6:C:350:ARG:HG2	6:C:353:ARG:HH21	1.74	0.52
18:P:84:PRO:HB2	18:P:87:SER:HB3	1.92	0.52
49:v:262:GLY:O	49:v:264:ARG:NE	2.41	0.52
51:9:942:G:N2	66:OO:137:SER:OG	2.41	0.52
57:FF:51:HIS:CE1	68:QQ:82:TYR:HH	2.25	0.52
70:SS:61:GLU:HA	70:SS:64:VAL:HG22	1.91	0.52
1:5:196:C:H4'	27:Y:126:ARG:HB3	1.90	0.52
1:5:450:G:H1	1:5:1297:U:H3	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1942:A:H2'	1:5:1943:A:C8	2.45	0.52
1:5:4618:G:H5''	24:V:15:ARG:HB2	1.91	0.52
15:M:125:ASN:HA	15:M:128:LYS:HG2	1.92	0.52
31:c:101:ASP:N	31:c:101:ASP:OD1	2.41	0.52
49:v:484:THR:HG21	49:v:493:ASN:HA	1.92	0.52
49:v:527:LEU:HD13	49:v:534:VAL:HG11	1.90	0.52
50:w:283:LEU:HD22	62:KK:16:PHE:HD2	1.74	0.52
51:9:612:U:H2'	51:9:613:G:H8	1.75	0.52
51:9:872:A:N1	51:9:914:U:O4	2.43	0.52
1:5:1860:B8H:C5	1:5:1860:B8H:C2	2.85	0.52
1:5:2019:C:OP1	46:s:6:ARG:NH1	2.43	0.52
49:v:602:LEU:HG	49:v:707:VAL:HG12	1.91	0.52
51:9:1598:G:H3'	77:ZZ:80:ARG:HH21	1.74	0.52
52:AA:184:ARG:HD3	52:AA:191:ARG:HG2	1.92	0.52
58:GG:58:LYS:HA	58:GG:107:SER:HB2	1.92	0.52
24:V:71:GLU:O	24:V:75:LYS:NZ	2.43	0.52
26:X:151:ASN:HB3	26:X:156:ILE:HD13	1.93	0.52
38:j:19:CYS:SG	38:j:20:ARG:N	2.82	0.52
48:u:36:ILE:HB	48:u:165:LEU:HB3	1.91	0.52
48:u:148:VAL:HA	48:u:151:VAL:HG12	1.90	0.52
51:9:1017:U:H5'	65:NN:55:ARG:HG2	1.92	0.52
59:HH:57:ARG:NE	59:HH:89:GLY:O	2.40	0.52
1:5:432:U:O4	17:O:96:GLN:NE2	2.43	0.51
1:5:953:C:OP1	34:f:73:LYS:NZ	2.41	0.51
47:t:153:ASP:OD1	47:t:154:ASP:N	2.41	0.51
51:9:65:C:H4'	58:GG:172:LYS:HD3	1.93	0.51
51:9:1354:G:N2	51:9:1357:A:OP2	2.40	0.51
55:DD:23:GLU:OE1	62:KK:64:TRP:NE1	2.36	0.51
1:5:5002:U:OP2	5:B:385:LYS:NZ	2.41	0.51
31:c:48:LEU:HD11	31:c:60:ILE:HG21	1.91	0.51
35:g:61:PRO:HA	35:g:64:LEU:HD13	1.93	0.51
42:n:14:LYS:HD2	51:9:1172:U:H5''	1.92	0.51
49:v:489:GLU:OE2	49:v:490:HIS:ND1	2.40	0.51
49:v:748:GLU:HB3	49:v:811:GLN:HB2	1.92	0.51
58:GG:142:ARG:HA	58:GG:147:LEU:HD23	1.92	0.51
68:QQ:51:LEU:HD21	68:QQ:81:ILE:HB	1.92	0.51
71:TT:65:TYR:HE1	71:TT:128:GLN:HG3	1.75	0.51
75:XX:123:VAL:HG12	75:XX:124:LYS:HG3	1.91	0.51
1:5:3951:G:C6	1:5:4062:A:N1	2.78	0.51
2:7:61:G:HO2'	7:D:279:ARG:HH12	1.57	0.51
19:Q:82:VAL:HG12	19:Q:84:GLY:H	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:v:262:GLY:H	49:v:264:ARG:HH21	1.59	0.51
51:9:962:A:N1	51:9:1055:A:O2'	2.43	0.51
61:JJ:136:ARG:NH1	61:JJ:159:PHE:O	2.42	0.51
1:5:116:G:OP1	16:N:2:GLY:N	2.43	0.51
17:O:157:GLU:HA	17:O:160:ARG:HG2	1.92	0.51
19:Q:57:ASN:O	19:Q:143:ARG:NH2	2.44	0.51
51:9:1144:A:H5'	51:9:1355:C:H41	1.74	0.51
55:DD:55:THR:HA	55:DD:58:VAL:HG12	1.92	0.51
56:EE:17:HIS:HB2	56:EE:108:ARG:HA	1.93	0.51
56:EE:212:ASP:OD1	56:EE:216:ASN:N	2.43	0.51
57:FF:182:LYS:HD2	57:FF:184:SER:HB2	1.93	0.51
80:cc:10:LYS:HE3	80:cc:34:PHE:HB3	1.92	0.51
1:5:1919:G:N2	21:S:163:HIS:O	2.43	0.51
50:w:195:ARG:N	51:9:1701:C:O2	2.44	0.51
84:gg:165:ILE:HG12	84:gg:177:TRP:HB2	1.93	0.51
1:5:4872:2MG:N2	17:O:201:LEU:O	2.41	0.51
7:D:41:LYS:HD2	22:T:93:ILE:HG12	1.92	0.51
8:E:287:HIS:CD2	34:f:38:GLU:HB3	2.46	0.51
49:v:103:ILE:HD12	49:v:118:ALA:HB1	1.92	0.51
49:v:476:ASP:O	49:v:529:LYS:NZ	2.43	0.51
51:9:28:U:H2'	51:9:29:G:H8	1.76	0.51
51:9:621:C:H5'	75:XX:107:ARG:HH22	1.74	0.51
51:9:1245:G:O2'	51:9:1492:U:OP1	2.28	0.51
63:LL:96:ILE:HD12	75:XX:10:ALA:HB1	1.93	0.51
64:MM:54:SER:HB3	64:MM:80:ASP:HA	1.93	0.51
5:B:165:HIS:ND1	5:B:166:THR:O	2.38	0.51
10:G:191:ALA:O	10:G:195:THR:OG1	2.29	0.51
14:L:161:PHE:CG	29:a:105:ARG:HD2	2.46	0.51
28:Z:50:PRO:HD3	28:Z:68:ILE:HG12	1.91	0.51
48:u:60:ARG:O	48:u:62:LYS:N	2.43	0.51
51:9:1665:G:H5''	71:TT:89:PRO:HD2	1.93	0.51
56:EE:70:ILE:HG22	56:EE:92:ILE:HG12	1.92	0.51
1:5:135:G:N2	36:h:95:LEU:O	2.37	0.51
1:5:1328:G:O2'	1:5:2349:A:OP1	2.28	0.51
1:5:1503:A:H4'	1:5:1504:G:H5'	1.93	0.51
14:L:130:LYS:NZ	14:L:132:SER:OG	2.42	0.51
27:Y:80:ILE:HD11	27:Y:104:VAL:HG21	1.92	0.51
49:v:398:ILE:HD11	49:v:479:LEU:HD11	1.93	0.51
50:w:282:THR:O	62:KK:89:ILE:HG22	2.11	0.51
51:9:649:U:H2'	51:9:650:A:H8	1.76	0.51
51:9:1661:A:OP2	81:dd:32:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:UU:26:SER:HB3	72:UU:32:LEU:HD22	1.93	0.51
79:bb:67:THR:OG1	79:bb:70:LYS:O	2.28	0.51
83:ff:132:MET:HG2	83:ff:141:CYS:HB2	1.92	0.51
1:5:4080:C:H2'	1:5:4081:G:H8	1.76	0.51
17:O:55:LEU:HD23	17:O:58:LEU:HD12	1.93	0.51
48:u:22:GLN:HA	48:u:25:ARG:HG2	1.93	0.51
49:v:121:VAL:HG13	49:v:415:ARG:HG3	1.93	0.51
51:9:18:C:O2'	75:XX:107:ARG:NH1	2.44	0.51
51:9:1452:A:H61	51:9:1473:G:N2	2.08	0.51
77:ZZ:48:VAL:HG22	77:ZZ:80:ARG:HE	1.75	0.51
84:gg:35:SER:OG	84:gg:36:ARG:N	2.44	0.51
1:5:4212:A:OP2	12:I:15:LYS:NZ	2.43	0.51
1:5:4476:C:O2'	1:5:4478:G:OP2	2.25	0.51
5:B:189:THR:O	5:B:193:LYS:HB2	2.10	0.51
15:M:35:ARG:NH2	21:S:99:ASP:OD1	2.43	0.51
48:u:31:THR:HA	48:u:171:HIS:HA	1.93	0.51
49:v:9:ILE:HD13	49:v:12:ILE:HD12	1.91	0.51
51:9:1599:U:OP2	77:ZZ:46:ASN:ND2	2.44	0.51
52:AA:198:MET:HE2	69:RR:89:SER:HB3	1.93	0.51
56:EE:100:ARG:HB2	56:EE:114:ILE:HD13	1.93	0.51
71:TT:126:GLN:HG2	71:TT:129:ARG:HH21	1.76	0.51
76:YY:44:LEU:HD11	76:YY:55:ILE:HD13	1.93	0.51
1:5:667:A:O2'	6:C:29:LYS:NZ	2.41	0.50
1:5:5047:C:O2'	1:5:5050:C:OP2	2.28	0.50
47:t:80:LEU:HD13	47:t:83:LYS:HD3	1.92	0.50
51:9:959:G:OP1	66:OO:104:ARG:NH2	2.42	0.50
51:9:1375:G:OP2	69:RR:67:ARG:NH2	2.44	0.50
55:DD:134:CYS:SG	55:DD:135:GLU:N	2.83	0.50
84:gg:256:ILE:HB	84:gg:270:LEU:HB2	1.92	0.50
1:5:423:G:OP1	18:P:62:ARG:NH2	2.42	0.50
1:5:4622:A:H4'	5:B:13:SER:HB2	1.93	0.50
9:F:100:VAL:HG13	9:F:138:TYR:HE2	1.76	0.50
19:Q:33:ARG:HE	19:Q:52:PHE:HZ	1.59	0.50
28:Z:57:MET:HE3	28:Z:62:ILE:HG22	1.93	0.50
29:a:90:ALA:HB3	29:a:120:GLN:HE21	1.75	0.50
47:t:17:CYS:SG	47:t:18:THR:N	2.84	0.50
51:9:5:U:H2'	51:9:6:G:H8	1.76	0.50
51:9:606:G:H4'	82:ee:130:ALA:HA	1.93	0.50
51:9:860:G:H21	74:WW:107:SER:HB3	1.75	0.50
51:9:1228:A:H2'	51:9:1229:G:C8	2.46	0.50
84:gg:217:MET:HG2	84:gg:229:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1427:A:OP2	1:5:1457:G:N2	2.38	0.50
1:5:1506:G:N3	6:C:116:ASN:ND2	2.58	0.50
1:5:3762:B8H:C5	1:5:3762:B8H:C2	2.85	0.50
1:5:4657:U:O2'	1:5:4659:G:OP2	2.29	0.50
5:B:384:GLU:OE2	25:W:14:TYR:OH	2.30	0.50
16:N:160:GLU:HG2	16:N:161:MET:HG3	1.93	0.50
25:W:4:GLU:OE2	25:W:30:GLN:NE2	2.45	0.50
50:w:195:ARG:CA	51:9:1701:C:O2	2.55	0.50
53:BB:103:MET:H	53:BB:215:VAL:HB	1.77	0.50
53:BB:144:LYS:HD3	53:BB:208:HIS:HB3	1.93	0.50
58:GG:192:ILE:HD12	58:GG:195:LYS:HD2	1.94	0.50
62:KK:1:MET:HB3	62:KK:3:MET:HG3	1.93	0.50
66:OO:105:THR:HG22	66:OO:107:THR:H	1.76	0.50
70:SS:132:ARG:HB2	70:SS:134:GLN:HE22	1.77	0.50
73:VV:1:MET:N	73:VV:1:MET:SD	2.82	0.50
1:5:102:G:OP1	14:L:71:ARG:NH1	2.45	0.50
1:5:2010:A:O2'	1:5:2011:C:O4'	2.29	0.50
1:5:4163:U:OP1	10:G:106:ARG:NH1	2.44	0.50
6:C:146:GLU:OE2	6:C:178:ASN:ND2	2.45	0.50
51:9:1204:A:H5''	54:CC:117:ARG:HE	1.76	0.50
51:9:1325:G:O2'	51:9:1327:G:OP1	2.29	0.50
51:9:1549:U:OP1	81:dd:34:TYR:OH	2.24	0.50
51:9:1679:A:H2'	57:FF:60:ARG:HD2	1.93	0.50
56:EE:57:THR:OG1	56:EE:60:GLU:OE1	2.26	0.50
1:5:3802:U:O4	1:5:4502:C:N4	2.37	0.50
51:9:476:A:N3	51:9:488:U:O2'	2.38	0.50
51:9:1124:C:O2'	69:RR:126:MET:O	2.29	0.50
57:FF:102:LEU:HD11	77:ZZ:100:VAL:HG11	1.92	0.50
58:GG:121:ILE:HD12	58:GG:122:PRO:HD2	1.92	0.50
64:MM:81:ASP:HB2	64:MM:84:LYS:HE3	1.94	0.50
70:SS:128:GLY:O	70:SS:144:ARG:NH1	2.44	0.50
1:5:2845:A:N6	1:5:3843:C:H42	2.09	0.50
1:5:3969:G:H1'	48:u:166:ALA:HB3	1.94	0.50
19:Q:81:VAL:HG22	19:Q:101:CYS:HB3	1.94	0.50
35:g:11:LEU:O	35:g:18:ASN:ND2	2.45	0.50
51:9:144:U:OP2	58:GG:139:SER:OG	2.30	0.50
55:DD:40:ARG:HH22	72:UU:106:ILE:HG23	1.77	0.50
61:JJ:42:GLU:HA	61:JJ:45:ARG:HG2	1.93	0.50
1:5:2780:C:H2'	1:5:2781:G:H8	1.76	0.50
2:7:11:A:O2'	2:7:13:A:OP2	2.30	0.50
11:H:104:VAL:HG13	11:H:113:GLU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:36:ARG:NH1	28:Z:38:TYR:OH	2.39	0.50
46:s:141:LEU:HD11	46:s:171:GLU:HG3	1.94	0.50
61:JJ:179:LYS:HA	61:JJ:182:GLN:HG2	1.92	0.50
67:PP:17:TYR:HE2	67:PP:37:TYR:HB3	1.75	0.50
68:QQ:8:GLN:HB3	68:QQ:95:TYR:HE1	1.77	0.50
1:5:32:G:H21	1:5:50:C:H5	1.60	0.50
1:5:3661:G:O3'	4:A:156:LYS:NZ	2.43	0.50
1:5:4627:U:H4'	5:B:373:LYS:HD2	1.94	0.50
19:Q:66:MET:HE2	19:Q:98:LEU:HD13	1.94	0.50
23:U:28:PRO:HB2	23:U:34:MET:HG2	1.94	0.50
51:9:1018:U:H5''	65:NN:71:ILE:HD12	1.94	0.50
51:9:1232:U:H2'	51:9:1233:G:H8	1.77	0.50
51:9:1593:C:OP1	77:ZZ:103:HIS:NE2	2.42	0.50
51:9:1864:U:O2'	51:9:1866:A:N7	2.41	0.50
83:ff:139:HIS:HB2	83:ff:148:TYR:HB2	1.94	0.50
1:5:158:A:H5''	1:5:159:C:H2'	1.94	0.50
1:5:1736:A:N3	2:7:78:C:O2'	2.41	0.50
1:5:2083:C:OP2	19:Q:14:ARG:NH2	2.44	0.50
1:5:2835:A:O2'	5:B:228:TYR:O	2.29	0.50
6:C:284:MET:HE3	19:Q:124:ASP:HB3	1.94	0.50
29:a:132:ARG:HA	29:a:135:GLU:HG2	1.94	0.50
46:s:31:GLY:HA3	46:s:190:GLN:HE22	1.77	0.50
46:s:126:GLN:H	46:s:154:ILE:HB	1.77	0.50
49:v:20:ARG:NE	49:v:358:LEU:O	2.45	0.50
49:v:706:ASP:N	49:v:706:ASP:OD1	2.44	0.50
51:9:1374:5MC:O2'	51:9:1464:C:O2	2.29	0.50
56:EE:184:THR:N	56:EE:224:ASN:O	2.43	0.50
57:FF:25:THR:OG1	57:FF:41:VAL:O	2.29	0.50
59:HH:30:LEU:O	59:HH:34:SER:HB3	2.12	0.50
71:TT:60:THR:HG23	71:TT:75:MET:HE2	1.93	0.50
1:5:2869:U:O2'	1:5:2881:A:N7	2.43	0.49
13:J:95:ARG:NH2	13:J:177:GLY:O	2.45	0.49
37:i:6:PRO:HB3	37:i:16:LYS:HD3	1.94	0.49
48:u:59:PRO:O	48:u:171:HIS:ND1	2.37	0.49
49:v:21:ASN:OD1	49:v:21:ASN:N	2.42	0.49
49:v:404:THR:OG1	49:v:406:ASP:OD1	2.29	0.49
57:FF:35:LEU:HD12	57:FF:117:ILE:HG22	1.93	0.49
1:5:115:C:O2'	1:5:276:C:OP1	2.27	0.49
1:5:1836:G:O5'	22:T:129:LYS:NZ	2.45	0.49
1:5:2287:G:O6	29:a:10:LYS:NZ	2.42	0.49
1:5:3893:C:O2'	1:5:4979:A:N1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3969:G:H22	1:5:4053:A:H2	1.58	0.49
5:B:254:ILE:HD13	5:B:268:ARG:HH22	1.77	0.49
17:O:9:LEU:HD23	17:O:118:MET:HB2	1.93	0.49
20:R:99:MET:HE2	20:R:127:VAL:HG12	1.94	0.49
21:S:8:ARG:NH1	21:S:35:PRO:O	2.45	0.49
36:h:4:ILE:O	36:h:56:ARG:NH1	2.45	0.49
38:j:14:LYS:NZ	40:l:51:LEU:OXT	2.45	0.49
49:v:200:MET:HE3	49:v:203:ILE:HG21	1.94	0.49
49:v:545:ILE:HD12	49:v:575:PRO:HB3	1.93	0.49
84:gg:113:PHE:HA	84:gg:120:ILE:HG22	1.94	0.49
1:5:1906:U:H2'	1:5:1907:A:H8	1.77	0.49
1:5:4860:G:H5'	17:O:169:ARG:HH11	1.77	0.49
12:I:66:GLU:HG3	12:I:69:ARG:HH11	1.77	0.49
51:9:1385:G:H4'	51:9:1484:A:H5'	1.94	0.49
65:NN:39:LYS:HA	65:NN:42:LYS:HG2	1.93	0.49
1:5:1914:C:H4'	17:O:89:PRO:HD3	1.93	0.49
1:5:2007:G:H21	1:5:2012:A:H62	1.60	0.49
1:5:2090:U:OP2	6:C:307:LYS:NZ	2.45	0.49
1:5:2406:G:N7	40:l:2:SER:N	2.59	0.49
10:G:139:VAL:HG11	10:G:238:LYS:HE2	1.92	0.49
20:R:8:LYS:HB2	20:R:24:LEU:HD11	1.93	0.49
21:S:80:ILE:HG12	21:S:129:VAL:HG22	1.95	0.49
53:BB:90:ASP:OD2	53:BB:92:GLN:NE2	2.45	0.49
54:CC:70:VAL:HG11	54:CC:93:ILE:HG12	1.94	0.49
57:FF:171:GLU:HG2	77:ZZ:106:GLN:HE22	1.77	0.49
1:5:1317:U:OP1	29:a:21:ARG:NH1	2.45	0.49
3:8:102:G:OP2	3:8:104:A:O2'	2.28	0.49
5:B:89:ILE:HD11	5:B:150:PHE:HE1	1.75	0.49
58:GG:26:THR:O	58:GG:30:LYS:NZ	2.39	0.49
84:gg:124:SER:OG	84:gg:126:ASP:OD1	2.24	0.49
1:5:382:G:N1	1:5:385:A:OP2	2.43	0.49
1:5:4474:A:H5'	41:m:99:LYS:HB2	1.93	0.49
28:Z:11:VAL:HG22	28:Z:82:PRO:HA	1.95	0.49
43:o:9:ARG:HA	43:o:20:PRO:HA	1.95	0.49
51:9:68:A:OP2	58:GG:164:LYS:NZ	2.44	0.49
51:9:454:U:H5''	58:GG:94:ARG:HG2	1.93	0.49
51:9:1299:A:O2'	51:9:1301:A:OP1	2.25	0.49
53:BB:46:LYS:HE3	66:OO:20:GLN:HB2	1.95	0.49
60:II:13:LYS:NZ	63:LL:108:ASN:O	2.44	0.49
75:XX:72:VAL:O	75:XX:80:LYS:HA	2.13	0.49
1:5:2489:C:H4'	1:5:2490:U:H5	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:187:SER:H	16:N:190:ALA:HB3	1.78	0.49
21:S:19:THR:HG23	21:S:22:CYS:H	1.77	0.49
33:e:89:LEU:HD23	33:e:118:LEU:HD22	1.94	0.49
52:AA:80:ARG:NH1	52:AA:126:ASP:OD2	2.45	0.49
58:GG:44:GLU:HB2	58:GG:119:LYS:HE2	1.95	0.49
74:WW:93:LEU:HB3	74:WW:102:ILE:HD11	1.94	0.49
79:bb:36:LYS:HB3	79:bb:43:ILE:HG12	1.95	0.49
1:5:511:C:OP2	14:L:163:LYS:NZ	2.45	0.49
1:5:1327:C:H2'	1:5:1328:G:H8	1.78	0.49
1:5:1787:A:N3	1:5:4210:U:O2'	2.43	0.49
3:8:29:G:H5''	14:L:27:ASN:HB3	1.94	0.49
5:B:55:HIS:HB2	5:B:369:ASP:HB3	1.95	0.49
49:v:70:ILE:HG22	49:v:404:THR:HA	1.93	0.49
49:v:607:ARG:NH1	49:v:703:ASP:OD2	2.45	0.49
49:v:714:ILE:HG21	50:w:199:SER:C	2.37	0.49
51:9:43:U:OP2	51:9:485:A:N6	2.45	0.49
51:9:1189:A:H4'	75:XX:34:THR:HG21	1.94	0.49
51:9:1566:G:OP2	71:TT:102:ARG:NH1	2.46	0.49
55:DD:193:ASP:OD2	55:DD:195:SER:OG	2.28	0.49
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.95	0.49
83:ff:140:TYR:HA	83:ff:146:LEU:O	2.12	0.49
1:5:2353:U:H5''	6:C:89:GLN:HG2	1.93	0.49
1:5:4380:A:OP1	43:o:58:LYS:NZ	2.45	0.49
4:A:101:VAL:HG22	4:A:163:ARG:HB3	1.94	0.49
4:A:177:LYS:HB2	44:p:29:ILE:HG21	1.94	0.49
15:M:12:VAL:HG22	15:M:60:PHE:HB2	1.95	0.49
51:9:923:G:H2'	51:9:924:G:H8	1.78	0.49
53:BB:136:ARG:HB3	53:BB:216:LYS:HB3	1.95	0.49
68:QQ:16:LYS:HG3	68:QQ:17:LYS:H	1.77	0.49
1:5:1390:G:N2	1:5:1393:G:OP2	2.44	0.49
1:5:4635:A:H8	1:5:5048:A:H61	1.60	0.49
11:H:37:ASP:OD1	11:H:39:ASN:ND2	2.46	0.49
17:O:54:TYR:HD2	17:O:145:VAL:HG21	1.78	0.49
47:t:90:ARG:HD3	47:t:95:GLN:H	1.78	0.49
58:GG:218:LYS:HA	58:GG:221:LYS:HG2	1.93	0.49
1:5:1077:C:OP1	1:5:1215:C:O2'	2.31	0.48
1:5:1332:C:H2'	1:5:1333:A:H8	1.78	0.48
1:5:1686:C:O2'	30:b:18:ARG:NH1	2.42	0.48
1:5:2337:C:H4'	45:r:19:LYS:HB2	1.94	0.48
12:I:12:CYS:HB3	12:I:128:ARG:HH21	1.78	0.48
17:O:77:SER:HB2	17:O:104:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:41:ILE:HD13	18:P:150:LEU:HD21	1.95	0.48
43:o:44:LYS:HE3	43:o:52:THR:HB	1.95	0.48
49:v:309:LYS:HA	49:v:312:THR:HG22	1.95	0.48
53:BB:120:MET:HG3	53:BB:142:PHE:HE1	1.76	0.48
63:LL:111:VAL:HG11	63:LL:128:VAL:HG11	1.95	0.48
66:OO:27:VAL:HB	66:OO:90:ILE:HA	1.95	0.48
83:ff:118:ARG:HH21	83:ff:134:SER:H	1.60	0.48
49:v:804:THR:HG22	49:v:807:GLN:HB2	1.94	0.48
51:9:628:A:O4'	55:DD:178:ARG:NH2	2.45	0.48
52:AA:81:ASN:HA	52:AA:84:GLN:HB2	1.94	0.48
1:5:14:C:H5''	26:X:56:ARG:HD3	1.95	0.48
1:5:3959:U:H2'	1:5:3960:A:H8	1.78	0.48
1:5:3963:A:O2'	1:5:3965:A:OP2	2.31	0.48
1:5:5038:A:OP1	25:W:61:LYS:NZ	2.40	0.48
5:B:218:ASP:OD2	5:B:348:ARG:NH1	2.45	0.48
46:s:108:PRO:HA	46:s:184:SER:HA	1.95	0.48
51:9:635:G:H4'	82:ee:94:LYS:HA	1.96	0.48
54:CC:264:SER:O	54:CC:268:GLU:HB2	2.12	0.48
71:TT:38:LYS:NZ	71:TT:40:ALA:O	2.37	0.48
1:5:1631:A:C8	4:A:199:VAL:HG21	2.48	0.48
1:5:4454:G:O2'	1:5:4500:PSU:O2'	2.30	0.48
4:A:64:ARG:NH2	10:G:95:GLY:O	2.44	0.48
14:L:43:ALA:O	14:L:149:GLN:NE2	2.40	0.48
23:U:84:LYS:HB2	23:U:110:TYR:CZ	2.49	0.48
49:v:607:ARG:O	49:v:701:ARG:HB3	2.13	0.48
51:9:1854:U:H2'	51:9:1855:G:H8	1.78	0.48
60:II:150:ASP:HA	60:II:153:LYS:HG2	1.96	0.48
64:MM:58:GLU:HB3	64:MM:61:TYR:HB3	1.95	0.48
67:PP:108:LYS:HD3	67:PP:110:GLU:H	1.79	0.48
1:5:305:A:OP2	16:N:15:GLN:NE2	2.36	0.48
1:5:1309:C:O2	34:f:21:GLN:NE2	2.46	0.48
1:5:1480:C:O2'	1:5:1482:G:OP2	2.32	0.48
9:F:70:MET:HA	9:F:73:MET:HG2	1.95	0.48
32:d:64:ILE:HG23	32:d:68:LEU:HD23	1.94	0.48
33:e:99:ILE:HD13	33:e:108:ARG:HG3	1.96	0.48
48:u:93:LEU:HD21	48:u:99:LEU:HD12	1.95	0.48
54:CC:171:GLY:O	74:WW:98:GLN:NE2	2.42	0.48
61:JJ:176:LYS:HA	61:JJ:179:LYS:HD3	1.96	0.48
1:5:4472:B8W:O2'	41:m:74:TYR:O	2.32	0.48
47:t:132:ILE:O	47:t:135:THR:OG1	2.29	0.48
50:w:195:ARG:HB2	51:9:1701:C:N3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1863:A:OP2	78:aa:4:LYS:NZ	2.42	0.48
74:WW:57:ARG:HH12	79:bb:26:GLN:HB3	1.77	0.48
84:gg:40:ILE:HG23	84:gg:59:LEU:HB2	1.96	0.48
1:5:742:G:H1	1:5:922(A):G:H21	1.61	0.48
1:5:965:G:N2	1:5:966:A:N7	2.61	0.48
1:5:2520:C:H2'	1:5:2521:G:H8	1.79	0.48
1:5:3853:U:O2'	1:5:4979:A:N3	2.47	0.48
1:5:4873:G:C8	17:O:179:LYS:HE3	2.49	0.48
6:C:330:PRO:HB3	9:F:46:ARG:HH21	1.78	0.48
49:v:610:PRO:HD2	49:v:613:LEU:HD21	1.94	0.48
51:9:616:A:N6	51:9:625:G:H21	2.11	0.48
1:5:2529:A:O2'	1:5:2531:C:OP2	2.31	0.48
1:5:2587:A:H5'	1:5:2770:C:H5'	1.96	0.48
1:5:5055:G:N2	32:d:118:GLN:OE1	2.37	0.48
4:A:27:ALA:O	4:A:128:ARG:NH2	2.47	0.48
5:B:231:VAL:HG21	5:B:251:VAL:HG23	1.94	0.48
10:G:215:ASP:OD1	10:G:215:ASP:N	2.36	0.48
18:P:32:THR:HG23	18:P:91:LEU:HD21	1.95	0.48
49:v:454:MET:N	49:v:454:MET:SD	2.86	0.48
51:9:56:G:OP2	76:YY:115:LYS:NZ	2.40	0.48
51:9:1589:A:N3	51:9:1653:U:O2'	2.46	0.48
54:CC:134:ASN:OD1	54:CC:167:ARG:NH1	2.47	0.48
54:CC:142:LYS:HB2	54:CC:157:LEU:HD12	1.96	0.48
74:WW:18:GLU:HG3	74:WW:69:LEU:HD23	1.95	0.48
74:WW:115:GLU:HA	74:WW:118:ARG:HG2	1.94	0.48
1:5:664:G:O2'	1:5:668:C:N4	2.46	0.48
1:5:2265:G:OP1	45:r:35:ARG:NH1	2.41	0.48
1:5:3759:A:N6	1:5:3765:G:O2'	2.47	0.48
1:5:3930:U:H3	1:5:4180:G:H1	1.62	0.48
1:5:4492:U:O2'	1:5:4512:U:O2	2.28	0.48
1:5:4541:G:N2	1:5:4544:A:OP2	2.42	0.48
5:B:276:HIS:O	5:B:277:ARG:NH1	2.47	0.48
6:C:305:PRO:HB3	19:Q:38:ARG:HH12	1.79	0.48
17:O:8:VAL:HG12	17:O:117:ARG:HG3	1.96	0.48
38:j:2:THR:O	38:j:7:SER:OG	2.28	0.48
49:v:686:ALA:O	49:v:726:ARG:NH1	2.46	0.48
51:9:1060:A:O2'	51:9:1062:A:N7	2.43	0.48
76:YY:91:LEU:HD22	76:YY:96:LEU:HD11	1.94	0.48
84:gg:137:VAL:HB	84:gg:139:LYS:HZ2	1.78	0.48
1:5:4076:G:OP1	10:G:126:ARG:NE	2.32	0.48
14:L:7:GLY:O	29:a:49:HIS:NE2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:16:ILE:HB	24:V:88:TYR:HB2	1.95	0.48
32:d:27:ILE:HD12	32:d:84:ILE:HD11	1.96	0.48
51:9:106:C:H2'	51:9:107:A:H8	1.79	0.48
51:9:587:A:H5'	51:9:592:C:H41	1.79	0.48
52:AA:16:LEU:HD21	69:RR:116:ASN:HD21	1.78	0.48
54:CC:60:TRP:O	54:CC:71:LYS:NZ	2.38	0.48
59:HH:143:ARG:HD2	74:WW:53:ILE:HG12	1.95	0.48
63:LL:75:GLY:HA3	63:LL:88:ILE:HD12	1.96	0.48
84:gg:300:ALA:O	84:gg:307:VAL:HA	2.14	0.48
1:5:85:G:O2'	1:5:97:G:O6	2.23	0.47
8:E:155:ILE:O	8:E:162:GLY:N	2.43	0.47
26:X:129:ARG:HD3	26:X:135:LYS:HE3	1.96	0.47
42:n:10:MET:HE1	51:9:1170:A:H4'	1.96	0.47
50:w:283:LEU:HD12	62:KK:89:ILE:HD13	1.96	0.47
70:SS:104:ASP:OD1	70:SS:104:ASP:N	2.46	0.47
70:SS:121:ARG:O	70:SS:125:HIS:ND1	2.44	0.47
1:5:2345:G:OP2	29:a:12:ARG:NH1	2.47	0.47
1:5:2362:U:H2'	1:5:2363:A2M:H8	1.96	0.47
1:5:4215:C:O2	22:T:60:LYS:NZ	2.45	0.47
1:5:4704:C:H2'	1:5:4705:A:H8	1.79	0.47
16:N:68:ARG:NH1	16:N:124:ASP:O	2.39	0.47
49:v:42:LYS:HD3	49:v:43:ALA:HB2	1.96	0.47
49:v:452:LEU:HD23	49:v:461:ILE:HD13	1.96	0.47
49:v:557:CYS:HA	49:v:561:LEU:HD23	1.95	0.47
53:BB:48:LEU:HB2	66:OO:51:GLU:HG2	1.96	0.47
54:CC:187:ARG:NH2	54:CC:189:GLY:O	2.47	0.47
61:JJ:70:ARG:HH21	61:JJ:94:LEU:HD21	1.78	0.47
84:gg:32:LEU:HD13	84:gg:42:MET:HB3	1.96	0.47
1:5:152:U:P	16:N:49:ARG:HH12	2.37	0.47
1:5:280:G:N2	1:5:306:A:OP2	2.36	0.47
1:5:668:C:H4'	6:C:6:PRO:HB3	1.96	0.47
1:5:1849:U:H3'	14:L:5:ARG:HH12	1.79	0.47
1:5:2637:U:OP1	35:g:28:ASN:ND2	2.42	0.47
5:B:300:LYS:HG2	5:B:313:SER:HB3	1.96	0.47
10:G:307:GLU:HA	10:G:310:LYS:HG2	1.96	0.47
49:v:584:SER:OG	49:v:737:GLN:NE2	2.46	0.47
50:w:282:THR:O	62:KK:89:ILE:CG2	2.63	0.47
51:9:420:G:H2'	51:9:660:C:H42	1.80	0.47
51:9:1563:G:H5''	71:TT:121:ARG:HH22	1.79	0.47
55:DD:158:ILE:HG12	55:DD:189:MET:HE1	1.95	0.47
1:5:1460:C:H5''	19:Q:144:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4693:C:OP1	11:H:64:ARG:NH2	2.47	0.47
1:5:4735:G:N1	1:5:4965:U:N3	2.54	0.47
12:I:36:LEU:HD13	12:I:73:ASN:ND2	2.29	0.47
21:S:15:ARG:HH12	21:S:18:PRO:HG3	1.79	0.47
51:9:218:U:O2	60:II:184:ARG:NH2	2.48	0.47
51:9:951:C:O2'	66:OO:50:LYS:NZ	2.39	0.47
54:CC:209:VAL:HG21	54:CC:233:LEU:HD21	1.97	0.47
62:KK:15:LEU:HG	62:KK:71:LEU:HD22	1.95	0.47
68:QQ:41:MET:N	68:QQ:41:MET:SD	2.87	0.47
1:5:163:A:H2'	1:5:164:G:H8	1.79	0.47
1:5:2411:C:H2'	1:5:2412:A:C8	2.50	0.47
6:C:315:LYS:HD2	9:F:167:ALA:HB1	1.97	0.47
11:H:176:LEU:HD23	41:m:60:ALA:HB3	1.96	0.47
16:N:116:LEU:HD22	16:N:135:ILE:HD11	1.95	0.47
25:W:82:ILE:HD11	58:GG:158:VAL:HG21	1.95	0.47
31:c:44:LYS:NZ	31:c:97:ILE:O	2.39	0.47
1:5:74:G:O3'	14:L:71:ARG:NH2	2.48	0.47
1:5:2072:C:O2'	9:F:212:LEU:O	2.30	0.47
1:5:2566:G:H2'	1:5:2567:G:H8	1.80	0.47
1:5:4225:G:OP1	12:I:24:ARG:NH2	2.47	0.47
8:E:181:PRO:HD2	8:E:184:LEU:HD12	1.97	0.47
12:I:189:ARG:NH2	12:I:199:TYR:OH	2.47	0.47
25:W:101:ARG:HA	25:W:104:GLN:HG2	1.95	0.47
48:u:68:LEU:HG	48:u:116:LEU:HD22	1.95	0.47
49:v:714:ILE:CG2	50:w:200:ASP:CA	2.92	0.47
51:9:1455:A:OP1	69:RR:5:ARG:NH1	2.48	0.47
54:CC:183:LYS:HD3	54:CC:194:ARG:HH21	1.79	0.47
1:5:1207:C:H2'	1:5:1208:G:H8	1.79	0.47
1:5:4391:G:OP1	6:C:75:ARG:NH1	2.46	0.47
1:5:5016:A:N6	1:5:5033:G:O2'	2.47	0.47
5:B:165:HIS:HA	5:B:179:HIS:O	2.14	0.47
8:E:156:LEU:HD11	8:E:198:ILE:HG13	1.96	0.47
9:F:178:LEU:HD21	9:F:203:ALA:HA	1.96	0.47
21:S:13:VAL:HA	21:S:28:TYR:O	2.14	0.47
31:c:47:ILE:HD12	31:c:94:LEU:HD11	1.97	0.47
43:o:3:ASN:ND2	43:o:95:GLY:O	2.48	0.47
49:v:179:GLN:HA	49:v:182:VAL:HG22	1.96	0.47
51:9:126:G:H2'	58:GG:199:THR:HG21	1.96	0.47
51:9:1010:G:H2'	51:9:1011:A:H8	1.80	0.47
59:HH:7:LYS:NZ	59:HH:40:LEU:O	2.34	0.47
1:5:375:G:N7	38:j:56:ARG:NH1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1498:G:OP1	19:Q:150:ARG:NH1	2.47	0.47
1:5:4057:C:OP1	48:u:202:ARG:NH1	2.46	0.47
1:5:4129:B8W:O6	1:5:4156:G:N2	2.47	0.47
3:8:141:C:H5'	16:N:60:VAL:HG11	1.97	0.47
27:Y:34:LEU:HD23	27:Y:38:LEU:HB3	1.97	0.47
48:u:97:LYS:HB3	48:u:128:LEU:HD11	1.97	0.47
50:w:286:TRP:CD2	62:KK:86:PRO:HG2	2.47	0.47
55:DD:74:GLN:NE2	55:DD:79:PHE:O	2.36	0.47
56:EE:182:MET:N	56:EE:226:PHE:O	2.43	0.47
58:GG:56:ASN:HB2	58:GG:108:VAL:HG12	1.97	0.47
58:GG:57:ASP:OD2	58:GG:72:ARG:NH1	2.46	0.47
66:OO:98:ARG:HH21	66:OO:134:PRO:HG3	1.80	0.47
1:5:2706:G:O2'	1:5:2709:C:N4	2.38	0.47
1:5:4594:U:H2'	1:5:4595:G:H8	1.79	0.47
45:r:65:LYS:O	45:r:102:TYR:OH	2.23	0.47
48:u:112:ALA:HB2	48:u:135:PRO:HB2	1.97	0.47
51:9:163:U:OP2	58:GG:87:ARG:NH1	2.40	0.47
51:9:220:U:H2'	51:9:221:A:C8	2.49	0.47
55:DD:46:THR:HB	55:DD:84:VAL:HG12	1.97	0.47
1:5:440:U:O2'	34:f:91:ASN:O	2.29	0.47
1:5:4184:G:H5'	4:A:233:ARG:HB2	1.97	0.47
1:5:4612:C:C2	11:H:120:GLU:HB2	2.49	0.47
11:H:120:GLU:OE2	11:H:124:ARG:NH2	2.44	0.47
14:L:121:ARG:HA	14:L:124:LEU:HD22	1.96	0.47
47:t:123:ARG:HG3	47:t:124:GLU:H	1.80	0.47
49:v:215:GLY:HA3	49:v:222:ALA:HA	1.96	0.47
49:v:667:LYS:HD2	49:v:667:LYS:HA	1.68	0.47
52:AA:88:LEU:HD13	52:AA:100:ALA:HB2	1.96	0.47
61:JJ:114:VAL:HG13	61:JJ:119:LEU:HB2	1.97	0.47
64:MM:40:LYS:HE2	83:ff:130:VAL:HA	1.96	0.47
64:MM:94:ILE:HB	64:MM:101:ARG:HD2	1.96	0.47
67:PP:44:ARG:HH21	67:PP:53:GLN:HE22	1.63	0.47
84:gg:20:GLN:HG2	84:gg:69:VAL:H	1.79	0.47
1:5:1907:A:H4'	9:F:222:LYS:HE3	1.97	0.46
1:5:2616:C:OP1	20:R:60:ARG:NH1	2.48	0.46
7:D:232:THR:OG1	7:D:234:ASP:OD1	2.31	0.46
19:Q:172:ARG:NH1	29:a:56:VAL:O	2.46	0.46
34:f:59:THR:OG1	34:f:65:ASN:OD1	2.33	0.46
51:9:621:C:H5'	75:XX:107:ARG:NH2	2.30	0.46
51:9:981:A:H2'	51:9:982:G:C8	2.49	0.46
54:CC:264:SER:H	54:CC:267:GLN:HE21	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:II:64:ASN:OD1	60:II:73:THR:OG1	2.31	0.46
74:WW:49:GLU:H	74:WW:64:ASN:HB2	1.79	0.46
77:ZZ:73:VAL:HG13	77:ZZ:77:LEU:HD12	1.96	0.46
78:aa:7:ASN:O	78:aa:9:GLY:N	2.48	0.46
1:5:66:A:N6	1:5:282:C:O2'	2.44	0.46
1:5:337:U:H2'	1:5:338:A:H8	1.79	0.46
1:5:509:A:H4'	14:L:163:LYS:HE2	1.98	0.46
1:5:709:C:H5''	34:f:46:ARG:HH22	1.80	0.46
1:5:1563:A:N6	51:9:1028:A:N1	2.63	0.46
1:5:3970:G:O3'	48:u:60:ARG:NH1	2.49	0.46
5:B:317:LEU:HB2	5:B:372:SER:HB2	1.96	0.46
10:G:219:LEU:HD21	16:N:45:PRO:HG2	1.98	0.46
49:v:692:LEU:HD11	49:v:738:PRO:HG2	1.97	0.46
51:9:434:G:H2'	51:9:435:A:C8	2.50	0.46
51:9:677:G:H21	51:9:1028:A:H62	1.62	0.46
51:9:692:G:H2'	51:9:693:A:H8	1.80	0.46
56:EE:11:ARG:HA	56:EE:28:ALA:HB2	1.97	0.46
57:FF:53:ALA:O	68:QQ:125:ARG:NH2	2.48	0.46
1:5:97:G:N7	14:L:13:HIS:NE2	2.63	0.46
1:5:1500:A:H5''	1:5:1501:C:H5'	1.97	0.46
1:5:1952:G:OP1	21:S:139:ARG:NE	2.37	0.46
1:5:3933:G:H2'	1:5:3934:G:H8	1.81	0.46
1:5:4996:C:H4'	32:d:26:THR:HG23	1.97	0.46
18:P:127:ARG:HH21	18:P:139:TYR:HE2	1.64	0.46
49:v:279:SER:HB2	49:v:285:LEU:HD21	1.97	0.46
51:9:377:G:H5'	60:II:98:LYS:HB3	1.97	0.46
51:9:1461:G:O2'	51:9:1464:C:N4	2.45	0.46
51:9:1607:A:H5'	71:TT:87:VAL:HG21	1.97	0.46
1:5:151:G:N7	10:G:194:ASN:ND2	2.57	0.46
1:5:163:A:H2'	1:5:164:G:C8	2.51	0.46
1:5:510:U:H5'	29:a:85:GLN:HG3	1.96	0.46
1:5:1481:C:O2'	1:5:1482:G:N3	2.47	0.46
1:5:4991:U:H2'	1:5:4992:G:H8	1.80	0.46
6:C:170:LEU:HD23	6:C:221:PHE:HZ	1.80	0.46
13:J:97:ASN:ND2	13:J:177:GLY:O	2.49	0.46
23:U:24:ASP:HB2	23:U:26:THR:HG23	1.98	0.46
47:t:66:ASN:HB2	47:t:67:ARG:HH11	1.80	0.46
50:w:286:TRP:CZ2	62:KK:86:PRO:CD	2.94	0.46
51:9:1013:U:OP1	51:9:1129:G:O2'	2.34	0.46
51:9:1542:C:OP1	71:TT:62:ARG:NH1	2.48	0.46
63:LL:102:PHE:HB2	75:XX:8:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:108:A:N1	1:5:333:U:O2'	2.39	0.46
1:5:1548:G:O2'	1:5:2812:A:N3	2.43	0.46
1:5:1633:G:C6	4:A:207:VAL:HG21	2.50	0.46
1:5:2739:C:H4'	44:p:52:VAL:HG21	1.96	0.46
1:5:4991:U:H2'	1:5:4992:G:C8	2.50	0.46
16:N:104:GLU:HA	16:N:160:GLU:HG3	1.96	0.46
21:S:127:MET:HE1	22:T:155:PRO:HA	1.98	0.46
43:o:6:LYS:NZ	43:o:93:LEU:O	2.44	0.46
47:t:146:ARG:HE	47:t:147:HIS:H	1.62	0.46
49:v:32:LYS:N	87:v:900:GDP:O1B	2.46	0.46
53:BB:181:LEU:HA	53:BB:184:VAL:HG22	1.98	0.46
76:YY:81:TYR:HA	76:YY:84:LYS:HG2	1.98	0.46
1:5:1341:U:O3'	16:N:204:ARG:NH1	2.48	0.46
1:5:3967:G:H1'	48:u:162:VAL:HG11	1.97	0.46
4:A:58:LEU:HD13	4:A:75:LEU:HD23	1.98	0.46
19:Q:66:MET:HB2	19:Q:66:MET:HE3	1.79	0.46
51:9:98:C:OP2	51:9:426:A:O2'	2.30	0.46
57:FF:34:SER:HA	80:cc:55:VAL:HB	1.96	0.46
61:JJ:21:GLU:OE1	61:JJ:24:ARG:N	2.44	0.46
61:JJ:53:ILE:HG23	61:JJ:77:LEU:HD11	1.98	0.46
76:YY:20:ARG:NH1	76:YY:76:TYR:OH	2.48	0.46
79:bb:56:CYS:SG	79:bb:57:VAL:N	2.88	0.46
1:5:724:C:H1'	6:C:343:GLN:HG2	1.96	0.46
1:5:3759:A:OP2	1:5:3765:G:N1	2.41	0.46
1:5:4056:A:H1'	48:u:164:CYS:HB3	1.97	0.46
1:5:4635:A:H2	1:5:4663:G:H21	1.62	0.46
2:7:92:C:H2'	2:7:93:G:H8	1.81	0.46
4:A:124:GLY:O	4:A:128:ARG:NH1	2.48	0.46
8:E:168:LEU:HD11	8:E:179:THR:HG22	1.98	0.46
39:k:26:LYS:HD3	39:k:69:LEU:HD22	1.97	0.46
44:p:47:MET:HE2	44:p:71:TYR:HE1	1.80	0.46
46:s:13:TYR:HA	46:s:16:LYS:HG2	1.98	0.46
51:9:640:A:H2'	51:9:641:A:C8	2.50	0.46
62:KK:3:MET:HG2	62:KK:44:HIS:CD2	2.51	0.46
63:LL:69:ARG:HH21	63:LL:132:ARG:HA	1.80	0.46
75:XX:105:PHE:HD1	75:XX:121:LYS:HD3	1.80	0.46
1:5:1332:C:H2'	1:5:1333:A:C8	2.51	0.46
1:5:1481:C:O2'	1:5:1482:G:O4'	2.34	0.46
1:5:2492:C:H2'	1:5:2493:G:C8	2.51	0.46
1:5:3717:A:H2'	1:5:3718:A2M:H8	1.97	0.46
2:7:61:G:O2'	7:D:279:ARG:NH1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:234:LYS:HG2	4:A:238:ILE:HD12	1.96	0.46
6:C:13:GLU:OE1	6:C:161:TYR:OH	2.29	0.46
23:U:23:LEU:HA	23:U:110:TYR:O	2.16	0.46
49:v:302:ASP:OD1	49:v:306:ASN:ND2	2.49	0.46
51:9:1523:C:H2'	51:9:1524:G:H8	1.81	0.46
56:EE:97:GLU:OE2	56:EE:113:ARG:NE	2.38	0.46
59:HH:60:ILE:O	59:HH:92:VAL:HA	2.16	0.46
60:II:48:VAL:HG21	60:II:54:LYS:HG3	1.98	0.46
62:KK:59:LYS:O	62:KK:69:TRP:HA	2.15	0.46
64:MM:101:ARG:HG2	64:MM:102:LYS:HG3	1.97	0.46
73:VV:40:ASP:HB3	73:VV:43:THR:HB	1.98	0.46
1:5:2407:G:OP2	1:5:2407:G:N2	2.40	0.46
1:5:3952:A:N1	1:5:4061:G:C6	2.84	0.46
1:5:4519:C:H5''	1:5:4520:G:H5''	1.97	0.46
1:5:4629:U:H2'	1:5:4630:G:H8	1.81	0.46
1:5:4693:C:O2'	1:5:4695:C:N4	2.44	0.46
3:8:27:U:H4'	6:C:53:ALA:HB3	1.98	0.46
6:C:28:PHE:HA	6:C:129:ALA:HA	1.97	0.46
9:F:126:LYS:HB2	22:T:133:ALA:HB3	1.98	0.46
22:T:121:GLU:HG2	22:T:122:LYS:HD2	1.97	0.46
49:v:266:PHE:HB2	49:v:288:THR:HB	1.98	0.46
50:w:286:TRP:CE2	62:KK:86:PRO:HD2	2.50	0.46
51:9:872:A:N1	51:9:914:U:C4	2.83	0.46
51:9:941:C:H2'	51:9:942:G:H8	1.81	0.46
51:9:948:C:H2'	51:9:949:G:H8	1.81	0.46
51:9:1597:C:OP2	77:ZZ:85:ARG:NH1	2.44	0.46
59:HH:130:LEU:HD23	59:HH:142:LYS:HE2	1.98	0.46
64:MM:35:ILE:HG12	64:MM:61:TYR:HE1	1.81	0.46
71:TT:40:ALA:HB3	71:TT:43:LYS:HG2	1.97	0.46
1:5:1866:UR3:OP1	12:I:4:ARG:NH2	2.49	0.46
6:C:292:ILE:HG21	19:Q:31:LEU:HD11	1.98	0.46
12:I:182:GLU:HA	12:I:185:VAL:HG12	1.98	0.46
16:N:5:LYS:HD3	16:N:8:GLN:HE21	1.81	0.46
21:S:95:ARG:NH2	21:S:112:ASP:OD2	2.40	0.46
51:9:165:G:OP2	51:9:165:G:N2	2.41	0.46
64:MM:36:ARG:HD2	83:ff:102:VAL:HG22	1.96	0.46
84:gg:41:ILE:HG22	84:gg:58:ALA:HA	1.98	0.46
1:5:483:G:H3'	1:5:484:U:H2'	1.97	0.45
1:5:3811:G:O2'	1:5:3814:U:OP2	2.33	0.45
14:L:106:SER:OG	14:L:109:SER:OG	2.34	0.45
51:9:302:A:N3	60:II:64:ASN:ND2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:633:C:H4'	75:XX:134:TYR:HE2	1.81	0.45
51:9:1228:A:H2'	51:9:1229:G:H8	1.81	0.45
53:BB:98:THR:O	53:BB:232:HIS:NE2	2.43	0.45
56:EE:183:VAL:HG11	56:EE:188:ASN:HB2	1.98	0.45
57:FF:49:LEU:HD23	68:QQ:49:TYR:HB2	1.99	0.45
84:gg:23:THR:HG22	84:gg:31:ILE:HD11	1.97	0.45
1:5:175:C:H2'	1:5:176:G:H8	1.81	0.45
1:5:1940:G:N2	1:5:4434:C:OP1	2.48	0.45
5:B:226:LYS:HD2	5:B:272:LYS:HE3	1.99	0.45
6:C:333:MLZ:HCM3	8:E:57:GLY:H	1.81	0.45
47:t:117:ARG:HH11	47:t:125:LEU:HB2	1.82	0.45
49:v:517:LEU:O	75:XX:97:ASN:ND2	2.44	0.45
51:9:382:C:H2'	51:9:383:G:H8	1.80	0.45
51:9:616:A:H5'	75:XX:68:LYS:HE2	1.99	0.45
51:9:637:U:H2'	51:9:638:C:O4'	2.16	0.45
51:9:649:U:H2'	51:9:650:A:C8	2.50	0.45
51:9:1446:A:H5''	72:UU:58:THR:HG23	1.97	0.45
51:9:1550:G:O2'	51:9:1558:C:O2	2.30	0.45
55:DD:65:ARG:HA	55:DD:68:GLU:HG2	1.98	0.45
68:QQ:49:TYR:HA	68:QQ:52:LEU:HB2	1.98	0.45
74:WW:55:ASP:N	74:WW:55:ASP:OD1	2.46	0.45
78:aa:12:LYS:HD3	78:aa:16:GLY:H	1.80	0.45
1:5:1655:C:OP2	29:a:26:ARG:NH1	2.50	0.45
5:B:56:ILE:HD11	5:B:74:GLU:HB2	1.97	0.45
9:F:93:ARG:NH2	9:F:95:ARG:O	2.49	0.45
24:V:132:ILE:HA	24:V:132:ILE:HD12	1.75	0.45
49:v:680:VAL:HA	49:v:683:PHE:HB3	1.98	0.45
51:9:690:G:H2'	51:9:691:G:H8	1.81	0.45
51:9:1215:C:O2'	51:9:1645:C:OP2	2.32	0.45
62:KK:80:ARG:HG3	62:KK:85:LEU:HB2	1.97	0.45
1:5:1488:G:OP1	14:L:183:ARG:NH1	2.49	0.45
1:5:1964:A:H3'	1:5:1965:G:H8	1.82	0.45
1:5:2407:G:H2'	40:l:13:LEU:HD22	1.98	0.45
3:8:8:U:H2'	3:8:9:A:H8	1.81	0.45
5:B:89:ILE:HG21	5:B:197:ALA:HB1	1.97	0.45
17:O:15:LEU:HB2	17:O:18:ARG:HB3	1.99	0.45
24:V:42:VAL:HA	24:V:61:VAL:HG23	1.99	0.45
43:o:2:VAL:N	43:o:90:HIS:O	2.50	0.45
43:o:36:GLN:OE1	43:o:39:ARG:NH2	2.50	0.45
51:9:527:C:H2'	51:9:528:A:H8	1.82	0.45
51:9:1142:G:OP2	54:CC:187:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:131:HIS:HA	52:AA:134:LEU:HD12	1.99	0.45
53:BB:113:MET:HB3	53:BB:142:PHE:HE2	1.80	0.45
56:EE:181:CYS:HA	56:EE:227:VAL:HA	1.97	0.45
57:FF:201:LYS:HA	57:FF:204:ARG:NH1	2.32	0.45
67:PP:56:LEU:HD13	67:PP:80:LEU:HD12	1.97	0.45
76:YY:87:PRO:HG2	76:YY:90:ARG:HH21	1.81	0.45
84:gg:216:ALA:HB3	84:gg:230:LEU:HD12	1.98	0.45
1:5:1502:G:H22	29:a:77:LYS:HE2	1.82	0.45
1:5:3597:G:H5''	1:5:3598:C:H5	1.82	0.45
1:5:3697:U:H5''	1:5:3698:G:H5'	1.98	0.45
1:5:3897:B8K:O2'	1:5:3898:G:OP2	2.34	0.45
1:5:4642:U:H2'	1:5:4643:G:H8	1.81	0.45
1:5:4736:C:H2'	1:5:4737:G:H8	1.82	0.45
3:8:8:U:H2'	3:8:9:A:C8	2.51	0.45
16:N:114:ARG:NH1	16:N:151:ILE:O	2.43	0.45
49:v:27:HIS:HB3	49:v:30:HIS:CE1	2.52	0.45
51:9:382:C:H2'	51:9:383:G:C8	2.52	0.45
52:AA:120:ARG:CZ	54:CC:267:GLN:HB3	2.47	0.45
66:OO:74:ALA:HB1	66:OO:115:ALA:HB2	1.98	0.45
73:VV:21:ASN:HB3	74:WW:67:GLY:HA3	1.99	0.45
1:5:1743:A:H5'	7:D:11:ALA:HB1	1.98	0.45
9:F:91:VAL:O	9:F:119:GLY:HA2	2.17	0.45
17:O:10:ASP:OD2	17:O:37:ARG:NH2	2.50	0.45
20:R:136:ARG:HA	20:R:139:MET:HG2	1.99	0.45
47:t:65:GLN:NE2	47:t:68:GLN:O	2.50	0.45
51:9:681:U:H4'	75:XX:9:THR:HG22	1.97	0.45
51:9:989:C:OP2	53:BB:155:TYR:OH	2.31	0.45
51:9:1375:G:H2'	51:9:1376:A:H8	1.82	0.45
52:AA:72:ALA:O	52:AA:97:THR:OG1	2.29	0.45
53:BB:49:VAL:HG21	53:BB:62:LEU:HB2	1.99	0.45
67:PP:72:LYS:HD3	67:PP:93:MET:HE3	1.98	0.45
67:PP:75:VAL:HG22	67:PP:93:MET:HB3	1.99	0.45
84:gg:292:SER:HB2	84:gg:299:PHE:HE2	1.80	0.45
1:5:280:G:H5''	16:N:14:LYS:HE2	1.99	0.45
2:7:113:G:N2	7:D:72:ASP:O	2.48	0.45
4:A:133:TYR:HB3	4:A:168:VAL:HG12	1.98	0.45
7:D:217:ASP:OD1	7:D:217:ASP:N	2.50	0.45
10:G:190:ARG:HB2	10:G:256:ALA:HB3	1.99	0.45
21:S:7:LEU:HD23	21:S:107:THR:HA	1.98	0.45
34:f:54:LYS:O	34:f:66:LYS:NZ	2.42	0.45
34:f:77:ALA:HA	34:f:84:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:44:TRP:O	40:l:48:LYS:NZ	2.42	0.45
51:9:5:U:H2'	51:9:6:G:C8	2.51	0.45
51:9:1112:U:H2'	51:9:1113:A:H8	1.82	0.45
65:NN:4:MET:HE3	65:NN:121:ARG:HG2	1.99	0.45
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	1.97	0.45
67:PP:18:ARG:HD2	70:SS:88:LYS:HG2	1.99	0.45
69:RR:31:ASN:HD21	69:RR:55:THR:HG22	1.82	0.45
83:ff:137:ASP:N	83:ff:137:ASP:OD1	2.49	0.45
1:5:373:OMG:HM21	1:5:1645:C:H4'	1.98	0.45
1:5:1398:A:H62	1:5:1419:G:H21	1.65	0.45
1:5:2108:G:OP2	9:F:30:LYS:NZ	2.42	0.45
1:5:4239:A:H2'	1:5:4240:G:C8	2.51	0.45
3:8:26:C:O2'	6:C:53:ALA:O	2.30	0.45
20:R:13:SER:OG	20:R:38:ARG:NH1	2.36	0.45
33:e:69:MET:HA	33:e:75:ARG:HD3	1.99	0.45
46:s:133:GLU:HG2	46:s:134:LYS:HG3	1.99	0.45
51:9:302:A:H1'	60:II:73:THR:HG23	1.98	0.45
51:9:831:G:O6	76:YY:11:LYS:NZ	2.49	0.45
51:9:996:A:H2'	51:9:997:A:C8	2.52	0.45
51:9:1585:U:O2'	51:9:1587:G:OP2	2.34	0.45
1:5:68:U:OP1	16:N:178:HIS:ND1	2.37	0.45
1:5:651:C:H2'	1:5:652:G:H8	1.82	0.45
1:5:1420:A:N7	29:a:116:LYS:NZ	2.64	0.45
1:5:2796:G:H5'	40:l:45:ARG:NH2	2.32	0.45
1:5:4943:A:OP1	8:E:157:THR:OG1	2.30	0.45
4:A:59:ALA:HB2	4:A:78:ALA:HB2	1.99	0.45
19:Q:61:LEU:HD22	19:Q:82:VAL:HG21	1.97	0.45
22:T:51:GLY:HA3	22:T:92:ARG:HB2	1.99	0.45
24:V:21:PRO:HA	24:V:54:ALA:HA	1.97	0.45
49:v:395:MET:O	49:v:417:PHE:N	2.49	0.45
50:w:283:LEU:HD23	62:KK:17:LYS:CB	2.40	0.45
51:9:511:U:O2'	51:9:576:A:N6	2.50	0.45
51:9:941:C:H2'	51:9:942:G:C8	2.52	0.45
51:9:1017:U:O2'	65:NN:48:SER:O	2.35	0.45
70:SS:51:ASP:OD1	70:SS:51:ASP:N	2.50	0.45
84:gg:8:ARG:HB2	84:gg:309:VAL:HG23	1.98	0.45
1:5:4661:G:N2	1:5:5004:C:O3'	2.50	0.45
6:C:143:ARG:HG2	6:C:182:LYS:HD2	1.98	0.45
18:P:122:ALA:HB3	18:P:143:PRO:HG2	1.99	0.45
42:n:1:MET:HB2	51:9:1706:G:H5'	1.99	0.45
49:v:831:PRO:HA	49:v:834:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1232:U:H2'	51:9:1233:G:C8	2.52	0.45
51:9:1579:A:O2'	51:9:1581:C:OP2	2.31	0.45
53:BB:144:LYS:HB2	53:BB:208:HIS:HB3	1.99	0.45
62:KK:3:MET:HG2	62:KK:44:HIS:HD2	1.79	0.45
64:MM:64:LEU:HD11	83:ff:106:TYR:HD2	1.82	0.45
67:PP:92:SER:HB3	67:PP:107:ILE:HD13	1.99	0.45
76:YY:74:MET:N	76:YY:74:MET:SD	2.90	0.45
1:5:328:A:OP2	37:i:30:ARG:NH1	2.42	0.44
1:5:940:C:OP1	9:F:241:ARG:NH2	2.49	0.44
1:5:1338:G:H4'	1:5:1339:U:C6	2.53	0.44
1:5:1523:A:N3	1:5:4389:C:O2'	2.46	0.44
1:5:1573:G:OP1	20:R:92:LYS:NZ	2.48	0.44
1:5:2696:A:H5'	39:k:26:LYS:HE2	1.99	0.44
1:5:3860:A:H2	18:P:131:ARG:HH22	1.66	0.44
1:5:4086:G:C4	10:G:104:LEU:HD21	2.52	0.44
1:5:4617:G:O2'	24:V:13:LYS:O	2.34	0.44
46:s:192:VAL:HB	46:s:199:TYR:HB3	2.00	0.44
49:v:517:LEU:HA	49:v:520:LEU:HG	1.98	0.44
49:v:655:ASP:N	49:v:684:GLN:OE1	2.48	0.44
51:9:495:U:O2'	56:EE:27:PHE:O	2.32	0.44
51:9:540:U:H1'	51:9:543:C:H41	1.82	0.44
51:9:639:C:OP1	82:ee:114:ARG:NH1	2.50	0.44
1:5:914:U:N3	1:5:918:G:N7	2.64	0.44
1:5:2338:C:O2	6:C:245:HIS:NE2	2.51	0.44
1:5:3709:U:H6	1:5:3711:A:H61	1.64	0.44
1:5:3749:C:O2'	4:A:220:GLY:O	2.35	0.44
9:F:226:PHE:CG	9:F:235:ARG:HG2	2.52	0.44
20:R:38:ARG:HA	20:R:41:ILE:HG12	1.99	0.44
49:v:715:DDE:HAB2	49:v:715:DDE:HAU3	1.84	0.44
52:AA:66:VAL:HG21	52:AA:185:MET:HB2	1.98	0.44
1:5:736:C:OP1	15:M:74:ARG:NH1	2.50	0.44
1:5:2491:C:H2'	1:5:2492:C:C6	2.53	0.44
1:5:2647:A:H62	1:5:2686:G:H8	1.64	0.44
1:5:4265:U:N3	7:D:17:GLN:O	2.51	0.44
3:8:11:C:O2'	18:P:5:SER:O	2.33	0.44
4:A:225:ILE:HD13	4:A:234:LYS:HA	1.99	0.44
17:O:22:ILE:HG23	21:S:166:ARG:HH11	1.82	0.44
32:d:19:GLU:OE2	32:d:92:ARG:NH2	2.51	0.44
51:9:65:C:OP1	58:GG:136:LYS:NZ	2.44	0.44
51:9:829:C:OP1	56:EE:22:LYS:N	2.48	0.44
51:9:1171:G:O2'	51:9:1187:G:O6	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BB:57:ILE:HG23	53:BB:60:ASP:HB2	1.98	0.44
65:NN:29:THR:OG1	65:NN:30:SER:N	2.51	0.44
1:5:1590:C:H4'	1:5:2857:A:H5'	1.99	0.44
1:5:2600:A:N6	1:5:2745:A:OP2	2.42	0.44
1:5:4537:C:H2'	1:5:4538:G:C8	2.51	0.44
1:5:4677:U:O2'	1:5:4713:G:N2	2.39	0.44
9:F:178:LEU:HB3	9:F:183:ILE:HB	1.99	0.44
47:t:128:THR:HA	47:t:131:GLU:HG2	1.98	0.44
49:v:24:VAL:O	49:v:105:SER:OG	2.35	0.44
49:v:742:GLU:HG3	49:v:820:LEU:HG	1.99	0.44
51:9:1016:U:OP2	79:bb:20:LYS:NZ	2.47	0.44
51:9:1488:C:O2'	51:9:1490:G:OP2	2.27	0.44
52:AA:147:LEU:O	52:AA:165:ASN:ND2	2.50	0.44
59:HH:69:LEU:HG	59:HH:96:ALA:HB2	1.98	0.44
60:II:67:TRP:NE1	60:II:191:GLU:OE2	2.50	0.44
72:UU:21:ARG:HE	72:UU:88:LEU:HD13	1.82	0.44
1:5:703:G:O2'	33:e:5:ARG:NH2	2.50	0.44
1:5:929:A:H3'	1:5:930:G:H8	1.82	0.44
1:5:1461:C:H2'	1:5:1462:A:C8	2.52	0.44
1:5:4405:G:O6	1:5:4439:U:O2	2.35	0.44
29:a:82:VAL:HG21	29:a:101:ILE:HG12	1.98	0.44
46:s:125:ALA:N	46:s:157:ASP:OD1	2.50	0.44
57:FF:100:ILE:HG23	57:FF:174:ALA:HB1	1.99	0.44
62:KK:49:MET:HA	62:KK:52:LEU:HB2	1.99	0.44
70:SS:40:TYR:CZ	70:SS:97:GLN:HG2	2.52	0.44
1:5:2812:A:OP1	20:R:83:GLY:N	2.43	0.44
1:5:4174:U:H2'	1:5:4175:G:H8	1.82	0.44
1:5:4322:G:N2	1:5:4325:A:OP2	2.45	0.44
14:L:186:ARG:HE	37:i:9:VAL:HG11	1.82	0.44
43:o:8:ARG:HD2	43:o:70:LEU:HD21	2.00	0.44
51:9:161:U:O2'	58:GG:87:ARG:NH2	2.51	0.44
51:9:220:U:H2'	51:9:221:A:H8	1.83	0.44
51:9:813:A:OP1	56:EE:16:LYS:NZ	2.43	0.44
51:9:1117:C:O2'	51:9:1118:C:O4'	2.35	0.44
51:9:1156:U:OP1	74:WW:71:LYS:NZ	2.43	0.44
53:BB:67:PHE:O	53:BB:85:LYS:HA	2.16	0.44
55:DD:29:LEU:HB2	55:DD:34:TYR:HB2	1.99	0.44
84:gg:114:SER:OG	84:gg:117:ASN:N	2.50	0.44
1:5:1558:A:H2'	1:5:1559:G:H8	1.83	0.44
1:5:1824:G:H2'	1:5:1825:A:C8	2.53	0.44
1:5:2745:A:H2'	1:5:2746:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:96:C:H5''	36:h:66:LYS:HD3	2.00	0.44
4:A:10:LYS:HA	4:A:16:PHE:HD2	1.82	0.44
11:H:34:LEU:HD21	11:H:150:ASP:HB3	2.00	0.44
13:J:22:LEU:HD22	13:J:130:PHE:CD1	2.52	0.44
19:Q:63:LEU:HA	19:Q:66:MET:HG2	1.99	0.44
49:v:194:GLU:OE2	49:v:197:SER:OG	2.35	0.44
51:9:155:G:H2'	51:9:156:G:H8	1.83	0.44
51:9:1213:C:H2'	51:9:1214:A:C8	2.53	0.44
55:DD:21:LEU:HD21	55:DD:48:ILE:HD11	2.00	0.44
57:FF:30:ILE:HD12	57:FF:36:GLN:HA	2.00	0.44
59:HH:62:ILE:HD12	59:HH:94:PHE:HE1	1.82	0.44
59:HH:79:LEU:HD22	59:HH:94:PHE:HZ	1.83	0.44
65:NN:60:VAL:HG23	65:NN:66:VAL:HG21	2.00	0.44
71:TT:110:LEU:HD23	71:TT:112:MET:HE2	1.99	0.44
73:VV:73:ALA:HB1	73:VV:78:ILE:HB	2.00	0.44
76:YY:58:PHE:HE1	76:YY:74:MET:HE1	1.82	0.44
1:5:739:G:H2'	1:5:740:G:H8	1.83	0.44
1:5:2735:G:H2'	1:5:2736:G:H8	1.81	0.44
5:B:43:LEU:HB2	5:B:210:VAL:HG22	2.00	0.44
13:J:89:VAL:HG23	67:PP:12:PHE:HB3	2.00	0.44
13:J:104:ASN:HD22	13:J:134:LEU:H	1.65	0.44
17:O:94:ARG:HE	34:f:97:ILE:HG21	1.82	0.44
18:P:4:TYR:HE2	18:P:16:LYS:HB3	1.83	0.44
33:e:30:LYS:HG3	33:e:31:ILE:HD12	2.00	0.44
38:j:18:LEU:HA	38:j:25:LYS:HA	1.98	0.44
46:s:139:GLN:HG2	49:v:180:ARG:HH11	1.83	0.44
51:9:1438:A:H2'	51:9:1439:A:C8	2.52	0.44
57:FF:125:SER:HB2	57:FF:136:ARG:HB3	1.99	0.44
1:5:1199:G:H2'	1:5:1200:G:H8	1.83	0.44
3:8:60:G:O6	36:h:62:ASN:ND2	2.49	0.44
9:F:41:LEU:HD11	30:b:102:PRO:HB3	1.99	0.44
15:M:12:VAL:HA	15:M:25:VAL:O	2.17	0.44
29:a:81:LEU:HD21	29:a:103:VAL:HG23	2.00	0.44
33:e:22:ARG:HB2	33:e:35:TRP:HA	1.99	0.44
35:g:44:SER:OG	35:g:46:CYS:SG	2.72	0.44
43:o:4:VAL:HG23	43:o:93:LEU:HD23	1.99	0.44
50:w:196:HIS:CE1	51:9:1702:G:OP1	2.71	0.44
51:9:639:C:H2'	51:9:640:A:C8	2.48	0.44
51:9:941:C:H5''	53:BB:136:ARG:NH2	2.32	0.44
52:AA:145:ILE:HG13	52:AA:159:ILE:HB	1.99	0.44
55:DD:67:ARG:O	55:DD:70:THR:OG1	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:KK:32:HIS:CE1	62:KK:34:GLU:HB3	2.51	0.44
62:KK:79:LEU:HD12	62:KK:79:LEU:HA	1.88	0.44
68:QQ:67:ASP:OD1	68:QQ:67:ASP:N	2.49	0.44
1:5:478:G:H2'	1:5:479:G:H8	1.83	0.43
1:5:2399:G:O2'	1:5:2822:G:O2'	2.31	0.43
1:5:4301:U:OP1	22:T:78:LYS:NZ	2.50	0.43
5:B:90:VAL:HG22	5:B:104:THR:HG23	2.00	0.43
5:B:160:ILE:HD12	5:B:193:LYS:HD2	2.00	0.43
51:9:74:G:N2	51:9:78:C:OP2	2.51	0.43
51:9:808:A:H2	51:9:855:G:H22	1.66	0.43
51:9:1596:U:OP2	77:ZZ:85:ARG:NH2	2.51	0.43
54:CC:207:ALA:O	54:CC:211:LYS:HB2	2.18	0.43
65:NN:90:HIS:HA	65:NN:93:LYS:HG2	2.00	0.43
70:SS:49:ASP:OD1	70:SS:49:ASP:N	2.51	0.43
84:gg:174:VAL:HG13	84:gg:195:LEU:HD13	2.00	0.43
1:5:1905:U:O2	9:F:214:SER:OG	2.28	0.43
1:5:5053:U:OP1	1:5:5054:C:N4	2.51	0.43
4:A:95:GLN:O	4:A:100:ASN:ND2	2.49	0.43
4:A:113:VAL:HB	4:A:164:ALA:HB1	2.00	0.43
4:A:116:LEU:N	4:A:126:LEU:O	2.47	0.43
4:A:126:LEU:HD13	4:A:150:LEU:HD21	2.00	0.43
6:C:152:LEU:HD23	6:C:251:ILE:HG12	2.00	0.43
49:v:464:VAL:HG21	49:v:470:VAL:HB	1.99	0.43
51:9:611:G:H21	82:ee:85:VAL:HG13	1.83	0.43
51:9:1648:G:O2'	51:9:1674:G:O6	2.28	0.43
51:9:1740:C:OP1	60:II:44:HIS:ND1	2.46	0.43
54:CC:176:LYS:O	54:CC:200:ARG:NH1	2.44	0.43
59:HH:36:LEU:HB2	59:HH:40:LEU:HD13	1.99	0.43
61:JJ:130:ILE:HG12	61:JJ:135:ILE:HD11	2.00	0.43
62:KK:4:PRO:HD2	62:KK:7:ASN:HD22	1.83	0.43
66:OO:34:PHE:HB3	66:OO:41:PHE:HB2	1.99	0.43
66:OO:136:PRO:HG3	66:OO:139:SER:HB3	2.00	0.43
70:SS:124:ARG:HE	70:SS:129:LEU:HB2	1.82	0.43
1:5:1933:G:H2'	1:5:1934:A:C8	2.52	0.43
1:5:4633:G:N2	1:5:4664:A:OP2	2.34	0.43
1:5:4992:G:H2'	1:5:4993:G:C8	2.52	0.43
10:G:143:GLN:HA	10:G:146:THR:HG22	2.00	0.43
19:Q:61:LEU:HD21	19:Q:66:MET:HB3	2.00	0.43
28:Z:22:LYS:NZ	28:Z:129:TRP:O	2.39	0.43
36:h:103:LYS:NZ	36:h:111:GLU:OE1	2.34	0.43
47:t:119:ARG:NH1	47:t:121:LEU:H	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:v:701:ARG:NE	49:v:703:ASP:OD1	2.42	0.43
51:9:1332:A:N3	55:DD:141:LYS:NZ	2.63	0.43
57:FF:41:VAL:HG23	57:FF:42:LYS:HB2	2.01	0.43
58:GG:116:LYS:HE2	58:GG:125:THR:HG21	1.99	0.43
61:JJ:97:ILE:HA	61:JJ:100:LEU:HD13	2.00	0.43
74:WW:49:GLU:O	74:WW:64:ASN:ND2	2.51	0.43
1:5:1538:U:H2'	1:5:1539:G:H8	1.83	0.43
1:5:3974:G:H1'	48:u:27:LYS:HE2	2.00	0.43
1:5:4153:C:H2'	1:5:4154:G:C8	2.53	0.43
1:5:4479:A:OP1	1:5:4610:A:O2'	2.36	0.43
1:5:4507:A:H2'	1:5:4508:C:C6	2.54	0.43
3:8:67:U:H2'	3:8:68:G:H8	1.84	0.43
7:D:289:ARG:HH21	7:D:293:ARG:HH22	1.67	0.43
49:v:204:MET:HE3	49:v:204:MET:HB3	1.93	0.43
49:v:714:ILE:N	50:w:198:GLY:O	2.50	0.43
51:9:687:C:O3'	59:HH:121:THR:OG1	2.35	0.43
51:9:1658:G:OP2	51:9:1660:C:N4	2.51	0.43
59:HH:36:LEU:H	59:HH:36:LEU:HG	1.68	0.43
84:gg:118:ARG:NH2	84:gg:134:THR:OG1	2.51	0.43
1:5:8:U:OP1	16:N:41:ARG:NH1	2.51	0.43
1:5:307:A:N3	1:5:310:G:O2'	2.47	0.43
1:5:710:G:H2'	1:5:711:A:H8	1.83	0.43
1:5:1081:C:N4	1:5:1219:G:O6	2.51	0.43
1:5:1868:A:H61	12:I:115:MET:HE3	1.83	0.43
1:5:2082:G:H5''	19:Q:12:LYS:HG2	1.99	0.43
1:5:2519:U:O2'	1:5:2530:U:O2	2.32	0.43
16:N:103:GLU:OE2	16:N:165:THR:OG1	2.29	0.43
19:Q:179:GLY:H	29:a:51:GLY:HA2	1.82	0.43
45:r:117:ILE:O	45:r:121:GLN:HB2	2.19	0.43
49:v:278:THR:OG1	49:v:283:LYS:O	2.36	0.43
49:v:550:GLY:H	49:v:553:HIS:HB3	1.82	0.43
49:v:856:ASP:OD1	49:v:856:ASP:N	2.49	0.43
53:BB:104:ASP:N	53:BB:104:ASP:OD1	2.52	0.43
55:DD:208:VAL:HG13	69:RR:41:ILE:HG13	2.00	0.43
58:GG:34:THR:O	58:GG:51:ARG:HA	2.18	0.43
61:JJ:109:ARG:HH22	61:JJ:127:ARG:HH12	1.65	0.43
74:WW:105:THR:HG23	74:WW:124:LYS:HB2	2.00	0.43
84:gg:163:PRO:O	84:gg:178:ASN:OD1	2.37	0.43
1:5:245:C:O2'	1:5:246:G:OP2	2.34	0.43
1:5:2556:G:H2'	1:5:2557:G:H8	1.84	0.43
1:5:2589:C:O2'	1:5:2767:U:O2'	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2809:G:O2'	1:5:4644:G:OP1	2.30	0.43
1:5:3717:A:H2'	1:5:3718:A2M:C8	2.48	0.43
1:5:3868:G:H22	1:5:3900:G:H1'	1.83	0.43
1:5:3928:A:O2'	16:N:77:LYS:O	2.34	0.43
1:5:4620:OMU:HM23	1:5:4620:OMU:H1'	1.72	0.43
11:H:58:ASP:OD1	11:H:58:ASP:N	2.50	0.43
16:N:15:GLN:O	16:N:20:ARG:NH1	2.52	0.43
44:p:37:TYR:CD2	44:p:71:TYR:HB2	2.54	0.43
48:u:34:LEU:HB3	48:u:167:VAL:HB	2.00	0.43
49:v:327:ASP:N	49:v:327:ASP:OD1	2.52	0.43
49:v:343:TRP:CD2	49:v:344:LEU:HD13	2.52	0.43
51:9:894:G:H2'	51:9:895:G:C8	2.53	0.43
51:9:1010:G:H2'	51:9:1011:A:C8	2.54	0.43
52:AA:141:ASN:OD1	52:AA:141:ASN:N	2.51	0.43
53:BB:175:GLU:OE1	53:BB:187:LYS:NZ	2.45	0.43
66:OO:81:VAL:O	66:OO:85:CYS:HB2	2.19	0.43
77:ZZ:63:PRO:HG3	77:ZZ:91:LEU:HD21	2.00	0.43
1:5:983:U:OP1	8:E:75:TYR:OH	2.29	0.43
1:5:2389:A:H5'	32:d:70:LYS:HE2	1.99	0.43
1:5:3839:G:N2	1:5:3843:C:O2'	2.51	0.43
1:5:3928:A:H5'	16:N:89:VAL:HG13	2.01	0.43
1:5:4626:A:H4'	5:B:53:MET:HG3	2.00	0.43
22:T:106:LEU:HA	22:T:109:VAL:HG12	2.00	0.43
49:v:119:LEU:HA	49:v:122:THR:HG22	1.99	0.43
49:v:461:ILE:HD11	49:v:464:VAL:HB	2.00	0.43
51:9:126:G:H8	58:GG:199:THR:HG21	1.83	0.43
51:9:154:U:O2	58:GG:4:ASN:ND2	2.42	0.43
51:9:367:U:H4'	51:9:371:A:C8	2.54	0.43
51:9:690:G:H2'	51:9:691:G:C8	2.53	0.43
51:9:1588:A:H2'	51:9:1589:A:C8	2.53	0.43
53:BB:164:ILE:HD12	53:BB:207:LEU:HD22	2.01	0.43
74:WW:15:ASN:HD21	74:WW:71:LYS:HG3	1.84	0.43
1:5:1787:A:H2'	1:5:1788:A:C8	2.54	0.43
1:5:2081:C:O2'	19:Q:10:ASP:O	2.32	0.43
1:5:4239:A:H2'	1:5:4240:G:H8	1.83	0.43
12:I:91:LEU:HD12	12:I:135:ILE:HG23	2.01	0.43
47:t:105:THR:HA	47:t:143:VAL:HG13	2.01	0.43
49:v:91:GLN:HG2	49:v:363:THR:HG21	2.01	0.43
49:v:665:ILE:HB	49:v:705:HIS:HA	2.01	0.43
62:KK:6:LYS:HE2	62:KK:6:LYS:HB3	1.89	0.43
1:5:1198:G:H2'	1:5:1199:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1591:U:OP2	1:5:2856:C:O2'	2.30	0.43
1:5:2638:G:H22	1:5:2697:A:H61	1.67	0.43
1:5:2743:A:H2'	1:5:2744:A:C8	2.54	0.43
1:5:4274:A:H2'	1:5:4275:G:H8	1.83	0.43
1:5:4564:M7A:OP1	17:O:68:ARG:NH2	2.52	0.43
1:5:4611:A:H2	11:H:120:GLU:HB3	1.83	0.43
1:5:4704:C:H2'	1:5:4705:A:C8	2.53	0.43
1:5:4933:C:OP2	8:E:265:LYS:NZ	2.52	0.43
11:H:80:MET:HE3	11:H:80:MET:HB2	1.85	0.43
19:Q:167:VAL:HG12	19:Q:169:SER:H	1.84	0.43
28:Z:92:ASP:N	28:Z:92:ASP:OD1	2.52	0.43
32:d:59:THR:HG22	32:d:61:ASP:H	1.83	0.43
45:r:47:LYS:HB2	45:r:102:TYR:CZ	2.54	0.43
49:v:586:GLU:HG2	49:v:605:LYS:HE3	2.01	0.43
51:9:611:G:N2	51:9:633:C:H42	2.17	0.43
70:SS:7:GLU:HG2	70:SS:8:LYS:HG3	2.01	0.43
72:UU:94:PRO:HD2	72:UU:97:ILE:HD12	2.01	0.43
84:gg:31:ILE:HG22	84:gg:43:TRP:HB2	2.00	0.43
1:5:150:U:OP2	10:G:253:THR:OG1	2.33	0.43
1:5:907:C:H2'	1:5:908:G:H8	1.83	0.43
1:5:1461:C:H2'	1:5:1462:A:H8	1.84	0.43
1:5:1484:G:O2'	1:5:1486:C:OP2	2.37	0.43
1:5:2875:C:OP1	44:p:23:ARG:NH1	2.39	0.43
1:5:3972:A:OP2	48:u:62:LYS:NZ	2.43	0.43
1:5:4891:G:H1	1:5:4928:C:N4	2.17	0.43
9:F:102:PRO:HA	9:F:105:ARG:HG2	2.00	0.43
10:G:308:LYS:HE2	10:G:308:LYS:HB3	1.92	0.43
14:L:10:LEU:O	29:a:34:ASN:ND2	2.46	0.43
21:S:127:MET:HA	22:T:153:PRO:HD2	2.01	0.43
49:v:839:ARG:HG3	49:v:844:LEU:HG	2.01	0.43
51:9:352:U:O2	63:LL:71:ARG:NE	2.39	0.43
51:9:793:G:H2'	51:9:794:A:H8	1.84	0.43
52:AA:30:LEU:HB2	52:AA:47:TYR:CE2	2.54	0.43
64:MM:26:LEU:HB3	64:MM:31:LEU:HD21	2.01	0.43
65:NN:101:HIS:NE2	65:NN:108:ASP:OD2	2.41	0.43
68:QQ:22:VAL:HG11	68:QQ:71:ARG:HH21	1.84	0.43
76:YY:35:VAL:HG13	76:YY:40:ILE:HD11	2.01	0.43
1:5:1169:G:H2'	1:5:1170:G:H8	1.84	0.42
1:5:2457:G:HO2'	1:5:3672:G:HO2'	1.67	0.42
1:5:2627:C:H41	1:5:4649:G:H1	1.66	0.42
1:5:3785:A2M:H8	1:5:3785:A2M:H2'	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:37:A:OP2	36:h:89:ARG:NH1	2.41	0.42
10:G:204:LYS:O	10:G:258:THR:OG1	2.34	0.42
34:f:76:ARG:HD2	34:f:85:ARG:HD2	2.01	0.42
43:o:74:GLU:HA	43:o:75:PRO:HD3	1.92	0.42
48:u:38:LEU:HA	48:u:202:ARG:H	1.84	0.42
48:u:171:HIS:CE1	48:u:174:MET:HE2	2.54	0.42
49:v:669:VAL:HG11	49:v:707:VAL:HG22	2.01	0.42
51:9:62:G:O2'	51:9:172:U:OP1	2.37	0.42
51:9:106:C:H2'	51:9:107:A:C8	2.53	0.42
51:9:148:U:H2'	51:9:149:A:H8	1.84	0.42
51:9:1013:U:H2'	51:9:1014:G:H8	1.84	0.42
59:HH:15:LYS:HD3	59:HH:16:PRO:HD2	2.01	0.42
70:SS:25:LYS:O	70:SS:29:ALA:N	2.50	0.42
84:gg:82:SER:OG	84:gg:83:TRP:N	2.52	0.42
84:gg:238:ALA:H	84:gg:251:ALA:HB3	1.83	0.42
1:5:137:G:H2'	1:5:138:G:H8	1.83	0.42
1:5:510:U:OP2	29:a:85:GLN:NE2	2.45	0.42
1:5:1382:G:H2'	1:5:1383:G:H8	1.84	0.42
1:5:1463:C:H5''	30:b:31:SER:HB3	2.01	0.42
1:5:2002:A:N6	47:t:138:SER:OG	2.52	0.42
1:5:2309:G:O2'	3:8:18:U:O2	2.37	0.42
1:5:3598:C:H2'	1:5:3599:A:C8	2.54	0.42
1:5:3951:G:C2	1:5:4062:A:H2	2.32	0.42
1:5:4055:U:H3'	1:5:4056:A:C8	2.54	0.42
1:5:4174:U:H2'	1:5:4175:G:C8	2.54	0.42
1:5:4274:A:H2'	1:5:4275:G:C8	2.54	0.42
10:G:159:THR:OG1	10:G:162:GLU:OE1	2.31	0.42
14:L:91:ALA:HB1	14:L:96:ILE:HB	2.01	0.42
14:L:207:VAL:O	14:L:211:LYS:HB2	2.19	0.42
51:9:618:C:H41	75:XX:67:ARG:NH1	2.17	0.42
51:9:1216:C:N4	51:9:1342:U:OP1	2.38	0.42
51:9:1536:G:H2'	51:9:1537:A:C8	2.54	0.42
53:BB:34:LYS:HB2	53:BB:97:LEU:HD13	2.01	0.42
56:EE:151:ASP:OD2	58:GG:216:ARG:NH1	2.50	0.42
75:XX:68:LYS:HE3	82:ee:82:VAL:HB	2.01	0.42
1:5:229:G:OP1	27:Y:11:ARG:NH1	2.47	0.42
1:5:1862:U:O2'	1:5:4212:A:OP1	2.36	0.42
1:5:1994:C:H2'	1:5:1995:G:C8	2.54	0.42
1:5:2756:G:O6	28:Z:51:ARG:NH2	2.46	0.42
5:B:80:GLU:HG3	5:B:326:VAL:HG13	2.02	0.42
13:J:20:LEU:HD13	13:J:132:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:71:LYS:HA	37:i:74:LYS:HG2	2.00	0.42
47:t:133:LEU:HD22	47:t:147:HIS:CD2	2.54	0.42
49:v:18:ASN:ND2	49:v:94:ASP:O	2.51	0.42
49:v:507:VAL:HG22	49:v:554:LEU:HD13	2.01	0.42
51:9:1304:U:H5''	83:ff:93:HIS:HB2	2.02	0.42
55:DD:176:LEU:HG	55:DD:181:VAL:HG22	2.02	0.42
58:GG:45:TRP:HE1	58:GG:121:ILE:HD13	1.83	0.42
73:VV:11:LEU:HD12	73:VV:12:TYR:HD1	1.83	0.42
76:YY:21:LYS:O	76:YY:75:ILE:N	2.47	0.42
84:gg:120:ILE:HD11	84:gg:132:TRP:HB2	2.00	0.42
84:gg:215:GLN:OE1	84:gg:231:ASP:OD1	2.37	0.42
1:5:93:G:OP2	29:a:54:GLY:N	2.50	0.42
1:5:175:C:H2'	1:5:176:G:C8	2.55	0.42
1:5:469:C:H42	8:E:108:ARG:HH21	1.67	0.42
1:5:1866:UR3:H3U2	1:5:4405:G:H8	1.83	0.42
1:5:3621:A:O2'	1:5:4658:G:O2'	2.34	0.42
1:5:4587:G:N2	5:B:15:GLY:O	2.37	0.42
2:7:120:U:OP1	7:D:259:ARG:NH1	2.52	0.42
22:T:121:GLU:OE2	22:T:122:LYS:NZ	2.41	0.42
23:U:22:THR:HB	23:U:69:LYS:HE2	2.01	0.42
50:w:283:LEU:CD1	62:KK:89:ILE:HD13	2.50	0.42
51:9:559:G:O2'	51:9:560:A:O4'	2.37	0.42
51:9:906:U:H2'	51:9:907:G:C8	2.55	0.42
62:KK:14:LEU:HD12	62:KK:14:LEU:HA	1.84	0.42
67:PP:82:ASP:OD1	67:PP:82:ASP:N	2.51	0.42
84:gg:277:THR:HG23	84:gg:281:ALA:HB3	2.01	0.42
1:5:1202:C:H2'	1:5:1203:G:C8	2.54	0.42
1:5:1326:A2M:HM'3	1:5:1326:A2M:H1'	1.94	0.42
1:5:1690:C:OP2	19:Q:11:ARG:NH2	2.53	0.42
1:5:3619:G:H22	1:5:3624:A:H1'	1.83	0.42
1:5:3932:U:H2'	1:5:3933:G:H8	1.84	0.42
1:5:4319:C:H2'	1:5:4320:G:H8	1.84	0.42
49:v:224:THR:HG23	49:v:226:LYS:HG2	2.00	0.42
51:9:155:G:H2'	51:9:156:G:C8	2.55	0.42
51:9:183:G:O2'	51:9:184:G:O4'	2.34	0.42
56:EE:44:LEU:HD11	56:EE:70:ILE:HD13	2.00	0.42
72:UU:51:LYS:HB2	72:UU:90:ASP:HB2	2.02	0.42
1:5:517:C:H2'	1:5:518:G:H8	1.85	0.42
1:5:937:U:H5	15:M:46:ARG:HH11	1.67	0.42
1:5:1354:A:N1	1:5:1385:G:O2'	2.48	0.42
1:5:1646:A:O2'	38:j:49:TRP:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1866:UR3:H3U2	1:5:4405:G:C8	2.54	0.42
1:5:3910:C:O2'	1:5:4196:OMG:N2	2.51	0.42
1:5:4629:U:H2'	1:5:4630:G:C8	2.54	0.42
3:8:135:C:OP1	26:X:63:LYS:NZ	2.44	0.42
7:D:61:ILE:HG23	7:D:79:TYR:HE1	1.84	0.42
7:D:125:VAL:HG21	7:D:199:ILE:HG21	2.01	0.42
8:E:217:ASP:N	8:E:217:ASP:OD1	2.50	0.42
20:R:99:MET:HE1	20:R:128:LYS:HA	2.02	0.42
27:Y:50:ARG:HG2	27:Y:51:LYS:H	1.84	0.42
47:t:11:LYS:HB2	47:t:64:ILE:HG23	2.01	0.42
49:v:613:LEU:HD13	49:v:635:LEU:HD21	2.01	0.42
51:9:453:C:O2'	58:GG:92:ARG:O	2.34	0.42
51:9:943:U:H2'	51:9:944:A:C8	2.55	0.42
54:CC:137:VAL:HG21	54:CC:244:ILE:HD12	2.01	0.42
57:FF:50:PRO:HB3	57:FF:69:VAL:HG13	2.01	0.42
1:5:32:G:OP1	16:N:73:ARG:NH1	2.53	0.42
1:5:57:G:H5''	16:N:154:PRO:HB2	2.01	0.42
1:5:1188:C:H2'	1:5:1189:G:C8	2.54	0.42
1:5:4087:G:N7	4:A:67:TYR:OH	2.52	0.42
3:8:47:C:H1'	3:8:61:A:H2'	2.02	0.42
13:J:115:LEU:HD11	13:J:130:PHE:HZ	1.83	0.42
48:u:35:GLN:HA	48:u:166:ALA:HA	2.02	0.42
48:u:184:HIS:HD2	48:u:185:LEU:HD12	1.84	0.42
49:v:748:GLU:OE1	49:v:785:LYS:HE2	2.20	0.42
50:w:196:HIS:CD2	50:w:196:HIS:H	2.38	0.42
50:w:286:TRP:NE1	62:KK:86:PRO:HD3	2.34	0.42
51:9:181:A:OP2	51:9:182:C:O2'	2.30	0.42
51:9:434:G:OP2	60:II:25:ARG:NH1	2.43	0.42
51:9:851:C:O2'	51:9:852:G:N2	2.48	0.42
51:9:1503:C:H2'	51:9:1504:U:C6	2.55	0.42
53:BB:149:GLN:HE22	53:BB:154:SER:HB2	1.84	0.42
81:dd:17:GLY:O	81:dd:27:ARG:NH2	2.52	0.42
84:gg:35:SER:OG	84:gg:37:ASP:OD1	2.34	0.42
1:5:1199:G:H2'	1:5:1200:G:C8	2.54	0.42
2:7:2:U:O2	2:7:117:G:O6	2.38	0.42
4:A:82:ILE:HG22	44:p:65:ALA:HB3	2.02	0.42
4:A:224:THR:HG21	4:A:243:THR:HG21	2.01	0.42
21:S:76:LYS:HD2	21:S:131:GLU:HG3	2.01	0.42
33:e:92:ASN:ND2	33:e:119:ALA:O	2.39	0.42
48:u:171:HIS:CE1	48:u:174:MET:HB3	2.55	0.42
49:v:279:SER:OG	49:v:281:GLU:OE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:581:U:H4'	76:YY:66:GLY:HA3	2.02	0.42
51:9:1356:G:O3'	54:CC:125:LYS:NZ	2.51	0.42
51:9:1413:G:H2'	51:9:1414:A:C8	2.55	0.42
68:QQ:89:SER:OG	68:QQ:119:LEU:O	2.35	0.42
69:RR:52:GLY:O	69:RR:55:THR:OG1	2.36	0.42
1:5:74:G:H1'	14:L:62:PRO:HG3	2.00	0.42
1:5:941:C:OP2	9:F:241:ARG:NE	2.44	0.42
1:5:950:G:H2'	1:5:951:G:H8	1.84	0.42
1:5:1298:C:H2'	1:5:1299:G:H8	1.84	0.42
1:5:3944:G:H2'	1:5:3945:A:C8	2.55	0.42
1:5:4764:A:O2'	11:H:43:VAL:O	2.31	0.42
6:C:124:ILE:H	6:C:124:ILE:HG13	1.76	0.42
9:F:165:ARG:HD2	9:F:208:TRP:CE2	2.55	0.42
19:Q:91:ARG:HB2	29:a:76:ASP:HB2	2.01	0.42
49:v:13:MET:HB2	49:v:468:ASN:ND2	2.35	0.42
49:v:26:ALA:HB2	49:v:128:VAL:HB	2.02	0.42
49:v:255:ASP:OD2	49:v:259:LYS:NZ	2.53	0.42
49:v:713:ALA:CB	50:w:199:SER:HA	2.40	0.42
49:v:751:CYS:SG	49:v:759:ILE:HD11	2.60	0.42
51:9:1395:C:OP2	68:QQ:15:ARG:NH1	2.51	0.42
52:AA:68:ILE:HD11	52:AA:121:LEU:HD13	2.01	0.42
53:BB:146:ARG:HB2	53:BB:149:GLN:HB2	2.01	0.42
56:EE:19:MET:HE1	56:EE:108:ARG:CZ	2.49	0.42
58:GG:61:PHE:HA	58:GG:62:PRO:HD3	1.93	0.42
1:5:456:C:H2'	1:5:457:G:H8	1.85	0.42
1:5:1340:C:OP2	29:a:6:ARG:NH1	2.44	0.42
1:5:1481:C:O2'	1:5:1482:G:O5'	2.38	0.42
1:5:3599:A:H2'	1:5:3600:G:C8	2.55	0.42
1:5:4188:U:H2'	1:5:4189:U:C6	2.55	0.42
1:5:4419:U:H5''	1:5:4420:U:H5	1.85	0.42
1:5:4690:B8K:O2'	11:H:72:THR:OG1	2.30	0.42
3:8:141:C:H2'	3:8:142:U:C6	2.55	0.42
5:B:55:HIS:CE1	25:W:16:GLY:HA3	2.55	0.42
7:D:155:THR:HG23	7:D:179:ARG:HA	2.01	0.42
9:F:79:ASN:HA	22:T:143:THR:HG22	2.02	0.42
20:R:67:THR:HA	20:R:70:ARG:HB2	2.01	0.42
20:R:69:ALA:HB1	20:R:74:ARG:HB2	2.02	0.42
26:X:143:ASP:N	26:X:143:ASP:OD1	2.53	0.42
27:Y:36:LYS:HA	27:Y:39:ARG:HG2	2.02	0.42
41:m:72:MLZ:O	41:m:74:TYR:N	2.41	0.42
45:r:10:VAL:HG13	45:r:14:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:65:C:N4	58:GG:134:GLY:O	2.49	0.42
51:9:115:U:H2'	51:9:116:U:C6	2.55	0.42
51:9:385:G:O2'	60:II:10:LYS:NZ	2.53	0.42
51:9:420:G:O2'	51:9:660:C:N3	2.48	0.42
51:9:1098:C:H2'	51:9:1099:G:C8	2.55	0.42
51:9:1253:A:OP2	51:9:1526:G:N2	2.40	0.42
51:9:1406:G:H2'	51:9:1407:U:C6	2.55	0.42
54:CC:180:VAL:HG22	54:CC:219:ILE:HD13	2.01	0.42
55:DD:164:VAL:HA	55:DD:168:VAL:HG22	2.02	0.42
56:EE:18:TRP:HB3	56:EE:20:LEU:HD13	2.01	0.42
56:EE:139:LEU:HB2	56:EE:150:PRO:HG3	2.02	0.42
61:JJ:108:ARG:NH2	61:JJ:149:VAL:O	2.53	0.42
1:5:709:C:H1'	1:5:4942:C:H5	1.85	0.41
1:5:4293:PSU:H5'	43:o:83:LEU:HD11	2.02	0.41
4:A:225:ILE:HD11	4:A:238:ILE:HD13	2.02	0.41
14:L:64:VAL:HA	14:L:67:HIS:CD2	2.54	0.41
33:e:7:LEU:HB2	33:e:93:LYS:HB3	2.02	0.41
33:e:22:ARG:HG3	33:e:36:ARG:H	1.84	0.41
33:e:90:MET:HG2	45:r:33:LYS:HG2	2.02	0.41
39:k:10:ASP:OD1	39:k:10:ASP:N	2.52	0.41
49:v:110:ASP:OD2	49:v:553:HIS:N	2.47	0.41
49:v:713:ALA:HB3	50:w:199:SER:CA	2.42	0.41
50:w:201:ARG:HH12	51:9:627:U:P	2.43	0.41
51:9:67:C:H41	58:GG:163:ASN:HA	1.86	0.41
51:9:1866:A:H61	78:aa:85:ARG:H	1.68	0.41
60:II:11:ARG:NH1	60:II:15:GLY:O	2.49	0.41
1:5:478:G:H2'	1:5:479:G:C8	2.54	0.41
1:5:1952:G:H4'	21:S:93:MET:HG2	2.02	0.41
1:5:3663:A:N6	1:5:4168:G:O2'	2.53	0.41
1:5:3726:A:H2'	1:5:3727:A:C8	2.54	0.41
1:5:3848:U:H2'	1:5:3849:A:C8	2.55	0.41
1:5:4630:G:H2'	1:5:4631:G:H8	1.85	0.41
1:5:4699:U:H1'	1:5:4700:A:H5''	2.01	0.41
5:B:49:TYR:OH	5:B:179:HIS:ND1	2.37	0.41
26:X:150:ALA:HB1	26:X:155:ILE:HG13	2.01	0.41
37:i:86:LYS:HA	37:i:89:GLU:HG2	2.02	0.41
49:v:66:ARG:HH12	49:v:449:ARG:HH12	1.67	0.41
49:v:580:ARG:HB2	49:v:696:ASN:O	2.20	0.41
51:9:548:C:H5'	51:9:549:C:H5''	2.02	0.41
51:9:980:A:H2'	51:9:981:A:C8	2.54	0.41
51:9:1535:U:O3'	57:FF:88:MET:HE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:FF:122:ARG:HG3	57:FF:146:ARG:HH11	1.85	0.41
61:JJ:32:ILE:HB	61:JJ:37:LEU:HB2	2.02	0.41
84:gg:230:LEU:HD13	84:gg:259:TRP:CE2	2.56	0.41
1:5:709:C:H1'	1:5:4942:C:C5	2.56	0.41
6:C:287:THR:HG21	45:r:5:LEU:HB2	2.02	0.41
7:D:3:PHE:HB3	7:D:4:VAL:H	1.68	0.41
16:N:101:VAL:HA	16:N:104:GLU:HG2	2.01	0.41
26:X:129:ARG:HH21	26:X:129:ARG:HD2	1.74	0.41
44:p:14:TYR:OH	44:p:30:GLU:OE2	2.29	0.41
49:v:105:SER:HB2	49:v:115:VAL:HG13	2.03	0.41
49:v:300:VAL:HG11	49:v:340:MET:HE3	2.01	0.41
49:v:352:GLN:O	49:v:356:ILE:HG12	2.21	0.41
49:v:582:THR:HG23	49:v:741:MET:HG2	2.01	0.41
51:9:560:A:H5'	61:JJ:174:LYS:HB3	2.02	0.41
58:GG:16:ILE:HG22	58:GG:18:VAL:HG23	2.02	0.41
82:ee:101:ARG:HD3	82:ee:105:ALA:HB1	2.01	0.41
1:5:709:C:OP1	34:f:89:ARG:NH1	2.53	0.41
1:5:951:G:H2'	1:5:952:G:H8	1.85	0.41
1:5:1088:C:H2'	1:5:1089:G:H8	1.85	0.41
1:5:1346:C:H2'	1:5:1347:G:H8	1.86	0.41
1:5:1688:G:H2'	1:5:1689:G:C8	2.55	0.41
1:5:2397:G:O6	35:g:4:ARG:NH2	2.50	0.41
1:5:3898:G:N2	5:B:260:ALA:O	2.44	0.41
2:7:23:A:N3	2:7:118:C:O2'	2.45	0.41
39:k:54:GLU:HA	39:k:57:LYS:HG2	2.01	0.41
44:p:46:LYS:HE3	44:p:58:GLY:HA3	2.03	0.41
46:s:128:THR:HG23	46:s:130:LEU:H	1.86	0.41
47:t:104:ILE:HG23	47:t:143:VAL:HG22	2.02	0.41
51:9:1712:A:H2'	51:9:1713:C:C6	2.56	0.41
54:CC:67:GLY:HA2	54:CC:70:VAL:HG12	2.02	0.41
59:HH:58:LYS:HB2	59:HH:90:LYS:HG3	2.01	0.41
63:LL:128:VAL:HA	63:LL:141:ASN:O	2.20	0.41
67:PP:53:GLN:HB3	67:PP:83:MET:HE1	2.02	0.41
1:5:2288:G:O6	29:a:10:LYS:NZ	2.54	0.41
4:A:33:ASP:O	4:A:37:ARG:HB2	2.19	0.41
7:D:209:ARG:HA	7:D:212:MET:HG2	2.02	0.41
9:F:103:LYS:HD3	9:F:134:ILE:HD11	2.03	0.41
33:e:44:ARG:HG3	33:e:49:PHE:CD2	2.55	0.41
51:9:960:U:O2'	51:9:962:A:N7	2.49	0.41
51:9:1351:G:C2	51:9:1379:A:C5	3.09	0.41
51:9:1395:C:H2'	51:9:1396:A:N3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DD:22:ASN:O	55:DD:26:THR:OG1	2.35	0.41
57:FF:142:SER:OG	80:cc:49:PRO:O	2.36	0.41
64:MM:54:SER:OG	64:MM:55:ASN:N	2.53	0.41
66:OO:31:CYS:HA	66:OO:43:HIS:O	2.19	0.41
76:YY:82:ALA:O	76:YY:86:GLU:CB	2.68	0.41
83:ff:135:HIS:CD2	83:ff:138:ARG:HH22	2.38	0.41
1:5:453:G:O2'	1:5:705:G:OP1	2.34	0.41
1:5:1525:A:O2'	1:5:3916:G:O2'	2.31	0.41
2:7:7:G:N2	7:D:70:GLU:O	2.43	0.41
24:V:87:SER:HA	24:V:97:TYR:HB3	2.03	0.41
25:W:82:ILE:HG22	58:GG:131:ARG:HB2	2.01	0.41
26:X:65:ALA:HB2	36:h:69:LEU:HD11	2.01	0.41
31:c:11:LEU:HA	31:c:14:ILE:HG22	2.02	0.41
51:9:652:U:H2'	51:9:653:A:C8	2.56	0.41
51:9:792:C:H2'	51:9:793:G:H8	1.85	0.41
55:DD:136:VAL:HG23	55:DD:186:VAL:HG22	2.02	0.41
57:FF:14:THR:N	68:QQ:57:LEU:O	2.53	0.41
60:II:70:GLU:OE2	63:LL:21:LYS:NZ	2.39	0.41
68:QQ:16:LYS:HE3	68:QQ:82:TYR:HD2	1.85	0.41
1:5:27:C:O2'	1:5:60:A:N3	2.44	0.41
1:5:287:U:H2'	1:5:288:G:C8	2.55	0.41
1:5:4478:G:O2'	1:5:4602:A:N1	2.44	0.41
4:A:112:ILE:HG13	44:p:79:VAL:HG22	2.02	0.41
11:H:151:ILE:O	11:H:155:SER:OG	2.33	0.41
28:Z:88:ASP:OD1	28:Z:88:ASP:N	2.53	0.41
47:t:115:GLN:HA	47:t:118:HIS:CG	2.56	0.41
49:v:412:ALA:HB3	49:v:472:LEU:HB2	2.02	0.41
50:w:193:PHE:N	50:w:193:PHE:CD1	2.89	0.41
51:9:527:C:H2'	51:9:528:A:C8	2.55	0.41
51:9:1240:A:C5	67:PP:100:LYS:HB2	2.56	0.41
51:9:1599:U:H2'	57:FF:166:ILE:HD11	2.02	0.41
66:OO:67:ASP:HB2	66:OO:70:SER:HB3	2.02	0.41
76:YY:23:MET:N	76:YY:23:MET:SD	2.94	0.41
82:ee:125:LYS:NZ	82:ee:126:LYS:O	2.47	0.41
1:5:1072:C:H42	1:5:1239:C:H42	1.69	0.41
1:5:2485:U:H2'	1:5:2486:G:C8	2.56	0.41
1:5:4537:C:H2'	1:5:4538:G:H8	1.85	0.41
1:5:4745:G:H1	1:5:4955:A:H61	1.69	0.41
1:5:4902:C:H2'	1:5:4903:G:H8	1.85	0.41
2:7:96:U:O2'	9:F:136:GLU:OE1	2.37	0.41
7:D:53:VAL:HG11	7:D:159:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:88:ASP:O	28:Z:121:ARG:NH2	2.54	0.41
43:o:61:LYS:HE2	43:o:61:LYS:HB3	1.93	0.41
51:9:72:C:H41	58:GG:170:ARG:NH1	2.18	0.41
51:9:143:U:N3	51:9:314:U:OP1	2.54	0.41
51:9:954:U:H2'	51:9:955:A:H8	1.86	0.41
51:9:1324:G:O6	51:9:1504:U:O4	2.39	0.41
51:9:1829:G:H1'	51:9:1850:A:H2	1.86	0.41
68:QQ:104:SER:HA	68:QQ:107:GLU:HG2	2.02	0.41
1:5:114:G:N2	1:5:276:C:O2'	2.53	0.41
1:5:1234:G:H1'	1:5:1235:G:H5'	2.02	0.41
1:5:1245:C:N4	1:5:1246:G:O6	2.54	0.41
1:5:1436:C:H5''	1:5:1437:C:H5'	2.03	0.41
1:5:2335:C:H2'	1:5:2336:G:H8	1.85	0.41
1:5:2778:G:N2	3:8:113:C:OP2	2.53	0.41
1:5:3848:U:H2'	1:5:3849:A:H8	1.85	0.41
1:5:4457:U:OP1	24:V:50:ASN:ND2	2.54	0.41
1:5:4467:A:O2'	1:5:4510:A:N3	2.39	0.41
1:5:4723:A:H2'	1:5:4724:A:C8	2.56	0.41
1:5:4861:G:H2'	1:5:4862:G:C8	2.55	0.41
1:5:4935:C:H2'	1:5:4936:G:C8	2.56	0.41
6:C:336:ARG:HA	6:C:339:THR:HG22	2.02	0.41
10:G:247:VAL:HB	10:G:249:ARG:HE	1.85	0.41
11:H:103:VAL:HG21	11:H:144:LEU:HD11	2.03	0.41
13:J:13:ARG:HB3	13:J:136:ARG:HH11	1.85	0.41
24:V:69:LYS:HA	24:V:70:PRO:HD3	1.89	0.41
25:W:97:LYS:HE3	25:W:98:PRO:HD2	2.03	0.41
27:Y:31:SER:HA	27:Y:48:PRO:HA	2.03	0.41
32:d:27:ILE:O	32:d:83:ARG:HA	2.20	0.41
48:u:68:LEU:HA	48:u:85:MET:HB3	2.02	0.41
49:v:81:LEU:HG	49:v:86:LEU:HD12	2.03	0.41
49:v:635:LEU:HD13	49:v:639:TYR:HB2	2.03	0.41
51:9:49:C:H2'	51:9:472:C:H41	1.86	0.41
51:9:1220:A:N3	51:9:1677:U:O2'	2.44	0.41
51:9:1277:C:H2'	51:9:1278:A:H8	1.86	0.41
51:9:1372:U:P	51:9:1385:G:H1	2.44	0.41
51:9:1683:C:H2'	51:9:1684:C:H6	1.85	0.41
56:EE:87:MET:HE1	56:EE:236:ILE:HD13	2.03	0.41
70:SS:35:GLY:O	70:SS:97:GLN:NE2	2.53	0.41
70:SS:125:HIS:CE1	70:SS:131:VAL:HG21	2.55	0.41
78:aa:33:ASP:OD1	78:aa:33:ASP:N	2.54	0.41
78:aa:45:VAL:HB	78:aa:49:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:ff:118:ARG:NH2	83:ff:134:SER:H	2.19	0.41
84:gg:40:ILE:O	84:gg:59:LEU:HB2	2.21	0.41
84:gg:176:VAL:HB	84:gg:186:THR:HG22	2.03	0.41
1:5:442:G:OP1	34:f:68:ARG:NH1	2.51	0.41
1:5:1743:A:N1	1:5:1789:C:O2'	2.52	0.41
1:5:3893:C:H2'	1:5:3894:A:H8	1.86	0.41
1:5:4890:G:H2'	1:5:4891:G:H8	1.86	0.41
2:7:110:G:H2'	2:7:111:C:C6	2.56	0.41
5:B:33:PRO:O	5:B:186:ASN:ND2	2.53	0.41
7:D:208:MET:HB2	7:D:208:MET:HE3	1.71	0.41
16:N:64:ILE:HD11	16:N:66:VAL:HG23	2.02	0.41
33:e:26:ASP:OD1	33:e:26:ASP:N	2.54	0.41
42:n:12:ARG:HG2	42:n:15:ARG:HH22	1.85	0.41
48:u:63:PHE:HZ	48:u:109:ALA:HB3	1.86	0.41
50:w:199:SER:OG	50:w:202:SER:O	2.39	0.41
51:9:114:G:N7	63:LL:69:ARG:NH2	2.69	0.41
51:9:618:C:H41	75:XX:67:ARG:HH11	1.67	0.41
51:9:925:G:N2	51:9:1017:U:O2	2.46	0.41
51:9:1413:G:H2'	51:9:1414:A:H8	1.85	0.41
56:EE:105:THR:HG23	56:EE:106:LYS:HD2	2.03	0.41
56:EE:199:GLU:HB2	56:EE:207:VAL:HG23	2.03	0.41
72:UU:48:LEU:HD21	72:UU:93:SER:HB3	2.02	0.41
84:gg:57:ARG:HH21	84:gg:95:GLY:HA3	1.86	0.41
1:5:710:G:H2'	1:5:711:A:C8	2.55	0.40
1:5:1984:A:H2'	1:5:2011:C:H5'	2.03	0.40
1:5:2745:A:H2'	1:5:2746:A:C8	2.55	0.40
1:5:4046:A:OP2	48:u:98:LYS:NZ	2.49	0.40
5:B:74:GLU:OE1	5:B:285:TYR:OH	2.26	0.40
6:C:228:THR:HG21	6:C:239:LYS:HG2	2.04	0.40
7:D:81:HIS:HA	7:D:92:LEU:HD13	2.03	0.40
7:D:156:GLY:HA2	7:D:181:PRO:HD3	2.03	0.40
12:I:152:LEU:HD23	12:I:152:LEU:HA	1.90	0.40
14:L:8:MET:HE3	19:Q:168:ARG:HB3	2.03	0.40
22:T:17:ARG:HD2	22:T:17:ARG:HA	1.92	0.40
22:T:30:TYR:HE1	22:T:94:GLU:HB3	1.86	0.40
29:a:100:ILE:HG12	29:a:123:ILE:HB	2.02	0.40
32:d:29:ILE:HD13	32:d:29:ILE:HG21	1.86	0.40
46:s:159:GLN:NE2	46:s:161:ILE:O	2.41	0.40
47:t:93:LYS:H	47:t:93:LYS:HG2	1.69	0.40
49:v:419:GLY:N	49:v:466:CYS:SG	2.93	0.40
51:9:172:U:O5'	51:9:314:U:O2'	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1560:U:H2'	51:9:1561:A:H8	1.87	0.40
51:9:1643:U:H2'	51:9:1644:C:C6	2.56	0.40
53:BB:97:LEU:HD12	53:BB:232:HIS:CG	2.56	0.40
57:FF:69:VAL:O	57:FF:73:THR:OG1	2.36	0.40
69:RR:14:ARG:HG2	69:RR:69:ILE:HD11	2.03	0.40
71:TT:134:ILE:HD13	71:TT:134:ILE:HA	1.96	0.40
1:5:8:U:H5''	16:N:40:PRO:HG3	2.03	0.40
1:5:741:C:H42	1:5:922(B):C:H42	1.70	0.40
1:5:956:A:H1'	1:5:2076:G:H5''	2.03	0.40
1:5:1471:U:H2'	1:5:1472:C:H6	1.86	0.40
1:5:2739:C:O2	4:A:174:ARG:NH1	2.51	0.40
1:5:3610:A:H2'	1:5:3611:A:H8	1.86	0.40
1:5:3612:C:H1'	1:5:5016:A:C8	2.56	0.40
1:5:3867:A2M:HM'3	1:5:3867:A2M:H1'	1.97	0.40
1:5:3892:U:O2'	18:P:80:GLN:OE1	2.31	0.40
1:5:3944:G:H2'	1:5:3945:A:H8	1.86	0.40
1:5:4729:A:H5''	1:5:4965:U:H1'	2.02	0.40
4:A:33:ASP:N	4:A:33:ASP:OD1	2.53	0.40
10:G:212:HIS:ND1	10:G:238:LYS:HA	2.37	0.40
10:G:214:VAL:HG23	10:G:217:ILE:HA	2.02	0.40
48:u:53:VAL:HG22	48:u:155:ILE:HB	2.03	0.40
57:FF:34:SER:OG	80:cc:55:VAL:O	2.34	0.40
58:GG:59:GLN:OE1	58:GG:72:ARG:NH1	2.45	0.40
61:JJ:88:ASP:OD1	61:JJ:88:ASP:N	2.54	0.40
1:5:62:A:N3	1:5:77:U:O2'	2.39	0.40
1:5:1306:C:H2'	1:5:1307:A:H8	1.87	0.40
1:5:1327:C:H2'	1:5:1328:G:C8	2.56	0.40
1:5:1329:G:H2'	1:5:3865:A:H5'	2.04	0.40
1:5:1406:G:N3	1:5:1411(A):G:N2	2.70	0.40
1:5:1444:G:H21	1:5:2110:G:H1	1.69	0.40
1:5:3607:U:H2'	1:5:3608:A:C8	2.56	0.40
1:5:4260:U:H2'	1:5:4261:C:C6	2.56	0.40
4:A:98:ILE:HD11	44:p:80:LYS:HA	2.03	0.40
5:B:189:THR:OG1	5:B:190:VAL:N	2.54	0.40
6:C:149:GLU:HB3	45:r:72:LYS:HG2	2.04	0.40
8:E:122:GLU:OE2	33:e:94:SER:OG	2.33	0.40
19:Q:172:ARG:HD2	29:a:57:GLY:HA3	2.03	0.40
22:T:40:VAL:HG22	22:T:96:ILE:HG12	2.03	0.40
30:b:102:PRO:HA	30:b:109:ARG:HH22	1.86	0.40
48:u:113:SER:HA	48:u:138:LEU:HG	2.02	0.40
51:9:28:U:H2'	51:9:29:G:C8	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:493:A:H1'	51:9:574:A:H5'	2.04	0.40
51:9:1144:A:H2'	51:9:1145:A:C8	2.57	0.40
51:9:1382:A:H2'	51:9:1383:A:H8	1.86	0.40
51:9:1775:U:H2'	51:9:1776:G:C8	2.57	0.40
59:HH:33:ASN:OD1	59:HH:34:SER:N	2.55	0.40
59:HH:34:SER:OG	59:HH:35:ASP:N	2.55	0.40
60:II:81:VAL:HG22	60:II:102:VAL:HG12	2.03	0.40
64:MM:85:LEU:HA	64:MM:88:TRP:HB2	2.01	0.40
70:SS:20:ILE:HD11	70:SS:33:ILE:HD11	2.03	0.40
77:ZZ:73:VAL:HG12	77:ZZ:79:ILE:HD11	2.02	0.40
1:5:20:U:OP2	3:8:36:G:N1	2.53	0.40
1:5:469:C:H2'	1:5:470:A:H8	1.87	0.40
1:5:713:C:H2'	1:5:714:G:H8	1.86	0.40
1:5:1202:C:H2'	1:5:1203:G:H8	1.86	0.40
1:5:2864:A:H2'	1:5:2865:U:C6	2.56	0.40
13:J:37:ALA:HA	13:J:70:VAL:HG11	2.03	0.40
49:v:689:GLU:O	49:v:730:TYR:OH	2.30	0.40
51:9:916:A:C5	65:NN:73:ARG:HD3	2.57	0.40
51:9:1084:A:OP1	51:9:1858:G:O2'	2.32	0.40
51:9:1808:U:H2'	51:9:1809:A:C8	2.57	0.40
55:DD:74:GLN:HG2	55:DD:79:PHE:HB2	2.02	0.40
62:KK:74:GLU:HA	62:KK:77:GLN:HG2	2.02	0.40
63:LL:5:GLN:NE2	63:LL:11:GLN:HB2	2.37	0.40
63:LL:111:VAL:HG12	63:LL:140:PHE:HB2	2.04	0.40
67:PP:56:LEU:HD22	67:PP:83:MET:HE3	2.04	0.40
72:UU:20:ILE:HG12	72:UU:98:VAL:HG11	2.03	0.40
84:gg:197:THR:HG21	84:gg:238:ALA:HA	2.03	0.40
1:5:266:C:H6	1:5:266:C:H2'	1.75	0.40
1:5:1833:G:N2	1:5:1835:G:O4'	2.55	0.40
1:5:3604:A:H5''	20:R:71:ARG:HH22	1.87	0.40
1:5:3664:G:H2'	1:5:3665:G:H8	1.86	0.40
1:5:3944:G:H1	1:5:4069:U:H3	1.70	0.40
1:5:4935:C:H2'	1:5:4936:G:H8	1.86	0.40
1:5:4967:A:H2'	1:5:4968:A:H8	1.86	0.40
1:5:4994:G:H2'	1:5:4995:U:C6	2.56	0.40
2:7:48:G:OP1	7:D:226:TYR:OH	2.38	0.40
4:A:45:VAL:HG22	4:A:61:VAL:HG22	2.04	0.40
5:B:213:GLN:NE2	5:B:285:TYR:O	2.38	0.40
6:C:221:PHE:HB3	6:C:227:ILE:HG21	2.03	0.40
11:H:129:ARG:HD2	11:H:156:ASN:HB3	2.04	0.40
46:s:10:LYS:HG2	46:s:60:MET:HE1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1580:A:OP1	72:UU:86:LYS:NZ	2.41	0.40
55:DD:31:GLU:O	55:DD:54:ARG:NH2	2.42	0.40
76:YY:82:ALA:O	76:YY:86:GLU:HB3	2.22	0.40
77:ZZ:69:THR:HG22	77:ZZ:72:VAL:HG12	2.04	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	
4	A	246/248 (99%)	225 (92%)	21 (8%)	0	100	100
5	B	392/394 (100%)	367 (94%)	25 (6%)	0	100	100
6	C	359/362 (99%)	342 (95%)	17 (5%)	0	100	100
7	D	291/293 (99%)	277 (95%)	14 (5%)	0	100	100
8	E	208/291 (72%)	195 (94%)	13 (6%)	0	100	100
9	F	223/225 (99%)	212 (95%)	11 (5%)	0	100	100
10	G	229/319 (72%)	218 (95%)	11 (5%)	0	100	100
11	H	188/190 (99%)	179 (95%)	9 (5%)	0	100	100
12	I	201/214 (94%)	192 (96%)	9 (4%)	0	100	100
13	J	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
14	L	208/210 (99%)	202 (97%)	6 (3%)	0	100	100
15	M	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
16	N	201/203 (99%)	188 (94%)	13 (6%)	0	100	100
17	O	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
18	P	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
19	Q	185/187 (99%)	176 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	R	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
21	S	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	21	52
22	T	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
23	U	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
24	V	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
25	W	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
26	X	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
27	Y	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
28	Z	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	16	45
29	a	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
30	b	100/245 (41%)	94 (94%)	6 (6%)	0	100	100
31	c	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
32	d	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
33	e	126/128 (98%)	116 (92%)	10 (8%)	0	100	100
34	f	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
35	g	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
36	h	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
37	i	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
38	j	84/86 (98%)	75 (89%)	9 (11%)	0	100	100
39	k	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
40	l	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
41	m	49/52 (94%)	43 (88%)	5 (10%)	1 (2%)	6	27
42	n	23/25 (92%)	23 (100%)	0	0	100	100
43	o	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
44	p	89/91 (98%)	89 (100%)	0	0	100	100
45	r	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
46	s	194/196 (99%)	176 (91%)	18 (9%)	0	100	100
47	t	151/153 (99%)	132 (87%)	18 (12%)	1 (1%)	18	49
48	u	204/206 (99%)	178 (87%)	24 (12%)	2 (1%)	12	40
49	v	834/839 (99%)	754 (90%)	78 (9%)	2 (0%)	43	71
50	w	22/26 (85%)	22 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	AA	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
53	BB	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
54	CC	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
55	DD	226/228 (99%)	216 (96%)	10 (4%)	0	100	100
56	EE	260/262 (99%)	248 (95%)	12 (5%)	0	100	100
57	FF	181/204 (89%)	165 (91%)	15 (8%)	1 (1%)	21	52
58	GG	235/237 (99%)	230 (98%)	5 (2%)	0	100	100
59	HH	181/194 (93%)	174 (96%)	7 (4%)	0	100	100
60	II	204/206 (99%)	191 (94%)	12 (6%)	1 (0%)	24	55
61	JJ	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
62	KK	94/96 (98%)	85 (90%)	9 (10%)	0	100	100
63	LL	139/158 (88%)	130 (94%)	9 (6%)	0	100	100
64	MM	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
65	NN	147/149 (99%)	142 (97%)	5 (3%)	0	100	100
66	OO	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
67	PP	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
68	QQ	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
69	RR	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
70	SS	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
71	TT	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
72	UU	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
73	VV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
74	WW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
75	XX	139/141 (99%)	133 (96%)	3 (2%)	3 (2%)	5	26
76	YY	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
77	ZZ	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
78	aa	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
79	bb	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
80	cc	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
81	dd	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
82	ee	53/55 (96%)	51 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
83	ff	66/68 (97%)	59 (89%)	7 (11%)	0	100	100
84	gg	311/313 (99%)	283 (91%)	28 (9%)	0	100	100
All	All	12576/13168 (96%)	11879 (94%)	684 (5%)	13 (0%)	49	75

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	m	73	CYS
48	u	61	PRO
49	v	288	THR
21	S	166	ARG
49	v	481	LYS
75	XX	62	PRO
47	t	98	ILE
75	XX	86	PRO
57	FF	20	PHE
48	u	60	ARG
28	Z	90	PRO
60	II	131	PRO
75	XX	61	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	190/190 (100%)	186 (98%)	4 (2%)	47	67
5	B	342/342 (100%)	339 (99%)	3 (1%)	70	78
6	C	301/301 (100%)	299 (99%)	2 (1%)	76	80
7	D	247/247 (100%)	244 (99%)	3 (1%)	63	75
8	E	190/251 (76%)	189 (100%)	1 (0%)	81	83
9	F	196/196 (100%)	196 (100%)	0	100	100
10	G	200/272 (74%)	198 (99%)	2 (1%)	68	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	H	169/169 (100%)	168 (99%)	1 (1%)	78	81
12	I	175/181 (97%)	175 (100%)	0	100	100
13	J	143/143 (100%)	143 (100%)	0	100	100
14	L	175/175 (100%)	170 (97%)	5 (3%)	37	62
15	M	117/117 (100%)	117 (100%)	0	100	100
16	N	171/171 (100%)	170 (99%)	1 (1%)	78	81
17	O	171/171 (100%)	170 (99%)	1 (1%)	78	81
18	P	134/134 (100%)	134 (100%)	0	100	100
19	Q	164/164 (100%)	164 (100%)	0	100	100
20	R	159/159 (100%)	158 (99%)	1 (1%)	78	81
21	S	157/157 (100%)	156 (99%)	1 (1%)	78	81
22	T	139/139 (100%)	139 (100%)	0	100	100
23	U	89/89 (100%)	87 (98%)	2 (2%)	45	66
24	V	101/101 (100%)	101 (100%)	0	100	100
25	W	86/126 (68%)	86 (100%)	0	100	100
26	X	106/106 (100%)	106 (100%)	0	100	100
27	Y	124/124 (100%)	124 (100%)	0	100	100
28	Z	117/117 (100%)	117 (100%)	0	100	100
29	a	119/119 (100%)	118 (99%)	1 (1%)	73	79
30	b	84/184 (46%)	84 (100%)	0	100	100
31	c	84/84 (100%)	83 (99%)	1 (1%)	63	75
32	d	98/98 (100%)	98 (100%)	0	100	100
33	e	114/114 (100%)	112 (98%)	2 (2%)	51	70
34	f	88/88 (100%)	87 (99%)	1 (1%)	65	76
35	g	98/98 (100%)	96 (98%)	2 (2%)	48	68
36	h	109/109 (100%)	109 (100%)	0	100	100
37	i	86/86 (100%)	85 (99%)	1 (1%)	63	75
38	j	73/73 (100%)	73 (100%)	0	100	100
39	k	64/64 (100%)	64 (100%)	0	100	100
40	l	47/47 (100%)	46 (98%)	1 (2%)	47	67
41	m	47/47 (100%)	46 (98%)	1 (2%)	47	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	n	24/24 (100%)	24 (100%)	0	100	100
43	o	91/91 (100%)	91 (100%)	0	100	100
44	p	74/74 (100%)	74 (100%)	0	100	100
45	r	108/108 (100%)	107 (99%)	1 (1%)	70	78
46	s	164/164 (100%)	163 (99%)	1 (1%)	78	81
47	t	126/126 (100%)	124 (98%)	2 (2%)	55	72
48	u	186/186 (100%)	184 (99%)	2 (1%)	65	76
49	v	713/713 (100%)	706 (99%)	7 (1%)	68	76
50	w	23/23 (100%)	21 (91%)	2 (9%)	9	32
52	AA	180/181 (99%)	178 (99%)	2 (1%)	65	76
53	BB	194/194 (100%)	194 (100%)	0	100	100
54	CC	187/187 (100%)	185 (99%)	2 (1%)	65	76
55	DD	190/190 (100%)	189 (100%)	1 (0%)	81	83
56	EE	224/224 (100%)	222 (99%)	2 (1%)	70	78
57	FF	158/170 (93%)	155 (98%)	3 (2%)	50	68
58	GG	207/207 (100%)	205 (99%)	2 (1%)	68	76
59	HH	165/174 (95%)	162 (98%)	3 (2%)	51	70
60	II	178/178 (100%)	178 (100%)	0	100	100
61	JJ	161/161 (100%)	160 (99%)	1 (1%)	78	81
62	KK	87/87 (100%)	87 (100%)	0	100	100
63	LL	130/142 (92%)	130 (100%)	0	100	100
64	MM	99/99 (100%)	97 (98%)	2 (2%)	48	68
65	NN	130/130 (100%)	129 (99%)	1 (1%)	73	79
66	OO	106/106 (100%)	105 (99%)	1 (1%)	70	78
67	PP	109/109 (100%)	108 (99%)	1 (1%)	70	78
68	QQ	117/117 (100%)	114 (97%)	3 (3%)	40	64
69	RR	119/119 (100%)	117 (98%)	2 (2%)	53	71
70	SS	125/125 (100%)	121 (97%)	4 (3%)	34	60
71	TT	111/111 (100%)	111 (100%)	0	100	100
72	UU	92/92 (100%)	91 (99%)	1 (1%)	65	76
73	VV	67/67 (100%)	65 (97%)	2 (3%)	36	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	WW	112/112 (100%)	111 (99%)	1 (1%)	70	78
75	XX	113/113 (100%)	113 (100%)	0	100	100
76	YY	107/107 (100%)	105 (98%)	2 (2%)	50	68
77	ZZ	66/66 (100%)	66 (100%)	0	100	100
78	aa	88/88 (100%)	87 (99%)	1 (1%)	65	76
79	bb	75/75 (100%)	74 (99%)	1 (1%)	61	74
80	cc	55/55 (100%)	54 (98%)	1 (2%)	51	70
81	dd	48/48 (100%)	48 (100%)	0	100	100
82	ee	46/46 (100%)	46 (100%)	0	100	100
83	ff	61/61 (100%)	61 (100%)	0	100	100
84	gg	272/272 (100%)	268 (98%)	4 (2%)	57	72
All	All	10962/11275 (97%)	10867 (99%)	95 (1%)	68	78

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	4	VAL
4	A	225	ILE
4	A	242	ARG
4	A	243	THR
5	B	17	LEU
5	B	66	LYS
5	B	262	VAL
6	C	57	LEU
6	C	180	ILE
7	D	10	LYS
7	D	36	LEU
7	D	64	ILE
8	E	178	VAL
10	G	122	ILE
10	G	215	ASP
11	H	161	ILE
14	L	58	ILE
14	L	59	VAL
14	L	63	THR
14	L	124	LEU
14	L	154	VAL
16	N	64	ILE

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Mol	Chain	Res	Type
17	O	22	ILE
20	R	105	LEU
21	S	70	LYS
23	U	40	GLU
23	U	47	ILE
29	a	7	LYS
31	c	93	THR
33	e	21	ILE
33	e	31	ILE
34	f	33	VAL
35	g	5	LEU
35	g	59	VAL
37	i	29	ARG
40	l	33	ASN
41	m	69	ILE
45	r	106	LEU
46	s	30	VAL
47	t	61	LYS
47	t	125	LEU
48	u	53	VAL
48	u	93	LEU
49	v	39	LEU
49	v	154	VAL
49	v	167	LEU
49	v	350	LEU
49	v	534	VAL
49	v	626	GLN
49	v	635	LEU
50	w	191	ARG
50	w	196	HIS
52	AA	197	VAL
52	AA	211	GLU
54	CC	233	LEU
54	CC	248	TYR
55	DD	44	THR
56	EE	102	ILE
56	EE	129	ILE
57	FF	92	ILE
57	FF	99	ILE
57	FF	154	LEU
58	GG	191	ARG
58	GG	226	GLU

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Mol	Chain	Res	Type
59	HH	31	GLU
59	HH	36	LEU
59	HH	95	ILE
61	JJ	79	ARG
64	MM	35	ILE
64	MM	80	ASP
65	NN	60	VAL
66	OO	116	LEU
67	PP	126	VAL
68	QQ	34	VAL
68	QQ	70	VAL
68	QQ	88	ILE
69	RR	69	ILE
69	RR	71	ILE
70	SS	36	VAL
70	SS	52	LEU
70	SS	59	LEU
70	SS	65	GLU
72	UU	101	ILE
73	VV	59	ILE
73	VV	70	LEU
74	WW	103	VAL
76	YY	17	LEU
76	YY	25	ILE
78	aa	21	ILE
79	bb	17	ARG
80	cc	31	ARG
84	gg	18	VAL
84	gg	40	ILE
84	gg	230	LEU
84	gg	257	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	140	ASN
4	A	187	HIS
5	B	145	GLN
5	B	167	GLN
5	B	204	GLN
5	B	289	GLN
6	C	38	ASN

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Mol	Chain	Res	Type
6	C	61	GLN
6	C	142	HIS
6	C	212	ASN
6	C	282	HIS
6	C	329	ASN
7	D	122	GLN
7	D	131	ASN
7	D	282	GLN
8	E	287	HIS
10	G	134	ASN
10	G	259	GLN
10	G	278	ASN
12	I	59	GLN
12	I	73	ASN
13	J	46	GLN
14	L	19	GLN
14	L	104	ASN
14	L	113	ASN
15	M	20	HIS
15	M	33	GLN
15	M	48	GLN
15	M	120	ASN
16	N	32	GLN
16	N	109	HIS
16	N	182	HIS
16	N	196	ASN
17	O	26	GLN
17	O	50	ASN
17	O	180	GLN
18	P	64	ASN
19	Q	7	HIS
19	Q	44	ASN
20	R	141	HIS
21	S	156	HIS
22	T	77	ASN
22	T	98	HIS
23	U	27	HIS
24	V	36	ASN
25	W	50	ASN
25	W	79	GLN
26	X	57	GLN
26	X	107	HIS

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Mol	Chain	Res	Type
26	X	111	GLN
27	Y	43	ASN
27	Y	127	GLN
29	a	44	ASN
31	c	15	ASN
31	c	72	HIS
32	d	79	ASN
33	e	52	GLN
33	e	102	ASN
34	f	56	ASN
36	h	98	HIS
37	i	80	HIS
38	j	76	HIS
43	o	3	ASN
43	o	45	GLN
44	p	92	GLN
46	s	71	ASN
47	t	65	GLN
48	u	22	GLN
49	v	535	GLN
49	v	660	ASN
49	v	705	HIS
49	v	803	ASN
50	w	196	HIS
53	BB	177	GLN
54	CC	235	ASN
54	CC	267	GLN
55	DD	101	GLN
57	FF	79	HIS
57	FF	95	HIS
57	FF	101	HIS
57	FF	118	ASN
57	FF	179	ASN
57	FF	203	ASN
58	GG	177	GLN
59	HH	97	GLN
61	JJ	154	GLN
61	JJ	156	HIS
62	KK	7	ASN
62	KK	28	HIS
62	KK	61	GLN
65	NN	62	GLN

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Mol	Chain	Res	Type
66	OO	32	HIS
66	OO	113	GLN
67	PP	53	GLN
67	PP	114	HIS
67	PP	128	HIS
68	QQ	77	HIS
69	RR	116	ASN
74	WW	15	ASN
74	WW	92	ASN
79	bb	19	HIS
79	bb	26	GLN
80	cc	29	GLN
84	gg	14	HIS
84	gg	296	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3556/3597 (98%)	848 (23%)	64 (1%)
2	7	119/120 (99%)	15 (12%)	0
3	8	149/151 (98%)	26 (17%)	1 (0%)
51	9	1682/1698 (99%)	407 (24%)	30 (1%)
All	All	5506/5566 (98%)	1296 (23%)	95 (1%)

All (1296) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	8	U
1	5	12	A
1	5	13	U
1	5	25	A
1	5	35	U
1	5	36	U
1	5	39	A
1	5	42	A
1	5	43	U
1	5	48	G
1	5	49	U
1	5	56	A
1	5	58	G
1	5	59	A

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Mol	Chain	Res	Type
1	5	64	A
1	5	65	A
1	5	71	C
1	5	72	C
1	5	73	A
1	5	74	G
1	5	76	A
1	5	84	A
1	5	91	G
1	5	98	A
1	5	104	G
1	5	108	A
1	5	109	G
1	5	110	C
1	5	116	G
1	5	119	G
1	5	120	A
1	5	126	C
1	5	134	G
1	5	135	G
1	5	136	C
1	5	142	G
1	5	151	G
1	5	157	U
1	5	159	C
1	5	167	C
1	5	172	C
1	5	173	C
1	5	179	G
1	5	182	G
1	5	195	C
1	5	200	U
1	5	201	C
1	5	202	C
1	5	203	U
1	5	205	C
1	5	209	U
1	5	210	C
1	5	216	C
1	5	218	A
1	5	220	C
1	5	224	U

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Mol	Chain	Res	Type
1	5	233	U
1	5	234	G
1	5	237	B9B
1	5	245	C
1	5	246	G
1	5	250	C
1	5	265	C
1	5	266	C
1	5	267	G
1	5	275	C
1	5	276	C
1	5	280	G
1	5	297	U
1	5	306	A
1	5	309	C
1	5	310	G
1	5	315	G
1	5	316	U
1	5	326	C
1	5	328	A
1	5	334	A
1	5	340	C
1	5	345	C
1	5	350	C
1	5	357	U
1	5	362	A
1	5	363	A
1	5	379	G
1	5	386	A
1	5	387	G
1	5	398	A2M
1	5	406	C
1	5	407	A
1	5	408	A
1	5	410	A
1	5	412	G
1	5	413	G
1	5	414	C
1	5	433	A
1	5	440	U
1	5	449	C
1	5	450	G

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Mol	Chain	Res	Type
1	5	451	C
1	5	452	A
1	5	453	G
1	5	454	U
1	5	455	C
1	5	463	A
1	5	467	U
1	5	468	U
1	5	482	G
1	5	484	U
1	5	485	C
1	5	486	C
1	5	492	U
1	5	493	G
1	5	496	G
1	5	497	G
1	5	498	C
1	5	499	G
1	5	505	G
1	5	506	C
1	5	510	U
1	5	646	G
1	5	666	G
1	5	667	A
1	5	669	C
1	5	685	C
1	5	686	A
1	5	687	U
1	5	688	U
1	5	691	C
1	5	696	C
1	5	697	G
1	5	704	C
1	5	705	G
1	5	708	G
1	5	719	C
1	5	729	2MG
1	5	731	G
1	5	742	G
1	5	744	G
1	5	747	A
1	5	748	G

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Mol	Chain	Res	Type
1	5	749	G
1	5	758	G
1	5	914	U
1	5	916	C
1	5	917	A
1	5	918	G
1	5	925	C
1	5	926	G
1	5	929	A
1	5	931	C
1	5	932	A
1	5	933	G
1	5	934	C
1	5	938	C
1	5	939	G
1	5	941	C
1	5	943	A
1	5	945	U
1	5	956	A
1	5	959	G
1	5	960	A
1	5	961	G
1	5	964	A
1	5	965	G
1	5	966	A
1	5	967	C
1	5	968	C
1	5	969	C
1	5	971(A)	G
1	5	972	C
1	5	973	C
1	5	980	C
1	5	983	U
1	5	1070	G
1	5	1072	C
1	5	1073	G
1	5	1078	A
1	5	1079	C
1	5	1080	C
1	5	1081	C
1	5	1082	C
1	5	1083	U

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Mol	Chain	Res	Type
1	5	1098	G
1	5	1175	A
1	5	1179	U
1	5	1180	C
1	5	1187	G
1	5	1193	C
1	5	1195	G
1	5	1204	C
1	5	1210	C
1	5	1211	G
1	5	1212	G
1	5	1214	C
1	5	1215	C
1	5	1216	C
1	5	1234	G
1	5	1235	G
1	5	1236	C
1	5	1237	C
1	5	1238	A
1	5	1239	C
1	5	1272	C
1	5	1273	G
1	5	1275	G
1	5	1276	C
1	5	1279	A
1	5	1284	G
1	5	1285	U
1	5	1287	G
1	5	1292	C
1	5	1293	G
1	5	1295	U
1	5	1296	G
1	5	1301	C
1	5	1303	A
1	5	1304	C
1	5	1314	C
1	5	1320	U
1	5	1326	A2M
1	5	1330	A
1	5	1337	A
1	5	1348	P4U
1	5	1354	A

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Mol	Chain	Res	Type
1	5	1358	G
1	5	1359	G
1	5	1370	G
1	5	1371	A
1	5	1372	A
1	5	1377	G
1	5	1378	C
1	5	1380	G
1	5	1381	U
1	5	1387	A
1	5	1394	G
1	5	1397	A
1	5	1398	A
1	5	1406(C)	G
1	5	1411(C)	C
1	5	1412	G
1	5	1415	G
1	5	1419	G
1	5	1421	G
1	5	1429	C
1	5	1436	C
1	5	1437	C
1	5	1438	U
1	5	1440	U
1	5	1441	C
1	5	1443	A
1	5	1445	U
1	5	1446	C
1	5	1456	B8Q
1	5	1457	G
1	5	1458	C
1	5	1465	G
1	5	1475	G
1	5	1482	G
1	5	1483	C
1	5	1497	A
1	5	1498	G
1	5	1502	G
1	5	1516	G
1	5	1518	A
1	5	1523	A
1	5	1534	A2M

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Mol	Chain	Res	Type
1	5	1547	A
1	5	1563	A
1	5	1566	C
1	5	1578	U
1	5	1582	PSU
1	5	1591	U
1	5	1596	U
1	5	1602	U
1	5	1612	G
1	5	1613	A
1	5	1624	G
1	5	1625	OMG
1	5	1626	G
1	5	1627	G
1	5	1631	A
1	5	1633	G
1	5	1634	A
1	5	1638	A
1	5	1640	C
1	5	1641	G
1	5	1649	U
1	5	1650	A
1	5	1654	G
1	5	1661	C
1	5	1671	U
1	5	1676	C
1	5	1677	PSU
1	5	1678	C
1	5	1679	A
1	5	1691	G
1	5	1734	G
1	5	1741	G
1	5	1742	A
1	5	1750	G
1	5	1751	A
1	5	1755	C
1	5	1756	U
1	5	1757	U
1	5	1764	G
1	5	1768	C
1	5	1772	C
1	5	1773	U

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Mol	Chain	Res	Type
1	5	1776	A
1	5	1781	U
1	5	1787	A
1	5	1797	E7G
1	5	1804	A
1	5	1805	A
1	5	1806	G
1	5	1815	G
1	5	1819	G
1	5	1821	G
1	5	1828	C
1	5	1833	G
1	5	1834	U
1	5	1835	G
1	5	1836	G
1	5	1837	A
1	5	1840	G
1	5	1842	G
1	5	1843	A
1	5	1855	G
1	5	1869	G
1	5	1873	A
1	5	1881	C
1	5	1888	A
1	5	1897	A
1	5	1898	C
1	5	1915	C
1	5	1916	G
1	5	1918	U
1	5	1920	C
1	5	1921	C
1	5	1922	G
1	5	1928	C
1	5	1930	U
1	5	1931	C
1	5	1932	A
1	5	1938	C
1	5	1940	G
1	5	1945	G
1	5	1951	G
1	5	1957	U
1	5	1958	A

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Mol	Chain	Res	Type
1	5	1961	G
1	5	1962	A
1	5	1964	A
1	5	1967	A
1	5	1971	U
1	5	1974	U
1	5	1976	G
1	5	1978	C
1	5	1979	A
1	5	1980	U
1	5	1981	G
1	5	1983	A
1	5	1984	A
1	5	1986	U
1	5	1987	C
1	5	1991	A
1	5	1992	U
1	5	1993	C
1	5	1997	U
1	5	2001	G
1	5	2002	A
1	5	2003	G
1	5	2004	U
1	5	2007	G
1	5	2008	U
1	5	2009	A
1	5	2011	C
1	5	2021	G
1	5	2025	A
1	5	2026	A
1	5	2029	A
1	5	2033	A
1	5	2043	A
1	5	2046	G
1	5	2047	A
1	5	2048	U
1	5	2052	G
1	5	2055	G
1	5	2056	G
1	5	2064	G
1	5	2069	A
1	5	2070	U

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Mol	Chain	Res	Type
1	5	2084	U
1	5	2090	U
1	5	2092	G
1	5	2093	G
1	5	2094	C
1	5	2097	A
1	5	2098	G
1	5	2100	G
1	5	2101	A
1	5	2102	G
1	5	2104	A
1	5	2105	A
1	5	2106	G
1	5	2108	G
1	5	2259	G
1	5	2260	C
1	5	2261	G
1	5	2267	U
1	5	2268	A
1	5	2269	C
1	5	2270	G
1	5	2275	G
1	5	2289	C
1	5	2300	A
1	5	2301	G
1	5	2306	G
1	5	2313	A
1	5	2314	G
1	5	2316	G
1	5	2332	A
1	5	2333	G
1	5	2335	C
1	5	2347	A
1	5	2348	G
1	5	2351	C
1	5	2357	G
1	5	2360	A
1	5	2364	OMG
1	5	2380	B8W
1	5	2395	A
1	5	2396	A
1	5	2408	U

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Mol	Chain	Res	Type
1	5	2410	C
1	5	2417	A
1	5	2422	OMC
1	5	2424	OMG
1	5	2425	U
1	5	2433	G
1	5	2434	G
1	5	2441	C
1	5	2447	U
1	5	2450	G
1	5	2471	G
1	5	2474	G
1	5	2475	G
1	5	2488	C
1	5	2489	C
1	5	2490	U
1	5	2491	C
1	5	2503	G
1	5	2504	C
1	5	2505	C
1	5	2506	G
1	5	2513	A
1	5	2529	A
1	5	2530	U
1	5	2537	A
1	5	2544	G
1	5	2546	G
1	5	2547	G
1	5	2553	A
1	5	2554	U
1	5	2560	C
1	5	2566	G
1	5	2568	C
1	5	2571	C
1	5	2575	U
1	5	2583	C
1	5	2586	G
1	5	2587	A
1	5	2588	C
1	5	2589	C
1	5	2601	A
1	5	2611	A

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Mol	Chain	Res	Type
1	5	2616	C
1	5	2618	G
1	5	2620	G
1	5	2628	U
1	5	2638	G
1	5	2639	U
1	5	2649	G
1	5	2653	C
1	5	2659	A
1	5	2661	U
1	5	2662	G
1	5	2663	G
1	5	2669	C
1	5	2670	C
1	5	2676	A
1	5	2680	G
1	5	2686	G
1	5	2687	U
1	5	2695	A
1	5	2696	A
1	5	2700	G
1	5	2707	U
1	5	2708	U
1	5	2709	C
1	5	2710	C
1	5	2711	G
1	5	2714	G
1	5	2715	G
1	5	2716	C
1	5	2721	G
1	5	2724	G
1	5	2725	A
1	5	2726	G
1	5	2740	U
1	5	2743	A
1	5	2744	A
1	5	2754	B9B
1	5	2764	A
1	5	2769	U
1	5	2773	OMG
1	5	2787	A
1	5	2788	U

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Mol	Chain	Res	Type
1	5	2790	U
1	5	2794	C
1	5	2798	A
1	5	2803	U
1	5	2826	U
1	5	2827	G
1	5	2829	U
1	5	2842	G
1	5	2855	G
1	5	2856	C
1	5	2867	C
1	5	2869	U
1	5	2884	G
1	5	3598	C
1	5	3605	C
1	5	3606	U
1	5	3616	U
1	5	3620	G
1	5	3625	G
1	5	3626	G
1	5	3630	A
1	5	3635	A
1	5	3649	A
1	5	3650	C
1	5	3658	C
1	5	3662	A
1	5	3663	A
1	5	3664	G
1	5	3673	C
1	5	3674	G
1	5	3691	G
1	5	3692	A
1	5	3696	C
1	5	3698	G
1	5	3711	A
1	5	3712	A
1	5	3714	G
1	5	3729	PSU
1	5	3740	G
1	5	3743	G
1	5	3753	G
1	5	3759	A

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Mol	Chain	Res	Type
1	5	3760	A
1	5	3761	C
1	5	3762	B8H
1	5	3764	PSU
1	5	3765	G
1	5	3773	U
1	5	3774	A
1	5	3776	G
1	5	3777	G
1	5	3783	A
1	5	3784	A
1	5	3786	U
1	5	3787	G
1	5	3792	OMG
1	5	3798	U
1	5	3799	A
1	5	3810	C
1	5	3811	G
1	5	3812	C
1	5	3813	A
1	5	3814	U
1	5	3817	A
1	5	3819	G
1	5	3822	U
1	5	3838	U
1	5	3839	G
1	5	3840	U
1	5	3851	U
1	5	3867	A2M
1	5	3868	G
1	5	3876	A
1	5	3877	A
1	5	3878	C
1	5	3879	G
1	5	3880	P7G
1	5	3889	G
1	5	3892	U
1	5	3897	B8K
1	5	3898	G
1	5	3899	BGH
1	5	3901	A
1	5	3904	G

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Mol	Chain	Res	Type
1	5	3905	A
1	5	3906	A
1	5	3907	G
1	5	3908	A
1	5	3915	U
1	5	3916	G
1	5	3927	U
1	5	3938	G
1	5	3939	G
1	5	3941	G
1	5	3955	A
1	5	3957	U
1	5	3962	A
1	5	3970	G
1	5	3972	A
1	5	3973	G
1	5	3974	G
1	5	3975	C
1	5	3976	C
1	5	4042	G
1	5	4047	A
1	5	4049	U
1	5	4050	A
1	5	4051	C
1	5	4053	A
1	5	4054	C
1	5	4055	U
1	5	4066	U
1	5	4073	A
1	5	4076	G
1	5	4085	A
1	5	4086	G
1	5	4097	G
1	5	4100	C
1	5	4116	C
1	5	4119	C
1	5	4120	U
1	5	4122	G
1	5	4125	C
1	5	4127	A
1	5	4151	G
1	5	4158	C

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Mol	Chain	Res	Type
1	5	4166	G
1	5	4170	A
1	5	4173	G
1	5	4183	G
1	5	4184	G
1	5	4191	G
1	5	4194	I4U
1	5	4203	A
1	5	4212	A
1	5	4225	G
1	5	4229	U
1	5	4233	A
1	5	4243	C
1	5	4249	G
1	5	4251	A
1	5	4254	G
1	5	4255	A
1	5	4256	A
1	5	4265	U
1	5	4266	G
1	5	4268	A
1	5	4271	A
1	5	4273	A
1	5	4281	A
1	5	4282	A
1	5	4291	G
1	5	4293	PSU
1	5	4304	A
1	5	4305	G
1	5	4306	OMU
1	5	4308	C
1	5	4313	A
1	5	4314	C
1	5	4317	A
1	5	4318	C
1	5	4319	C
1	5	4326	G
1	5	4329	G
1	5	4330	G
1	5	4332	C
1	5	4348	A
1	5	4349	C

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Mol	Chain	Res	Type
1	5	4354	U
1	5	4355	E6G
1	5	4368	G
1	5	4371	MHG
1	5	4373	G
1	5	4377	G
1	5	4378	A
1	5	4380	A
1	5	4387	C
1	5	4393	G
1	5	4394	A
1	5	4395	U
1	5	4396	A
1	5	4398	C
1	5	4401	G
1	5	4413	C
1	5	4415	1MA
1	5	4419	U
1	5	4420	U
1	5	4422	A
1	5	4426	C
1	5	4433	G
1	5	4440	G
1	5	4448	G
1	5	4449	A
1	5	4450	PSU
1	5	4464	A
1	5	4475	G
1	5	4476	C
1	5	4495	G
1	5	4500	PSU
1	5	4502	C
1	5	4510	A
1	5	4511	A
1	5	4512	U
1	5	4513	A
1	5	4515	G
1	5	4518	A
1	5	4520	G
1	5	4522	G
1	5	4523	A2M
1	5	4524	G

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Mol	Chain	Res	Type
1	5	4530	UR3
1	5	4548	A
1	5	4549	G
1	5	4560	C
1	5	4567	G
1	5	4570	G
1	5	4573	G
1	5	4574	U
1	5	4575	G
1	5	4582	C
1	5	4584	A
1	5	4586	G
1	5	4587	G
1	5	4589	A
1	5	4590	A
1	5	4599	A
1	5	4606	G
1	5	4627	U
1	5	4629	U
1	5	4635	A
1	5	4636	PSU
1	5	4637	OMG
1	5	4639	G
1	5	4652	G
1	5	4656	A
1	5	4657	U
1	5	4661	G
1	5	4664	A
1	5	4670	C
1	5	4672	A
1	5	4677	U
1	5	4687	A
1	5	4690	B8K
1	5	4693	C
1	5	4694	G
1	5	4695	C
1	5	4700	A
1	5	4709	U
1	5	4719	G
1	5	4720	C
1	5	4738	C
1	5	4750	G

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Mol	Chain	Res	Type
1	5	4751	G
1	5	4754	G
1	5	4756	C
1	5	4757	C
1	5	4759	C
1	5	4761	G
1	5	4765	G
1	5	4771	C
1	5	4772	C
1	5	4868	G
1	5	4870	OMG
1	5	4872	2MG
1	5	4873	G
1	5	4875	G
1	5	4877	G
1	5	4881	U
1	5	4882	U
1	5	4883	C
1	5	4885	U
1	5	4887	C
1	5	4895	C
1	5	4902	C
1	5	4904	G
1	5	4906	C
1	5	4910	A
1	5	4912	G
1	5	4914	G
1	5	4915	G
1	5	4918	C
1	5	4919	G
1	5	4921	C
1	5	4922	C
1	5	4923	U
1	5	4925	U
1	5	4926	C
1	5	4927	G
1	5	4928	C
1	5	4929	C
1	5	4931	G
1	5	4934	A
1	5	4937	C
1	5	4938	A

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Mol	Chain	Res	Type
1	5	4940	C
1	5	4944	C
1	5	4948	C
1	5	4949	G
1	5	4950	U
1	5	4951	G
1	5	4956	A
1	5	4958	C
1	5	4960	G
1	5	4961	G
1	5	4964	C
1	5	4965	U
1	5	4966	A
1	5	4967	A
1	5	4975	G
1	5	4976	U
1	5	4985	U
1	5	4988	U
1	5	4990	C
1	5	4993	G
1	5	4999	G
1	5	5006	U
1	5	5014	A
1	5	5017	G
1	5	5022	U
1	5	5040	U
1	5	5041	G
1	5	5047	C
1	5	5050	C
1	5	5052	C
1	5	5053	U
1	5	5054	C
1	5	5058	A
1	5	5061	A
1	5	5062	G
1	5	5069	U
2	7	7	G
2	7	13	A
2	7	22	A
2	7	25	G
2	7	29	C
2	7	33	U

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Mol	Chain	Res	Type
2	7	53	U
2	7	54	A
2	7	64	G
2	7	97	G
2	7	100	A
2	7	102	U
2	7	110	G
2	7	111	C
2	7	120	U
3	8	2	G
3	8	32	C
3	8	34	U
3	8	35	C
3	8	38	U
3	8	39	G
3	8	49	G
3	8	59	A
3	8	62	A
3	8	63	U
3	8	75	G
3	8	87	G
3	8	99	U
3	8	103	A
3	8	105	C
3	8	109	C
3	8	110	U
3	8	111	U
3	8	114	G
3	8	123	U
3	8	125	C
3	8	126	C
3	8	127	U
3	8	137	A
3	8	147	G
3	8	153	C
51	9	2	A
51	9	3	C
51	9	4	C
51	9	17	C
51	9	23	G
51	9	25	A
51	9	26	U

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Mol	Chain	Res	Type
51	9	33	G
51	9	37	C
51	9	41	G
51	9	42	A
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	60	A
51	9	65	C
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	73	C
51	9	74	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	103	A
51	9	104	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	129	C
51	9	130	G
51	9	141	A
51	9	143	U
51	9	146	G
51	9	147	A
51	9	155	G
51	9	158	A
51	9	162	C
51	9	163	U
51	9	167	G
51	9	168	C

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Mol	Chain	Res	Type
51	9	180	G
51	9	183	G
51	9	184	G
51	9	187	G
51	9	188	C
51	9	189	U
51	9	190	G
51	9	192	C
51	9	202	G
51	9	206	G
51	9	215	G
51	9	302	A
51	9	307	G
51	9	308	G
51	9	309	G
51	9	312	G
51	9	314	U
51	9	318	A
51	9	319	C
51	9	332	G
51	9	335	G
51	9	339	A
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	369	C
51	9	370	G
51	9	376	A
51	9	380	G
51	9	381	C
51	9	385	G
51	9	386	C
51	9	398	A
51	9	400	C
51	9	408	A
51	9	409	C
51	9	418	A
51	9	420	G
51	9	421	G

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Mol	Chain	Res	Type
51	9	426	A
51	9	428	U
51	9	435	A
51	9	438	G
51	9	448	A
51	9	450	C
51	9	455	A
51	9	456	C
51	9	464	A
51	9	465	A
51	9	466	G
51	9	471	G
51	9	472	C
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	492	C
51	9	496	C
51	9	517	C
51	9	530	U
51	9	531	A
51	9	532	C
51	9	533	A
51	9	542	U
51	9	544	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	554	A
51	9	555	A
51	9	556	U
51	9	559	G
51	9	560	A
51	9	563	G
51	9	564	A
51	9	568	C
51	9	570	C
51	9	575	A
51	9	576	A

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Mol	Chain	Res	Type
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	599	A
51	9	600	G
51	9	601	G
51	9	603	C
51	9	606	G
51	9	608	C
51	9	609	U
51	9	611	G
51	9	614	C
51	9	615	C
51	9	617	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	631	U
51	9	632	C
51	9	633	C
51	9	637	U
51	9	643	A
51	9	644	G
51	9	655	A
51	9	660	C
51	9	663	C
51	9	668	A
51	9	669	A
51	9	671	A
51	9	672	A
51	9	673	G
51	9	684	G
51	9	688	U
51	9	689	U
51	9	690	G
51	9	752	G
51	9	753	C
51	9	754	G

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Mol	Chain	Res	Type
51	9	798	G
51	9	811	A
51	9	821	G
51	9	822	U
51	9	827	A
51	9	830	A
51	9	834	C
51	9	844	U
51	9	847	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	874	G
51	9	875	A
51	9	876	C
51	9	878	G
51	9	879	C
51	9	881	G
51	9	887	U
51	9	888	U
51	9	889	U
51	9	890	U
51	9	892	U
51	9	907	G
51	9	909	G
51	9	913	A
51	9	914	U
51	9	920	A
51	9	933	G
51	9	934	G
51	9	971	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1002	U
51	9	1017	U
51	9	1023	A
51	9	1026	C
51	9	1040	G
51	9	1041	G
51	9	1045	U

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Mol	Chain	Res	Type
51	9	1050	A
51	9	1060	A
51	9	1062	A
51	9	1067	C
51	9	1083	A
51	9	1084	A
51	9	1085	C
51	9	1086	G
51	9	1099	G
51	9	1100	A
51	9	1109	C
51	9	1114	U
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1121	G
51	9	1123	C
51	9	1126	G
51	9	1131	G
51	9	1133	A
51	9	1138	C
51	9	1139	C
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1155	U
51	9	1161	U
51	9	1170	A
51	9	1171	G
51	9	1195	A
51	9	1207	G
51	9	1208	A
51	9	1215	C
51	9	1221	G
51	9	1224	G
51	9	1242	U
51	9	1243	PSU
51	9	1248	B8N
51	9	1250	A
51	9	1251	A

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Mol	Chain	Res	Type
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1259	A
51	9	1264	C
51	9	1265	A
51	9	1274	G
51	9	1275	G
51	9	1281	G
51	9	1282	A
51	9	1283	C
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1288	U
51	9	1289	U
51	9	1299	A
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1307	U
51	9	1308	U
51	9	1309	C
51	9	1310	U
51	9	1312	G
51	9	1313	A
51	9	1314	U
51	9	1318	G
51	9	1327	G
51	9	1333	U
51	9	1342	U
51	9	1348	G
51	9	1363	C
51	9	1364	U
51	9	1371	U
51	9	1372	U
51	9	1376	A
51	9	1378	A
51	9	1382	A
51	9	1393	G
51	9	1395	C

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Mol	Chain	Res	Type
51	9	1396	A
51	9	1397	U
51	9	1401	A
51	9	1402	A
51	9	1406	G
51	9	1428	G
51	9	1431	G
51	9	1449	G
51	9	1454	A
51	9	1462	U
51	9	1463	U
51	9	1464	C
51	9	1466	G
51	9	1474	A
51	9	1475	G
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1480	A
51	9	1483	A
51	9	1484	A
51	9	1485	U
51	9	1486	A
51	9	1488	C
51	9	1489	A
51	9	1490	G
51	9	1495	G
51	9	1497	G
51	9	1498	A
51	9	1507	G
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1531	A
51	9	1533	A
51	9	1535	U
51	9	1536	G
51	9	1544	C
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1554	C

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Mol	Chain	Res	Type
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G
51	9	1574	C
51	9	1580	A
51	9	1584	G
51	9	1585	U
51	9	1586	U
51	9	1587	G
51	9	1588	A
51	9	1598	G
51	9	1601	A
51	9	1604	G
51	9	1606	G
51	9	1621	U
51	9	1623	A
51	9	1624	U
51	9	1634	A
51	9	1637	A
51	9	1638	G
51	9	1646	C
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1680	G
51	9	1683	C
51	9	1695	A
51	9	1698	C
51	9	1699	A
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1726	G
51	9	1732	G
51	9	1734	G
51	9	1744	G
51	9	1748	G
51	9	1753	C
51	9	1783	C

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Mol	Chain	Res	Type
51	9	1785	C
51	9	1799	G
51	9	1819	A
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1837	G
51	9	1838	U
51	9	1849	G
51	9	1851	A
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1864	U
51	9	1865	C
51	9	1866	A
51	9	1867	U
51	9	1869	A

All (95) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	12	A
1	5	47	A
1	5	48	G
1	5	125	C
1	5	134	G
1	5	217	C
1	5	233	U
1	5	245	C
1	5	265	C
1	5	266	C
1	5	275	C
1	5	385	A
1	5	406	C
1	5	449	C
1	5	485	C
1	5	492	U

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Mol	Chain	Res	Type
1	5	504	G
1	5	684	G
1	5	930	G
1	5	959	G
1	5	1072	C
1	5	1174	G
1	5	1211	G
1	5	1236	C
1	5	1238	A
1	5	1291	G
1	5	1329	G
1	5	1370	G
1	5	1406(B)	C
1	5	1440	U
1	5	1445	U
1	5	1625	OMG
1	5	1633	G
1	5	1804	A
1	5	1818	G
1	5	1979	A
1	5	2046	G
1	5	2089	G
1	5	2266	C
1	5	2474	G
1	5	2502	A
1	5	2546	G
1	5	2587	A
1	5	2661	U
1	5	2695	A
1	5	3625	G
1	5	3697	U
1	5	3760	A
1	5	3876	A
1	5	3888	G
1	5	3904	G
1	5	3954	A
1	5	4053	A
1	5	4065	G
1	5	4119	C
1	5	4232	U
1	5	4254	G
1	5	4448	G

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Mol	Chain	Res	Type
1	5	4699	U
1	5	4719	G
1	5	4884	G
1	5	4925	U
1	5	4936	G
1	5	4947	U
3	8	124	U
51	9	110	U
51	9	182	C
51	9	434	G
51	9	465	A
51	9	532	C
51	9	553	U
51	9	555	A
51	9	599	A
51	9	606	G
51	9	642	U
51	9	688	U
51	9	752	G
51	9	870	A
51	9	872	A
51	9	874	G
51	9	1137	U
51	9	1207	G
51	9	1253	A
51	9	1264	C
51	9	1363	C
51	9	1394	G
51	9	1395	C
51	9	1483	A
51	9	1484	A
51	9	1489	A
51	9	1520	G
51	9	1637	A
51	9	1664	A
51	9	1665	G
51	9	1835	A

5.4 Non-standard residues in protein, DNA, RNA chains

110 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
51	B8N	9	1248	51	25,29,30	3.08	8 (32%)	28,42,45	2.06	7 (25%)
51	PSU	9	1243	51	18,21,22	1.19	1 (5%)	21,30,33	1.44	4 (19%)
1	OMG	5	1883	1	23,26,27	2.42	8 (34%)	32,38,41	2.06	7 (21%)
1	PSU	5	1677	1	18,21,22	1.11	3 (16%)	21,30,33	2.03	6 (28%)
1	2MG	5	4872	1	23,26,27	2.82	9 (39%)	33,38,41	3.35	16 (48%)
1	I4U	5	4194	1	20,24,25	5.00	14 (70%)	27,34,37	1.90	3 (11%)
6	MLZ	C	333	6	8,9,10	0.84	0	4,9,11	0.72	0
1	5MC	5	4447	1	19,22,23	3.81	8 (42%)	26,32,35	1.15	2 (7%)
1	B8T	5	4671	1	19,22,23	3.04	8 (42%)	25,31,34	0.93	1 (4%)
1	A2M	5	3867	1	22,25,26	3.92	12 (54%)	30,36,39	2.30	9 (30%)
1	B8W	5	4529	85,1	23,26,27	3.38	12 (52%)	33,38,41	5.77	22 (66%)
1	PSU	5	4293	1	18,21,22	1.08	2 (11%)	21,30,33	1.99	4 (19%)
1	A2M	5	1524	1	22,25,26	3.89	11 (50%)	30,36,39	2.52	11 (36%)
1	OMG	5	4196	1	23,26,27	2.38	9 (39%)	32,38,41	1.97	8 (25%)
1	A2M	5	4523	85,1	22,25,26	3.89	12 (54%)	30,36,39	2.34	12 (40%)
1	PSU	5	4403	1	18,21,22	1.02	1 (5%)	21,30,33	1.87	5 (23%)
1	OMC	5	2861	1	19,22,23	2.90	7 (36%)	25,31,34	0.92	1 (4%)
1	PSU	5	3729	1	18,21,22	1.06	1 (5%)	21,30,33	1.85	4 (19%)
1	OMG	5	1522	1	23,26,27	2.40	9 (39%)	32,38,41	1.98	8 (25%)
1	B9B	5	1574	1	25,28,29	3.72	9 (36%)	35,40,43	2.39	16 (45%)
51	A2M	9	1678	51	22,25,26	3.98	12 (54%)	30,36,39	2.39	11 (36%)
1	OMG	5	1625	85,1	23,26,27	2.40	9 (39%)	32,38,41	1.93	8 (25%)
1	PSU	5	4500	1	18,21,22	1.03	2 (11%)	21,30,33	2.05	4 (19%)
1	PSU	5	3715	1	18,21,22	1.01	1 (5%)	21,30,33	1.77	4 (19%)
1	UR3	5	4597	1	19,22,23	2.65	7 (36%)	26,32,35	1.59	4 (15%)
1	PSU	5	3764	1	18,21,22	1.07	1 (5%)	21,30,33	1.77	4 (19%)
1	B8H	5	4296	1	19,22,23	6.85	6 (31%)	21,32,35	2.55	5 (23%)
1	PSU	5	4636	1	18,21,22	1.07	2 (11%)	21,30,33	2.08	5 (23%)
1	OMG	5	1316	1	23,26,27	2.40	9 (39%)	32,38,41	1.95	8 (25%)
1	B8W	5	2380	1	23,26,27	3.34	12 (52%)	33,38,41	5.62	19 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	5	2508	1	18,21,22	1.00	1 (5%)	21,30,33	1.74	3 (14%)
1	B9H	5	2786	1	21,25,26	3.15	3 (14%)	22,35,38	2.07	4 (18%)
51	B8Q	9	1219	51	18,22,23	2.95	4 (22%)	21,32,35	2.81	7 (33%)
1	5MC	5	4335	1	19,22,23	3.84	8 (42%)	26,32,35	1.24	3 (11%)
1	A2M	5	1326	1	22,25,26	3.89	12 (54%)	30,36,39	2.30	9 (30%)
1	A2M	5	1871	85,1	22,25,26	3.93	12 (54%)	30,36,39	2.44	11 (36%)
1	A2M	5	4571	1	22,25,26	3.95	11 (50%)	30,36,39	2.38	11 (36%)
1	B8K	5	4690	1	24,28,29	4.93	17 (70%)	29,42,45	2.72	12 (41%)
1	E6G	5	4355	1	24,27,28	3.59	11 (45%)	34,39,42	2.44	13 (38%)
1	OMG	5	4870	1	23,26,27	2.38	8 (34%)	32,38,41	1.89	8 (25%)
1	PSU	5	1683	1	18,21,22	1.13	2 (11%)	21,30,33	1.93	4 (19%)
1	P4U	5	1348	85,1	21,24,25	3.28	7 (33%)	28,33,36	1.98	4 (14%)
1	OMG	5	3792	1	23,26,27	2.43	7 (30%)	32,38,41	2.08	9 (28%)
1	OMU	5	4306	1	19,22,23	2.85	8 (42%)	25,31,34	1.87	5 (20%)
1	7MG	5	1605	1	23,26,27	3.25	10 (43%)	27,39,42	2.17	10 (37%)
1	OMC	5	3701	85,1	19,22,23	2.81	7 (36%)	25,31,34	0.75	0
1	OMC	5	4536	1	19,22,23	2.86	7 (36%)	25,31,34	1.02	1 (4%)
1	PSU	5	1582	1	18,21,22	1.17	3 (16%)	21,30,33	1.83	4 (19%)
1	I4U	5	1659	1	20,24,25	4.97	13 (65%)	27,34,37	2.07	3 (11%)
1	OMG	5	2364	1	23,26,27	2.39	9 (39%)	32,38,41	1.88	7 (21%)
1	UR3	5	1866	1	19,22,23	2.57	6 (31%)	26,32,35	1.56	5 (19%)
1	OMG	5	4623	1	23,26,27	2.41	9 (39%)	32,38,41	1.92	8 (25%)
1	A2M	5	1534	85,1	22,25,26	3.98	13 (59%)	30,36,39	2.40	11 (36%)
1	OMC	5	2365	1	19,22,23	2.86	7 (36%)	25,31,34	0.68	0
1	B8W	5	4129	1	23,26,27	3.34	11 (47%)	33,38,41	5.54	20 (60%)
1	PSU	5	4450	85,1	18,21,22	1.08	2 (11%)	21,30,33	2.07	5 (23%)
1	7MG	5	2522	1	23,26,27	3.30	10 (43%)	27,39,42	2.12	10 (37%)
1	MHG	5	4371	1	29,32,33	3.65	11 (37%)	34,46,49	2.46	12 (35%)
1	A2M	5	2401	85,1	22,25,26	3.93	11 (50%)	30,36,39	2.43	9 (30%)
3	OMU	8	14	1,3	19,22,23	2.83	7 (36%)	25,31,34	2.10	7 (28%)
1	5MC	5	3782	1	19,22,23	3.80	8 (42%)	26,32,35	1.10	1 (3%)
1	P7G	5	3880	1	24,28,29	3.52	10 (41%)	25,41,44	1.36	2 (8%)
1	B8W	5	4185	1	23,26,27	3.35	11 (47%)	33,38,41	5.49	23 (69%)
1	B8Q	5	1456	1	18,22,23	2.71	5 (27%)	21,32,35	1.92	5 (23%)
1	E7G	5	2297	1	24,27,28	3.14	11 (45%)	28,40,43	2.28	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	1MA	5	4415	1	21,25,26	2.68	5 (23%)	30,37,40	1.77	7 (23%)
1	OMC	5	2804	1	19,22,23	2.84	7 (36%)	25,31,34	0.82	0
1	OMC	5	3869	1	19,22,23	2.83	7 (36%)	25,31,34	0.72	0
1	A2M	5	3825	1	22,25,26	3.96	10 (45%)	30,36,39	2.36	11 (36%)
1	E7G	5	1797	1	24,27,28	3.22	11 (45%)	28,40,43	2.31	10 (35%)
1	B8H	5	1860	1	19,22,23	6.84	6 (31%)	21,32,35	2.46	5 (23%)
1	OMC	5	3887	1	19,22,23	2.84	7 (36%)	25,31,34	0.91	1 (4%)
1	BGH	5	3899	85,1	25,29,30	4.19	15 (60%)	30,43,46	2.62	13 (43%)
1	PSU	5	4628	1	18,21,22	1.14	3 (16%)	21,30,33	2.15	5 (23%)
1	B9B	5	2754	85,1	25,28,29	3.80	9 (36%)	35,40,43	2.39	11 (31%)
1	P7G	5	1909	1	24,28,29	3.74	11 (45%)	25,41,44	1.47	2 (8%)
1	B8T	5	4483	1	19,22,23	3.08	8 (42%)	25,31,34	1.03	2 (8%)
1	OMG	5	2050	1	23,26,27	2.40	9 (39%)	32,38,41	1.85	8 (25%)
1	2MG	5	729	1	23,26,27	2.86	7 (30%)	33,38,41	2.27	7 (21%)
1	PSU	5	4531	1	18,21,22	1.06	1 (5%)	21,30,33	1.99	5 (23%)
1	A2M	5	2363	85,1	22,25,26	3.95	10 (45%)	30,36,39	2.42	11 (36%)
1	OMC	5	3909	1	19,22,23	2.86	7 (36%)	25,31,34	0.74	0
1	B9B	5	237	1	25,28,29	3.78	9 (36%)	35,40,43	2.54	14 (40%)
1	OMG	5	4494	1	23,26,27	2.40	8 (34%)	32,38,41	1.90	9 (28%)
41	MLZ	m	72	41	8,9,10	0.74	0	4,9,11	0.78	0
1	OMG	5	373	1	23,26,27	2.41	9 (39%)	32,38,41	1.95	9 (28%)
49	DDE	v	715	49	18,20,21	1.01	1 (5%)	17,28,30	0.92	1 (5%)
1	7MG	5	4550	1	23,26,27	3.28	10 (43%)	27,39,42	2.10	10 (37%)
1	1MA	5	1322	85,1	21,25,26	2.55	6 (28%)	30,37,40	1.80	6 (20%)
1	OMG	5	4370	1	23,26,27	2.44	9 (39%)	32,38,41	1.85	7 (21%)
1	OMG	5	2424	1	23,26,27	2.45	9 (39%)	32,38,41	1.85	7 (21%)
1	PSU	5	4442	1	18,21,22	1.10	2 (11%)	21,30,33	1.98	4 (19%)
51	4AC	9	1337	51	21,24,25	3.15	10 (47%)	28,34,37	1.17	4 (14%)
1	6MZ	5	4220	1	22,25,26	2.85	6 (27%)	29,36,39	4.12	12 (41%)
1	OMG	5	4637	1	23,26,27	2.35	9 (39%)	32,38,41	1.87	8 (25%)
1	OMU	5	4620	1	19,22,23	2.73	7 (36%)	25,31,34	1.81	5 (20%)
1	5MU	5	4083	1	19,22,23	4.82	7 (36%)	27,32,35	3.59	10 (37%)
1	A2M	5	3785	1	22,25,26	3.84	14 (63%)	30,36,39	2.50	12 (40%)
1	UR3	5	4530	1	19,22,23	2.68	7 (36%)	26,32,35	1.57	4 (15%)
1	B8K	5	3897	1	24,28,29	4.71	17 (70%)	29,42,45	2.69	12 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	M7A	5	4564	1	19,25,26	1.61	2 (10%)	25,37,40	4.07	8 (32%)
1	OMC	5	2422	85,1	19,22,23	2.93	7 (36%)	25,31,34	0.95	2 (8%)
1	B8H	5	3762	1	19,22,23	6.84	6 (31%)	21,32,35	2.54	5 (23%)
1	A2M	5	398	1	22,25,26	3.92	11 (50%)	30,36,39	2.30	9 (30%)
1	B8W	5	4472	1	23,26,27	3.39	12 (52%)	33,38,41	5.52	20 (60%)
51	5MC	9	1374	51	19,22,23	3.84	8 (42%)	26,32,35	1.10	2 (7%)
1	A2M	5	3723	1	22,25,26	3.92	11 (50%)	30,36,39	2.32	9 (30%)
1	A2M	5	3718	1	22,25,26	3.94	13 (59%)	30,36,39	2.14	9 (30%)
1	OMG	5	2773	1	23,26,27	2.43	8 (34%)	32,38,41	1.97	8 (25%)
1	2MG	5	1517	1	23,26,27	2.90	7 (30%)	33,38,41	2.66	10 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	B8N	9	1248	51	-	3/16/34/35	0/2/2/2
51	PSU	9	1243	51	-	2/7/25/26	0/2/2/2
1	OMG	5	1883	1	-	0/9/27/28	0/3/3/3
1	PSU	5	1677	1	-	0/7/25/26	0/2/2/2
1	2MG	5	4872	1	-	2/9/27/28	0/3/3/3
1	I4U	5	4194	1	-	3/9/29/30	0/2/2/2
6	MLZ	C	333	6	-	2/7/8/10	-
1	5MC	5	4447	1	-	4/7/25/26	0/2/2/2
1	B8T	5	4671	1	-	0/7/27/28	0/2/2/2
1	A2M	5	3867	1	-	2/9/27/28	0/3/3/3
1	B8W	5	4529	85,1	-	2/9/27/28	0/3/3/3
1	PSU	5	4293	1	-	0/7/25/26	0/2/2/2
1	A2M	5	1524	1	-	1/9/27/28	0/3/3/3
1	OMG	5	4196	1	-	0/9/27/28	0/3/3/3
1	A2M	5	4523	85,1	-	2/9/27/28	0/3/3/3
1	PSU	5	4403	1	-	2/7/25/26	0/2/2/2
1	OMC	5	2861	1	-	0/9/27/28	0/2/2/2
1	PSU	5	3729	1	-	2/7/25/26	0/2/2/2
1	OMG	5	1522	1	-	0/9/27/28	0/3/3/3
1	B9B	5	1574	1	-	2/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	A2M	9	1678	51	-	0/9/27/28	0/3/3/3
1	OMG	5	1625	85,1	-	3/9/27/28	0/3/3/3
1	PSU	5	4500	1	-	4/7/25/26	0/2/2/2
1	PSU	5	3715	1	-	0/7/25/26	0/2/2/2
1	UR3	5	4597	1	-	0/7/25/26	0/2/2/2
1	PSU	5	3764	1	-	1/7/25/26	0/2/2/2
1	B8H	5	4296	1	-	0/7/25/26	0/2/2/2
1	PSU	5	4636	1	-	3/7/25/26	0/2/2/2
1	OMG	5	1316	1	-	0/9/27/28	0/3/3/3
1	B8W	5	2380	1	-	5/9/27/28	0/3/3/3
1	PSU	5	2508	1	-	0/7/25/26	0/2/2/2
1	B9H	5	2786	1	-	4/12/47/48	0/2/2/2
51	B8Q	9	1219	51	-	1/7/42/43	0/2/2/2
1	5MC	5	4335	1	-	0/7/25/26	0/2/2/2
1	A2M	5	1326	1	-	0/9/27/28	0/3/3/3
1	A2M	5	1871	85,1	-	0/9/27/28	0/3/3/3
1	A2M	5	4571	1	-	0/9/27/28	0/3/3/3
1	B8K	5	4690	1	-	2/11/41/42	0/3/3/3
1	E6G	5	4355	1	-	3/10/28/29	0/3/3/3
1	OMG	5	4870	1	-	3/9/27/28	0/3/3/3
1	PSU	5	1683	1	-	0/7/25/26	0/2/2/2
1	P4U	5	1348	85,1	-	4/10/29/30	0/2/2/2
1	OMG	5	3792	1	-	2/9/27/28	0/3/3/3
1	OMU	5	4306	1	-	0/9/27/28	0/2/2/2
1	7MG	5	1605	1	-	0/7/37/38	0/3/3/3
1	OMC	5	3701	85,1	-	4/9/27/28	0/2/2/2
1	OMC	5	4536	1	-	1/9/27/28	0/2/2/2
1	PSU	5	1582	1	-	2/7/25/26	0/2/2/2
1	I4U	5	1659	1	-	2/9/29/30	0/2/2/2
1	OMG	5	2364	1	-	2/9/27/28	0/3/3/3
1	UR3	5	1866	1	-	1/7/25/26	0/2/2/2
1	OMG	5	4623	1	-	0/9/27/28	0/3/3/3
1	A2M	5	1534	85,1	-	1/9/27/28	0/3/3/3
1	OMC	5	2365	1	-	0/9/27/28	0/2/2/2
1	B8W	5	4129	1	-	3/9/27/28	0/3/3/3
1	PSU	5	4450	85,1	-	3/7/25/26	0/2/2/2
1	7MG	5	2522	1	-	0/7/37/38	0/3/3/3
1	MHG	5	4371	1	-	7/16/46/47	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	5	2401	85,1	-	0/9/27/28	0/3/3/3
3	OMU	8	14	1,3	-	1/9/27/28	0/2/2/2
1	5MC	5	3782	1	-	0/7/25/26	0/2/2/2
1	P7G	5	3880	1	-	3/10/40/41	0/3/3/3
1	B8W	5	4185	1	-	3/9/27/28	0/3/3/3
1	B8Q	5	1456	1	-	2/7/42/43	0/2/2/2
1	E7G	5	2297	1	-	1/9/39/40	0/3/3/3
1	1MA	5	4415	1	-	2/7/25/26	0/3/3/3
1	OMC	5	2804	1	-	0/9/27/28	0/2/2/2
1	OMC	5	3869	1	-	0/9/27/28	0/2/2/2
1	A2M	5	3825	1	-	0/9/27/28	0/3/3/3
1	E7G	5	1797	1	-	2/9/39/40	0/3/3/3
1	B8H	5	1860	1	-	0/7/25/26	0/2/2/2
1	OMC	5	3887	1	-	1/9/27/28	0/2/2/2
1	BGH	5	3899	85,1	-	2/13/43/44	0/3/3/3
1	PSU	5	4628	1	-	0/7/25/26	0/2/2/2
1	B9B	5	2754	85,1	-	3/11/29/30	0/3/3/3
1	P7G	5	1909	1	-	2/10/40/41	0/3/3/3
1	B8T	5	4483	1	-	0/7/27/28	0/2/2/2
1	OMG	5	2050	1	-	0/9/27/28	0/3/3/3
1	2MG	5	729	1	-	1/9/27/28	0/3/3/3
1	PSU	5	4531	1	-	0/7/25/26	0/2/2/2
1	A2M	5	2363	85,1	-	0/9/27/28	0/3/3/3
1	OMC	5	3909	1	-	0/9/27/28	0/2/2/2
1	B9B	5	237	1	-	4/11/29/30	0/3/3/3
1	OMG	5	4494	1	-	1/9/27/28	0/3/3/3
41	MLZ	m	72	41	-	3/7/8/10	-
1	OMG	5	373	1	-	1/9/27/28	0/3/3/3
49	DDE	v	715	49	-	11/20/21/23	0/1/1/1
1	7MG	5	4550	1	-	0/7/37/38	0/3/3/3
1	1MA	5	1322	85,1	-	0/7/25/26	0/3/3/3
1	OMG	5	4370	1	-	1/9/27/28	0/3/3/3
1	OMG	5	2424	1	-	2/9/27/28	0/3/3/3
1	PSU	5	4442	1	-	0/7/25/26	0/2/2/2
51	4AC	9	1337	51	-	0/11/29/30	0/2/2/2
1	6MZ	5	4220	1	-	0/9/27/28	0/3/3/3
1	OMG	5	4637	1	-	2/9/27/28	0/3/3/3
1	OMU	5	4620	1	-	1/9/27/28	0/2/2/2
1	5MU	5	4083	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	5	3785	1	-	2/9/27/28	0/3/3/3
1	UR3	5	4530	1	-	2/7/25/26	0/2/2/2
1	B8K	5	3897	1	-	3/11/41/42	0/3/3/3
1	M7A	5	4564	1	-	0/7/37/38	0/3/3/3
1	OMC	5	2422	85,1	-	0/9/27/28	0/2/2/2
1	B8H	5	3762	1	-	3/7/25/26	0/2/2/2
1	A2M	5	398	1	-	2/9/27/28	0/3/3/3
1	B8W	5	4472	1	-	2/9/27/28	0/3/3/3
51	5MC	9	1374	51	-	0/7/25/26	0/2/2/2
1	A2M	5	3723	1	-	0/9/27/28	0/3/3/3
1	A2M	5	3718	1	-	0/9/27/28	0/3/3/3
1	OMG	5	2773	1	-	2/9/27/28	0/3/3/3
1	2MG	5	1517	1	-	0/9/27/28	0/3/3/3

All (855) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4296	B8H	C6-C5	-15.90	1.12	1.35
1	5	1860	B8H	C6-C5	-15.77	1.12	1.35
1	5	3762	B8H	C6-C5	-15.74	1.12	1.35
1	5	1860	B8H	C4-N3	-14.94	1.10	1.38
1	5	4296	B8H	C4-N3	-14.89	1.11	1.38
1	5	3762	B8H	C4-N3	-14.55	1.11	1.38
1	5	3762	B8H	C4-C5	14.06	1.83	1.44
1	5	4296	B8H	C4-C5	13.88	1.82	1.44
1	5	1860	B8H	C4-C5	13.70	1.82	1.44
1	5	3762	B8H	C6-N1	13.47	1.69	1.36
1	5	1860	B8H	C6-N1	13.38	1.68	1.36
1	5	4296	B8H	C6-N1	13.18	1.68	1.36
1	5	4690	B8K	C3'-C4'	-11.65	1.23	1.53
1	5	1659	I4U	C3'-C2'	-11.46	1.22	1.53
1	5	3897	B8K	C3'-C4'	-11.37	1.24	1.53
1	5	4194	I4U	C3'-C2'	-11.30	1.22	1.53
1	5	4220	6MZ	C6-N6	11.18	1.47	1.34
1	5	4083	5MU	C2-N1	10.96	1.55	1.38
1	5	4083	5MU	C6-N1	10.63	1.56	1.38
1	5	1659	I4U	C4-N3	10.34	1.44	1.31
1	5	1909	P7G	C8-N9	10.33	1.52	1.45
1	5	3899	BGH	C3'-C4'	-10.29	1.26	1.53
1	5	237	B9B	O4'-C1'	10.02	1.65	1.42
1	5	4194	I4U	C4-N3	9.87	1.44	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1574	B9B	O4'-C1'	9.71	1.64	1.42
1	5	2754	B9B	O4'-C1'	9.70	1.64	1.42
1	5	3899	BGH	O4'-C4'	9.68	1.66	1.45
1	5	1348	P4U	C4-N3	9.67	1.43	1.31
1	5	4523	A2M	O4'-C1'	9.64	1.64	1.42
1	5	4083	5MU	C4-C5	9.59	1.60	1.44
1	5	3723	A2M	O4'-C1'	9.57	1.64	1.42
1	5	4447	5MC	C6-C5	9.57	1.50	1.34
51	9	1678	A2M	O4'-C1'	9.54	1.64	1.42
1	5	398	A2M	O4'-C1'	9.46	1.63	1.42
1	5	1871	A2M	O4'-C1'	9.41	1.63	1.42
1	5	4571	A2M	O4'-C1'	9.39	1.63	1.42
1	5	3718	A2M	O4'-C1'	9.39	1.63	1.42
51	9	1374	5MC	C6-C5	9.28	1.49	1.34
1	5	2363	A2M	O4'-C1'	9.28	1.63	1.42
1	5	3825	A2M	O4'-C1'	9.24	1.63	1.42
1	5	3880	P7G	C8-N9	9.22	1.51	1.45
1	5	2401	A2M	O4'-C1'	9.21	1.63	1.42
1	5	2786	B9H	C2-N3	9.20	1.49	1.37
1	5	1524	A2M	O4'-C1'	9.13	1.63	1.42
1	5	1534	A2M	O4'-C1'	9.07	1.63	1.42
1	5	1326	A2M	O4'-C1'	9.00	1.62	1.42
1	5	3782	5MC	C6-C5	8.99	1.49	1.34
1	5	4335	5MC	C6-C5	8.97	1.49	1.34
1	5	4371	MHG	C8-N9	8.94	1.51	1.45
51	9	1219	B8Q	C6-C5	8.87	1.51	1.33
1	5	3867	A2M	O4'-C1'	8.85	1.62	1.42
1	5	3785	A2M	O4'-C1'	8.81	1.62	1.42
1	5	4355	E6G	O4'-C1'	8.81	1.62	1.42
1	5	1534	A2M	C2'-C1'	-8.74	1.31	1.53
1	5	1456	B8Q	C6-C5	8.69	1.51	1.33
1	5	4415	1MA	C2-N3	8.66	1.46	1.30
1	5	2754	B9B	C2'-C1'	-8.64	1.26	1.53
1	5	3825	A2M	C2'-C1'	-8.62	1.31	1.53
1	5	1574	B9B	C2'-C1'	-8.56	1.26	1.53
1	5	237	B9B	C2'-C1'	-8.46	1.26	1.53
1	5	3867	A2M	C2'-C1'	-8.45	1.32	1.53
1	5	1909	P7G	C5-N7	8.37	1.46	1.35
1	5	4690	B8K	C8-N9	8.37	1.51	1.45
1	5	4194	I4U	O4'-C4'	-8.33	1.26	1.45
1	5	2363	A2M	C2'-C1'	-8.31	1.32	1.53
1	5	3897	B8K	C2'-C1'	-8.30	1.27	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1248	B8N	C4-N3	-8.29	1.25	1.40
1	5	4571	A2M	C2'-C1'	-8.23	1.32	1.53
1	5	4083	5MU	C4-N3	-8.22	1.23	1.38
51	9	1678	A2M	C2'-C1'	-8.20	1.32	1.53
1	5	1871	A2M	C2'-C1'	-8.20	1.32	1.53
1	5	1326	A2M	C2'-C1'	-8.19	1.32	1.53
1	5	1322	1MA	C2-N3	8.19	1.45	1.30
1	5	2401	A2M	C2'-C1'	-8.19	1.33	1.53
1	5	4690	B8K	C2'-C1'	-8.15	1.27	1.53
1	5	398	A2M	C2'-C1'	-8.10	1.33	1.53
1	5	3718	A2M	C2'-C1'	-8.09	1.33	1.53
1	5	4371	MHG	C2-N3	8.07	1.47	1.32
1	5	3785	A2M	C2'-C1'	-8.04	1.33	1.53
1	5	4523	A2M	C2'-C1'	-7.99	1.33	1.53
1	5	4355	E6G	O4'-C4'	-7.99	1.27	1.45
1	5	4371	MHG	C5-N7	7.98	1.45	1.35
1	5	3723	A2M	C2'-C1'	-7.95	1.33	1.53
1	5	1524	A2M	C2'-C1'	-7.93	1.33	1.53
1	5	4129	B8W	O4'-C1'	7.85	1.60	1.42
1	5	1659	I4U	O4'-C4'	-7.84	1.27	1.45
1	5	3867	A2M	O4'-C4'	-7.79	1.27	1.45
1	5	4472	B8W	O4'-C1'	7.76	1.59	1.42
1	5	2363	A2M	O4'-C4'	-7.74	1.27	1.45
1	5	4529	B8W	O4'-C1'	7.73	1.59	1.42
51	9	1678	A2M	O4'-C4'	-7.72	1.27	1.45
1	5	3880	P7G	C5-N7	7.71	1.45	1.35
1	5	4355	E6G	C2'-C1'	-7.65	1.29	1.53
1	5	1534	A2M	O4'-C4'	-7.65	1.28	1.45
1	5	1524	A2M	O4'-C4'	-7.62	1.28	1.45
1	5	2380	B8W	O4'-C1'	7.62	1.59	1.42
1	5	2401	A2M	O4'-C4'	-7.61	1.28	1.45
1	5	4571	A2M	O4'-C4'	-7.56	1.28	1.45
1	5	2786	B9H	C2-N1	7.53	1.48	1.38
1	5	3825	A2M	O4'-C4'	-7.52	1.28	1.45
1	5	1326	A2M	O4'-C4'	-7.46	1.28	1.45
1	5	3723	A2M	O4'-C4'	-7.44	1.28	1.45
1	5	4523	A2M	O4'-C4'	-7.43	1.28	1.45
1	5	2786	B9H	C6-C5	7.41	1.48	1.33
1	5	4185	B8W	O4'-C1'	7.41	1.59	1.42
1	5	398	A2M	O4'-C4'	-7.34	1.28	1.45
1	5	3718	A2M	O4'-C4'	-7.34	1.28	1.45
1	5	1871	A2M	O4'-C4'	-7.32	1.28	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2754	B9B	C2-N2	7.32	1.48	1.33
1	5	2754	B9B	O4'-C4'	-7.31	1.28	1.45
1	5	4550	7MG	C8-N9	7.31	1.50	1.45
1	5	237	B9B	C2-N2	7.31	1.48	1.33
51	9	1248	B8N	C6-N1	7.28	1.54	1.36
1	5	3782	5MC	C4-N3	7.23	1.45	1.34
1	5	3785	A2M	O4'-C4'	-7.22	1.28	1.45
1	5	3897	B8K	O4'-C4'	7.22	1.61	1.45
1	5	2297	E7G	C5-N7	7.20	1.44	1.35
1	5	1797	E7G	C5-N7	7.20	1.44	1.35
1	5	2522	7MG	C8-N9	7.20	1.50	1.45
1	5	237	B9B	O4'-C4'	-7.15	1.29	1.45
1	5	4690	B8K	O4'-C4'	7.15	1.60	1.45
1	5	1574	B9B	O4'-C4'	-7.13	1.29	1.45
1	5	4550	7MG	C5-N7	7.10	1.44	1.35
1	5	729	2MG	C2-N3	7.10	1.45	1.32
1	5	4185	B8W	C3'-C4'	-7.08	1.35	1.53
1	5	4335	5MC	C4-N3	7.02	1.45	1.34
1	5	1517	2MG	C2-N3	7.01	1.45	1.32
51	9	1337	4AC	C4-N3	7.00	1.44	1.32
1	5	1574	B9B	C2-N2	7.00	1.47	1.33
1	5	4472	B8W	C2'-C1'	-6.99	1.31	1.53
1	5	2522	7MG	C5-N7	6.98	1.44	1.35
1	5	1605	7MG	C5-N7	6.93	1.44	1.35
1	5	4530	UR3	C2-N1	6.86	1.48	1.38
1	5	4597	UR3	C2-N1	6.83	1.48	1.38
51	9	1374	5MC	C4-N3	6.81	1.45	1.34
1	5	4447	5MC	C4-N3	6.80	1.45	1.34
1	5	4671	B8T	C4-N3	6.79	1.44	1.32
1	5	4529	B8W	C3'-C4'	-6.78	1.35	1.53
1	5	4472	B8W	C3'-C4'	-6.76	1.35	1.53
1	5	4129	B8W	C3'-C4'	-6.75	1.35	1.53
1	5	4529	B8W	C2'-C1'	-6.75	1.32	1.53
1	5	1517	2MG	C4-N3	6.71	1.49	1.34
1	5	2380	B8W	C2'-C1'	-6.70	1.32	1.53
3	8	14	OMU	C2-N3	6.69	1.49	1.38
1	5	2380	B8W	C3'-C4'	-6.68	1.36	1.53
1	5	729	2MG	C4-N3	6.67	1.49	1.34
1	5	4483	B8T	C4-N3	6.66	1.44	1.32
1	5	1866	UR3	C2-N1	6.60	1.47	1.38
1	5	4185	B8W	C2'-C1'	-6.60	1.32	1.53
1	5	4129	B8W	C2'-C1'	-6.59	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1248	B8N	C4-C5	6.56	1.62	1.47
1	5	4335	5MC	C5-C4	6.55	1.49	1.44
1	5	4306	OMU	C2-N3	6.54	1.49	1.38
1	5	3897	B8K	C8-N9	6.53	1.50	1.45
1	5	3792	OMG	C4-N3	6.53	1.49	1.34
1	5	3867	A2M	C6-N6	6.50	1.50	1.34
1	5	4571	A2M	C6-N6	6.49	1.50	1.34
1	5	3718	A2M	C6-N6	6.48	1.50	1.34
1	5	398	A2M	C6-N6	6.48	1.50	1.34
1	5	4370	OMG	C4-N3	6.48	1.49	1.34
1	5	1605	7MG	C8-N9	6.47	1.50	1.45
1	5	2773	OMG	C4-N3	6.45	1.49	1.34
3	8	14	OMU	C2-N1	6.44	1.48	1.38
51	9	1678	A2M	C6-N6	6.44	1.50	1.34
1	5	2424	OMG	C4-N3	6.43	1.49	1.34
1	5	4620	OMU	C2-N3	6.43	1.49	1.38
1	5	3723	A2M	C6-N6	6.42	1.50	1.34
1	5	1326	A2M	C6-N6	6.41	1.50	1.34
1	5	1871	A2M	C6-N6	6.40	1.50	1.34
1	5	4196	OMG	C4-N3	6.40	1.48	1.34
1	5	1534	A2M	C6-N6	6.40	1.50	1.34
1	5	3825	A2M	C6-N6	6.40	1.50	1.34
1	5	1883	OMG	C4-N3	6.38	1.48	1.34
1	5	1517	2MG	C2-N2	6.37	1.46	1.33
1	5	4872	2MG	C2-N2	6.37	1.46	1.33
1	5	2401	A2M	C6-N6	6.36	1.50	1.34
1	5	1524	A2M	C6-N6	6.33	1.50	1.34
1	5	4523	A2M	C6-N6	6.33	1.50	1.34
1	5	2363	A2M	C6-N6	6.33	1.50	1.34
1	5	1625	OMG	C4-N3	6.33	1.48	1.34
1	5	2422	OMC	C2-N3	6.32	1.48	1.36
1	5	729	2MG	C2-N2	6.30	1.46	1.33
1	5	373	OMG	C4-N3	6.30	1.48	1.34
1	5	1522	OMG	C4-N3	6.29	1.48	1.34
1	5	4870	OMG	C4-N3	6.29	1.48	1.34
1	5	4371	MHG	C2-N1	6.28	1.46	1.36
1	5	4494	OMG	C4-N3	6.27	1.48	1.34
1	5	4637	OMG	C4-N3	6.26	1.48	1.34
1	5	3782	5MC	C2-N3	6.26	1.48	1.36
1	5	1797	E7G	C8-N9	6.25	1.49	1.45
51	9	1374	5MC	C2-N3	6.24	1.48	1.36
1	5	4335	5MC	C2-N3	6.22	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4306	OMU	C2-N1	6.21	1.48	1.38
1	5	2050	OMG	C4-N3	6.20	1.48	1.34
1	5	3869	OMC	C6-C5	6.19	1.49	1.35
1	5	4623	OMG	C4-N3	6.19	1.48	1.34
1	5	4371	MHG	C2-N2	6.18	1.46	1.33
1	5	4872	2MG	C2-N3	6.16	1.43	1.32
1	5	4536	OMC	C6-C5	6.16	1.49	1.35
1	5	2364	OMG	C4-N3	6.15	1.48	1.34
1	5	3785	A2M	C6-N6	6.15	1.49	1.34
1	5	1659	I4U	C2-N3	6.14	1.48	1.36
1	5	2804	OMC	C6-C5	6.14	1.49	1.35
1	5	2861	OMC	C2-N3	6.14	1.48	1.36
1	5	2422	OMC	C6-C5	6.13	1.49	1.35
1	5	4536	OMC	C2-N3	6.13	1.48	1.36
1	5	2861	OMC	C6-C5	6.12	1.49	1.35
1	5	4447	5MC	C2-N3	6.12	1.48	1.36
1	5	2365	OMC	C2-N3	6.11	1.48	1.36
1	5	4671	B8T	C2-N3	6.11	1.48	1.36
1	5	4530	UR3	C6-C5	6.10	1.49	1.35
1	5	3701	OMC	C6-C5	6.09	1.49	1.35
1	5	3909	OMC	C2-N3	6.07	1.48	1.36
1	5	1316	OMG	C4-N3	6.07	1.48	1.34
1	5	4483	B8T	C2-N3	6.04	1.48	1.36
1	5	1348	P4U	C6-C5	6.03	1.49	1.35
1	5	3887	OMC	C2-N3	6.03	1.48	1.36
51	9	1337	4AC	C6-C5	6.03	1.49	1.35
1	5	2804	OMC	C2-N3	6.02	1.48	1.36
1	5	3887	OMC	C6-C5	6.01	1.49	1.35
1	5	2365	OMC	C6-C5	6.00	1.49	1.35
1	5	3909	OMC	C6-C5	5.99	1.49	1.35
51	9	1337	4AC	C2-N3	5.98	1.48	1.36
1	5	1348	P4U	C2-N3	5.97	1.48	1.36
51	9	1219	B8Q	C2-N3	5.97	1.46	1.35
1	5	3701	OMC	C2-N3	5.91	1.48	1.36
1	5	4597	UR3	C6-C5	5.90	1.48	1.35
1	5	3869	OMC	C2-N3	5.88	1.48	1.36
1	5	1866	UR3	C6-C5	5.88	1.48	1.35
1	5	2422	OMC	C4-N3	5.86	1.46	1.34
1	5	4415	1MA	C4-N3	5.86	1.47	1.35
1	5	1797	E7G	C2-N3	5.84	1.47	1.33
1	5	4194	I4U	C6-C5	5.82	1.48	1.35
1	5	2861	OMC	C4-N3	5.82	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4483	B8T	C6-C5	5.82	1.48	1.35
1	5	4194	I4U	C1'-N1	-5.75	1.31	1.47
1	5	2297	E7G	C2-N3	5.74	1.47	1.33
1	5	3909	OMC	C4-N3	5.73	1.45	1.34
51	9	1374	5MC	C5-C4	5.73	1.48	1.44
1	5	1909	P7G	C2-N1	5.73	1.47	1.33
1	5	1574	B9B	O6-C6	5.73	1.43	1.34
1	5	2754	B9B	O6-C6	5.73	1.43	1.34
1	5	1909	P7G	C4-N3	5.72	1.47	1.37
1	5	4620	OMU	C2-N1	5.72	1.47	1.38
1	5	3880	P7G	C2-N1	5.69	1.47	1.33
1	5	2365	OMC	C4-N3	5.68	1.45	1.34
1	5	4194	I4U	C2-N3	5.67	1.47	1.36
1	5	4671	B8T	C6-C5	5.67	1.48	1.35
1	5	1659	I4U	C6-C5	5.66	1.48	1.35
1	5	237	B9B	O6-C6	5.65	1.43	1.34
1	5	4529	B8W	C2-N2	5.65	1.45	1.33
1	5	2297	E7G	C8-N9	5.64	1.49	1.45
1	5	3701	OMC	C4-N3	5.64	1.45	1.34
1	5	3880	P7G	C4-N3	5.61	1.47	1.37
1	5	2522	7MG	C4-N3	5.60	1.47	1.34
1	5	2804	OMC	C4-N3	5.58	1.45	1.34
1	5	3887	OMC	C4-N3	5.58	1.45	1.34
1	5	1605	7MG	C2-N3	5.56	1.46	1.33
1	5	4690	B8K	C4-N3	5.55	1.47	1.34
1	5	1605	7MG	C4-N3	5.54	1.46	1.34
1	5	4550	7MG	C2-N3	5.53	1.46	1.33
1	5	2522	7MG	C2-N3	5.53	1.46	1.33
1	5	4083	5MU	C6-C5	5.52	1.43	1.34
1	5	3869	OMC	C4-N3	5.50	1.45	1.34
1	5	4355	E6G	C2-N2	5.50	1.44	1.33
1	5	4690	B8K	C4-N9	5.48	1.44	1.37
1	5	4690	B8K	C2-N3	5.47	1.46	1.33
1	5	4306	OMU	C6-C5	5.46	1.47	1.35
1	5	4129	B8W	C2-N2	5.45	1.44	1.33
1	5	4690	B8K	C3'-C2'	5.45	1.68	1.53
1	5	2380	B8W	C2-N2	5.44	1.44	1.33
1	5	4371	MHG	C4-N3	5.42	1.46	1.34
1	5	1322	1MA	C4-N3	5.41	1.46	1.35
1	5	3782	5MC	C5-C4	5.41	1.48	1.44
1	5	3897	B8K	C4-N9	5.40	1.44	1.37
1	5	3762	B8H	C2-N3	5.38	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1248	B8N	C2-N1	5.37	1.54	1.39
1	5	4194	I4U	C3'-C4'	5.37	1.66	1.53
1	5	1522	OMG	C2-N3	5.35	1.46	1.33
1	5	4872	2MG	C4-N3	5.34	1.46	1.34
1	5	3899	BGH	C2-N3	5.33	1.46	1.33
1	5	4620	OMU	C6-C5	5.31	1.47	1.35
1	5	4550	7MG	C4-N3	5.31	1.46	1.34
1	5	2424	OMG	C2-N3	5.31	1.46	1.33
1	5	2773	OMG	C2-N3	5.31	1.46	1.33
1	5	3792	OMG	C2-N3	5.30	1.46	1.33
1	5	3897	B8K	C3'-C2'	5.29	1.67	1.53
1	5	4185	B8W	C2-N2	5.28	1.44	1.33
1	5	1909	P7G	C4-N9	5.28	1.43	1.35
1	5	3897	B8K	C2-N3	5.27	1.46	1.33
1	5	4370	OMG	C2-N3	5.27	1.46	1.33
1	5	3899	BGH	C4-N3	5.27	1.46	1.34
1	5	4536	OMC	C4-N3	5.27	1.44	1.34
51	9	1219	B8Q	C2-N1	5.25	1.45	1.38
1	5	1456	B8Q	C2-N3	5.24	1.44	1.35
1	5	1797	E7G	C4-N9	5.24	1.44	1.37
1	5	1625	OMG	C2-N3	5.23	1.45	1.33
1	5	4296	B8H	C2-N3	5.23	1.47	1.38
1	5	3897	B8K	C4-N3	5.23	1.46	1.34
1	5	3899	BGH	C8-N9	5.21	1.49	1.45
1	5	4472	B8W	C2-N2	5.19	1.44	1.33
1	5	373	OMG	C2-N3	5.18	1.45	1.33
1	5	4870	OMG	C2-N3	5.18	1.45	1.33
1	5	4623	OMG	C2-N3	5.16	1.45	1.33
1	5	1860	B8H	C2-N3	5.15	1.46	1.38
1	5	2297	E7G	C4-N9	5.15	1.44	1.37
1	5	3880	P7G	C4-N9	5.12	1.43	1.35
1	5	4196	OMG	C2-N3	5.12	1.45	1.33
1	5	2364	OMG	C2-N3	5.11	1.45	1.33
1	5	1883	OMG	C2-N3	5.09	1.45	1.33
1	5	4494	OMG	C2-N3	5.09	1.45	1.33
1	5	2050	OMG	C2-N3	5.09	1.45	1.33
1	5	4637	OMG	C2-N3	5.07	1.45	1.33
1	5	1316	OMG	C2-N3	5.05	1.45	1.33
1	5	4447	5MC	C5-C4	5.04	1.47	1.44
1	5	1659	I4U	C1'-N1	-5.02	1.33	1.47
3	8	14	OMU	C6-C5	4.98	1.46	1.35
1	5	1797	E7G	C4-N3	4.92	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	3899	BGH	O4'-C1'	-4.91	1.30	1.42
1	5	3782	5MC	C4-N4	4.82	1.46	1.34
1	5	4597	UR3	C2-N3	4.81	1.48	1.39
1	5	2522	7MG	C2-N2	4.80	1.45	1.34
51	9	1374	5MC	C4-N4	4.79	1.46	1.34
1	5	1883	OMG	C2-N2	4.77	1.45	1.34
1	5	4872	2MG	C2-N1	4.76	1.44	1.36
1	5	1605	7MG	C2-N2	4.75	1.45	1.34
1	5	4447	5MC	C4-N4	4.74	1.46	1.34
1	5	2424	OMG	C2-N2	4.73	1.45	1.34
1	5	4335	5MC	C4-N4	4.73	1.46	1.34
1	5	2773	OMG	C2-N2	4.73	1.45	1.34
1	5	4447	5MC	C6-N1	4.73	1.46	1.38
1	5	4370	OMG	C2-N2	4.73	1.45	1.34
1	5	2364	OMG	C2-N2	4.72	1.45	1.34
1	5	373	OMG	C2-N2	4.70	1.45	1.34
1	5	4623	OMG	C2-N2	4.70	1.45	1.34
1	5	2297	E7G	C4-N3	4.70	1.45	1.34
1	5	3880	P7G	C2-N2	4.69	1.45	1.34
1	5	4371	MHG	C4-N9	4.68	1.43	1.37
1	5	4690	B8K	O4'-C1'	4.68	1.52	1.42
1	5	1625	OMG	C2-N2	4.65	1.45	1.34
1	5	4550	7MG	C2-N2	4.64	1.45	1.34
1	5	3792	OMG	C2-N2	4.64	1.45	1.34
1	5	1909	P7G	C2-N2	4.63	1.45	1.34
1	5	4196	OMG	C2-N2	4.62	1.45	1.34
1	5	4870	OMG	C2-N2	4.60	1.44	1.34
1	5	1316	OMG	C2-N2	4.59	1.44	1.34
1	5	4494	OMG	C2-N2	4.57	1.44	1.34
1	5	4530	UR3	C2-N3	4.55	1.48	1.39
1	5	1524	A2M	O3'-C3'	-4.55	1.31	1.43
1	5	2050	OMG	C2-N2	4.54	1.44	1.34
1	5	3897	B8K	C2-N2	4.54	1.44	1.34
1	5	4690	B8K	C2-N2	4.52	1.44	1.34
51	9	1248	B8N	C6-C5	4.52	1.41	1.35
1	5	1522	OMG	C2-N2	4.51	1.44	1.34
1	5	1605	7MG	C4-N9	4.51	1.43	1.37
1	5	3899	BGH	C2-N2	4.50	1.44	1.34
1	5	398	A2M	O3'-C3'	-4.49	1.31	1.43
1	5	4483	B8T	C4-N4	4.49	1.45	1.36
1	5	3899	BGH	O2'-C2'	-4.49	1.31	1.42
1	5	1659	I4U	C3'-C4'	4.48	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1374	5MC	C6-N1	4.47	1.45	1.38
1	5	3825	A2M	O3'-C3'	-4.47	1.31	1.43
1	5	1326	A2M	O3'-C3'	-4.46	1.31	1.43
1	5	3782	5MC	C2-N1	4.44	1.49	1.40
1	5	4415	1MA	C2-N1	4.39	1.44	1.35
1	5	4571	A2M	O3'-C3'	-4.38	1.32	1.43
1	5	1866	UR3	C2-N3	4.37	1.47	1.39
51	9	1374	5MC	C2-N1	4.36	1.49	1.40
51	9	1678	A2M	O3'-C3'	-4.35	1.32	1.43
1	5	3782	5MC	C6-N1	4.34	1.45	1.38
1	5	4690	B8K	C71-N7	4.32	1.49	1.39
1	5	4637	OMG	C2-N2	4.30	1.44	1.34
1	5	3718	A2M	O3'-C3'	-4.30	1.32	1.43
1	5	4690	B8K	C5-N7	4.28	1.48	1.39
1	5	4564	M7A	C6-N6	4.27	1.45	1.34
1	5	2522	7MG	C4-N9	4.27	1.43	1.37
1	5	2401	A2M	O3'-C3'	-4.27	1.32	1.43
1	5	1871	A2M	O3'-C3'	-4.27	1.32	1.43
1	5	3723	A2M	O3'-C3'	-4.27	1.32	1.43
1	5	1659	I4U	O4'-C1'	4.26	1.51	1.42
51	9	1337	4AC	C7-N4	4.25	1.45	1.37
1	5	3867	A2M	O3'-C3'	-4.24	1.32	1.43
1	5	2363	A2M	O3'-C3'	-4.23	1.32	1.43
1	5	1348	P4U	C2-N1	4.23	1.48	1.40
1	5	4550	7MG	C4-N9	4.20	1.43	1.37
1	5	4671	B8T	C4-N4	4.18	1.44	1.36
1	5	3897	B8K	O4'-C1'	4.15	1.51	1.42
1	5	1797	E7G	C2-N2	4.11	1.43	1.34
51	9	1337	4AC	C2-N1	4.10	1.48	1.40
1	5	2297	E7G	C2-N2	4.06	1.43	1.34
1	5	3897	B8K	C5-N7	4.04	1.47	1.39
1	5	4671	B8T	C2-N1	4.04	1.48	1.40
51	9	1337	4AC	C4-N4	4.03	1.45	1.39
1	5	4564	M7A	C5-N7	4.02	1.48	1.39
1	5	4529	B8W	O6-C6	4.02	1.41	1.35
1	5	4335	5MC	C6-N1	4.01	1.44	1.38
1	5	1517	2MG	C2-N1	3.99	1.43	1.36
1	5	3899	BGH	C4-N9	3.98	1.42	1.37
1	5	4335	5MC	C2-N1	3.97	1.48	1.40
1	5	1534	A2M	O3'-C3'	-3.95	1.33	1.43
1	5	1348	P4U	O4-C4	3.92	1.39	1.35
1	5	4447	5MC	C2-N1	3.92	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	729	2MG	C2-N1	3.91	1.42	1.36
1	5	4523	A2M	O3'-C3'	-3.91	1.33	1.43
1	5	4185	B8W	O6-C6	3.91	1.41	1.35
1	5	3897	B8K	C71-N7	3.90	1.48	1.39
1	5	2422	OMC	C2-N1	3.84	1.48	1.40
1	5	4194	I4U	C2-N1	3.84	1.48	1.40
1	5	4483	B8T	C2-N1	3.81	1.48	1.40
1	5	3880	P7G	C2-N3	3.80	1.46	1.37
1	5	237	B9B	O3'-C3'	-3.80	1.33	1.43
1	5	4536	OMC	C2-N1	3.79	1.48	1.40
1	5	2861	OMC	C4-N4	3.78	1.43	1.33
1	5	2422	OMC	C4-N4	3.76	1.43	1.33
1	5	4129	B8W	O4'-C4'	3.76	1.53	1.45
1	5	4472	B8W	O6-C6	3.75	1.40	1.35
1	5	2365	OMC	C4-N4	3.75	1.43	1.33
1	5	4529	B8W	O4'-C4'	3.75	1.53	1.45
1	5	1517	2MG	C5-N7	-3.73	1.31	1.39
3	8	14	OMU	C4-N3	3.73	1.45	1.38
1	5	3869	OMC	C4-N4	3.72	1.42	1.33
51	9	1243	PSU	C6-C5	3.71	1.39	1.35
1	5	4355	E6G	O6-C6	3.71	1.40	1.34
1	5	2754	B9B	O3'-C3'	-3.69	1.33	1.43
1	5	1797	E7G	C5-C6	3.69	1.52	1.43
1	5	1322	1MA	C2-N1	3.68	1.43	1.35
1	5	3785	A2M	C5-C4	-3.68	1.32	1.39
1	5	4536	OMC	C4-N4	3.68	1.42	1.33
1	5	3899	BGH	C5-C6	3.67	1.52	1.43
51	9	1678	A2M	O2'-C2'	3.67	1.51	1.42
1	5	2380	B8W	C3'-C2'	3.67	1.63	1.53
1	5	3723	A2M	O2'-C2'	3.66	1.51	1.42
1	5	3909	OMC	C4-N4	3.66	1.42	1.33
1	5	2363	A2M	C5-N7	-3.66	1.32	1.39
1	5	4220	6MZ	C5-C4	-3.65	1.32	1.39
1	5	4306	OMU	C4-N3	3.64	1.44	1.38
1	5	2804	OMC	C4-N4	3.64	1.42	1.33
1	5	3718	A2M	C5-N7	-3.64	1.32	1.39
1	5	3701	OMC	C4-N4	3.64	1.42	1.33
1	5	2297	E7G	C5-C6	3.64	1.52	1.43
1	5	3887	OMC	C4-N4	3.63	1.42	1.33
1	5	3785	A2M	O3'-C3'	-3.63	1.34	1.43
1	5	1659	I4U	C2-N1	3.62	1.47	1.40
1	5	4194	I4U	O4'-C1'	3.62	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2380	B8W	O4'-C4'	3.62	1.53	1.45
1	5	3897	B8K	C2-N1	3.61	1.46	1.37
1	5	1456	B8Q	C2-N1	3.61	1.43	1.38
51	9	1337	4AC	C5-C4	3.61	1.49	1.41
1	5	4129	B8W	O6-C6	3.61	1.40	1.35
1	5	3909	OMC	O2-C2	-3.60	1.17	1.23
1	5	1534	A2M	C5-C4	-3.60	1.32	1.39
1	5	1909	P7G	C2-N3	3.60	1.46	1.37
1	5	4472	B8W	O4'-C4'	3.60	1.53	1.45
1	5	729	2MG	C5-N7	-3.58	1.31	1.39
1	5	4620	OMU	C4-N3	3.58	1.44	1.38
1	5	3785	A2M	C5-N7	-3.57	1.32	1.39
1	5	4690	B8K	C2-N1	3.56	1.46	1.37
1	5	1574	B9B	O3'-C3'	-3.55	1.34	1.43
1	5	2365	OMC	C6-N1	3.55	1.46	1.38
1	5	1582	PSU	C6-C5	3.55	1.39	1.35
1	5	2861	OMC	C2-N1	3.55	1.47	1.40
1	5	1605	7MG	C2-N1	3.55	1.46	1.37
1	5	3718	A2M	O2'-C2'	3.55	1.51	1.42
1	5	4872	2MG	O6-C6	-3.54	1.16	1.23
1	5	1683	PSU	C6-C5	3.53	1.39	1.35
1	5	4129	B8W	C3'-C2'	3.53	1.62	1.53
1	5	1517	2MG	O6-C6	-3.53	1.16	1.23
1	5	1534	A2M	C5-N7	-3.53	1.32	1.39
1	5	1326	A2M	O2'-C2'	3.52	1.51	1.42
1	5	1326	A2M	C5-N7	-3.51	1.32	1.39
1	5	3825	A2M	O2'-C2'	3.50	1.51	1.42
1	5	2522	7MG	C5-C6	3.50	1.52	1.43
1	5	1797	E7G	C2-N1	3.49	1.46	1.37
1	5	4185	B8W	O4'-C4'	3.49	1.52	1.45
1	5	2297	E7G	C2-N1	3.49	1.46	1.37
1	5	2804	OMC	C2-N1	3.48	1.47	1.40
1	5	4371	MHG	C5-C6	3.48	1.52	1.43
1	5	1871	A2M	C5-N7	-3.48	1.32	1.39
1	5	3785	A2M	O2'-C2'	3.47	1.51	1.42
1	5	2380	B8W	C5-C4	-3.47	1.32	1.39
1	5	398	A2M	O2'-C2'	3.47	1.51	1.42
1	5	4472	B8W	C5-C4	-3.47	1.32	1.39
1	5	2401	A2M	O2'-C2'	3.46	1.51	1.42
1	5	1605	7MG	C5-C6	3.46	1.52	1.43
1	5	1534	A2M	C8-N9	-3.45	1.31	1.37
1	5	4523	A2M	C5-C4	-3.44	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4550	7MG	C5-C6	3.43	1.52	1.43
1	5	3764	PSU	C6-C5	3.43	1.39	1.35
1	5	1871	A2M	C5-C4	-3.43	1.33	1.39
1	5	3701	OMC	C2-N1	3.43	1.47	1.40
1	5	3899	BGH	C5-N7	3.43	1.46	1.39
1	5	729	2MG	O6-C6	-3.42	1.17	1.23
1	5	2522	7MG	C2-N1	3.42	1.45	1.37
1	5	1625	OMG	C5-N7	-3.41	1.32	1.39
1	5	3869	OMC	C6-N1	3.40	1.46	1.38
1	5	3887	OMC	C2-N1	3.40	1.47	1.40
1	5	4536	OMC	C6-N1	3.40	1.46	1.38
1	5	4623	OMG	C5-N7	-3.39	1.32	1.39
1	5	4690	B8K	O6-C6	-3.39	1.17	1.23
1	5	3867	A2M	C5-C4	-3.38	1.33	1.39
1	5	2297	E7G	C8-N7	3.37	1.51	1.45
1	5	4571	A2M	O2'-C2'	3.37	1.50	1.42
1	5	1871	A2M	O2'-C2'	3.37	1.50	1.42
1	5	4185	B8W	C5-C4	-3.36	1.33	1.39
1	5	2363	A2M	O2'-C2'	3.36	1.50	1.42
1	5	3869	OMC	C2-N1	3.35	1.47	1.40
1	5	1909	P7G	C5-C4	3.35	1.45	1.36
1	5	4690	B8K	C5-C6	3.35	1.51	1.43
1	5	4335	5MC	O2-C2	-3.35	1.17	1.23
1	5	4355	E6G	C5-C4	-3.35	1.33	1.39
1	5	1797	E7G	C8-N7	3.35	1.51	1.45
1	5	4571	A2M	C5-C4	-3.35	1.33	1.39
1	5	4194	I4U	O4-C41	-3.34	1.39	1.47
1	5	1524	A2M	O2'-C2'	3.31	1.50	1.42
1	5	1524	A2M	C5-N7	-3.31	1.33	1.39
1	5	3887	OMC	C6-N1	3.31	1.46	1.38
1	5	2363	A2M	C5-C4	-3.31	1.33	1.39
1	5	4529	B8W	C3'-C2'	3.31	1.62	1.53
1	5	3867	A2M	O2'-C2'	3.30	1.50	1.42
1	5	3887	OMC	O2-C2	-3.30	1.17	1.23
1	5	3701	OMC	C6-N1	3.30	1.45	1.38
1	5	1524	A2M	C5-C4	-3.29	1.33	1.39
1	5	2050	OMG	C5-N7	-3.29	1.32	1.39
1	5	3899	BGH	C2-N1	3.29	1.45	1.37
1	5	3792	OMG	C5-N7	-3.29	1.32	1.39
1	5	2401	A2M	C5-N7	-3.29	1.33	1.39
1	5	1322	1MA	C5-C6	3.28	1.52	1.43
1	5	4571	A2M	C5-N7	-3.28	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4447	5MC	O2-C2	-3.27	1.17	1.23
1	5	2422	OMC	C6-N1	3.26	1.45	1.38
1	5	4523	A2M	O2'-C2'	3.26	1.50	1.42
1	5	4185	B8W	C3'-C2'	3.26	1.62	1.53
1	5	2365	OMC	C2-N1	3.26	1.46	1.40
1	5	2861	OMC	C6-N1	3.26	1.45	1.38
1	5	4371	MHG	C8-N7	3.26	1.51	1.45
1	5	4872	2MG	C5-N7	-3.25	1.32	1.39
1	5	4523	A2M	C5-N7	-3.25	1.33	1.39
1	5	398	A2M	C5-N7	-3.24	1.33	1.39
1	5	2773	OMG	C5-N7	-3.24	1.32	1.39
1	5	2401	A2M	C5-C4	-3.24	1.33	1.39
1	5	1326	A2M	C5-C4	-3.24	1.33	1.39
1	5	1316	OMG	C5-N7	-3.24	1.32	1.39
3	8	14	OMU	O4-C4	-3.23	1.18	1.24
1	5	2804	OMC	C6-N1	3.23	1.45	1.38
1	5	4306	OMU	O4-C4	-3.23	1.18	1.24
1	5	4550	7MG	C2-N1	3.23	1.45	1.37
1	5	4296	B8H	O4-C4	-3.22	1.17	1.23
1	5	1860	B8H	O4-C4	-3.22	1.17	1.23
1	5	1522	OMG	C5-N7	-3.22	1.32	1.39
1	5	1883	OMG	C5-N7	-3.21	1.32	1.39
1	5	4483	B8T	C6-N1	3.21	1.45	1.38
1	5	2861	OMC	O2-C2	-3.20	1.17	1.23
1	5	4370	OMG	C5-N7	-3.20	1.32	1.39
1	5	4355	E6G	O2'-C2'	3.20	1.50	1.43
1	5	4293	PSU	C6-C5	3.20	1.38	1.35
1	5	2424	OMG	C5-N7	-3.20	1.32	1.39
51	9	1374	5MC	O2-C2	-3.19	1.17	1.23
1	5	3897	B8K	C5-C6	3.19	1.51	1.43
1	5	3723	A2M	C5-N7	-3.19	1.33	1.39
51	9	1678	A2M	C5-N7	-3.18	1.33	1.39
1	5	3909	OMC	C2-N1	3.18	1.46	1.40
1	5	3825	A2M	C5-C4	-3.17	1.33	1.39
1	5	3715	PSU	C6-C5	3.17	1.38	1.35
1	5	3909	OMC	C6-N1	3.17	1.45	1.38
1	5	4870	OMG	C5-N7	-3.17	1.32	1.39
1	5	2804	OMC	O2-C2	-3.17	1.17	1.23
1	5	4415	1MA	C5-C6	3.17	1.52	1.43
1	5	4628	PSU	C6-C5	3.16	1.38	1.35
1	5	4194	I4U	O2'-C2'	3.16	1.50	1.43
1	5	398	A2M	C5-C4	-3.15	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	373	OMG	C5-N7	-3.15	1.32	1.39
1	5	3729	PSU	C6-C5	3.15	1.38	1.35
1	5	3723	A2M	C5-C4	-3.15	1.33	1.39
1	5	4442	PSU	C6-C5	3.15	1.38	1.35
1	5	3718	A2M	C5-C4	-3.14	1.33	1.39
1	5	4355	E6G	C5-N7	-3.14	1.33	1.39
1	5	4529	B8W	C5-C4	-3.14	1.33	1.39
1	5	2508	PSU	C6-C5	3.13	1.38	1.35
1	5	4637	OMG	C5-N7	-3.13	1.32	1.39
1	5	1883	OMG	O6-C6	-3.13	1.17	1.23
1	5	3899	BGH	O6-C6	-3.13	1.17	1.23
1	5	2363	A2M	C8-N9	-3.11	1.32	1.37
1	5	4371	MHG	C6-N1	3.11	1.44	1.38
1	5	4196	OMG	C5-N7	-3.10	1.32	1.39
1	5	4536	OMC	O2-C2	-3.10	1.17	1.23
51	9	1678	A2M	C5-C4	-3.08	1.33	1.39
1	5	3825	A2M	C5-N7	-3.08	1.33	1.39
1	5	3880	P7G	C5-C4	3.07	1.44	1.36
1	5	3867	A2M	C5-N7	-3.07	1.33	1.39
1	5	4129	B8W	C5-C4	-3.07	1.33	1.39
1	5	3869	OMC	O2-C2	-3.07	1.18	1.23
1	5	1871	A2M	C8-N9	-3.07	1.32	1.37
1	5	4531	PSU	C6-C5	3.07	1.38	1.35
1	5	2364	OMG	C5-N7	-3.06	1.32	1.39
1	5	2401	A2M	C8-N9	-3.06	1.32	1.37
1	5	4494	OMG	C5-N7	-3.05	1.32	1.39
1	5	4620	OMU	O4-C4	-3.05	1.18	1.24
1	5	2365	OMC	O2-C2	-3.05	1.18	1.23
1	5	4483	B8T	C5-C4	3.05	1.47	1.41
1	5	4671	B8T	C5-C4	3.05	1.47	1.41
1	5	4355	E6G	O3'-C3'	-3.04	1.35	1.43
1	5	1659	I4U	C6-N1	3.04	1.45	1.38
1	5	2380	B8W	O6-C6	3.03	1.39	1.35
1	5	4472	B8W	C3'-C2'	3.01	1.61	1.53
1	5	3762	B8H	O4-C4	-3.00	1.17	1.23
1	5	3785	A2M	C3'-C4'	3.00	1.60	1.53
1	5	2422	OMC	O2-C2	-2.99	1.18	1.23
1	5	3718	A2M	C8-N9	-2.98	1.32	1.37
51	9	1337	4AC	C6-N1	2.98	1.45	1.38
1	5	1534	A2M	O2'-C2'	2.98	1.50	1.42
1	5	1348	P4U	O2-C2	-2.98	1.18	1.23
1	5	4194	I4U	O2-C2	-2.98	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1659	I4U	O2'-C2'	2.98	1.50	1.43
1	5	1659	I4U	O4-C41	-2.96	1.40	1.47
1	5	3825	A2M	C8-N9	-2.95	1.32	1.37
1	5	2522	7MG	C6-N1	2.94	1.44	1.38
1	5	2364	OMG	O6-C6	-2.94	1.18	1.23
1	5	4472	B8W	C5-N7	-2.94	1.33	1.39
1	5	3897	B8K	C6-N1	2.94	1.44	1.38
1	5	4530	UR3	C6-N1	2.93	1.45	1.38
1	5	4083	5MU	O4-C4	-2.93	1.18	1.23
1	5	3897	B8K	O6-C6	-2.93	1.18	1.23
1	5	4483	B8T	O2-C2	-2.93	1.18	1.23
1	5	4472	B8W	C8-N9	-2.92	1.32	1.37
1	5	4403	PSU	C6-C5	2.91	1.38	1.35
1	5	2754	B9B	C5-C4	-2.91	1.33	1.39
1	5	1659	I4U	O2-C2	-2.90	1.18	1.23
1	5	2380	B8W	C5-N7	-2.89	1.33	1.39
1	5	1524	A2M	C8-N9	-2.88	1.32	1.37
1	5	4671	B8T	O2-C2	-2.88	1.18	1.23
1	5	3899	BGH	C71-N7	2.87	1.46	1.39
1	5	3792	OMG	O6-C6	-2.87	1.18	1.23
1	5	1605	7MG	C6-N1	2.86	1.44	1.38
1	5	3782	5MC	O2-C2	-2.85	1.18	1.23
1	5	4872	2MG	C4-N9	-2.84	1.30	1.38
51	9	1678	A2M	C8-N9	-2.83	1.32	1.37
1	5	4306	OMU	O2-C2	-2.83	1.18	1.23
1	5	4571	A2M	C8-N9	-2.83	1.32	1.37
1	5	3723	A2M	C8-N9	-2.83	1.32	1.37
1	5	4597	UR3	C6-N1	2.82	1.44	1.38
1	5	1677	PSU	O4'-C1'	-2.82	1.39	1.43
1	5	1456	B8Q	O2-C2	-2.82	1.17	1.22
1	5	3867	A2M	C8-N9	-2.80	1.32	1.37
1	5	2050	OMG	O6-C6	-2.80	1.18	1.23
51	9	1219	B8Q	O2-C2	-2.80	1.17	1.22
1	5	4500	PSU	C6-C5	2.80	1.38	1.35
1	5	4636	PSU	C6-C5	2.79	1.38	1.35
1	5	4529	B8W	C5-N7	-2.79	1.34	1.39
1	5	4185	B8W	C4-N9	-2.78	1.31	1.37
1	5	4494	OMG	O6-C6	-2.78	1.18	1.23
1	5	4690	B8K	C6-N1	2.77	1.44	1.38
1	5	1605	7MG	O6-C6	-2.75	1.18	1.23
1	5	4620	OMU	O2-C2	-2.75	1.18	1.23
1	5	4623	OMG	O6-C6	-2.74	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1316	OMG	O6-C6	-2.74	1.18	1.23
1	5	3701	OMC	O2-C2	-2.74	1.18	1.23
1	5	2424	OMG	O6-C6	-2.74	1.18	1.23
1	5	4129	B8W	C5-N7	-2.73	1.34	1.39
1	5	398	A2M	C8-N9	-2.71	1.32	1.37
51	9	1337	4AC	O2-C2	-2.71	1.18	1.23
1	5	1316	OMG	C4-N9	-2.70	1.31	1.38
1	5	4220	6MZ	C4-N9	-2.70	1.32	1.37
1	5	4220	6MZ	C8-N9	-2.69	1.33	1.37
1	5	4370	OMG	O6-C6	-2.69	1.18	1.23
1	5	4870	OMG	O6-C6	-2.68	1.18	1.23
1	5	4196	OMG	O6-C6	-2.68	1.18	1.23
1	5	4083	5MU	O2-C2	-2.68	1.18	1.23
1	5	1625	OMG	O6-C6	-2.68	1.18	1.23
1	5	4194	I4U	C6-N1	2.68	1.44	1.38
1	5	1522	OMG	O6-C6	-2.67	1.18	1.23
1	5	4550	7MG	O6-C6	-2.67	1.18	1.23
1	5	2297	E7G	C6-N1	2.66	1.43	1.38
1	5	1326	A2M	C8-N9	-2.66	1.33	1.37
1	5	4550	7MG	C6-N1	2.65	1.43	1.38
1	5	373	OMG	O6-C6	-2.65	1.18	1.23
1	5	4371	MHG	O6-C6	-2.64	1.18	1.23
1	5	1866	UR3	C6-N1	2.64	1.44	1.38
1	5	4370	OMG	C2-N1	2.63	1.44	1.37
1	5	4637	OMG	O6-C6	-2.63	1.18	1.23
1	5	1797	E7G	C6-N1	2.63	1.43	1.38
1	5	4872	2MG	C6-N1	2.62	1.43	1.38
1	5	4671	B8T	C6-N1	2.61	1.44	1.38
1	5	4220	6MZ	C5-C6	-2.61	1.35	1.41
1	5	3899	BGH	C6-N1	2.60	1.43	1.38
1	5	4494	OMG	C4-N9	-2.60	1.31	1.38
1	5	4220	6MZ	C6-N1	-2.60	1.30	1.35
1	5	2773	OMG	C2-N1	2.60	1.43	1.37
1	5	2050	OMG	C2-N1	2.59	1.43	1.37
49	v	715	DDE	CD2-CG	2.59	1.41	1.36
1	5	4450	PSU	C6-C5	2.59	1.38	1.35
1	5	2522	7MG	O6-C6	-2.59	1.18	1.23
1	5	2424	OMG	C2-N1	2.58	1.43	1.37
1	5	3785	A2M	C8-N9	-2.58	1.33	1.37
1	5	4529	B8W	C8-N9	-2.58	1.33	1.37
1	5	2773	OMG	O6-C6	-2.58	1.18	1.23
1	5	2754	B9B	O2'-C2'	2.57	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2364	OMG	C2-N1	2.57	1.43	1.37
1	5	1574	B9B	C5-C4	-2.57	1.34	1.39
1	5	4185	B8W	C5-N7	-2.56	1.34	1.39
1	5	4355	E6G	C5-C6	-2.56	1.37	1.41
1	5	2380	B8W	C5-C6	-2.55	1.37	1.41
1	5	1348	P4U	C6-N1	2.52	1.44	1.38
1	5	1866	UR3	O4-C4	-2.52	1.18	1.23
1	5	2050	OMG	C4-N9	-2.52	1.31	1.38
3	8	14	OMU	O2-C2	-2.52	1.18	1.23
1	5	237	B9B	C5-C4	-2.51	1.34	1.39
1	5	373	OMG	C2-N1	2.51	1.43	1.37
1	5	237	B9B	O2'-C2'	2.51	1.49	1.43
1	5	4523	A2M	C8-N9	-2.50	1.33	1.37
1	5	1625	OMG	C2-N1	2.49	1.43	1.37
1	5	2380	B8W	C8-N9	-2.49	1.33	1.37
1	5	4129	B8W	C8-N9	-2.49	1.33	1.37
1	5	3880	P7G	O6-C6	-2.47	1.19	1.23
1	5	4185	B8W	C8-N9	-2.47	1.33	1.37
1	5	373	OMG	C4-N9	-2.47	1.31	1.38
1	5	1909	P7G	O6-C6	-2.47	1.19	1.23
1	5	1316	OMG	C2-N1	2.47	1.43	1.37
1	5	4472	B8W	C4-N9	-2.46	1.32	1.37
1	5	1574	B9B	O2'-C2'	2.45	1.49	1.43
1	5	4196	OMG	C2-N1	2.45	1.43	1.37
1	5	4623	OMG	C2-N1	2.45	1.43	1.37
1	5	4530	UR3	O4-C4	-2.44	1.18	1.23
1	5	4306	OMU	C6-N1	2.43	1.43	1.38
1	5	4872	2MG	C5-C6	2.43	1.53	1.44
1	5	3792	OMG	C2-N1	2.43	1.43	1.37
1	5	4355	E6G	C8-N9	-2.41	1.33	1.37
1	5	4494	OMG	C2-N1	2.41	1.43	1.37
1	5	4597	UR3	O4-C4	-2.41	1.18	1.23
1	5	4637	OMG	C2-N1	2.40	1.43	1.37
1	5	4450	PSU	C4-C5	-2.40	1.37	1.44
1	5	1797	E7G	O6-C6	-2.39	1.19	1.23
1	5	1522	OMG	C5-C6	2.39	1.53	1.44
1	5	4870	OMG	C2-N1	2.38	1.43	1.37
1	5	3897	B8K	C5-C4	2.37	1.45	1.37
1	5	3718	A2M	C5'-C4'	2.35	1.58	1.51
1	5	4637	OMG	C4-N9	-2.35	1.32	1.38
1	5	1909	P7G	C8-N7	2.34	1.49	1.45
1	5	4623	OMG	C4-N9	-2.34	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4690	B8K	C5-C4	2.33	1.44	1.37
1	5	2424	OMG	C4-N9	-2.33	1.32	1.38
1	5	4196	OMG	C5-C6	2.32	1.53	1.44
1	5	1322	1MA	C5-N7	-2.32	1.34	1.39
1	5	3867	A2M	C5'-C4'	2.32	1.58	1.51
1	5	1677	PSU	C6-C5	2.31	1.37	1.35
1	5	2364	OMG	C4-N9	-2.31	1.32	1.38
1	5	4415	1MA	C5-N7	-2.31	1.34	1.39
1	5	1522	OMG	C2-N1	2.31	1.43	1.37
1	5	4370	OMG	C4-N9	-2.30	1.32	1.38
1	5	4870	OMG	C4-N9	-2.30	1.32	1.38
1	5	3723	A2M	C3'-C4'	2.30	1.58	1.53
1	5	3792	OMG	C5-C6	2.29	1.53	1.44
1	5	1866	UR3	O2-C2	-2.29	1.18	1.22
1	5	3723	A2M	C5'-C4'	2.28	1.58	1.51
1	5	4636	PSU	C4-C5	-2.27	1.38	1.44
51	9	1248	B8N	O4-C4	-2.27	1.18	1.23
1	5	3785	A2M	C5'-C4'	2.26	1.58	1.51
1	5	3718	A2M	C4-N9	-2.26	1.33	1.37
1	5	1871	A2M	C5'-C4'	2.26	1.58	1.51
1	5	4494	OMG	C5-C6	2.26	1.52	1.44
1	5	2773	OMG	C5-C6	2.26	1.52	1.44
1	5	398	A2M	C5'-C4'	2.25	1.58	1.51
1	5	2424	OMG	C5-C6	2.25	1.52	1.44
1	5	4530	UR3	C4-N3	2.25	1.45	1.40
51	9	1678	A2M	C3'-C4'	2.25	1.58	1.53
3	8	14	OMU	C6-N1	2.24	1.43	1.38
1	5	237	B9B	C5'-C4'	2.24	1.58	1.51
1	5	4870	OMG	C5-C6	2.24	1.52	1.44
1	5	2297	E7G	O6-C6	-2.24	1.19	1.23
1	5	3718	A2M	C3'-C4'	2.24	1.58	1.53
1	5	4637	OMG	C5-C6	2.24	1.52	1.44
1	5	4523	A2M	C5'-C4'	2.23	1.58	1.51
1	5	4370	OMG	C5-C6	2.23	1.52	1.44
1	5	1883	OMG	C2-N1	2.22	1.43	1.37
1	5	1574	B9B	C5'-C4'	2.22	1.58	1.51
1	5	4623	OMG	C5-C6	2.22	1.52	1.44
51	9	1248	B8N	O2-C2	-2.21	1.18	1.22
1	5	4194	I4U	C5-C4	2.21	1.49	1.43
1	5	3880	P7G	C8-N7	2.21	1.49	1.45
1	5	4530	UR3	O2-C2	-2.21	1.18	1.22
1	5	2424	OMG	C6-N1	2.20	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1517	2MG	C5-C6	2.20	1.52	1.44
1	5	1316	OMG	C5-C6	2.20	1.52	1.44
1	5	4129	B8W	C4-N9	-2.19	1.33	1.37
1	5	1909	P7G	C6-N1	2.18	1.41	1.38
1	5	2380	B8W	C4-N9	-2.18	1.33	1.37
1	5	2050	OMG	C5-C6	2.18	1.52	1.44
1	5	4529	B8W	C4-N9	-2.18	1.33	1.37
1	5	373	OMG	C5-C6	2.17	1.52	1.44
1	5	3718	A2M	C6-N1	-2.17	1.29	1.35
1	5	1625	OMG	C4-N9	-2.17	1.32	1.38
1	5	1883	OMG	C4-N9	-2.17	1.32	1.38
1	5	4370	OMG	C6-N1	2.17	1.42	1.38
1	5	1316	OMG	C6-N1	2.16	1.42	1.38
1	5	2401	A2M	C5'-C4'	2.16	1.58	1.51
1	5	1522	OMG	C4-N9	-2.16	1.32	1.38
1	5	4597	UR3	O2-C2	-2.16	1.18	1.22
1	5	4620	OMU	C6-N1	2.15	1.43	1.38
1	5	1677	PSU	C4-C5	-2.15	1.38	1.44
1	5	4571	A2M	C5'-C4'	2.15	1.58	1.51
1	5	2754	B9B	C5'-C4'	2.14	1.58	1.51
1	5	4472	B8W	C5-C6	-2.14	1.37	1.41
1	5	3867	A2M	C4-N9	-2.14	1.33	1.37
1	5	3867	A2M	C3'-C4'	2.14	1.58	1.53
1	5	2364	OMG	C5-C6	2.13	1.52	1.44
1	5	398	A2M	C3'-C4'	2.13	1.58	1.53
1	5	729	2MG	C5-C6	2.13	1.52	1.44
1	5	1524	A2M	C5'-C4'	2.13	1.58	1.51
51	9	1678	A2M	C5'-C4'	2.13	1.58	1.51
1	5	4523	A2M	C3'-C4'	2.13	1.58	1.53
1	5	1322	1MA	C4-N9	-2.12	1.32	1.38
1	5	1326	A2M	C5'-C4'	2.12	1.57	1.51
1	5	4523	A2M	C4-N9	-2.11	1.33	1.37
1	5	4196	OMG	C6-N1	2.11	1.42	1.38
1	5	1683	PSU	C4-C5	-2.11	1.38	1.44
1	5	4628	PSU	O4'-C1'	-2.11	1.40	1.43
1	5	1871	A2M	C3'-C4'	2.11	1.58	1.53
1	5	4196	OMG	C4-N9	-2.11	1.32	1.38
1	5	2050	OMG	C6-N1	2.10	1.42	1.38
1	5	3825	A2M	C4-N9	-2.10	1.33	1.37
1	5	4623	OMG	C6-N1	2.10	1.42	1.38
1	5	373	OMG	C6-N1	2.10	1.42	1.38
1	5	2773	OMG	C6-N1	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1534	A2M	C3'-C4'	2.09	1.58	1.53
1	5	1326	A2M	C3'-C4'	2.09	1.58	1.53
1	5	1871	A2M	C6-N1	-2.09	1.29	1.35
1	5	1883	OMG	C5-C6	2.08	1.52	1.44
1	5	1625	OMG	C5-C6	2.08	1.52	1.44
1	5	3785	A2M	C4-N9	-2.08	1.33	1.37
1	5	4442	PSU	C4-C5	-2.06	1.38	1.44
1	5	4500	PSU	C4-C5	-2.06	1.38	1.44
1	5	2363	A2M	C5'-C4'	2.06	1.57	1.51
1	5	1522	OMG	C6-N1	2.06	1.42	1.38
1	5	1534	A2M	C6-N1	-2.06	1.30	1.35
1	5	4529	B8W	C5-C6	-2.06	1.37	1.41
1	5	4293	PSU	C4-C5	-2.06	1.38	1.44
1	5	1625	OMG	C6-N1	2.05	1.42	1.38
1	5	4571	A2M	C4-N9	-2.05	1.33	1.37
1	5	4597	UR3	C4-N3	2.05	1.44	1.40
1	5	2364	OMG	C6-N1	2.05	1.42	1.38
51	9	1678	A2M	C2-N3	2.05	1.37	1.33
1	5	4628	PSU	C4-C5	-2.04	1.38	1.44
1	5	1582	PSU	O4'-C1'	-2.04	1.41	1.43
1	5	1456	B8Q	C4-N3	-2.03	1.45	1.48
51	9	1248	B8N	O4'-C1'	-2.03	1.41	1.43
1	5	3785	A2M	C6-N1	-2.03	1.30	1.35
1	5	3785	A2M	C2-N3	2.03	1.37	1.33
1	5	2401	A2M	C6-N1	-2.03	1.30	1.35
1	5	1534	A2M	C2-N3	2.02	1.37	1.33
51	9	1337	4AC	O7-C7	-2.02	1.18	1.23
1	5	1582	PSU	C4-C5	-2.02	1.38	1.44
1	5	1524	A2M	C6-N1	-2.02	1.30	1.35
1	5	1534	A2M	C5'-C4'	2.01	1.57	1.51
1	5	4637	OMG	C6-N1	2.00	1.42	1.38
1	5	4306	OMU	C5-C4	2.00	1.48	1.43
1	5	1326	A2M	C4-N9	-2.00	1.33	1.37

All (787) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4529	B8W	N2-C2-N3	18.87	145.51	117.22
1	5	2380	B8W	N2-C2-N3	18.72	145.29	117.22
1	5	4129	B8W	N2-C2-N3	18.58	145.07	117.22
1	5	4185	B8W	N2-C2-N3	18.31	144.68	117.22
1	5	4472	B8W	N2-C2-N3	18.14	144.42	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2380	B8W	N2-C2-N1	-15.43	94.08	117.22
1	5	4529	B8W	N2-C2-N1	-15.24	94.37	117.22
1	5	4129	B8W	N2-C2-N1	-15.01	94.71	117.22
1	5	4472	B8W	N2-C2-N1	-14.89	94.89	117.22
1	5	4185	B8W	N2-C2-N1	-14.46	95.55	117.22
1	5	4564	M7A	C5-C6-N6	13.45	146.61	123.75
1	5	4220	6MZ	C4-N9-C8	12.08	118.43	105.74
1	5	2380	B8W	C1'-N9-C8	-11.81	100.89	127.09
1	5	4083	5MU	C5-C4-N3	11.58	125.39	115.32
1	5	4529	B8W	C1'-N9-C8	-11.53	101.50	127.09
1	5	4472	B8W	C1'-N9-C8	-11.52	101.52	127.09
1	5	4129	B8W	C1'-N9-C8	-11.21	102.22	127.09
1	5	4564	M7A	N6-C6-N1	-11.10	93.66	118.38
1	5	4872	2MG	N1-C2-N2	10.55	127.33	116.56
1	5	4185	B8W	C1'-N9-C8	-10.27	104.29	127.09
1	5	2380	B8W	C4-N9-C1'	10.10	150.25	126.63
1	5	4529	B8W	C4-N9-C1'	10.03	150.09	126.63
1	5	4472	B8W	C4-N9-C1'	9.87	149.71	126.63
1	5	4129	B8W	C4-N9-C1'	9.75	149.44	126.63
1	5	4220	6MZ	N9-C8-N7	-9.22	100.86	113.94
1	5	4220	6MZ	C5-C6-N1	9.00	127.81	118.15
1	5	4083	5MU	C5-C6-N1	-8.82	113.73	123.31
1	5	4185	B8W	C4-N9-C1'	8.49	146.49	126.63
1	5	1517	2MG	C2-N3-C4	7.98	121.98	112.00
1	5	1659	I4U	O4-C4-C5	7.70	120.91	115.45
1	5	4194	I4U	O4-C4-C5	7.67	120.90	115.45
1	5	2786	B9H	C31-N3-C2	7.55	126.57	117.29
1	5	4529	B8W	O6-C6-C5	7.51	126.23	117.17
1	5	237	B9B	C5-C4-N3	-7.49	119.29	127.18
1	5	4185	B8W	O6-C6-C5	7.36	126.05	117.17
1	5	1348	P4U	O4-C4-C5	7.27	120.61	115.45
1	5	4872	2MG	C2-N3-C4	7.24	121.05	112.00
1	5	4355	E6G	C5-C4-N3	-7.14	119.66	127.18
1	5	2754	B9B	C5-C4-N3	-7.09	119.71	127.18
1	5	1517	2MG	C5-C4-N3	-6.93	117.36	128.39
1	5	3762	B8H	C4-N3-C2	-6.89	118.31	127.34
1	5	4220	6MZ	N3-C4-N9	6.84	138.81	127.17
51	9	1219	B8Q	C1'-N1-C2	6.78	128.14	117.04
1	5	4296	B8H	C4-N3-C2	-6.74	118.50	127.34
1	5	1860	B8H	C4-N3-C2	-6.70	118.55	127.34
1	5	4296	B8H	N3-C2-N1	6.64	121.64	115.22
1	5	3762	B8H	N3-C2-N1	6.54	121.54	115.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	729	2MG	C2-N3-C4	6.52	120.15	112.00
1	5	729	2MG	C5-C4-N3	-6.44	118.14	128.39
3	8	14	OMU	C4-N3-C2	-6.42	118.64	126.61
1	5	2380	B8W	C5-C4-N3	-6.40	120.44	127.18
1	5	4872	2MG	N2-C2-N3	-6.32	112.46	120.51
1	5	4129	B8W	O6-C6-C5	6.25	124.71	117.17
1	5	1574	B9B	C5-C4-N3	-6.24	120.60	127.18
1	5	1871	A2M	N3-C2-N1	-6.17	119.24	128.58
1	5	4371	MHG	C2-N3-C4	6.16	119.70	112.00
1	5	1860	B8H	N3-C2-N1	6.16	121.17	115.22
1	5	1797	E7G	C4-C5-N7	6.14	109.92	104.94
1	5	4472	B8W	O6-C6-C5	6.13	124.56	117.17
1	5	4690	B8K	C72-C71-N7	6.13	127.84	118.80
1	5	4690	B8K	C5-C6-N1	6.03	121.56	110.94
1	5	2401	A2M	N3-C2-N1	-6.03	119.46	128.58
1	5	4564	M7A	N3-C4-N9	5.98	134.37	126.88
1	5	1524	A2M	N3-C2-N1	-5.97	119.55	128.58
1	5	3723	A2M	N3-C2-N1	-5.97	119.55	128.58
1	5	4529	B8W	C5-C4-N3	-5.96	120.90	127.18
1	5	3897	B8K	C72-C71-N7	5.96	127.59	118.80
1	5	4129	B8W	C5-C4-N3	-5.95	120.91	127.18
51	9	1219	B8Q	O2-C2-N3	-5.94	114.62	122.95
1	5	4564	M7A	N3-C2-N1	-5.92	119.62	128.58
1	5	4571	A2M	N3-C2-N1	-5.91	119.64	128.58
1	5	4472	B8W	C5-C4-N3	-5.86	121.00	127.18
1	5	2363	A2M	N3-C2-N1	-5.86	119.71	128.58
1	5	4306	OMU	C4-N3-C2	-5.85	119.35	126.61
1	5	1534	A2M	N3-C2-N1	-5.84	119.75	128.58
1	5	3792	OMG	C5-C4-N3	-5.83	119.11	128.39
51	9	1219	B8Q	C6-N1-C2	-5.81	117.05	121.80
1	5	3825	A2M	N3-C2-N1	-5.79	119.81	128.58
1	5	2297	E7G	C4-C5-N7	5.79	109.64	104.94
1	5	3899	BGH	C5-C6-N1	5.76	121.08	110.94
1	5	398	A2M	N3-C2-N1	-5.76	119.87	128.58
1	5	1326	A2M	N3-C2-N1	-5.74	119.89	128.58
51	9	1678	A2M	N3-C2-N1	-5.74	119.89	128.58
1	5	4628	PSU	N1-C2-N3	5.72	121.20	115.17
1	5	4523	A2M	N3-C2-N1	-5.69	119.97	128.58
1	5	4371	MHG	C4-C5-N7	5.69	109.55	104.94
1	5	4690	B8K	C4-C5-N7	5.67	109.52	104.93
1	5	4220	6MZ	N1-C2-N3	-5.67	120.00	128.58
1	5	3897	B8K	C4-C5-N7	5.64	109.49	104.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3897	B8K	C5-C6-N1	5.62	120.84	110.94
1	5	3785	A2M	N3-C2-N1	-5.54	120.20	128.58
1	5	3867	A2M	N3-C2-N1	-5.53	120.21	128.58
1	5	4196	OMG	C5-C4-N3	-5.51	119.61	128.39
1	5	1883	OMG	C5-C4-N3	-5.51	119.63	128.39
1	5	1522	OMG	C5-C4-N3	-5.47	119.69	128.39
1	5	2773	OMG	C5-C4-N3	-5.46	119.71	128.39
1	5	1534	A2M	C5-C4-N3	-5.45	119.22	126.72
1	5	4872	2MG	C2-N1-C6	-5.40	118.02	124.55
1	5	4636	PSU	C4-N3-C2	-5.40	118.93	126.37
1	5	3785	A2M	C5-C4-N3	-5.38	119.30	126.72
1	5	2401	A2M	C5-C4-N3	-5.37	119.32	126.72
1	5	4620	OMU	C4-N3-C2	-5.36	119.96	126.61
1	5	3899	BGH	C72-C71-N7	5.32	126.65	118.80
1	5	4500	PSU	C4-N3-C2	-5.32	119.05	126.37
1	5	1625	OMG	C5-C4-N3	-5.30	119.95	128.39
1	5	1871	A2M	C5-C4-N3	-5.30	119.42	126.72
1	5	4450	PSU	C4-N3-C2	-5.30	119.08	126.37
1	5	1524	A2M	C5-C4-N3	-5.29	119.43	126.72
1	5	2363	A2M	C5-C4-N3	-5.26	119.47	126.72
1	5	398	A2M	C5-C4-N3	-5.25	119.49	126.72
1	5	4371	MHG	C5-C6-N1	5.25	120.18	110.94
1	5	4083	5MU	N3-C2-N1	5.24	121.71	114.89
1	5	3718	A2M	C5-C4-N3	-5.22	119.53	126.72
1	5	1605	7MG	C5-C6-N1	5.21	120.11	110.94
1	5	4293	PSU	N1-C2-N3	5.20	120.65	115.17
1	5	4185	B8W	N9-C8-N7	-5.18	106.58	113.94
51	9	1678	A2M	C5-C4-N3	-5.14	119.64	126.72
1	5	1677	PSU	C4-N3-C2	-5.14	119.29	126.37
1	5	4529	B8W	C61-O6-C6	5.13	122.00	117.20
1	5	4500	PSU	N1-C2-N3	5.13	120.58	115.17
1	5	4220	6MZ	C5-C4-N9	-5.11	100.24	105.81
1	5	3723	A2M	C5-C4-N3	-5.11	119.69	126.72
1	5	1797	E7G	C5-C6-N1	5.10	119.92	110.94
1	5	4628	PSU	C4-N3-C2	-5.09	119.36	126.37
1	5	4531	PSU	N1-C2-N3	5.09	120.53	115.17
1	5	4623	OMG	C5-C4-N3	-5.08	120.30	128.39
1	5	1517	2MG	C2-N1-C6	-5.06	118.44	124.55
1	5	2297	E7G	C5-C6-N1	5.05	119.82	110.94
1	5	4450	PSU	N1-C2-N3	5.05	120.49	115.17
1	5	4571	A2M	C5-C4-N3	-5.04	119.78	126.72
1	5	1326	A2M	C5-C4-N3	-5.03	119.79	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4637	OMG	C5-C4-N3	-5.02	120.40	128.39
1	5	4442	PSU	N1-C2-N3	5.02	120.46	115.17
1	5	4870	OMG	C5-C4-N3	-5.01	120.41	128.39
1	5	4531	PSU	C4-N3-C2	-5.00	119.48	126.37
1	5	4355	E6G	C4-C5-C6	5.00	120.13	115.22
1	5	4370	OMG	C5-C4-N3	-4.99	120.45	128.39
1	5	4293	PSU	C4-N3-C2	-4.98	119.51	126.37
1	5	4636	PSU	N1-C2-N3	4.98	120.42	115.17
51	9	1248	B8N	C5-C4-N3	4.97	125.18	116.15
1	5	1883	OMG	C2-N3-C4	4.95	120.83	112.30
1	5	1322	1MA	N1-C2-N3	-4.95	120.12	126.00
1	5	2424	OMG	C5-C4-N3	-4.94	120.53	128.39
1	5	2522	7MG	C5-C6-N1	4.92	119.61	110.94
1	5	373	OMG	C5-C4-N3	-4.92	120.56	128.39
1	5	1534	A2M	N6-C6-N1	-4.91	107.43	118.38
1	5	2050	OMG	C5-C4-N3	-4.91	120.58	128.39
1	5	2364	OMG	C5-C4-N3	-4.89	120.60	128.39
1	5	4083	5MU	O4-C4-C5	-4.88	119.33	124.92
1	5	729	2MG	C2-N1-C6	-4.88	118.64	124.55
1	5	1316	OMG	C5-C4-N3	-4.88	120.62	128.39
1	5	2401	A2M	N6-C6-N1	-4.88	107.52	118.38
1	5	1683	PSU	N1-C2-N3	4.87	120.31	115.17
1	5	2363	A2M	N6-C6-N1	-4.87	107.53	118.38
1	5	4523	A2M	C5-C4-N3	-4.86	120.02	126.72
1	5	3825	A2M	C5-C4-N3	-4.86	120.02	126.72
1	5	4550	7MG	C5-C6-N1	4.86	119.49	110.94
1	5	3718	A2M	N3-C2-N1	-4.86	121.23	128.58
1	5	4442	PSU	C4-N3-C2	-4.85	119.69	126.37
1	5	3825	A2M	N6-C6-N1	-4.84	107.60	118.38
1	5	3792	OMG	C2-N3-C4	4.84	120.63	112.30
1	5	1326	A2M	N6-C6-N1	-4.83	107.61	118.38
1	5	4597	UR3	C4-N3-C2	-4.82	120.70	124.58
1	5	1677	PSU	N1-C2-N3	4.82	120.25	115.17
1	5	4415	1MA	C5-C4-N3	-4.80	120.20	127.27
1	5	4196	OMG	C2-N3-C4	4.79	120.56	112.30
1	5	237	B9B	N3-C4-N9	4.79	133.07	126.99
1	5	4415	1MA	N1-C2-N3	-4.79	120.31	126.00
1	5	1517	2MG	N9-C4-N3	4.79	135.52	125.95
1	5	1522	OMG	C2-N3-C4	4.78	120.53	112.30
1	5	1871	A2M	N6-C6-N1	-4.76	107.78	118.38
1	5	729	2MG	N9-C4-N3	4.76	135.46	125.95
1	5	2297	E7G	C2-N3-C4	4.75	120.48	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4083	5MU	C4-N3-C2	-4.73	121.14	127.34
1	5	3729	PSU	N1-C2-N3	4.72	120.14	115.17
1	5	3867	A2M	C5-C4-N3	-4.71	120.23	126.72
1	5	4494	OMG	C5-C4-N3	-4.69	120.92	128.39
1	5	4185	B8W	C5-C4-N3	-4.69	122.24	127.18
1	5	4403	PSU	N1-C2-N3	4.68	120.11	115.17
51	9	1678	A2M	N6-C6-N1	-4.66	108.00	118.38
1	5	4872	2MG	C1'-N9-C4	-4.66	112.73	126.49
1	5	3718	A2M	N6-C6-N1	-4.65	108.02	118.38
1	5	1524	A2M	N6-C6-N1	-4.64	108.04	118.38
1	5	1683	PSU	C4-N3-C2	-4.63	119.99	126.37
1	5	1582	PSU	N1-C2-N3	4.63	120.05	115.17
1	5	3899	BGH	C2-N3-C4	4.63	120.27	112.30
1	5	1574	B9B	O6-C6-C5	4.62	122.84	116.73
1	5	1582	PSU	C4-N3-C2	-4.62	120.00	126.37
51	9	1248	B8N	C4-N3-C2	-4.62	119.93	125.62
1	5	3715	PSU	C4-N3-C2	-4.62	120.01	126.37
1	5	4530	UR3	C4-N3-C2	-4.61	120.87	124.58
1	5	398	A2M	N6-C6-N1	-4.61	108.10	118.38
1	5	4403	PSU	C4-N3-C2	-4.61	120.02	126.37
1	5	1517	2MG	N1-C2-N2	4.61	121.26	116.56
1	5	4623	OMG	C2-N3-C4	4.58	120.19	112.30
1	5	4872	2MG	C5-C4-N3	-4.57	121.11	128.39
1	5	2773	OMG	C2-N3-C4	4.56	120.16	112.30
1	5	2508	PSU	C4-N3-C2	-4.56	120.08	126.37
1	5	1909	P7G	C4-C5-N7	4.56	109.78	106.71
1	5	4355	E6G	N3-C4-N9	4.56	132.78	126.99
1	5	4472	B8W	N9-C8-N7	-4.55	107.47	113.94
1	5	4523	A2M	N6-C6-N1	-4.55	108.24	118.38
1	5	4571	A2M	N6-C6-N1	-4.55	108.25	118.38
1	5	4872	2MG	C1'-N9-C8	4.54	139.64	126.73
1	5	2364	OMG	C2-N3-C4	4.54	120.12	112.30
1	5	1797	E7G	C2-N3-C4	4.54	120.12	112.30
1	5	3723	A2M	N6-C6-N1	-4.54	108.27	118.38
1	5	3729	PSU	C4-N3-C2	-4.53	120.13	126.37
1	5	4550	7MG	C2-N3-C4	4.53	120.10	112.30
1	5	3880	P7G	C4-C5-N7	4.52	109.76	106.71
1	5	2522	7MG	C2-N3-C4	4.52	120.08	112.30
1	5	1659	I4U	C5-C4-N3	-4.52	118.23	124.86
1	5	2380	B8W	N9-C8-N7	-4.52	107.53	113.94
51	9	1219	B8Q	N3-C2-N1	4.51	123.44	117.16
1	5	1316	OMG	C2-N3-C4	4.50	120.06	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2754	B9B	N3-C4-N9	4.50	132.70	126.99
1	5	373	OMG	C2-N3-C4	4.49	120.04	112.30
1	5	3867	A2M	N6-C6-N1	-4.49	108.38	118.38
1	5	1322	1MA	C5-C4-N3	-4.48	120.67	127.27
1	5	1605	7MG	C2-N3-C4	4.45	119.96	112.30
1	5	2424	OMG	C2-N3-C4	4.44	119.95	112.30
1	5	4690	B8K	C2-N3-C4	4.44	119.94	112.30
1	5	4870	OMG	C2-N3-C4	4.43	119.94	112.30
1	5	3715	PSU	N1-C2-N3	4.43	119.84	115.17
1	5	4529	B8W	N9-C8-N7	-4.43	107.65	113.94
1	5	3764	PSU	C4-N3-C2	-4.42	120.28	126.37
1	5	4370	OMG	C2-N3-C4	4.39	119.86	112.30
1	5	4371	MHG	N1-C2-N2	4.38	121.04	116.56
1	5	1574	B9B	N9-C8-N7	-4.38	107.72	113.94
1	5	4129	B8W	N9-C8-N7	-4.36	107.75	113.94
1	5	4494	OMG	C2-N3-C4	4.35	119.80	112.30
1	5	1625	OMG	C2-N3-C4	4.35	119.79	112.30
1	5	2380	B8W	O6-C6-C5	4.35	122.41	117.17
1	5	237	B9B	N2-C2-N3	4.34	123.74	117.22
1	5	4637	OMG	C2-N3-C4	4.34	119.78	112.30
1	5	2754	B9B	N9-C8-N7	-4.33	107.79	113.94
1	5	3785	A2M	N6-C6-N1	-4.33	108.74	118.38
1	5	2380	B8W	C4-C5-C6	4.32	119.46	115.22
1	5	2508	PSU	N1-C2-N3	4.29	119.70	115.17
1	5	3764	PSU	N1-C2-N3	4.28	119.68	115.17
1	5	1456	B8Q	C31-N3-C4	4.25	122.12	114.76
1	5	3899	BGH	C5-C4-N9	4.23	111.76	106.33
1	5	2754	B9B	N2-C2-N3	4.23	123.57	117.22
1	5	1456	B8Q	N3-C2-N1	4.23	123.06	117.16
1	5	4220	6MZ	C5-C4-N3	-4.22	120.90	126.72
3	8	14	OMU	C5-C4-N3	4.22	120.71	114.80
1	5	237	B9B	O6-C6-C5	4.19	122.27	116.73
51	9	1248	B8N	C1'-C5-C4	4.14	123.90	117.61
1	5	2754	B9B	C4-C5-C6	4.14	119.29	115.22
1	5	3897	B8K	C2-N3-C4	4.14	119.42	112.30
1	5	2380	B8W	N3-C4-N9	4.14	132.24	126.99
1	5	3867	A2M	N9-C8-N7	-4.13	108.07	113.94
1	5	4306	OMU	N3-C2-N1	4.13	120.27	114.89
1	5	2050	OMG	C2-N3-C4	4.13	119.41	112.30
1	5	237	B9B	N9-C8-N7	-4.12	108.09	113.94
51	9	1678	A2M	N9-C8-N7	-4.09	108.14	113.94
1	5	3899	BGH	C4-C5-N7	4.09	108.23	104.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4571	A2M	N9-C8-N7	-4.07	108.16	113.94
1	5	237	B9B	C4-C5-C6	4.06	119.21	115.22
1	5	4472	B8W	C4-C5-C6	4.04	119.19	115.22
1	5	4529	B8W	C4-C5-C6	4.04	119.19	115.22
51	9	1219	B8Q	C31-N3-C4	4.03	121.74	114.76
1	5	4296	B8H	O2-C2-N1	-4.02	118.71	122.78
1	5	1524	A2M	N9-C8-N7	-4.01	108.25	113.94
1	5	3825	A2M	N9-C8-N7	-4.00	108.26	113.94
1	5	1348	P4U	C5-C4-N3	-4.00	118.99	124.86
1	5	4355	E6G	N9-C8-N7	-4.00	108.27	113.94
1	5	2401	A2M	N9-C8-N7	-3.99	108.27	113.94
1	5	3792	OMG	N9-C4-N3	3.98	133.91	125.95
1	5	3785	A2M	N9-C8-N7	-3.97	108.31	113.94
1	5	4185	B8W	C61-O6-C6	3.93	120.88	117.20
1	5	4371	MHG	C2-N1-C6	-3.93	119.80	124.55
1	5	2297	E7G	C5-C4-N3	-3.92	120.77	128.13
1	5	1866	UR3	C6-N1-C2	-3.88	118.63	121.80
1	5	4083	5MU	C5M-C5-C6	-3.88	117.60	122.85
1	5	3897	B8K	N9-C8-N7	3.87	108.41	103.31
1	5	1909	P7G	N9-C8-N7	3.85	108.82	103.37
1	5	1797	E7G	C5-C4-N3	-3.84	120.92	128.13
1	5	4083	5MU	C5M-C5-C4	3.84	122.88	118.78
1	5	1605	7MG	C5-C4-N3	-3.84	120.93	128.13
1	5	1860	B8H	C5-C4-N3	3.83	124.99	116.55
1	5	1883	OMG	N9-C4-N3	3.83	133.61	125.95
1	5	4550	7MG	C5-C4-N3	-3.82	120.96	128.13
51	9	1248	B8N	N3-C2-N1	3.80	121.36	116.72
1	5	4529	B8W	O6-C6-N1	-3.79	113.92	118.96
1	5	1605	7MG	C4-C5-N7	3.79	109.85	105.38
1	5	4872	2MG	CM2-N2-C2	-3.79	115.52	123.65
1	5	1456	B8Q	O2-C2-N3	-3.78	117.64	122.95
1	5	2522	7MG	C4-C5-N7	3.77	109.84	105.38
1	5	4335	5MC	C5-C6-N1	-3.77	119.22	123.31
1	5	4220	6MZ	C9-N6-C6	-3.76	119.36	122.85
1	5	2363	A2M	N9-C8-N7	-3.75	108.62	113.94
1	5	4620	OMU	N3-C2-N1	3.73	119.75	114.89
1	5	4185	B8W	N1-C2-N3	-3.73	119.77	125.48
1	5	3723	A2M	N9-C8-N7	-3.73	108.65	113.94
1	5	2522	7MG	C5-C4-N3	-3.72	121.14	128.13
1	5	4355	E6G	N3-C2-N1	-3.71	119.79	125.48
1	5	4523	A2M	N9-C8-N7	-3.71	108.67	113.94
1	5	4415	1MA	C2-N3-C4	3.71	119.80	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2773	OMG	N9-C4-N3	3.71	133.36	125.95
1	5	4185	B8W	O4'-C1'-N9	3.71	115.21	108.09
1	5	4550	7MG	C5-C4-N9	3.70	111.08	106.33
1	5	4371	MHG	C5-C4-N3	-3.70	121.18	128.13
1	5	1326	A2M	N9-C8-N7	-3.70	108.69	113.94
1	5	3899	BGH	N9-C8-N7	3.70	108.18	103.31
1	5	398	A2M	N9-C8-N7	-3.69	108.69	113.94
1	5	1322	1MA	C2-N3-C4	3.66	119.70	112.53
1	5	2401	A2M	C2-N3-C4	3.66	120.76	111.83
1	5	1348	P4U	O2-C2-N3	-3.65	116.58	122.33
1	5	4129	B8W	C4-C5-C6	3.65	118.80	115.22
1	5	3762	B8H	C5-C4-N3	3.64	124.56	116.55
1	5	4129	B8W	O4'-C1'-N9	3.64	115.07	108.09
1	5	2786	B9H	C4-N3-C2	-3.63	115.46	122.00
1	5	4447	5MC	C5-C6-N1	-3.62	119.38	123.31
1	5	4690	B8K	N9-C8-N7	3.62	108.08	103.31
1	5	3762	B8H	O2-C2-N1	-3.61	119.13	122.78
1	5	1871	A2M	C2-N3-C4	3.60	120.63	111.83
1	5	1871	A2M	C5-C6-N6	3.60	132.21	123.29
1	5	1534	A2M	C2-N3-C4	3.60	120.62	111.83
1	5	2363	A2M	C2-N3-C4	3.60	120.61	111.83
1	5	1866	UR3	C4-N3-C2	-3.59	121.69	124.58
1	5	4472	B8W	O4'-C1'-N9	3.59	114.98	108.09
1	5	3825	A2M	C5-C6-N6	3.59	132.16	123.29
1	5	1871	A2M	N9-C8-N7	-3.58	108.85	113.94
1	5	1316	OMG	N9-C8-N7	-3.58	106.77	113.40
3	8	14	OMU	N3-C2-N1	3.57	119.54	114.89
1	5	4690	B8K	C5-C4-N9	3.57	110.91	106.33
1	5	4306	OMU	C5-C4-N3	3.56	119.79	114.80
1	5	1625	OMG	N9-C4-N3	3.56	133.06	125.95
1	5	3718	A2M	C5-C6-N6	3.55	132.08	123.29
1	5	4185	B8W	O6-C6-N1	-3.54	114.25	118.96
1	5	4296	B8H	C5-C4-N3	3.54	124.34	116.55
1	5	1524	A2M	C2-N3-C4	3.54	120.47	111.83
1	5	1326	A2M	C5-C6-N6	3.53	132.03	123.29
1	5	4220	6MZ	C2-N3-C4	3.53	120.44	111.83
1	5	4494	OMG	N9-C8-N7	-3.53	106.86	113.40
1	5	3785	A2M	N3-C4-N9	3.52	133.16	127.17
1	5	4550	7MG	C4-C5-N7	3.52	109.53	105.38
1	5	4529	B8W	C3'-C2'-C1'	3.51	108.11	101.46
1	5	3785	A2M	C2'-C1'-N9	-3.51	107.97	113.75
1	5	4529	B8W	N1-C2-N3	-3.50	120.12	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2363	A2M	C5-C6-N6	3.50	131.94	123.29
1	5	3723	A2M	C2-N3-C4	3.49	120.37	111.83
1	5	398	A2M	C2-N3-C4	3.49	120.35	111.83
1	5	4185	B8W	C2-N1-C6	3.49	120.81	115.96
1	5	237	B9B	N3-C2-N1	-3.49	120.14	125.48
1	5	3792	OMG	C2-N1-C6	-3.48	118.80	125.11
1	5	4571	A2M	C2-N3-C4	3.47	120.32	111.83
1	5	4220	6MZ	C5-N7-C8	3.47	108.91	103.45
1	5	2401	A2M	N3-C4-N9	3.47	133.07	127.17
1	5	1316	OMG	C2-N1-C6	-3.47	118.81	125.11
3	8	14	OMU	O4-C4-C5	-3.46	119.19	125.16
1	5	4196	OMG	N9-C4-N3	3.46	132.88	125.95
1	5	3825	A2M	C2-N3-C4	3.46	120.28	111.83
51	9	1678	A2M	C5-C6-N6	3.46	131.85	123.29
1	5	3785	A2M	C2-N3-C4	3.45	120.25	111.83
1	5	1326	A2M	C2-N3-C4	3.44	120.24	111.83
1	5	4129	B8W	N1-C2-N3	-3.44	120.21	125.48
1	5	4530	UR3	C5-C4-N3	3.43	119.56	115.04
51	9	1678	A2M	C2-N3-C4	3.43	120.20	111.83
1	5	2522	7MG	C5-C4-N9	3.42	110.71	106.33
1	5	1883	OMG	C2-N1-C6	-3.41	118.93	125.11
1	5	1574	B9B	N3-C4-N9	3.41	131.32	126.99
1	5	4196	OMG	C2-N1-C6	-3.41	118.93	125.11
1	5	2050	OMG	N9-C8-N7	-3.40	107.09	113.40
1	5	4185	B8W	C5-N7-C8	3.40	108.79	103.45
1	5	4523	A2M	C2-N3-C4	3.40	120.13	111.83
1	5	1534	A2M	N9-C8-N7	-3.40	109.12	113.94
1	5	2401	A2M	C5-C6-N6	3.39	131.69	123.29
1	5	3723	A2M	C5-C6-N6	3.39	131.67	123.29
1	5	4620	OMU	C5-C4-N3	3.39	119.54	114.80
1	5	4597	UR3	C5-C4-N3	3.39	119.50	115.04
1	5	4637	OMG	N9-C8-N7	-3.37	107.15	113.40
1	5	1522	OMG	C2-N1-C6	-3.37	119.00	125.11
1	5	2380	B8W	C3'-C2'-C1'	3.36	107.82	101.46
1	5	3785	A2M	O4'-C1'-N9	3.35	114.52	108.09
1	5	4690	B8K	C6-C5-C4	-3.35	116.52	122.40
1	5	1524	A2M	N3-C4-N9	3.34	132.85	127.17
1	5	3867	A2M	C5-C6-N6	3.34	131.55	123.29
1	5	1574	B9B	C4-C5-C6	3.33	118.50	115.22
1	5	1524	A2M	C5-C6-N6	3.33	131.53	123.29
1	5	1883	OMG	N9-C8-N7	-3.33	107.23	113.40
1	5	4523	A2M	C5-C6-N6	3.33	131.53	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	398	A2M	C5-C6-N6	3.32	131.52	123.29
1	5	3867	A2M	C2-N3-C4	3.32	119.94	111.83
1	5	4571	A2M	C5-C6-N6	3.32	131.50	123.29
1	5	2380	B8W	C61-O6-C6	-3.32	114.10	117.20
1	5	2754	B9B	N3-C2-N1	-3.32	120.40	125.48
1	5	1683	PSU	O2-C2-N1	-3.31	119.37	122.79
1	5	1534	A2M	C5-C6-N6	3.31	131.49	123.29
1	5	1522	OMG	N9-C4-N3	3.31	132.57	125.95
1	5	4185	B8W	C4-N9-C8	3.31	109.21	105.74
1	5	2050	OMG	C2-N1-C6	-3.30	119.13	125.11
1	5	1574	B9B	N2-C2-N3	3.29	122.15	117.22
1	5	4472	B8W	N3-C4-N9	3.28	131.16	126.99
1	5	3899	BGH	C5-C4-N3	-3.28	121.98	128.13
1	5	373	OMG	N9-C8-N7	-3.26	107.35	113.40
1	5	4872	2MG	N9-C8-N7	-3.26	107.35	113.40
1	5	2364	OMG	N9-C8-N7	-3.26	107.36	113.40
1	5	1860	B8H	O2-C2-N1	-3.26	119.48	122.78
1	5	1625	OMG	C2-N1-C6	-3.26	119.20	125.11
1	5	1574	B9B	O6-C6-N1	-3.25	115.68	120.02
1	5	4371	MHG	C5-C4-N9	3.25	110.50	106.33
1	5	4529	B8W	C5-N7-C8	3.24	108.54	103.45
1	5	1534	A2M	N3-C4-N9	3.24	132.67	127.17
1	5	3897	B8K	C6-C5-C4	-3.23	116.72	122.40
1	5	4628	PSU	C6-N1-C2	-3.23	119.69	122.69
51	9	1678	A2M	N3-C4-N9	3.23	132.66	127.17
1	5	1866	UR3	C1'-N1-C2	3.22	122.32	117.04
51	9	1248	B8N	C31-N3-C4	3.22	121.74	117.18
1	5	4637	OMG	C2-N1-C6	-3.22	119.28	125.11
1	5	4564	M7A	C2-N3-C4	3.21	119.68	111.83
1	5	2424	OMG	C2-N1-C6	-3.20	119.30	125.11
1	5	4185	B8W	C4-C5-N7	-3.20	106.92	110.58
1	5	1574	B9B	N3-C2-N1	-3.20	120.58	125.48
1	5	4623	OMG	C2-N1-C6	-3.20	119.31	125.11
1	5	4529	B8W	N3-C4-N9	3.19	131.03	126.99
1	5	2364	OMG	C2-N1-C6	-3.18	119.34	125.11
1	5	4690	B8K	C5-C4-N3	-3.18	122.16	128.13
1	5	3899	BGH	C6-C5-C4	-3.18	116.81	122.40
51	9	1374	5MC	C5-C6-N1	-3.17	119.87	123.31
1	5	2380	B8W	N1-C2-N3	-3.17	120.62	125.48
1	5	4530	UR3	C6-N1-C2	-3.17	119.21	121.80
1	5	4870	OMG	N9-C8-N7	-3.17	107.52	113.40
1	5	398	A2M	N3-C4-N9	3.17	132.55	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4450	PSU	C6-C5-C4	3.17	120.31	118.17
1	5	4529	B8W	C2-N1-C6	3.16	120.36	115.96
1	5	4185	B8W	C4'-O4'-C1'	-3.16	102.49	109.47
1	5	3782	5MC	C5-C6-N1	-3.16	119.88	123.31
1	5	1522	OMG	N9-C8-N7	-3.16	107.55	113.40
1	5	4472	B8W	C5-N7-C8	3.16	108.41	103.45
1	5	2363	A2M	N3-C4-N9	3.15	132.52	127.17
1	5	1605	7MG	C5-C4-N9	3.15	110.36	106.33
1	5	373	OMG	N9-C4-N3	3.14	132.24	125.95
51	9	1243	PSU	C6-N1-C2	-3.13	119.78	122.69
1	5	4472	B8W	N1-C2-N3	-3.13	120.68	125.48
1	5	2297	E7G	C5-C4-N9	3.13	110.34	106.33
1	5	3897	B8K	C5-C4-N9	3.12	110.33	106.33
51	9	1243	PSU	N1-C2-N3	3.12	118.45	115.17
1	5	3792	OMG	N9-C8-N7	-3.11	107.62	113.40
1	5	4494	OMG	C2-N1-C6	-3.11	119.47	125.11
1	5	4571	A2M	N3-C4-N9	3.11	132.46	127.17
1	5	1871	A2M	N3-C4-N9	3.11	132.45	127.17
1	5	4129	B8W	N3-C4-N9	3.10	130.93	126.99
1	5	4370	OMG	N9-C8-N7	-3.10	107.66	113.40
1	5	4371	MHG	C71-C72-C73	-3.09	105.86	114.13
1	5	4129	B8W	C5-N7-C8	3.09	108.31	103.45
1	5	4129	B8W	O6-C6-N1	-3.09	114.85	118.96
1	5	1866	UR3	C5-C4-N3	3.08	119.10	115.04
1	5	4623	OMG	N9-C8-N7	-3.07	107.70	113.40
1	5	4531	PSU	O2-C2-N1	-3.07	119.62	122.79
1	5	4370	OMG	C2-N1-C6	-3.07	119.54	125.11
1	5	3899	BGH	C2'-C1'-N9	-3.07	107.90	114.14
1	5	1883	OMG	C5-C6-N1	3.07	121.06	113.25
1	5	4623	OMG	N9-C4-N3	3.06	132.08	125.95
1	5	3718	A2M	C2-N3-C4	3.06	119.31	111.83
1	5	2364	OMG	N9-C4-N3	3.06	132.07	125.95
1	5	2773	OMG	C2-N1-C6	-3.06	119.56	125.11
1	5	3723	A2M	N3-C4-N9	3.04	132.34	127.17
1	5	2424	OMG	N9-C8-N7	-3.04	107.77	113.40
1	5	373	OMG	C2-N1-C6	-3.04	119.61	125.11
1	5	4628	PSU	O2-C2-N1	-3.03	119.67	122.79
1	5	1524	A2M	C4'-O4'-C1'	-3.03	102.78	109.47
1	5	1883	OMG	O6-C6-C5	-3.02	118.55	126.53
1	5	4500	PSU	O2-C2-N1	-3.02	119.67	122.79
1	5	4370	OMG	N9-C4-N3	3.02	131.99	125.95
1	5	2050	OMG	N9-C4-N3	3.02	131.99	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1797	E7G	C5-C4-N9	3.01	110.19	106.33
1	5	4529	B8W	O4'-C1'-N9	3.01	113.87	108.09
1	5	4870	OMG	N9-C4-N3	3.01	131.97	125.95
1	5	4196	OMG	N9-C8-N7	-3.00	107.83	113.40
51	9	1248	B8N	O4-C4-C5	-3.00	117.39	122.58
1	5	4870	OMG	C2-N1-C6	-3.00	119.67	125.11
1	5	1517	2MG	C5-C6-N1	3.00	120.89	113.25
1	5	4355	E6G	C2-N1-C6	2.99	120.11	115.96
1	5	1625	OMG	N9-C8-N7	-2.98	107.87	113.40
1	5	3729	PSU	O2-C2-N1	-2.98	119.72	122.79
1	5	3729	PSU	C6-N1-C2	-2.98	119.93	122.69
1	5	4597	UR3	C6-N1-C2	-2.97	119.37	121.80
1	5	4194	I4U	C5-C4-N3	-2.97	120.50	124.86
1	5	4185	B8W	C4-C5-C6	2.97	118.14	115.22
1	5	2380	B8W	C4-N9-C8	2.96	108.85	105.74
1	5	4637	OMG	N9-C4-N3	2.95	131.86	125.95
1	5	4872	2MG	C5-C6-N1	2.95	120.77	113.25
1	5	237	B9B	O6-C6-N1	-2.95	116.08	120.02
1	5	4620	OMU	O4-C4-C5	-2.95	120.08	125.16
1	5	4335	5MC	CM5-C5-C6	-2.94	118.88	122.85
1	5	2424	OMG	N9-C4-N3	2.93	131.81	125.95
1	5	1683	PSU	C6-N1-C2	-2.93	119.97	122.69
1	5	1322	1MA	N9-C8-N7	-2.92	107.98	113.40
1	5	2380	B8W	O4'-C1'-N9	2.92	113.69	108.09
1	5	4597	UR3	C1'-N1-C2	2.92	121.81	117.04
1	5	3792	OMG	C5-C6-N1	2.91	120.67	113.25
1	5	3897	B8K	C5-C4-N3	-2.91	122.67	128.13
1	5	1517	2MG	O6-C6-C5	-2.90	118.86	126.53
1	5	4083	5MU	O2-C2-N1	-2.89	119.04	122.80
1	5	4472	B8W	C4-N9-C8	2.88	108.77	105.74
1	5	2773	OMG	N9-C8-N7	-2.88	108.05	113.40
1	5	4636	PSU	O2-C2-N1	-2.88	119.81	122.79
1	5	1326	A2M	N3-C4-N9	2.88	132.07	127.17
1	5	4196	OMG	C5-C6-N1	2.88	120.58	113.25
1	5	1456	B8Q	C6-N1-C2	-2.88	119.45	121.80
1	5	1574	B9B	C4-N9-C1'	-2.87	119.93	126.63
1	5	1316	OMG	C5-C6-N1	2.86	120.54	113.25
1	5	4185	B8W	C5-C6-N1	-2.86	119.67	123.49
1	5	1605	7MG	N9-C8-N7	2.85	107.40	103.37
1	5	2297	E7G	C2-N1-C6	-2.85	119.95	125.11
1	5	4529	B8W	C4-C5-N7	-2.84	107.33	110.58
1	5	4355	E6G	N2-C2-N1	2.84	121.49	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1522	OMG	C5-C6-N1	2.84	120.49	113.25
1	5	4442	PSU	O2-C2-N1	-2.84	119.86	122.79
1	5	4442	PSU	C6-N1-C2	-2.83	120.06	122.69
1	5	3764	PSU	C6-N1-C2	-2.83	120.06	122.69
1	5	2364	OMG	C5-C6-N1	2.83	120.46	113.25
1	5	1574	B9B	C5-N7-C8	2.82	107.88	103.45
1	5	1871	A2M	C2'-C1'-N9	-2.82	109.11	113.75
1	5	2424	OMG	C5-C6-N1	2.82	120.42	113.25
1	5	4220	6MZ	C1'-N9-C8	-2.82	120.84	127.09
1	5	1534	A2M	O4'-C1'-C2'	-2.81	101.74	106.59
1	5	2364	OMG	O6-C6-C5	-2.81	119.12	126.53
1	5	4083	5MU	C6-N1-C2	-2.80	118.51	121.30
51	9	1219	B8Q	C1'-N1-C6	-2.80	114.79	120.78
1	5	4494	OMG	C5-C6-N1	2.79	120.35	113.25
1	5	3718	A2M	C5-C4-N9	2.78	108.85	105.81
1	5	1797	E7G	C2-N1-C6	-2.78	120.06	125.11
1	5	1316	OMG	N9-C4-N3	2.78	131.51	125.95
1	5	3764	PSU	O2-C2-N1	-2.78	119.92	122.79
1	5	1605	7MG	C2-N1-C6	-2.77	120.08	125.11
1	5	2522	7MG	N9-C8-N7	2.77	107.30	103.37
1	5	4623	OMG	C5-C6-N1	2.77	120.31	113.25
1	5	237	B9B	C5-N7-C8	2.77	107.80	103.45
1	5	3785	A2M	C5-C6-N6	2.76	130.13	123.29
1	5	3867	A2M	N3-C4-N9	2.75	131.85	127.17
1	5	4872	2MG	O6-C6-C5	-2.75	119.27	126.53
1	5	2380	B8W	C5-N7-C8	2.75	107.77	103.45
1	5	4129	B8W	C4-C5-N7	-2.75	107.44	110.58
1	5	4529	B8W	C5-C6-N1	-2.75	119.81	123.49
1	5	1625	OMG	O6-C6-C5	-2.75	119.28	126.53
1	5	4355	E6G	C5-N7-C8	2.74	107.76	103.45
1	5	4129	B8W	C2-N1-C6	2.74	119.78	115.96
1	5	1517	2MG	CM2-N2-C2	-2.74	117.77	123.65
1	5	2424	OMG	O6-C6-C5	-2.73	119.33	126.53
1	5	3825	A2M	N3-C4-N9	2.73	131.80	127.17
1	5	4371	MHG	C21-N2-C2	-2.72	117.80	123.65
51	9	1337	4AC	C6-C5-C4	2.72	120.28	117.00
1	5	1677	PSU	O2-C2-N1	-2.72	119.98	122.79
1	5	1866	UR3	O2-C2-N3	-2.72	117.57	121.33
1	5	4623	OMG	O6-C6-C5	-2.72	119.36	126.53
1	5	373	OMG	C5-C6-N1	2.71	120.16	113.25
1	5	729	2MG	C5-C6-N1	2.71	120.16	113.25
1	5	4494	OMG	N9-C4-N3	2.71	131.38	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4129	B8W	C3'-C2'-C1'	2.71	106.58	101.46
1	5	4415	1MA	N9-C8-N7	-2.70	108.40	113.40
1	5	4185	B8W	O4'-C4'-C3'	-2.70	99.80	105.15
1	5	2508	PSU	O2-C2-N1	-2.70	120.01	122.79
1	5	4472	B8W	C4-C5-N7	-2.69	107.50	110.58
1	5	4690	B8K	C2-N1-C6	-2.69	120.23	125.11
51	9	1243	PSU	C4-N3-C2	-2.69	122.66	126.37
49	v	715	DDE	CAU-CBW-CBI	-2.69	105.96	111.22
1	5	4293	PSU	C6-N1-C2	-2.69	120.20	122.69
1	5	4472	B8W	O6-C6-N1	-2.68	115.39	118.96
1	5	4370	OMG	C5-C6-N1	2.68	120.08	113.25
1	5	2363	A2M	C5-N7-C8	2.68	107.67	103.45
1	5	4637	OMG	C5-C6-N1	2.68	120.08	113.25
1	5	4620	OMU	O2-C2-N1	-2.68	119.31	122.80
51	9	1678	A2M	C5-N7-C8	2.68	107.66	103.45
1	5	4870	OMG	C5-C6-N1	2.68	120.07	113.25
1	5	1582	PSU	C6-N1-C2	-2.68	120.20	122.69
1	5	1625	OMG	C5-C6-N1	2.68	120.07	113.25
1	5	237	B9B	C2-N3-C4	2.68	120.68	113.51
1	5	4371	MHG	O6-C6-C5	-2.67	121.06	127.62
1	5	3899	BGH	C2-N1-C6	-2.67	120.27	125.11
1	5	4306	OMU	O4-C4-C5	-2.66	120.57	125.16
1	5	3718	A2M	N9-C8-N7	-2.66	110.16	113.94
1	5	1316	OMG	O6-C6-C5	-2.66	119.51	126.53
1	5	2754	B9B	C5-N7-C8	2.66	107.62	103.45
1	5	3715	PSU	O2-C2-N1	-2.65	120.05	122.79
1	5	2050	OMG	O6-C6-C5	-2.64	119.55	126.53
1	5	4196	OMG	O6-C6-C5	-2.64	119.57	126.53
1	5	4355	E6G	C5-C6-N1	-2.63	119.97	123.49
1	5	4293	PSU	O2-C2-N1	-2.62	120.08	122.79
1	5	1322	1MA	C1'-N9-C4	-2.62	118.74	126.49
1	5	3792	OMG	C1'-N9-C8	-2.62	119.29	126.73
1	5	3718	A2M	N3-C4-N9	2.62	131.62	127.17
1	5	373	OMG	CM2-O2'-C2'	-2.61	107.77	114.47
1	5	373	OMG	O6-C6-C5	-2.61	119.64	126.53
1	5	2380	B8W	C4'-O4'-C1'	-2.61	103.70	109.47
1	5	3880	P7G	N9-C8-N7	2.61	107.06	103.37
1	5	2773	OMG	C5-C6-N1	2.61	119.89	113.25
1	5	2050	OMG	C5-C6-N1	2.60	119.87	113.25
1	5	2401	A2M	C5-N7-C8	2.59	107.53	103.45
1	5	3792	OMG	O6-C6-C5	-2.59	119.69	126.53
1	5	4403	PSU	C6-N1-C2	-2.59	120.29	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3825	A2M	C5-N7-C8	2.59	107.51	103.45
1	5	4472	B8W	C5-C6-N1	-2.58	120.03	123.49
1	5	4531	PSU	C6-N1-C2	-2.58	120.30	122.69
1	5	4536	OMC	O2-C2-N3	-2.58	118.26	122.33
3	8	14	OMU	CM2-O2'-C2'	2.58	121.10	114.47
1	5	3897	B8K	C2-N1-C6	-2.57	120.44	125.11
1	5	4564	M7A	C71-N7-C5	-2.57	112.72	123.44
1	5	4083	5MU	O4-C4-N3	-2.57	115.28	120.11
1	5	1797	E7G	N9-C8-N7	2.56	107.00	103.37
1	5	2786	B9H	C1'-N1-C2	2.56	121.23	117.04
1	5	4370	OMG	O6-C6-C5	-2.56	119.78	126.53
1	5	4220	6MZ	C4-N9-C1'	-2.55	120.66	126.63
1	5	4872	2MG	C5-C4-N9	2.55	110.23	105.66
1	5	4872	2MG	C4-C5-N7	-2.55	106.63	110.67
1	5	729	2MG	O6-C6-C5	-2.55	119.80	126.53
1	5	1524	A2M	C2'-C1'-N9	-2.55	109.56	113.75
1	5	1582	PSU	O2-C2-N1	-2.55	120.16	122.79
1	5	1524	A2M	C5-N7-C8	2.55	107.45	103.45
1	5	4529	B8W	C4-N9-C8	2.54	108.41	105.74
1	5	2754	B9B	C4-N9-C8	2.54	108.41	105.74
1	5	4472	B8W	C2-N1-C6	2.54	119.50	115.96
1	5	1574	B9B	C4-N9-C8	2.54	108.41	105.74
1	5	4355	E6G	C2-N3-C4	2.54	120.32	113.51
1	5	4636	PSU	C6-C5-C4	2.53	119.88	118.17
1	5	4571	A2M	C5-N7-C8	2.53	107.43	103.45
1	5	1326	A2M	C5-N7-C8	2.53	107.42	103.45
1	5	4185	B8W	C2'-C1'-N9	-2.52	107.03	113.30
1	5	2754	B9B	C2-N3-C4	2.52	120.26	113.51
1	5	729	2MG	N9-C8-N7	-2.52	108.73	113.40
1	5	4472	B8W	C4'-O4'-C1'	-2.52	103.91	109.47
1	5	1860	B8H	O4-C4-N3	-2.52	115.38	120.11
1	5	3867	A2M	C5-N7-C8	2.51	107.40	103.45
1	5	2773	OMG	O6-C6-C5	-2.51	119.90	126.53
1	5	4523	A2M	N3-C4-N9	2.51	131.44	127.17
1	5	4550	7MG	N9-C8-N7	2.51	106.92	103.37
1	5	4523	A2M	C5-N7-C8	2.51	107.39	103.45
1	5	4523	A2M	C5-C4-N9	2.50	108.54	105.81
1	5	4296	B8H	O4-C4-N3	-2.48	115.45	120.11
1	5	398	A2M	C5-N7-C8	2.48	107.35	103.45
1	5	4531	PSU	C6-C5-C4	2.48	119.84	118.17
1	5	4129	B8W	C4-N9-C8	2.48	108.34	105.74
51	9	1337	4AC	C5-C4-N3	-2.47	118.73	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3718	A2M	C6-C5-C4	2.47	120.55	117.18
1	5	1456	B8Q	C31-N3-C2	2.46	121.57	117.70
1	5	3723	A2M	C5-N7-C8	2.46	107.32	103.45
1	5	1659	I4U	C5'-C4'-C3'	-2.46	106.36	115.21
1	5	4185	B8W	C5-C4-N9	2.46	108.49	105.81
1	5	1797	E7G	O6-C6-C5	-2.46	121.59	127.62
1	5	4690	B8K	O6-C6-C5	-2.46	121.59	127.62
1	5	4415	1MA	C1'-N9-C4	-2.45	119.25	126.49
1	5	4494	OMG	O6-C6-C5	-2.45	120.07	126.53
3	8	14	OMU	C1'-N1-C2	2.44	121.98	117.59
1	5	2297	E7G	O6-C6-C5	-2.44	121.62	127.62
1	5	1871	A2M	C5-N7-C8	2.43	107.27	103.45
1	5	3897	B8K	O6-C6-C5	-2.43	121.66	127.62
1	5	3897	B8K	O4'-C1'-C2'	-2.42	101.43	106.62
1	5	4637	OMG	O6-C6-C5	-2.42	120.14	126.53
1	5	4523	A2M	O4'-C1'-N9	2.42	112.73	108.09
1	5	1522	OMG	O6-C6-C5	-2.41	120.17	126.53
1	5	3762	B8H	O4-C4-N3	-2.41	115.59	120.11
1	5	1625	OMG	C1'-N9-C8	-2.41	119.89	126.73
1	5	3785	A2M	C5-N7-C8	2.41	107.23	103.45
1	5	237	B9B	C3'-C2'-C1'	2.40	106.01	101.46
1	5	1574	B9B	C2-N3-C4	2.40	119.95	113.51
1	5	4483	B8T	O2-C2-N3	-2.40	118.54	122.33
1	5	2773	OMG	C1'-N9-C8	-2.40	119.91	126.73
1	5	4671	B8T	C6-C5-C4	2.40	119.89	117.00
1	5	1517	2MG	N9-C8-N7	-2.40	108.95	113.40
1	5	4564	M7A	C5-C4-N3	-2.39	121.03	126.56
1	5	4185	B8W	C3'-C2'-C1'	2.39	105.99	101.46
1	5	2754	B9B	O6-C6-C5	2.39	119.89	116.73
1	5	3867	A2M	C4-N9-C8	2.39	108.24	105.74
1	5	1605	7MG	O6-C6-C5	-2.38	121.78	127.62
1	5	4129	B8W	C2-N3-C4	2.38	119.88	113.51
51	9	1374	5MC	O2-C2-N3	-2.37	118.59	122.33
51	9	1248	B8N	O4'-C1'-C2'	2.36	108.42	105.15
1	5	4450	PSU	O2-C2-N1	-2.36	120.35	122.79
1	5	4403	PSU	O4'-C1'-C2'	2.36	108.42	105.15
51	9	1243	PSU	O2-C2-N1	-2.35	120.36	122.79
1	5	1574	B9B	C4-C5-N7	-2.34	107.90	110.58
51	9	1678	A2M	C4-N9-C8	2.34	108.20	105.74
1	5	4306	OMU	O2-C2-N1	-2.34	119.75	122.80
1	5	2297	E7G	N9-C4-N3	2.34	128.89	125.46
1	5	1797	E7G	N9-C4-N3	2.34	128.88	125.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4523	A2M	C2'-C1'-N9	-2.33	109.91	113.75
1	5	4872	2MG	C6-C5-N7	2.33	134.53	130.29
1	5	4564	M7A	N9-C8-N7	-2.33	100.08	103.37
1	5	2522	7MG	C2-N1-C6	-2.32	120.91	125.11
1	5	2401	A2M	C4-N9-C8	2.31	108.17	105.74
1	5	2380	B8W	C2-N1-C6	2.31	119.17	115.96
1	5	4403	PSU	O2-C2-N1	-2.30	120.42	122.79
1	5	4129	B8W	C5-C6-N1	-2.29	120.42	123.49
1	5	4550	7MG	C2-N1-C6	-2.29	120.95	125.11
1	5	4571	A2M	C4-N9-C8	2.29	108.14	105.74
1	5	4500	PSU	C6-N1-C2	-2.28	120.57	122.69
1	5	1316	OMG	C8-N7-C5	2.28	108.33	104.26
1	5	3897	B8K	O3'-C3'-C4'	-2.28	104.54	111.08
1	5	4529	B8W	C2-N3-C4	2.28	119.61	113.51
1	5	4637	OMG	C8-N7-C5	2.28	108.32	104.26
1	5	3899	BGH	O6-C6-N1	-2.28	115.83	120.11
1	5	1348	P4U	C1'-N1-C2	2.27	123.45	118.44
1	5	4415	1MA	N9-C4-N3	2.27	132.07	126.90
1	5	4472	B8W	C2-N3-C4	2.27	119.58	113.51
1	5	4335	5MC	C1'-N1-C6	-2.26	117.42	121.15
1	5	237	B9B	C4-N9-C8	2.26	108.11	105.74
1	5	1677	PSU	C6-C5-C4	2.26	119.70	118.17
1	5	1534	A2M	C5-N7-C8	2.26	107.00	103.45
51	9	1219	B8Q	C31-N3-C2	2.26	121.25	117.70
1	5	3825	A2M	C4-C5-N7	-2.25	108.00	110.58
1	5	2786	B9H	O2-C2-N1	-2.25	117.76	122.78
1	5	2380	B8W	C2-N3-C4	2.25	119.54	113.51
1	5	3715	PSU	C6-N1-C2	-2.25	120.60	122.69
1	5	2422	OMC	O2-C2-N3	-2.24	118.80	122.33
1	5	1322	1MA	C1'-N9-C8	2.24	133.09	126.73
1	5	1677	PSU	C6-N1-C2	-2.24	120.61	122.69
1	5	4870	OMG	O6-C6-C5	-2.24	120.63	126.53
1	5	3899	BGH	C5'-C4'-C3'	-2.23	107.17	115.21
1	5	2297	E7G	N9-C8-N7	2.23	106.53	103.37
1	5	3887	OMC	O2-C2-N3	-2.23	118.82	122.33
1	5	4194	I4U	O4'-C1'-C2'	-2.22	101.86	106.62
1	5	4529	B8W	C5'-C4'-C3'	-2.22	107.21	115.21
1	5	4872	2MG	C8-N7-C5	2.22	108.22	104.26
1	5	2363	A2M	C3'-C2'-C1'	2.22	107.06	102.81
1	5	2522	7MG	O6-C6-C5	-2.22	122.17	127.62
1	5	1524	A2M	C4-N9-C8	2.22	108.07	105.74
1	5	1605	7MG	N9-C4-N3	2.21	128.71	125.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4494	OMG	C8-N7-C5	2.21	108.20	104.26
1	5	237	B9B	C2-N1-C6	2.21	119.03	115.96
1	5	3825	A2M	C4-N9-C8	2.20	108.05	105.74
1	5	4447	5MC	CM5-C5-C4	-2.20	116.89	120.51
1	5	237	B9B	C61-O6-C6	-2.20	113.83	117.66
1	5	4483	B8T	C6-C5-C4	2.19	119.64	117.00
1	5	1522	OMG	C8-N7-C5	2.19	108.16	104.26
1	5	4415	1MA	C1'-N9-C8	2.19	132.95	126.73
1	5	4185	B8W	C2-N3-C4	2.19	119.37	113.51
1	5	2754	B9B	C4-N9-C1'	-2.18	121.53	126.63
1	5	4472	B8W	O4'-C4'-C3'	-2.17	100.84	105.15
1	5	3825	A2M	C5-C4-N9	2.17	108.17	105.81
1	5	1517	2MG	N1-C2-N3	-2.16	120.03	123.68
1	5	2050	OMG	C8-N7-C5	2.16	108.11	104.26
1	5	4129	B8W	C5-C4-N9	2.16	108.16	105.81
3	8	14	OMU	O2-C2-N1	-2.15	120.00	122.80
1	5	4450	PSU	C6-N1-C2	-2.15	120.70	122.69
1	5	4571	A2M	C5'-C4'-C3'	-2.15	107.48	115.21
1	5	3785	A2M	C6-C5-C4	2.14	120.10	117.18
1	5	1326	A2M	C5-C4-N9	2.13	108.14	105.81
1	5	1871	A2M	C5-C4-N9	2.12	108.13	105.81
1	5	2522	7MG	C6-C5-C4	-2.12	118.67	122.40
1	5	4494	OMG	C2'-C1'-N9	-2.12	110.21	114.24
1	5	2861	OMC	C1'-N1-C2	2.11	123.11	118.44
1	5	4355	E6G	C6-C5-N7	-2.11	131.34	133.82
1	5	1534	A2M	C5-C4-N9	2.11	108.11	105.81
1	5	4870	OMG	C8-N7-C5	2.11	108.02	104.26
1	5	4355	E6G	C61-O6-C6	-2.11	115.48	117.57
1	5	1574	B9B	C2-N1-C6	2.11	118.89	115.96
1	5	4523	A2M	C4-C5-N7	-2.10	108.18	110.58
1	5	4628	PSU	C6-C5-C4	2.10	119.59	118.17
1	5	4550	7MG	O6-C6-C5	-2.10	122.47	127.62
1	5	4571	A2M	C2'-C1'-N9	-2.09	110.32	113.75
51	9	1337	4AC	O2-C2-N3	-2.08	119.04	122.33
1	5	1574	B9B	C5-C4-N9	2.08	108.08	105.81
51	9	1337	4AC	O7-C7-CM7	-2.08	118.35	122.05
1	5	2363	A2M	C4-C5-N7	-2.08	108.20	110.58
1	5	1871	A2M	C6-C5-C4	2.08	120.02	117.18
1	5	1605	7MG	C6-C5-C4	-2.08	118.75	122.40
1	5	3792	OMG	C8-N7-C5	2.08	107.96	104.26
1	5	4623	OMG	C8-N7-C5	2.07	107.95	104.26
1	5	4529	B8W	C5-C4-N9	2.07	108.07	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1678	A2M	C6-C5-C4	2.07	120.00	117.18
1	5	4872	2MG	N1-C2-N3	-2.07	120.20	123.68
1	5	1574	B9B	C1'-N9-C8	2.06	131.66	127.09
1	5	1677	PSU	O4'-C1'-C2'	2.06	108.00	105.15
1	5	4355	E6G	C4-N9-C8	2.05	107.89	105.74
1	5	4371	MHG	C6-C5-C4	-2.05	118.80	122.40
1	5	3899	BGH	N1-C2-N3	-2.04	119.59	123.32
1	5	2522	7MG	N1-C2-N3	-2.04	119.59	123.32
1	5	4690	B8K	C3'-C2'-C1'	2.04	105.31	101.46
1	5	4690	B8K	N1-C2-N3	-2.04	119.60	123.32
1	5	398	A2M	C6-C5-C4	2.03	119.96	117.18
1	5	2380	B8W	C5-C6-N1	-2.03	120.77	123.49
1	5	4196	OMG	C8-N7-C5	2.03	107.88	104.26
1	5	3723	A2M	C6-C5-C4	2.03	119.95	117.18
1	5	1797	E7G	C6-C5-C4	-2.03	118.83	122.40
1	5	4550	7MG	C6-C5-C4	-2.03	118.83	122.40
1	5	2363	A2M	C5-C4-N9	2.02	108.01	105.81
1	5	4371	MHG	N9-C8-N7	2.01	106.22	103.37
1	5	2422	OMC	C1'-N1-C2	2.01	122.88	118.44
51	9	1678	A2M	C4-C5-N7	-2.01	108.29	110.58
1	5	373	OMG	C8-N7-C5	2.01	107.84	104.26
1	5	4636	PSU	C6-N1-C2	-2.00	120.83	122.69
1	5	4550	7MG	N1-C2-N3	-2.00	119.65	123.32
1	5	3785	A2M	C4-N9-C8	2.00	107.84	105.74
1	5	1534	A2M	C6-C5-C4	2.00	119.91	117.18
1	5	4530	UR3	C1'-N1-C2	2.00	120.31	117.04

There are no chirality outliers.

All (155) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	333	MLZ	N-CA-CB-CG
6	C	333	MLZ	C-CA-CB-CG
49	v	715	DDE	O-C-CA-CB
49	v	715	DDE	CA-CB-CG-ND1
49	v	715	DDE	CBI-CBW-NCB-CAC
49	v	715	DDE	CBI-CBW-NCB-CAA
49	v	715	DDE	CAU-CBW-NCB-CAB
49	v	715	DDE	CAU-CBW-NCB-CAC
49	v	715	DDE	CAU-CBW-NCB-CAA
49	v	715	DDE	CAT-CAU-CBW-CBI
49	v	715	DDE	CAT-CAU-CBW-NCB

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Mol	Chain	Res	Type	Atoms
1	5	237	B9B	C5-C6-O6-C61
1	5	237	B9B	N1-C6-O6-C61
1	5	237	B9B	C3'-C4'-C5'-O5'
1	5	237	B9B	O4'-C4'-C5'-O5'
1	5	1348	P4U	N3-C4-O4-C41
1	5	1348	P4U	O4'-C4'-C5'-O5'
1	5	1574	B9B	C5-C6-O6-C61
1	5	1574	B9B	N1-C6-O6-C61
1	5	1909	P7G	C72-C71-N7-C5
1	5	2364	OMG	O4'-C4'-C5'-O5'
1	5	2380	B8W	C5-C6-O6-C61
1	5	2424	OMG	O4'-C4'-C5'-O5'
1	5	2773	OMG	O4'-C4'-C5'-O5'
1	5	2773	OMG	C3'-C4'-C5'-O5'
1	5	2786	B9H	C32-C31-N3-C2
1	5	3701	OMC	C2'-C1'-N1-C6
1	5	3762	B8H	O4'-C4'-C5'-O5'
1	5	3792	OMG	O4'-C4'-C5'-O5'
1	5	3880	P7G	O4'-C4'-C5'-O5'
1	5	3897	B8K	O4'-C4'-C5'-O5'
1	5	3899	BGH	C3'-C4'-C5'-O5'
1	5	3899	BGH	O4'-C4'-C5'-O5'
1	5	4129	B8W	C5-C6-O6-C61
1	5	4129	B8W	N1-C6-O6-C61
1	5	4185	B8W	C5-C6-O6-C61
1	5	4185	B8W	N1-C6-O6-C61
1	5	4194	I4U	O4'-C4'-C5'-O5'
1	5	4355	E6G	C5-C6-O6-C61
1	5	4355	E6G	N1-C6-O6-C61
1	5	4403	PSU	O4'-C1'-C5-C4
1	5	4403	PSU	O4'-C1'-C5-C6
1	5	4415	1MA	O4'-C4'-C5'-O5'
1	5	4447	5MC	C2'-C1'-N1-C6
1	5	4472	B8W	C5-C6-O6-C61
1	5	4472	B8W	N1-C6-O6-C61
1	5	4500	PSU	O4'-C4'-C5'-O5'
1	5	4523	A2M	O4'-C4'-C5'-O5'
1	5	4529	B8W	C5-C6-O6-C61
1	5	4529	B8W	N1-C6-O6-C61
1	5	4620	OMU	C1'-C2'-O2'-CM2
1	5	4637	OMG	O4'-C4'-C5'-O5'
1	5	4690	B8K	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	5	4870	OMG	O4'-C4'-C5'-O5'
1	5	4870	OMG	C3'-C4'-C5'-O5'
3	8	14	OMU	C1'-C2'-O2'-CM2
41	m	72	MLZ	N-CA-CB-CG
41	m	72	MLZ	CD-CE-NZ-CM
51	9	1248	B8N	O4'-C4'-C5'-O5'
1	5	3701	OMC	C2'-C1'-N1-C2
1	5	4447	5MC	C2'-C1'-N1-C2
1	5	398	A2M	O4'-C4'-C5'-O5'
1	5	1348	P4U	C3'-C4'-C5'-O5'
1	5	1582	PSU	C3'-C4'-C5'-O5'
1	5	1582	PSU	O4'-C4'-C5'-O5'
1	5	1625	OMG	C3'-C4'-C5'-O5'
1	5	1797	E7G	O4'-C4'-C5'-O5'
1	5	2364	OMG	C3'-C4'-C5'-O5'
1	5	2380	B8W	C3'-C4'-C5'-O5'
1	5	2380	B8W	O4'-C4'-C5'-O5'
1	5	2424	OMG	C3'-C4'-C5'-O5'
1	5	3729	PSU	O4'-C4'-C5'-O5'
1	5	3867	A2M	O4'-C4'-C5'-O5'
1	5	3867	A2M	C3'-C4'-C5'-O5'
1	5	4185	B8W	O4'-C4'-C5'-O5'
1	5	4415	1MA	C3'-C4'-C5'-O5'
1	5	4500	PSU	C3'-C4'-C5'-O5'
1	5	4872	2MG	O4'-C4'-C5'-O5'
51	9	1248	B8N	C3'-C4'-C5'-O5'
1	5	1348	P4U	O4-C41-C42-C43
1	5	2380	B8W	N1-C6-O6-C61
1	5	2786	B9H	O4'-C4'-C5'-O5'
1	5	3792	OMG	C3'-C4'-C5'-O5'
1	5	4371	MHG	O4'-C4'-C5'-O5'
1	5	4530	UR3	O4'-C4'-C5'-O5'
1	5	4530	UR3	C3'-C4'-C5'-O5'
1	5	4636	PSU	C3'-C4'-C5'-O5'
1	5	4636	PSU	O4'-C4'-C5'-O5'
51	9	1243	PSU	C3'-C4'-C5'-O5'
51	9	1243	PSU	O4'-C4'-C5'-O5'
1	5	4371	MHG	C2'-C1'-N9-C8
1	5	3762	B8H	C3'-C4'-C5'-O5'
1	5	3897	B8K	C3'-C4'-C5'-O5'
1	5	4523	A2M	C3'-C4'-C5'-O5'
1	5	4637	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	5	1797	E7G	C3'-C4'-C5'-O5'
1	5	3729	PSU	C3'-C4'-C5'-O5'
1	5	3880	P7G	C3'-C4'-C5'-O5'
1	5	4194	I4U	C3'-C4'-C5'-O5'
1	5	4450	PSU	C3'-C4'-C5'-O5'
1	5	4690	B8K	C3'-C4'-C5'-O5'
49	v	715	DDE	CA-CB-CG-CD2
1	5	729	2MG	O4'-C4'-C5'-O5'
1	5	1625	OMG	O4'-C4'-C5'-O5'
1	5	3785	A2M	O4'-C4'-C5'-O5'
1	5	3785	A2M	C3'-C4'-C5'-O5'
1	5	4450	PSU	O4'-C4'-C5'-O5'
1	5	4872	2MG	C3'-C4'-C5'-O5'
1	5	4371	MHG	C75-C73-C74-C76
1	5	4129	B8W	O4'-C4'-C5'-O5'
1	5	398	A2M	C3'-C4'-C5'-O5'
1	5	4371	MHG	C3'-C4'-C5'-O5'
1	5	2754	B9B	C5-C6-O6-C61
1	5	1909	P7G	C72-C71-N7-C8
1	5	1625	OMG	C4'-C5'-O5'-P
1	5	1866	UR3	O4'-C4'-C5'-O5'
1	5	4355	E6G	O4'-C4'-C5'-O5'
1	5	2297	E7G	C72-C71-N7-C8
49	v	715	DDE	NAD-CBI-CBW-NCB
41	m	72	MLZ	C-CA-CB-CG
51	9	1248	B8N	N3-C31-C32-C33
1	5	3701	OMC	O4'-C1'-N1-C2
1	5	4450	PSU	O4'-C1'-C5-C4
1	5	4500	PSU	O4'-C1'-C5-C4
1	5	2786	B9H	C3'-C4'-C5'-O5'
1	5	2786	B9H	C32-C31-N3-C4
1	5	1659	I4U	C43-C41-O4-C4
1	5	3701	OMC	O4'-C1'-N1-C6
1	5	4447	5MC	O4'-C1'-N1-C6
1	5	2754	B9B	N1-C6-O6-C61
1	5	4447	5MC	O4'-C1'-N1-C2
1	5	1534	A2M	C4'-C5'-O5'-P
1	5	3897	B8K	C4'-C5'-O5'-P
1	5	4870	OMG	C4'-C5'-O5'-P
1	5	373	OMG	C4'-C5'-O5'-P
1	5	3764	PSU	C4'-C5'-O5'-P
1	5	4371	MHG	C72-C73-C74-C76

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Mol	Chain	Res	Type	Atoms
1	5	2380	B8W	C4'-C5'-O5'-P
1	5	2754	B9B	C4'-C5'-O5'-P
1	5	3887	OMC	C4'-C5'-O5'-P
1	5	4371	MHG	C72-C71-N7-C5
1	5	4636	PSU	O4'-C1'-C5-C6
1	5	4370	OMG	C3'-C2'-O2'-CM2
1	5	1659	I4U	C42-C41-O4-C4
1	5	4194	I4U	C43-C41-O4-C4
1	5	3762	B8H	C4'-C5'-O5'-P
1	5	4500	PSU	C4'-C5'-O5'-P
1	5	3880	P7G	N7-C71-C72-C73
1	5	4494	OMG	C3'-C2'-O2'-CM2
1	5	1524	A2M	O4'-C1'-N9-C8
51	9	1219	B8Q	C2'-C1'-N1-C2
1	5	1456	B8Q	C3'-C4'-C5'-O5'
1	5	4371	MHG	C72-C71-N7-C8
1	5	1456	B8Q	O4'-C4'-C5'-O5'
1	5	4536	OMC	C3'-C4'-C5'-O5'

There are no ring outliers.

44 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5	1883	OMG	1	0
1	5	4872	2MG	1	0
1	5	4194	I4U	1	0
6	C	333	MLZ	1	0
1	5	3867	A2M	1	0
1	5	4293	PSU	2	0
1	5	4196	OMG	1	0
1	5	4523	A2M	2	0
1	5	1574	B9B	2	0
51	9	1678	A2M	2	0
1	5	4500	PSU	1	0
1	5	4296	B8H	6	0
1	5	1316	OMG	1	0
1	5	2380	B8W	1	0
1	5	1326	A2M	2	0
1	5	1871	A2M	2	0
1	5	4571	A2M	1	0
1	5	4690	B8K	1	0
1	5	1605	7MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5	1866	UR3	3	0
1	5	4129	B8W	1	0
1	5	2522	7MG	1	0
1	5	1860	B8H	5	0
1	5	3899	BGH	1	0
1	5	2754	B9B	1	0
1	5	729	2MG	1	0
1	5	2363	A2M	1	0
1	5	237	B9B	1	0
1	5	4494	OMG	1	0
41	m	72	MLZ	1	0
1	5	373	OMG	1	0
49	v	715	DDE	2	0
51	9	1337	4AC	1	0
1	5	4620	OMU	1	0
1	5	3785	A2M	1	0
1	5	3897	B8K	1	0
1	5	4564	M7A	1	0
1	5	2422	OMC	1	0
1	5	3762	B8H	6	0
1	5	398	A2M	1	0
1	5	4472	B8W	1	0
51	9	1374	5MC	2	0
1	5	3723	A2M	2	0
1	5	3718	A2M	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 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
87	GDP	v	900	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	9 (20%)

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
87	GDP	v	900	-	-	0/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	v	900	GDP	C5-C4	2.85	1.46	1.38
87	v	900	GDP	C6-N1	-2.72	1.33	1.38
87	v	900	GDP	C5-N7	-2.40	1.34	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	v	900	GDP	C5-C4-N3	-6.04	118.78	128.39
87	v	900	GDP	C2-N3-C4	4.89	120.72	112.30
87	v	900	GDP	N9-C4-N3	4.70	135.35	125.95
87	v	900	GDP	C6-C5-N7	3.07	135.88	130.29
87	v	900	GDP	O6-C6-C5	-2.33	120.38	126.53
87	v	900	GDP	C4-C5-N7	-2.31	107.00	110.67
87	v	900	GDP	C3'-C2'-C1'	2.06	105.36	101.46
87	v	900	GDP	C2'-C1'-N9	-2.06	107.51	113.25
87	v	900	GDP	C5-C6-N1	2.03	118.42	113.25

There are no chirality outliers.

There are no torsion outliers.

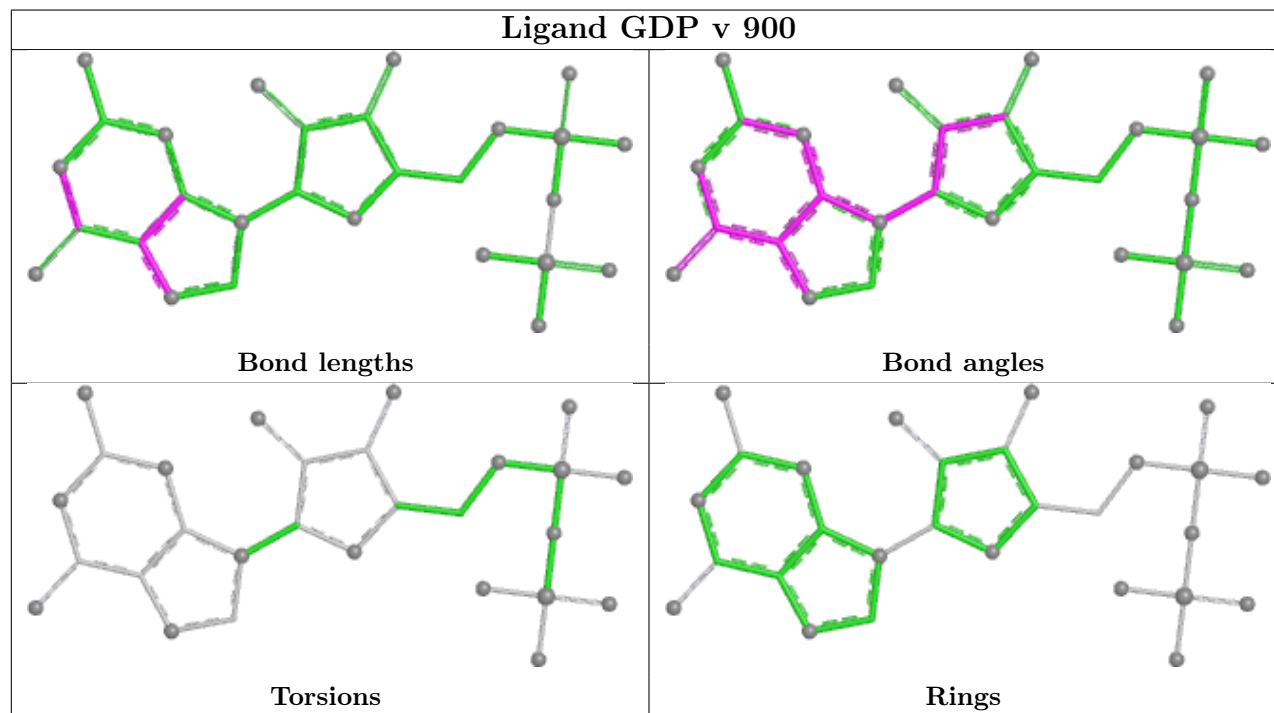
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	v	900	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	47
51	9	19
50	w	1
3	8	1
49	v	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	202:SER	C	282:THR	N	64.88
1	5	2113:G	O3'	2258:C	P	39.97
1	5	1252:C	O3'	1271:G	P	34.48
1	5	1406(C):G	O3'	1411:C	P	20.81
1	5	1405:C	O3'	1406:G	P	20.70
1	5	1219:G	O3'	1233:G	P	19.83
1	5	1411:C	O3'	1411(A):G	P	18.43
1	9	697:G	O3'	729:C	P	18.01
1	5	523:C	O3'	638:G	P	17.61
1	9	756:C	O3'	788:G	P	17.60
1	9	834:C	O3'	841:G	P	17.53
1	9	130:G	O3'	140:U	P	17.46
1	9	1761:U	O3'	1771:G	P	17.14
1	5	4777:C	O3'	4859:C	P	17.02
1	5	4138:C	O3'	4146:G	P	16.97
1	5	990:U	O3'	1064:G	P	16.68
1	9	323:C	O3'	329:G	P	16.58
1	5	4101:C	O3'	4107:G	P	15.93
1	5	3976:C	O3'	4039:G	P	15.04
1	5	1406:G	O3'	1406(A):G	P	14.94
1	9	1417:C	O3'	1423:C	P	14.94
1	5	1696:C	O3'	1720:C	P	14.48
1	5	5022:U	O3'	5028:G	P	14.45
1	5	760:G	O3'	904:C	P	14.02
1	5	922:C	O3'	922(A):G	P	13.55
1	5	1364:U	O3'	1368:A	P	13.55
1	5	2901:G	O3'	3597:G	P	13.23
1	5	182:G	O3'	189:G	P	12.86
1	8	79:G	O3'	85:U	P	12.75
1	5	738:C	O3'	738(A):C	P	12.46
1	v	47:ALA	C	66:ARG	N	12.04
1	5	921:C	O3'	922:C	P	11.51
1	5	922(B):C	O3'	923:C	P	8.98
1	5	4729:A	O3'	4735:G	P	8.54
1	5	1180:C	O3'	1183:C	P	8.41
1	9	225:G	O3'	287:U	P	8.05
1	5	512:U	O3'	515:C	P	8.00
1	5	738(A):C	O3'	739:G	P	7.72
1	5	935:A	O3'	935(A):G	P	7.65
1	5	935(A):G	O3'	936:C	P	7.35
1	9	745:C	O3'	749:U	P	6.96
1	5	3955:A	O3'	3956:G	P	6.68

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	500:G	O3'	504:G	P	6.36
1	5	737:C	O3'	738:C	P	6.23
1	5	481:G	O3'	481(A):C	P	5.81
1	5	480:C	O3'	481:G	P	5.65
1	5	4740:G	O3'	4743:G	P	4.97
1	9	736:C	O3'	743:U	P	4.95
1	9	1432:U	O3'	1438:A	P	4.93
1	5	1239:C	O3'	1244:G	P	4.73
1	9	309:G	O3'	310:C	P	4.66
1	9	322:C	O3'	323:C	P	4.66
1	5	170:C	O3'	171:U	P	4.49
1	5	4055:U	O3'	4056:A	P	4.39
1	5	1100:U	O3'	1168:G	P	4.38
1	5	934:C	O3'	935:A	P	4.26
1	9	304:C	O3'	305:U	P	4.14
1	9	798:G	O3'	799:U	P	4.08
1	5	3945:A	O3'	3946:G	P	3.55
1	5	1438:U	O3'	1440:U	P	3.46
1	5	3947:A	O3'	3948:C	P	3.29
1	9	903:A	O3'	904:A	P	3.25
1	5	751:G	O3'	752:G	P	3.24
1	5	4899:G	O3'	4902:C	P	3.23
1	9	1295:A	O3'	1296:U	P	3.23
1	9	902:G	O3'	903:A	P	3.22
1	5	5020:G	O3'	5021:C	P	3.21
1	9	1686:G	O3'	1687:C	P	3.20
1	5	267:G	O3'	268:G	P	3.16

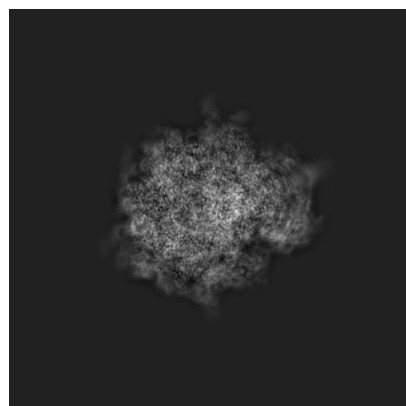
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9240. These allow visual inspection of the internal detail of the map and identification of artifacts.

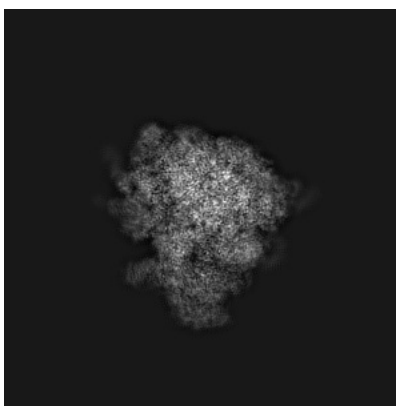
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

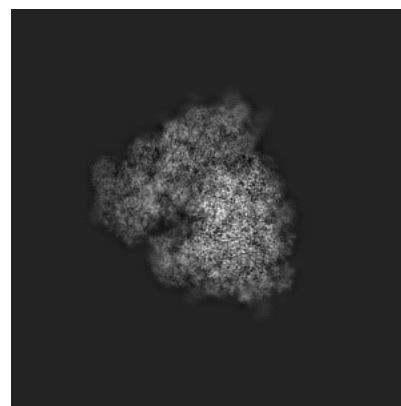
6.1.1 Primary map



X

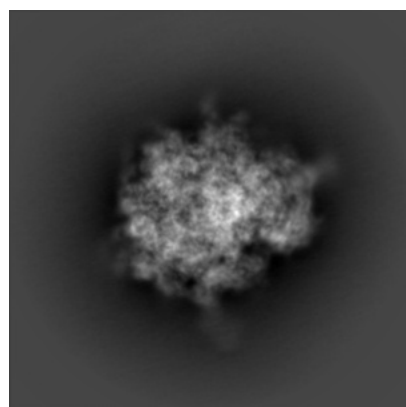


Y

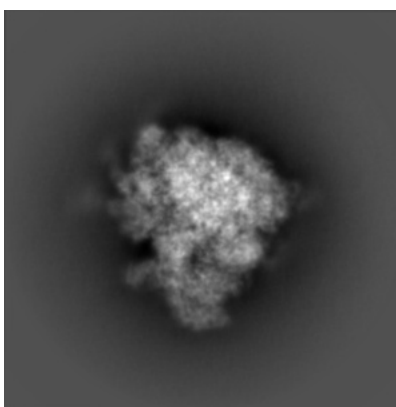


Z

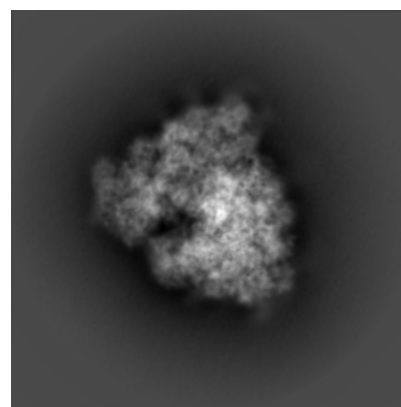
6.1.2 Raw map



X



Y

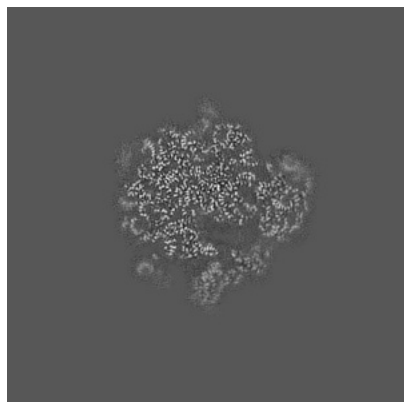


Z

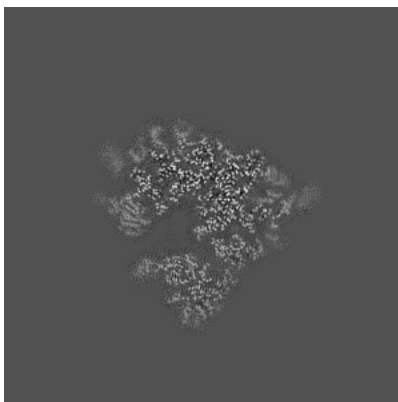
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

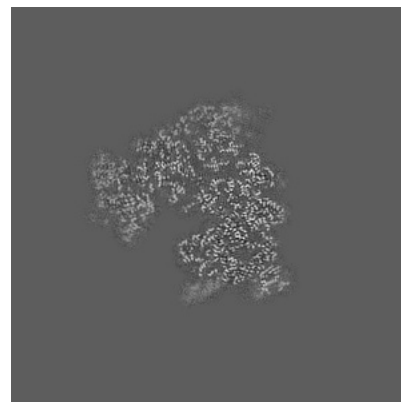
6.2.1 Primary map



X Index: 200

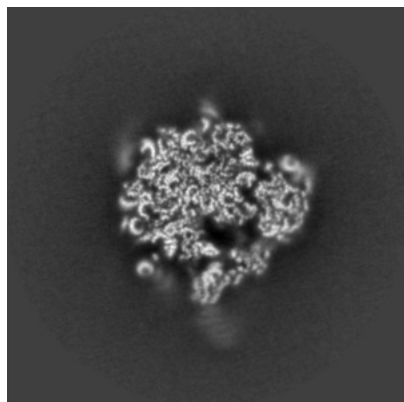


Y Index: 200

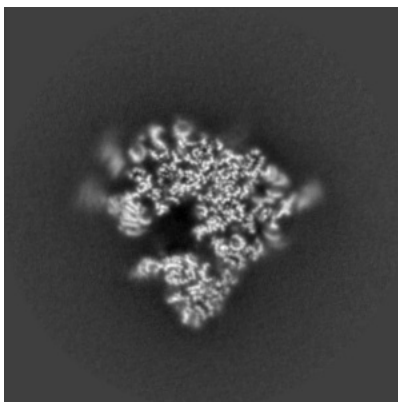


Z Index: 200

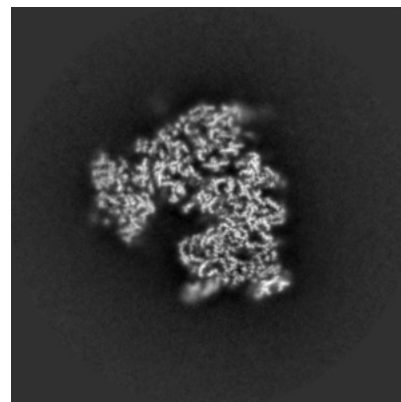
6.2.2 Raw map



X Index: 200



Y Index: 200

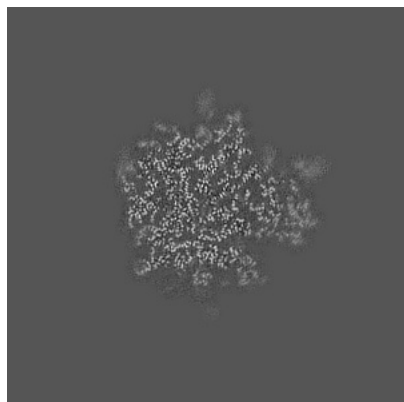


Z Index: 200

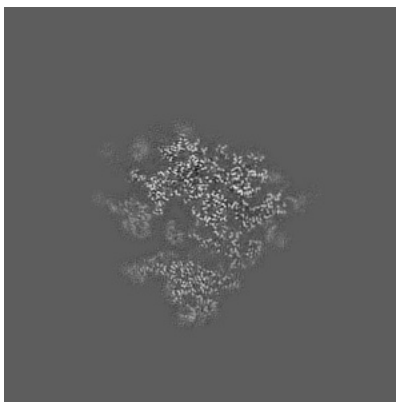
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

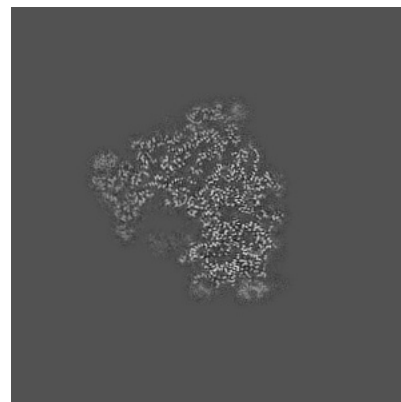
6.3.1 Primary map



X Index: 213

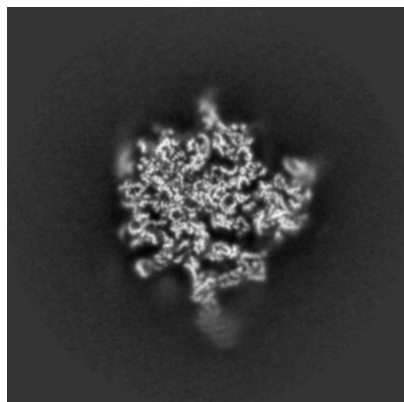


Y Index: 208

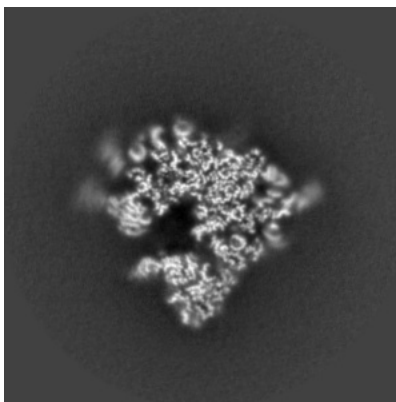


Z Index: 210

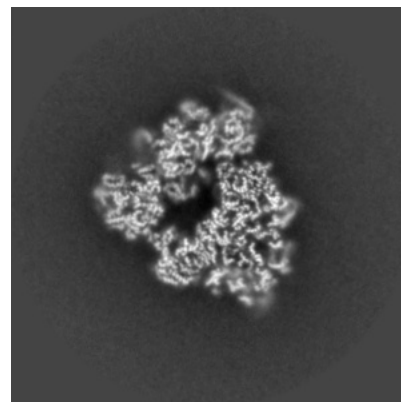
6.3.2 Raw map



X Index: 206



Y Index: 201

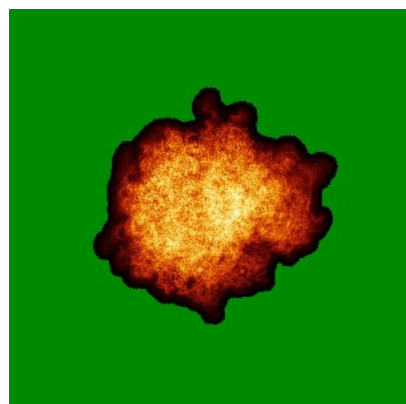


Z Index: 176

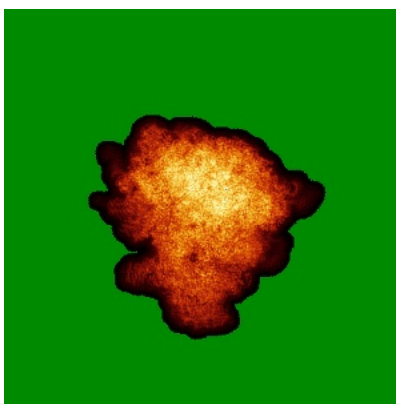
The images above show the largest variance slices of the map in three orthogonal directions.

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

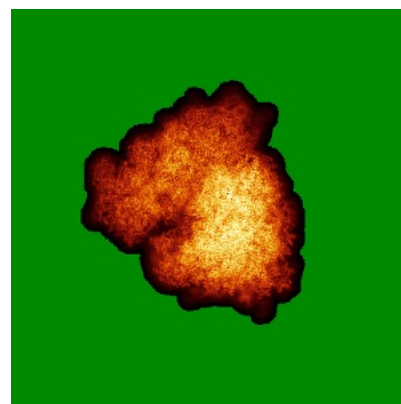
6.4.1 Primary map



X

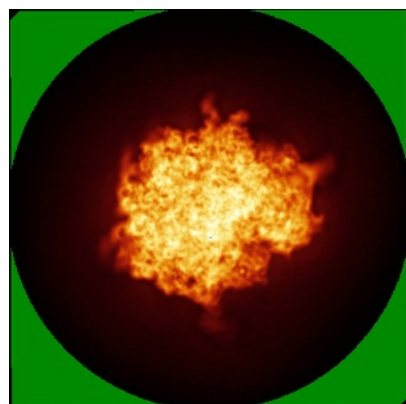


Y

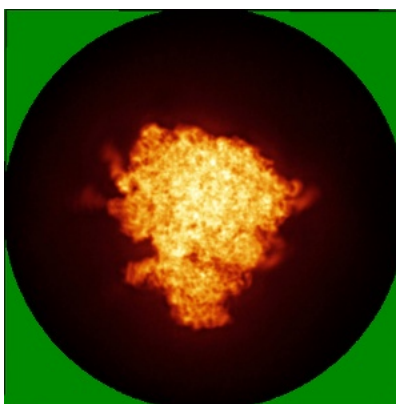


Z

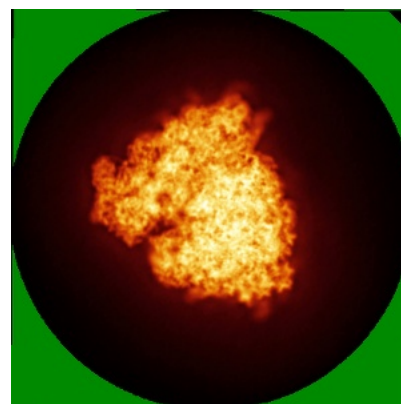
6.4.2 Raw map



X



Y

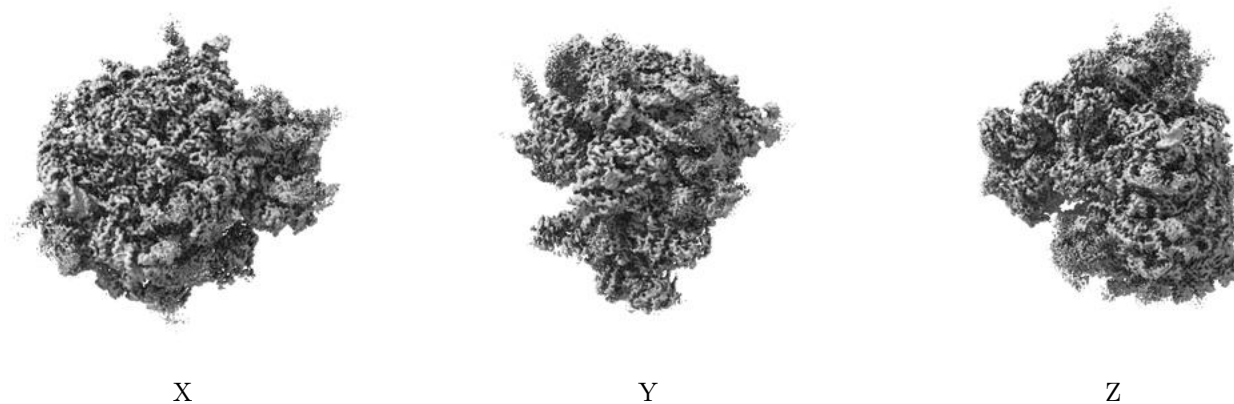


Z

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

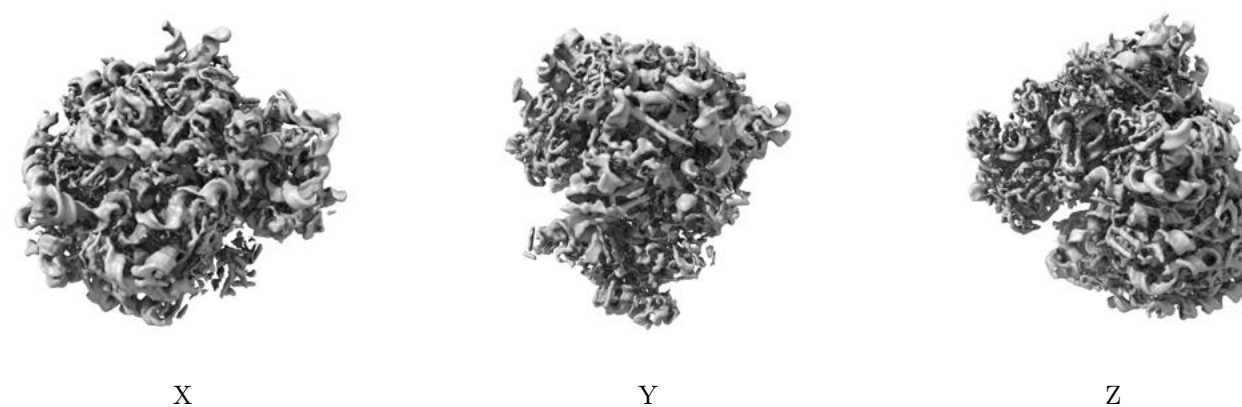
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

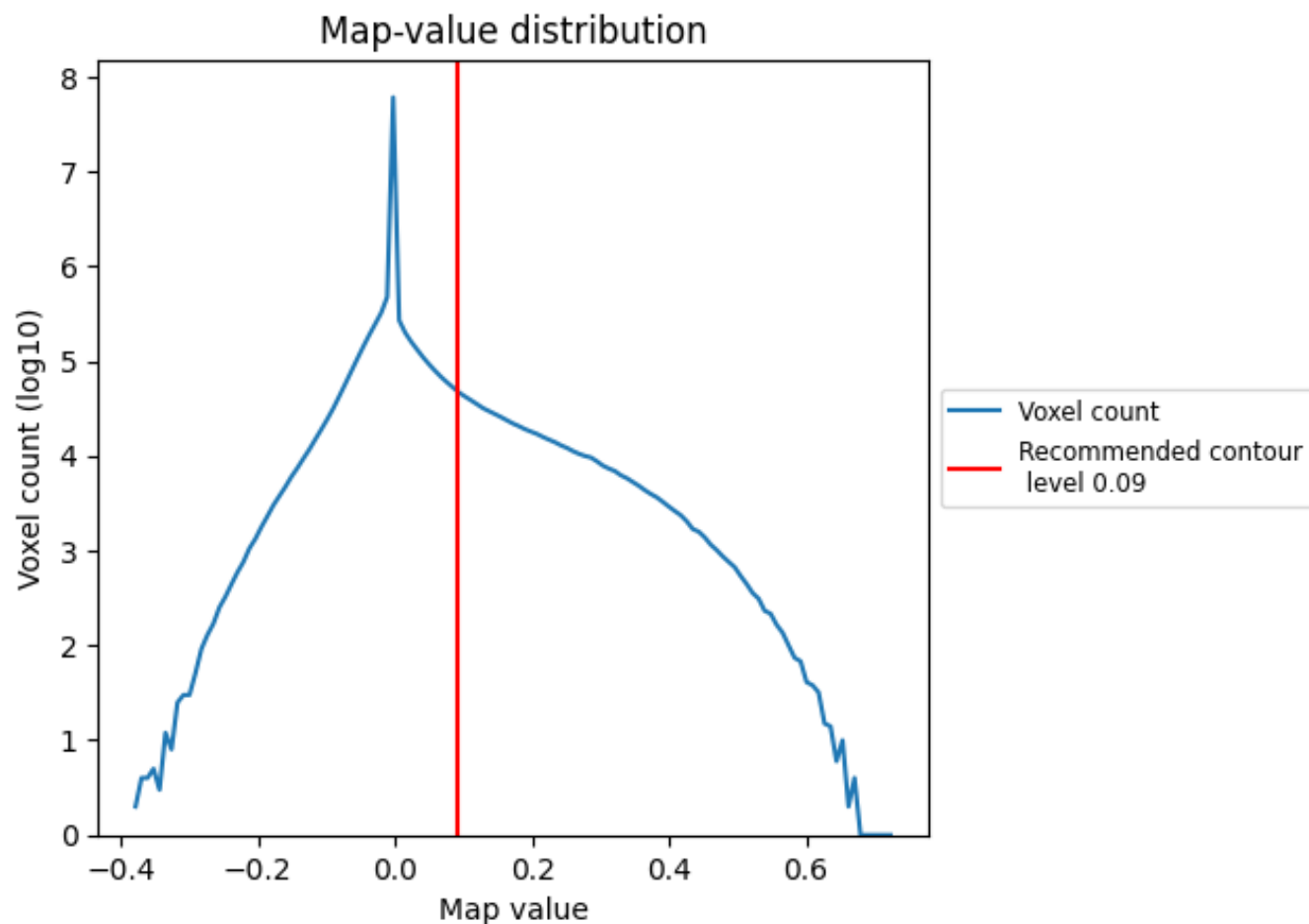
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

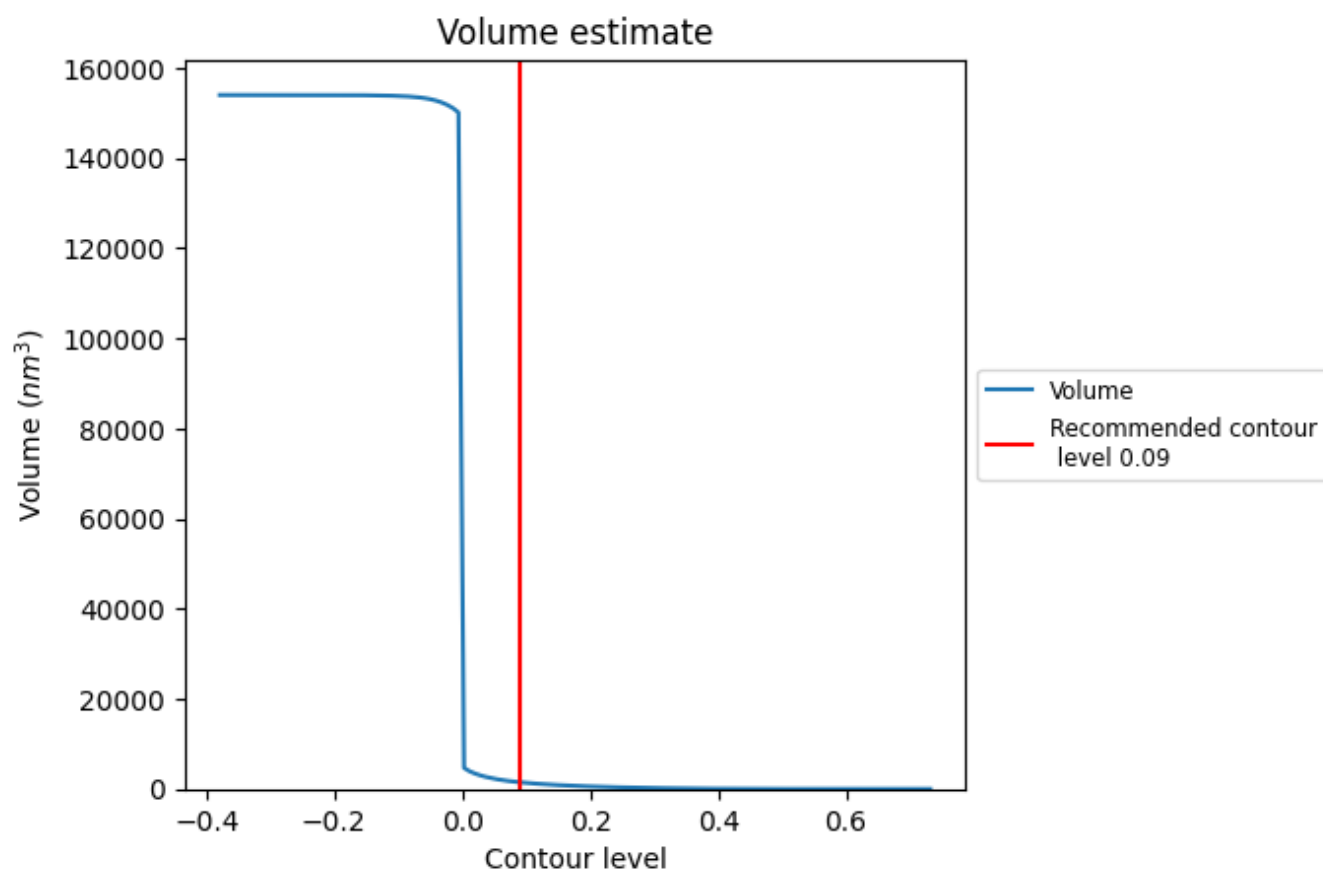
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

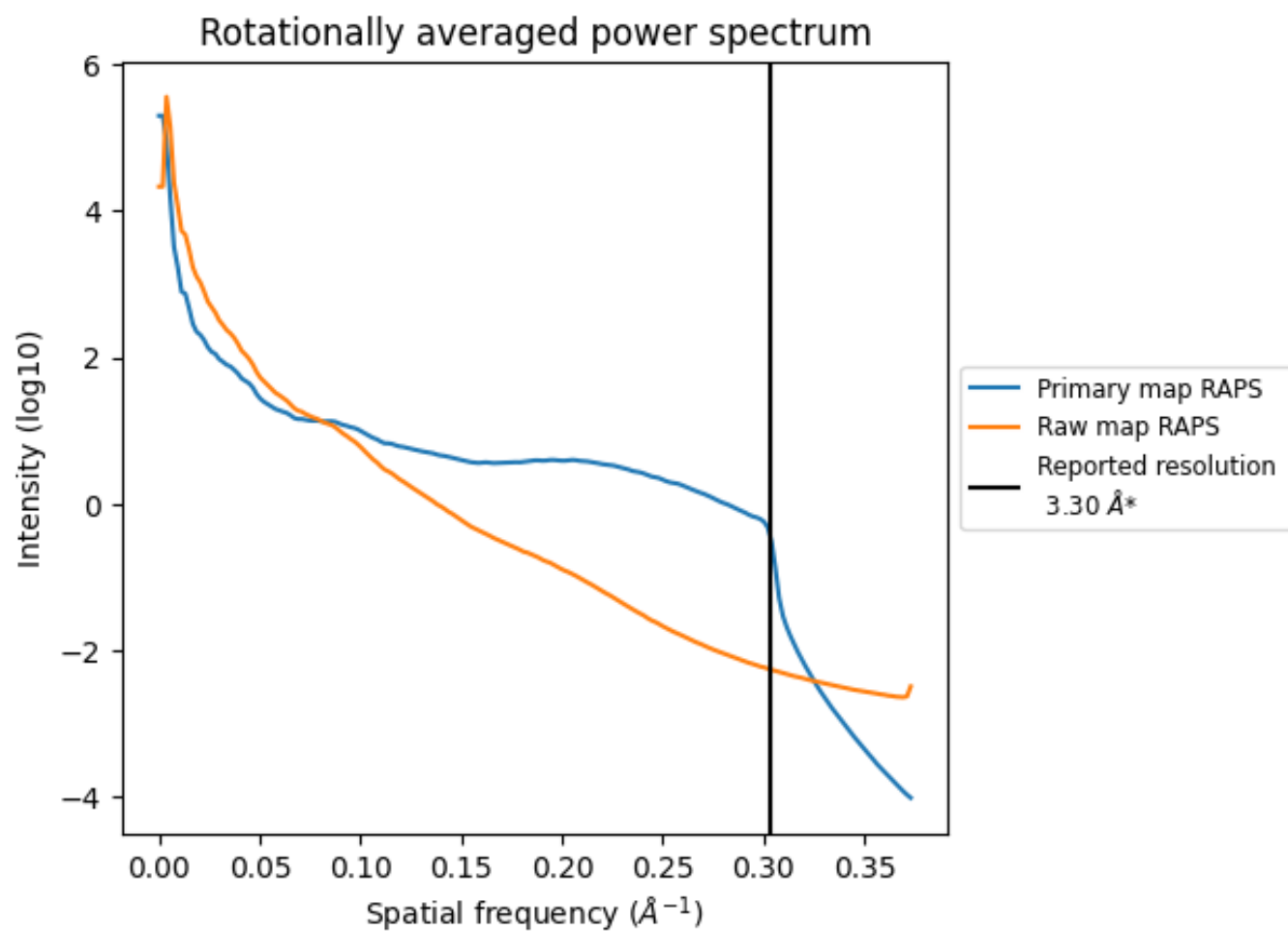
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1483 nm³; this corresponds to an approximate mass of 1340 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 ⓘ

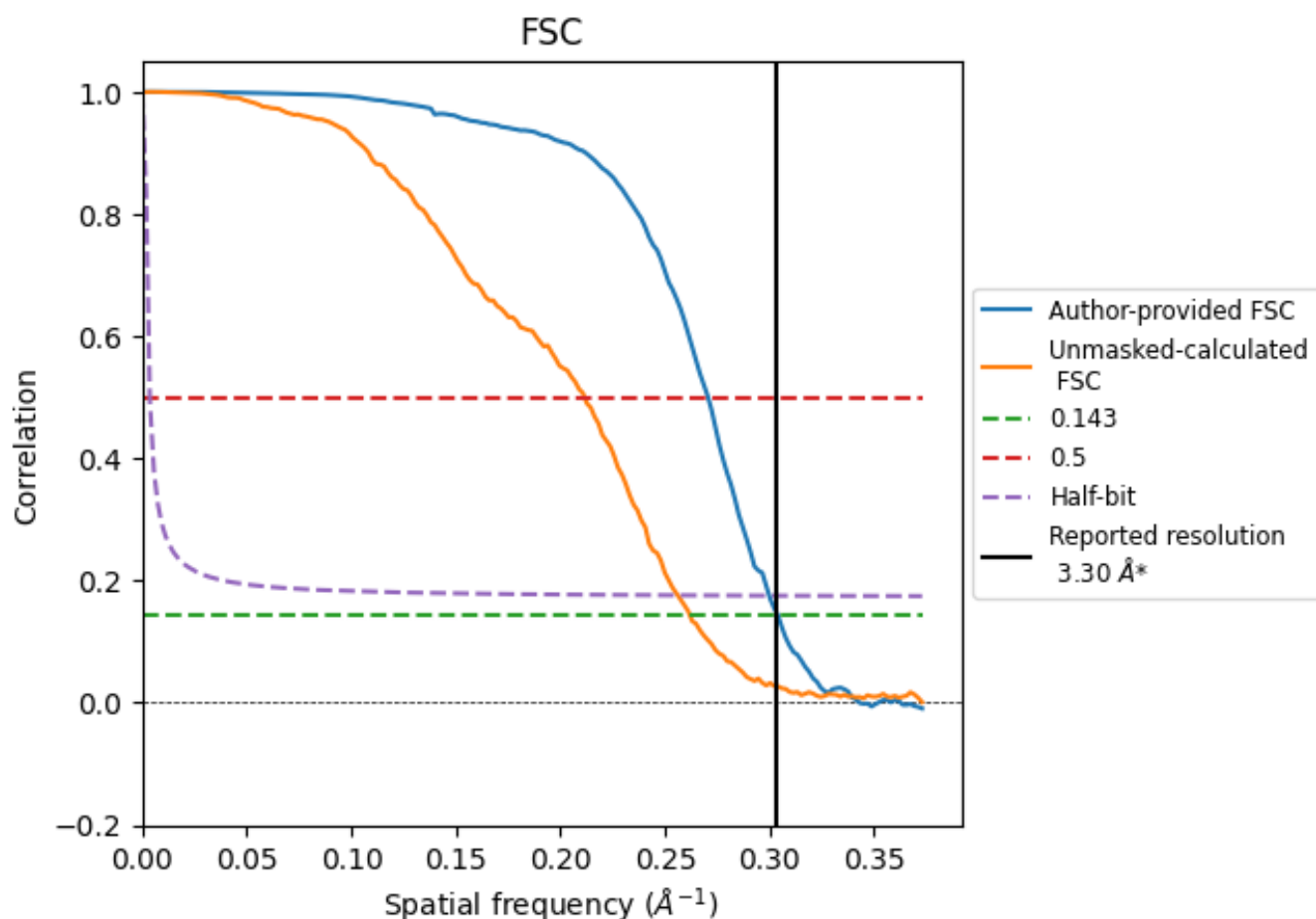


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

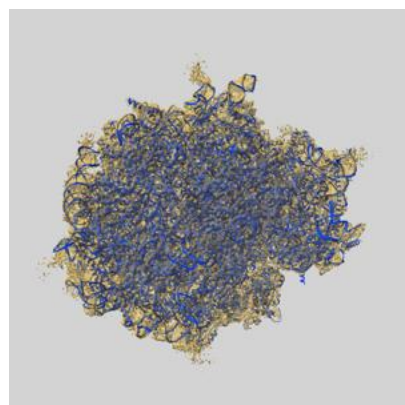
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.69	3.33
Unmasked-calculated*	3.82	4.73	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.3 by more than 10 %

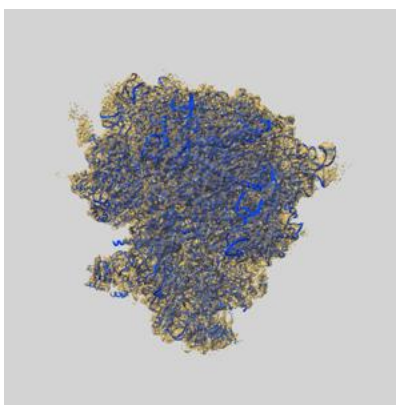
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9240 and PDB model 6MTD. Per-residue inclusion information can be found in section [3](#) on page [21](#).

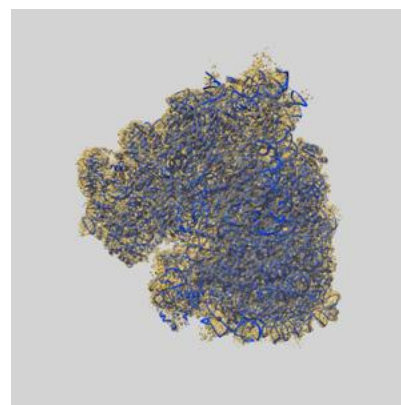
9.1 Map-model overlay [i](#)



X



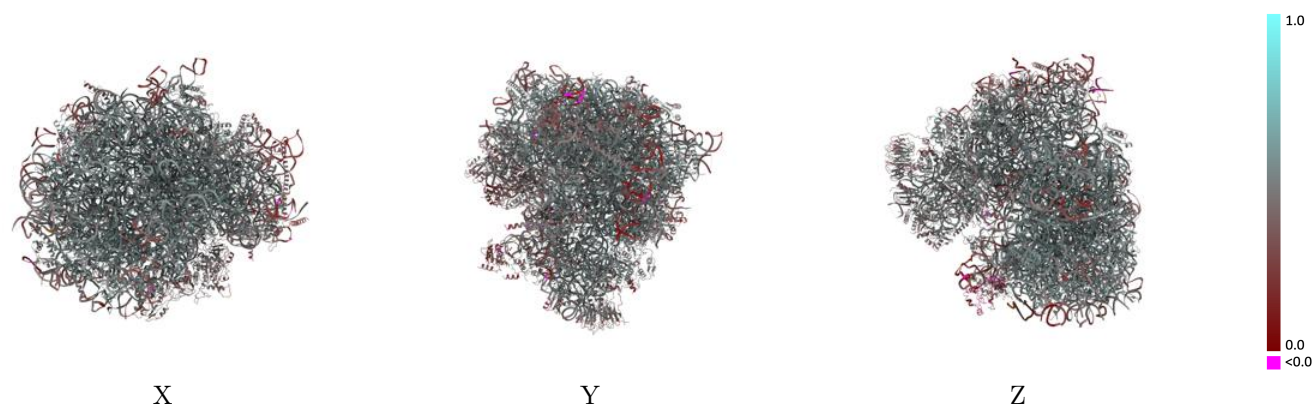
Y



Z

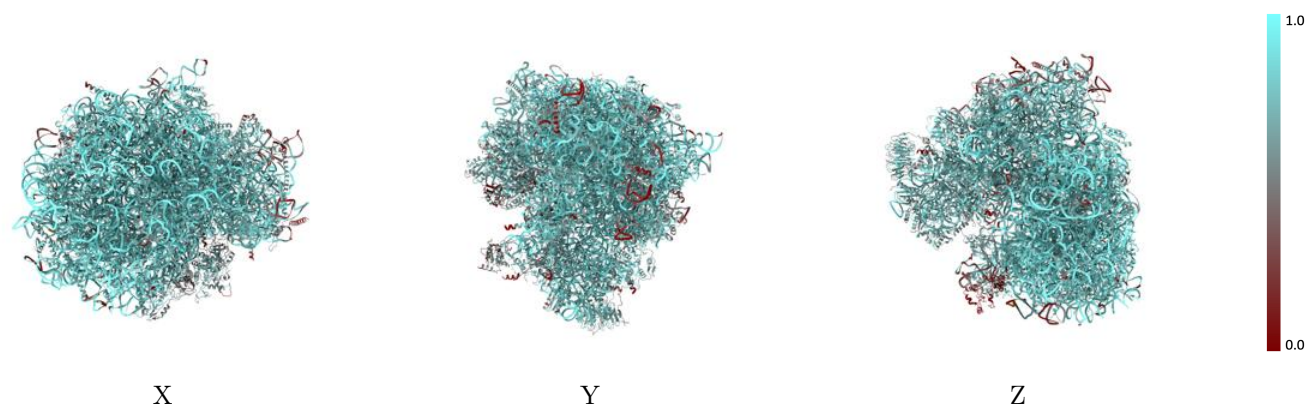
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



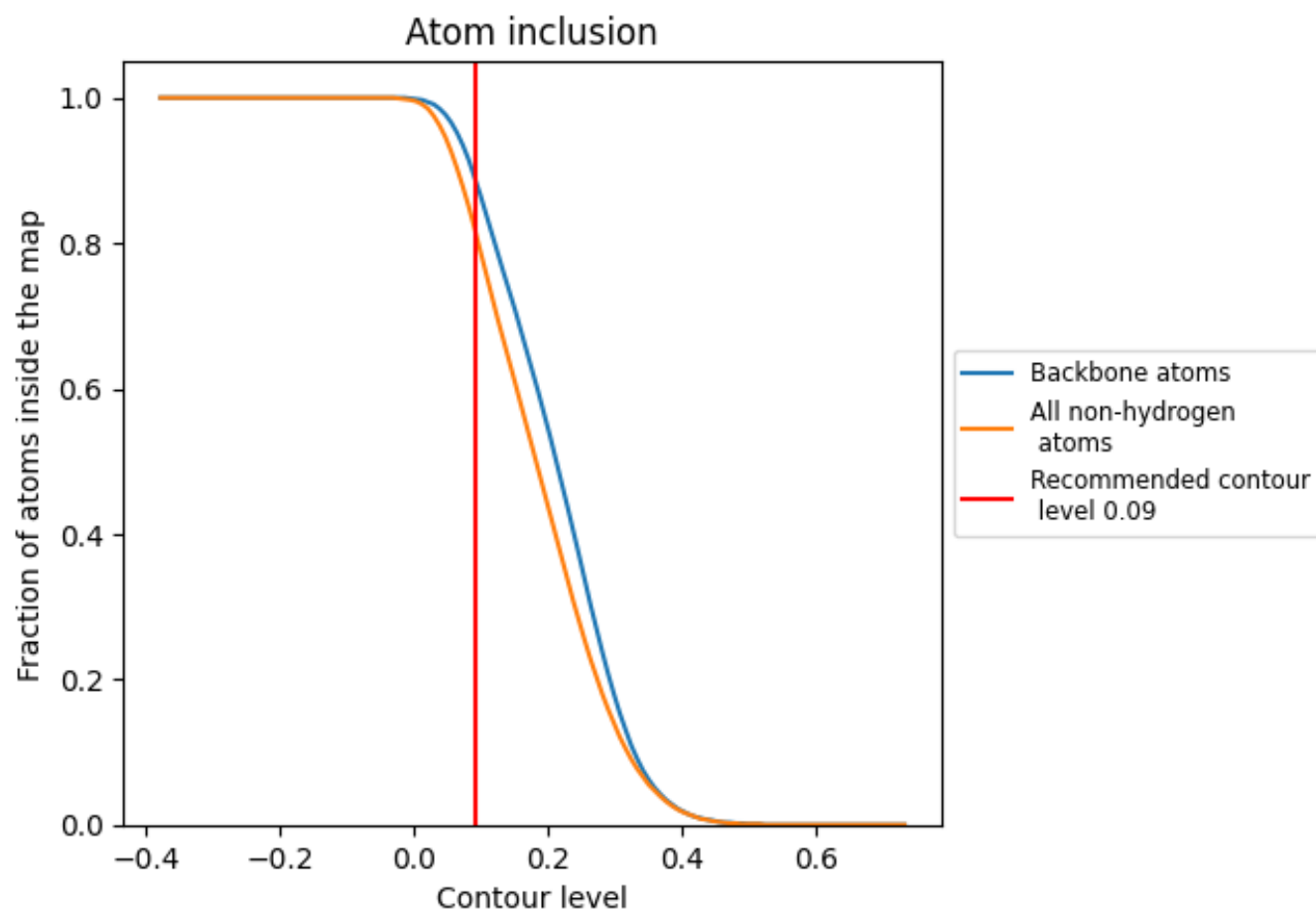
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.4860
5	 0.8940	 0.4930
7	 0.9460	 0.5210
8	 0.9100	 0.5010
9	 0.8650	 0.4680
A	 0.8390	 0.5480
AA	 0.7710	 0.4910
B	 0.8670	 0.5460
BB	 0.7200	 0.4820
C	 0.8430	 0.5400
CC	 0.7840	 0.5130
D	 0.8320	 0.5040
DD	 0.7010	 0.4740
E	 0.8150	 0.5160
EE	 0.7290	 0.4850
F	 0.8250	 0.5370
FF	 0.6960	 0.4600
G	 0.7730	 0.4990
GG	 0.6590	 0.4410
H	 0.7990	 0.5270
HH	 0.6650	 0.4530
I	 0.8170	 0.5310
II	 0.7470	 0.4970
J	 0.7830	 0.4970
JJ	 0.7210	 0.4760
KK	 0.7230	 0.4450
L	 0.8160	 0.5210
LL	 0.7710	 0.5210
M	 0.8440	 0.5210
MM	 0.4210	 0.2910
N	 0.8760	 0.5560
NN	 0.7670	 0.5110
O	 0.8530	 0.5390
OO	 0.7430	 0.4930
P	 0.8370	 0.5370



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Chain	Atom inclusion	Q-score
PP	 0.7100	 0.4520
Q	 0.8530	 0.5460
QQ	 0.7360	 0.4780
R	 0.7830	 0.5120
RR	 0.6930	 0.4710
S	 0.8560	 0.5410
SS	 0.6980	 0.4540
T	 0.8090	 0.5320
TT	 0.7300	 0.4610
U	 0.7620	 0.4700
UU	 0.7270	 0.4580
V	 0.8210	 0.5440
VV	 0.7540	 0.4930
W	 0.6410	 0.4420
WW	 0.7910	 0.5150
X	 0.8020	 0.5220
XX	 0.7530	 0.5140
Y	 0.8150	 0.5270
YY	 0.6980	 0.4510
Z	 0.8320	 0.5160
ZZ	 0.6380	 0.4220
a	 0.8670	 0.5540
aa	 0.7740	 0.5120
b	 0.7120	 0.4810
bb	 0.7000	 0.4820
c	 0.8080	 0.5110
cc	 0.6600	 0.4710
d	 0.8130	 0.5170
dd	 0.8400	 0.5150
e	 0.8150	 0.5450
ee	 0.6290	 0.4480
f	 0.8690	 0.5590
ff	 0.4920	 0.3380
g	 0.8000	 0.5260
gg	 0.6680	 0.4220
h	 0.7930	 0.5170
i	 0.7990	 0.5110
j	 0.8720	 0.5460
k	 0.7270	 0.4800
l	 0.8170	 0.5300
m	 0.8350	 0.5360
n	 0.7610	 0.5090

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Chain	Atom inclusion	Q-score
o	 0.8020	 0.5420
p	 0.7790	 0.5290
r	 0.8510	 0.5360
s	 0.6150	 0.4070
t	 0.3700	 0.2830
u	 0.1320	 0.2110
v	 0.5360	 0.3910
w	 0.3160	 0.3470