



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 12:13 PM EDT

PDB ID : 6MTB / pdb_00006mtb
EMDB ID : EMD-9237
Title : Rabbit 80S ribosome with P- and Z-site tRNAs (unrotated state)
Authors : Brown, A.; Baird, M.R.; Yip, M.C.J.; Murray, J.; Shao, S.
Deposited on : 2018-10-19
Resolution : 3.60 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:

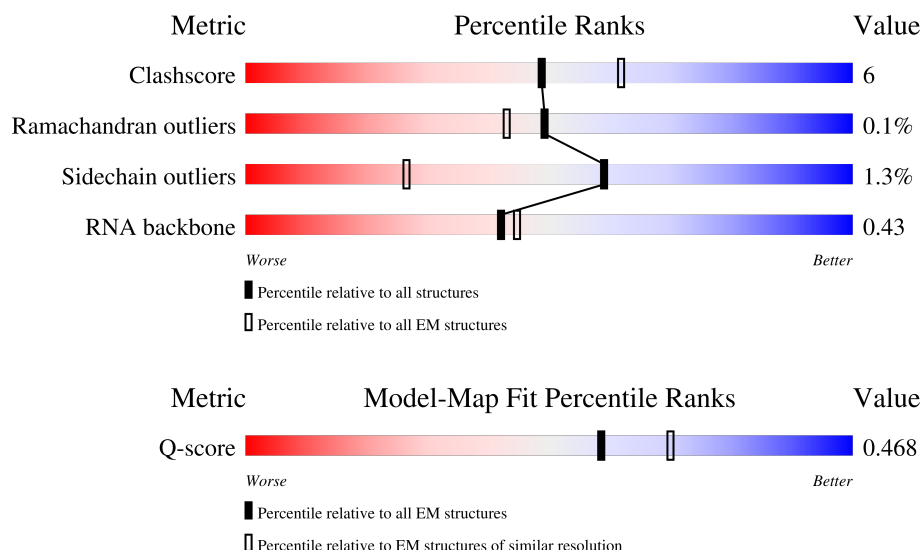
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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.



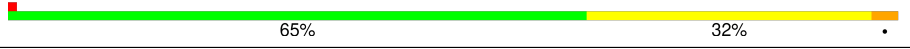
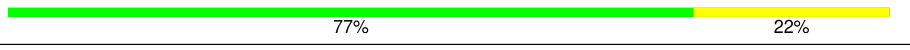
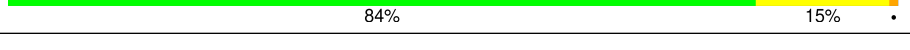
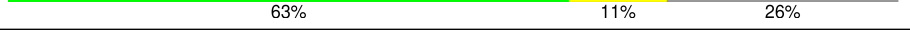
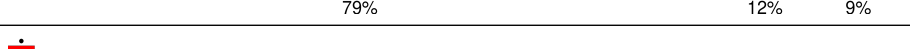
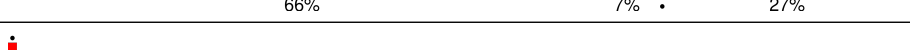
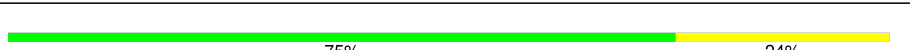
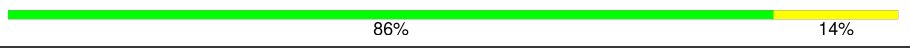
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	1	7	
2	2	76	
3	4	75	

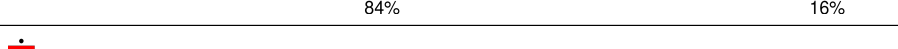
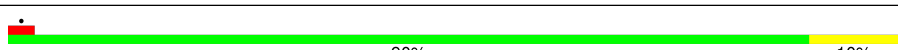
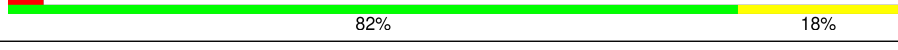
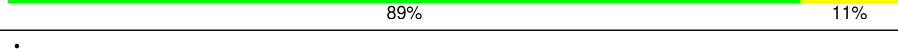
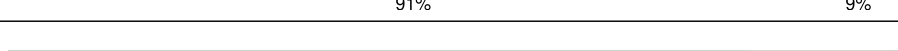
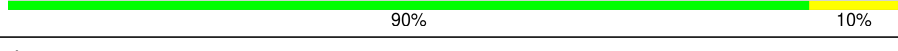
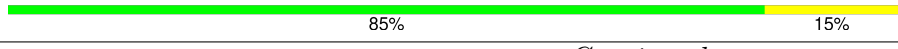
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Mol	Chain	Length	Quality of chain
4	5	3597	
5	7	120	
6	8	151	
7	A	248	
8	B	394	
9	C	362	
10	D	293	
11	E	291	
12	F	247	
13	G	319	
14	H	190	
15	I	214	
16	J	178	
17	L	210	
18	M	138	
19	N	203	
20	O	199	
21	P	153	
22	Q	187	
23	R	180	
24	S	176	
25	T	159	
26	U	99	
27	V	131	
28	W	157	

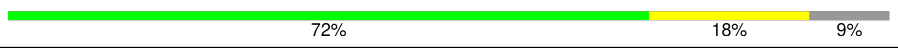
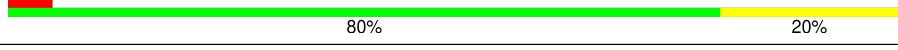
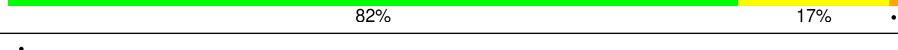
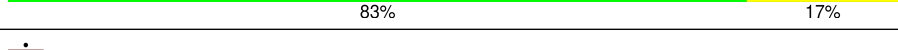
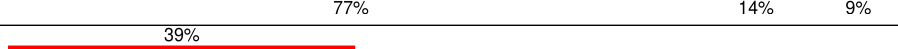
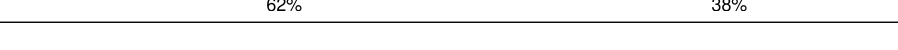
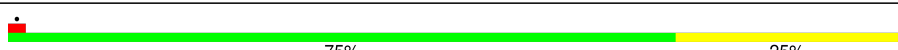
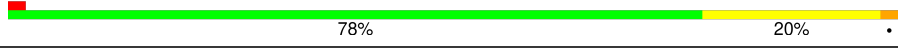
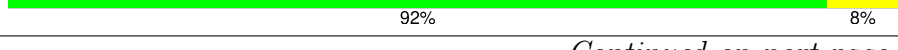
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Mol	Chain	Length	Quality of chain
29	X	118	
30	Y	134	
31	Z	135	
32	a	147	
33	b	245	
34	c	98	
35	d	107	
36	e	128	
37	f	109	
38	g	114	
39	h	122	
40	i	102	
41	j	86	
42	k	69	
43	l	50	
44	m	52	
45	n	25	
46	o	103	
47	p	91	
48	r	124	
49	u	206	
50	9	1698	
51	AA	217	
52	BB	213	
53	CC	221	

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

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Mol	Chain	Length	Quality of chain
79	cc	62	74%26%
80	dd	55	76%24%
81	ee	55	15%80%20%
82	ff	68	38%38%49%10%
83	gg	313	77%23%

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 216003 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	7	Total	C	N	O	P	0	0
			149	67	27	48	7		

- Molecule 2 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 3 is a RNA chain called Z-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	3597	Total	C	N	O	P	0	0
			77254	34469	14127	25061	3597		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	151	Total	C	N	O	P	0	0
			3209	1433	564	1062	150		

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

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

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

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

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

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

- Molecule 10 is a protein called 60S ribosomal protein L5.

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

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

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

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

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

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

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

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

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

- Molecule 15 is a protein called 60S ribosomal protein L10.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 28 is a protein called 60S ribosomal protein L24.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 45 is a protein called 60S ribosomal protein L41.

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

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

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

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

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

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

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

- Molecule 49 is a protein called 60S ribosomal protein L10a.

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

- Molecule 50 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	9	1698	Total	C	N	O	P	0	0
			36291	16217	6509	11868	1697		

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

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

- Molecule 52 is a protein called 40S ribosomal protein S3a.

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

- Molecule 53 is a protein called 40S ribosomal protein S2.

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

- Molecule 54 is a protein called 40S ribosomal protein S3.

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

- Molecule 55 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 56 is a protein called 40S ribosomal protein S5.

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

- Molecule 57 is a protein called 40S ribosomal protein S6.

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

- Molecule 58 is a protein called 40S ribosomal protein S7.

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

- Molecule 59 is a protein called 40S ribosomal protein S8.

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

- Molecule 60 is a protein called 40S ribosomal protein S9.

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

- Molecule 61 is a protein called 40S ribosomal protein S10.

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

- Molecule 62 is a protein called 40S ribosomal protein S11.

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

- Molecule 63 is a protein called 40S ribosomal protein S12.

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

- Molecule 64 is a protein called 40S ribosomal protein S13.

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

- Molecule 65 is a protein called 40S ribosomal protein S14.

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

- Molecule 66 is a protein called 40S ribosomal protein S15.

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

- Molecule 67 is a protein called 40S ribosomal protein S16.

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

- Molecule 68 is a protein called 40S ribosomal protein S17.

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

- Molecule 69 is a protein called 40S ribosomal protein S18.

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

- Molecule 70 is a protein called 40S ribosomal protein S19.

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

- Molecule 71 is a protein called 40S ribosomal protein S20.

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

- Molecule 72 is a protein called 40S ribosomal protein S21.

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

- Molecule 73 is a protein called 40S ribosomal protein S15a.

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

- Molecule 74 is a protein called 40S ribosomal protein S23.

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

- Molecule 75 is a protein called 40S ribosomal protein S24.

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

- Molecule 76 is a protein called 40S ribosomal protein S25.

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

- Molecule 77 is a protein called 40S ribosomal protein S26.

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

- Molecule 78 is a protein called 40S ribosomal protein S27.

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

- Molecule 79 is a protein called 40S ribosomal protein S28.

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

- Molecule 80 is a protein called 40S ribosomal protein S29.

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

- Molecule 81 is a protein called 40S ribosomal protein S30.

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

- Molecule 82 is a protein called 40S ribosomal protein S27a.

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

- Molecule 83 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	5	198	Total 198	Mg 198	0
84	7	7	Total 7	Mg 7	0
84	8	8	Total 8	Mg 8	0
84	A	1	Total 1	Mg 1	0
84	P	1	Total 1	Mg 1	0
84	V	1	Total 1	Mg 1	0
84	a	1	Total 1	Mg 1	0
84	j	1	Total 1	Mg 1	0
84	9	78	Total 78	Mg 78	0
84	TT	1	Total 1	Mg 1	0

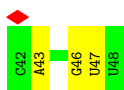
- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	g	1	Total 1	Zn 1	0
85	j	1	Total 1	Zn 1	0
85	m	1	Total 1	Zn 1	0
85	o	1	Total 1	Zn 1	0
85	p	1	Total 1	Zn 1	0
85	aa	1	Total 1	Zn 1	0
85	dd	1	Total 1	Zn 1	0
85	ff	1	Total 1	Zn 1	0

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.

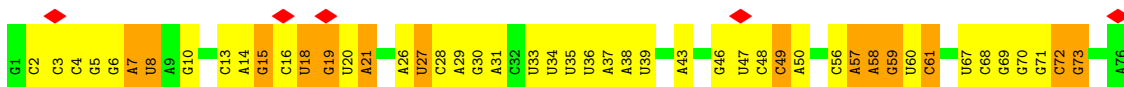
- Molecule 1: mRNA



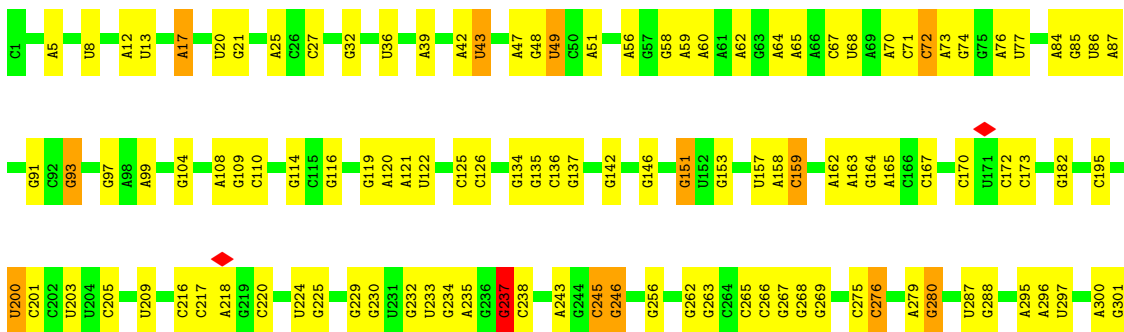
- Molecule 2: P-site tRNA



- Molecule 3: Z-site tRNA

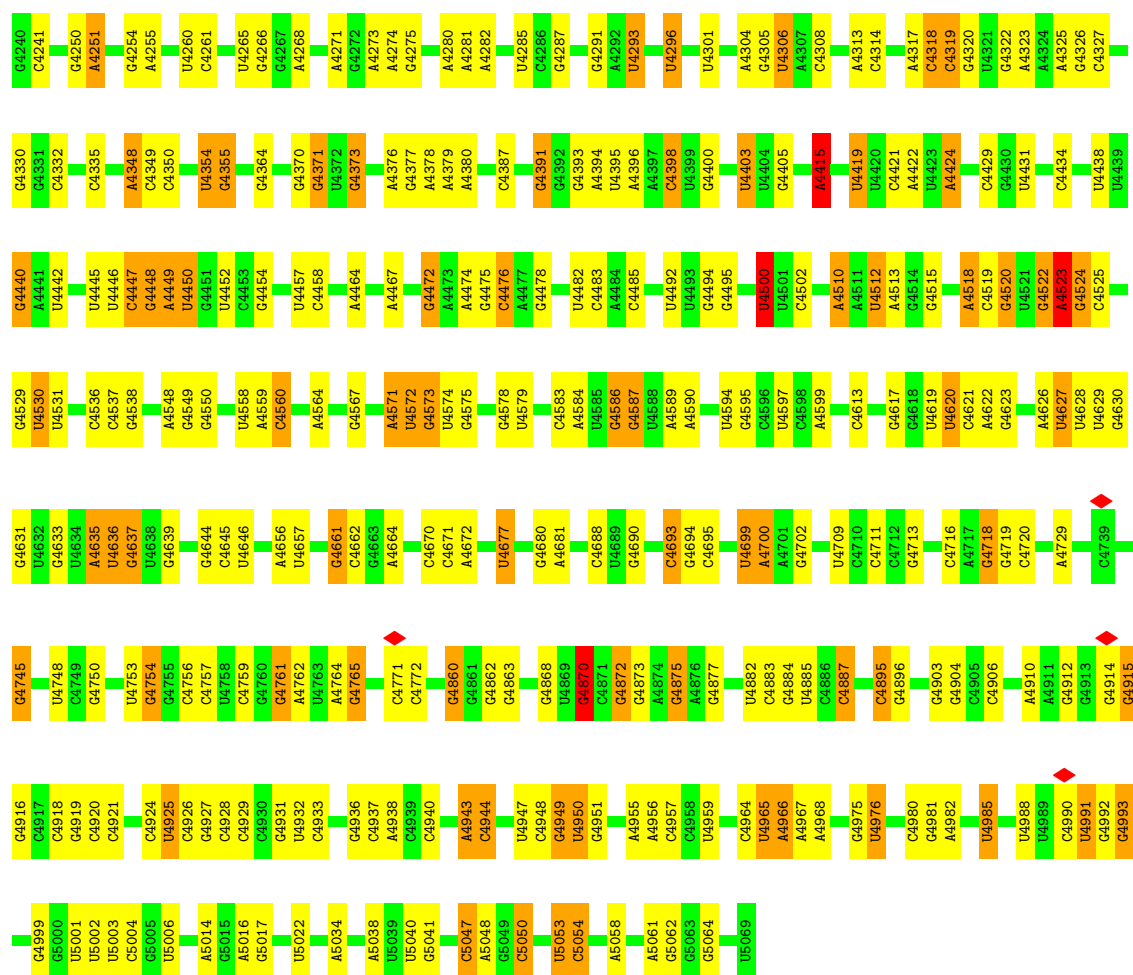


- Molecule 4: 28S rRNA









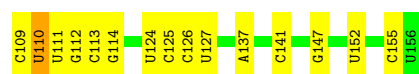
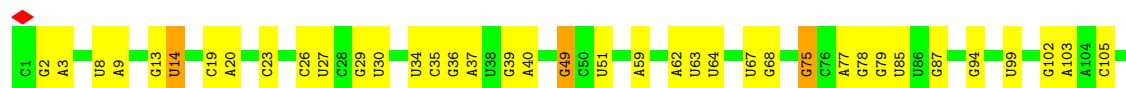
- Molecule 5: 5S rRNA

Chain 7: 72% 23%



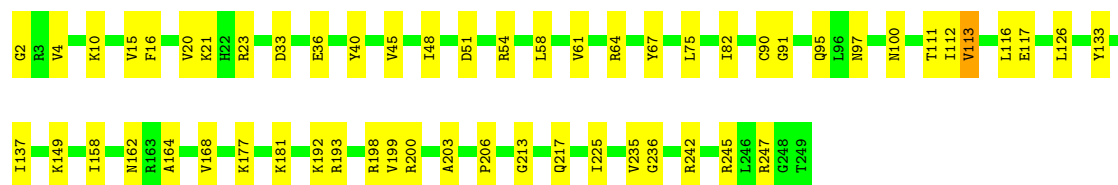
- Molecule 6: 5.8S rRNA

Chain 8: 65% 32%

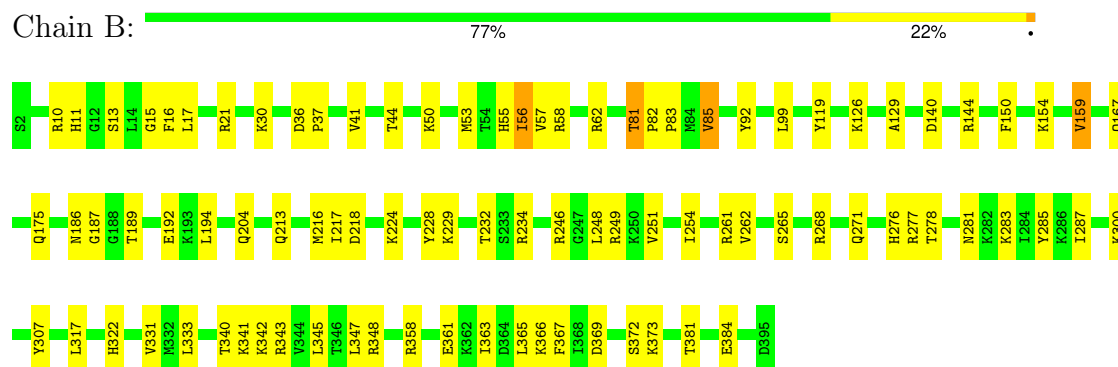


- Molecule 7: 60S ribosomal protein L8

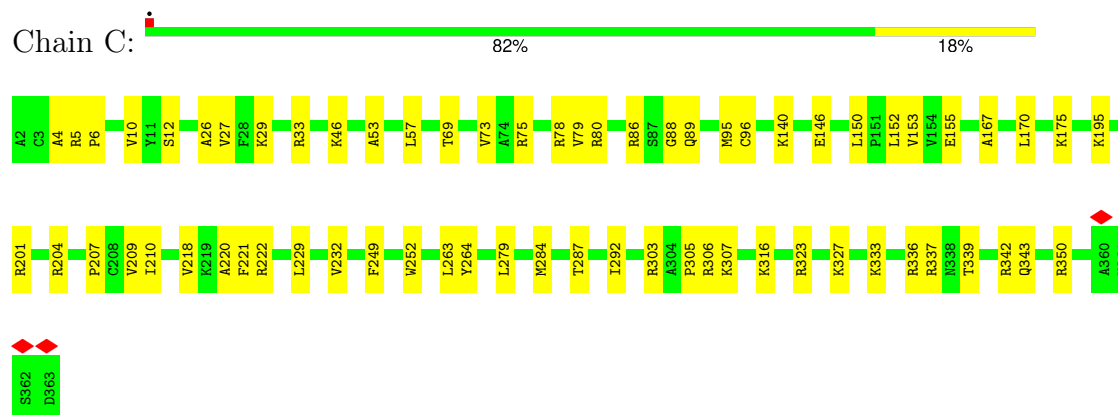
Chain A: 77% 22%



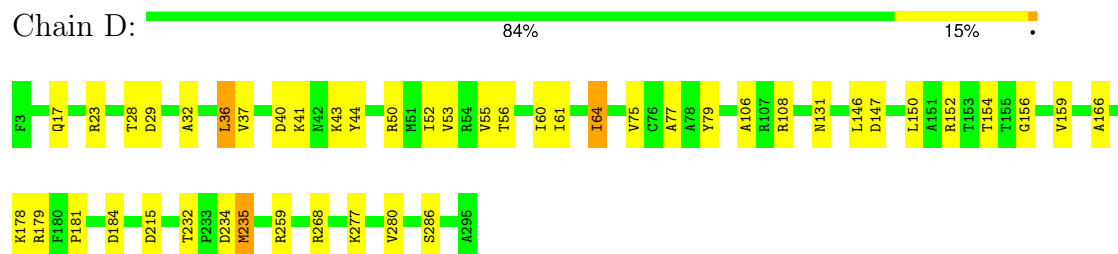
• Molecule 8: 60S ribosomal protein L3



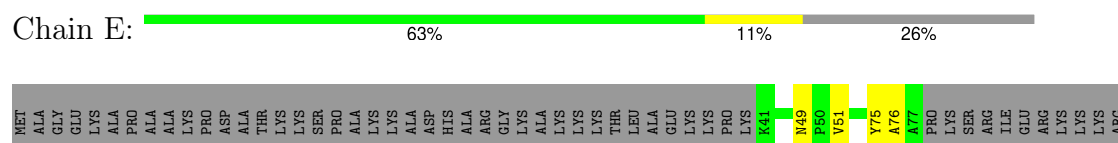
• Molecule 9: 60S ribosomal protein L4

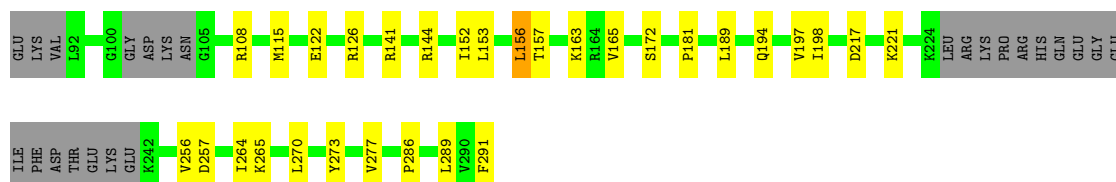


• Molecule 10: 60S ribosomal protein L5



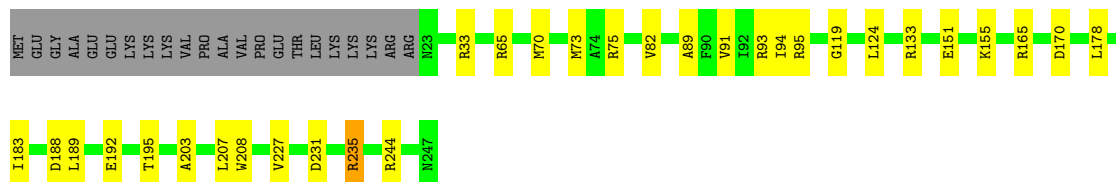
• Molecule 11: 60S ribosomal protein L6





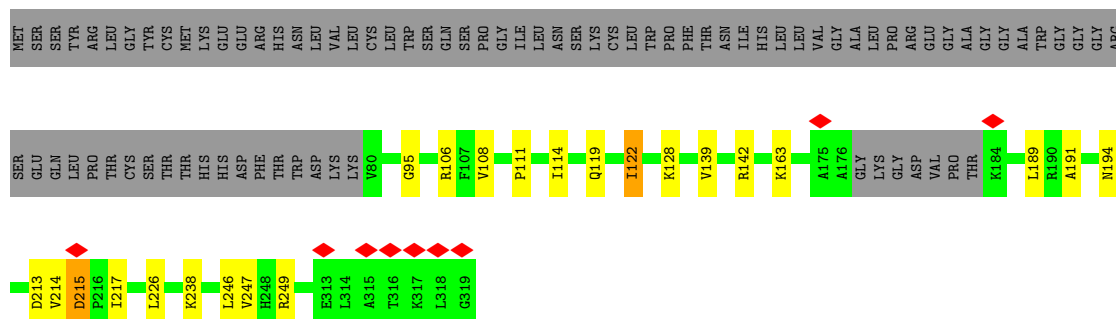
- Molecule 12: 60S ribosomal protein L7

Chain F:



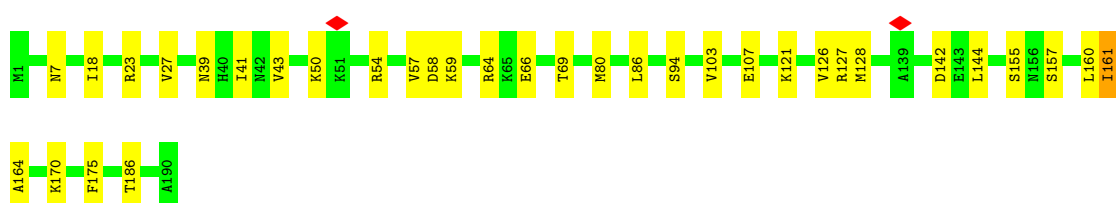
- Molecule 13: 60S ribosomal protein L7a

Chain G:



- Molecule 14: 60S ribosomal protein L9

Chain H:



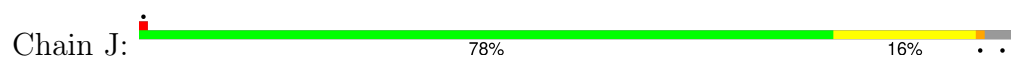
- Molecule 15: 60S ribosomal protein L10

Chain I:





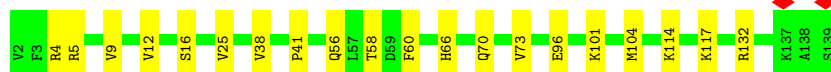
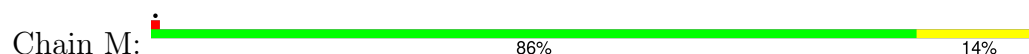
- Molecule 16: 60S ribosomal protein L11



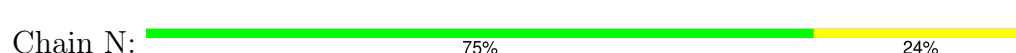
- Molecule 17: 60S ribosomal protein L13



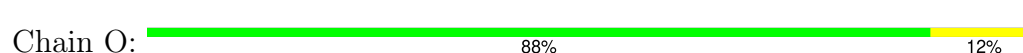
- Molecule 18: 60S ribosomal protein L14



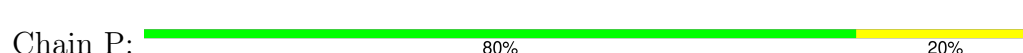
- Molecule 19: 60S ribosomal protein L15



- Molecule 20: 60S ribosomal protein L13a



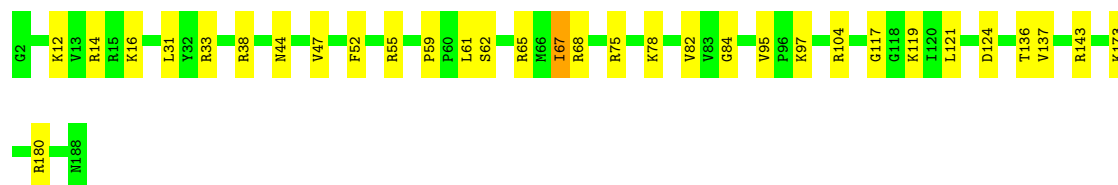
- Molecule 21: 60S ribosomal protein L17





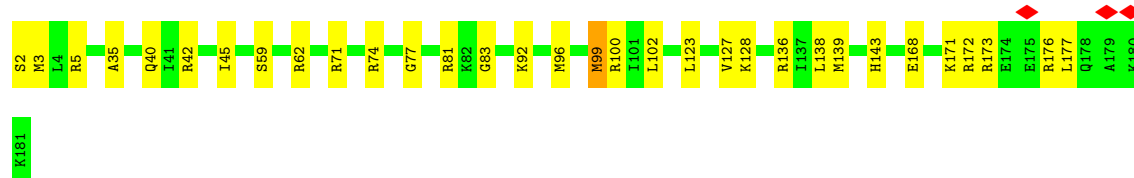
- Molecule 22: 60S ribosomal protein L18

Chain Q: 83% 17%



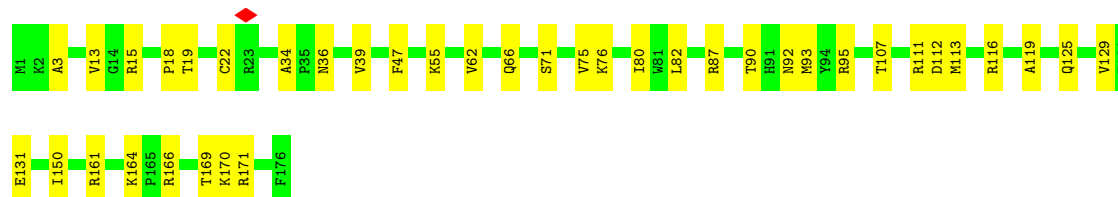
- Molecule 23: 60S ribosomal protein L19

Chain R: 82% 17%



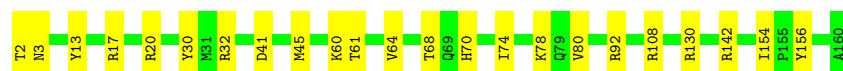
- Molecule 24: 60S ribosomal protein L18a

Chain S: 78% 22%



- Molecule 25: 60S ribosomal protein L21

Chain T: 86% 14%

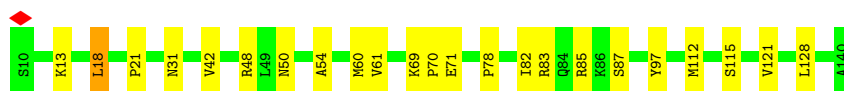
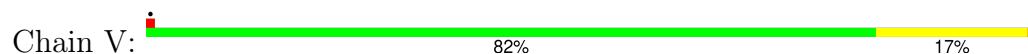


- Molecule 26: 60S ribosomal protein L22

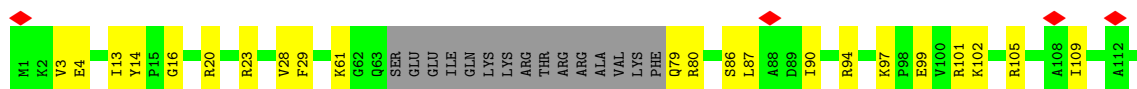
Chain U: 85% 13%



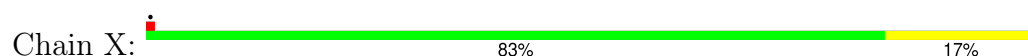
- Molecule 27: 60S ribosomal protein L23



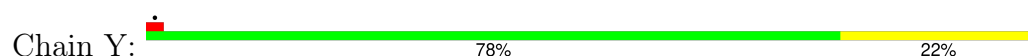
- Molecule 28: 60S ribosomal protein L24



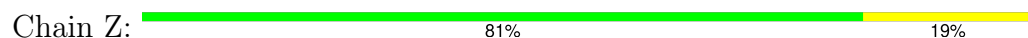
- Molecule 29: 60S ribosomal protein L23a



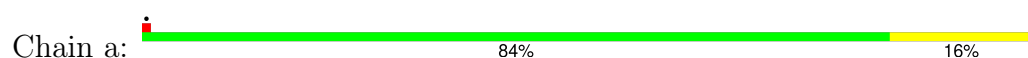
- Molecule 30: 60S ribosomal protein L26

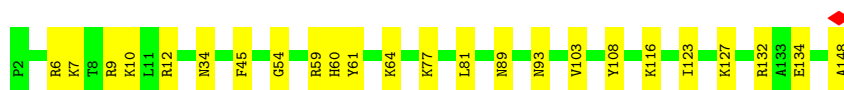


- Molecule 31: 60S ribosomal protein L27

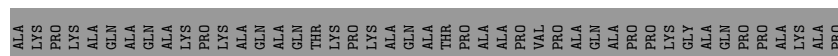
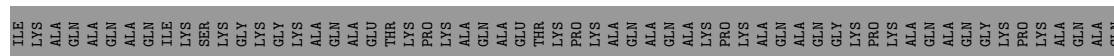
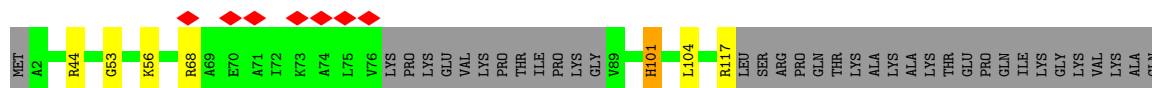


- Molecule 32: 60S ribosomal protein L27a

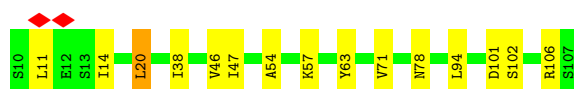
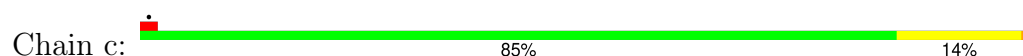




- Molecule 33: 60S ribosomal protein L29



- Molecule 34: 60S ribosomal protein L30



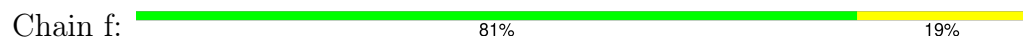
- Molecule 35: 60S ribosomal protein L31



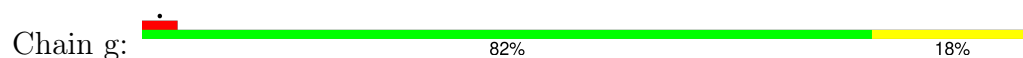
- Molecule 36: 60S ribosomal protein L32



- Molecule 37: 60S ribosomal protein L35a

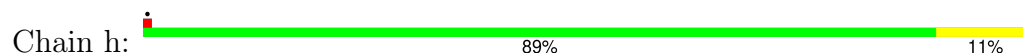


- Molecule 38: 60S ribosomal protein L34

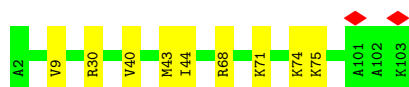




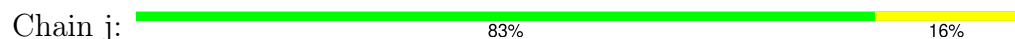
- Molecule 39: 60S ribosomal protein L35



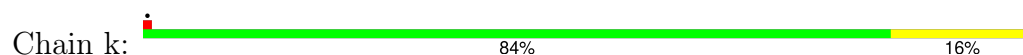
- Molecule 40: 60S ribosomal protein L36



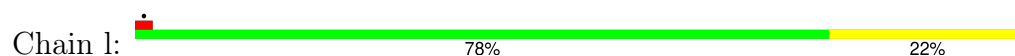
- Molecule 41: 60S ribosomal protein L37



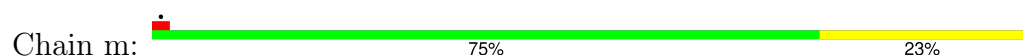
- Molecule 42: 60S ribosomal protein L38



- Molecule 43: 60S ribosomal protein L39

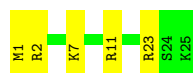


- Molecule 44: 60S ribosomal protein L40



- Molecule 45: 60S ribosomal protein L41

Chain n:  80% 20%



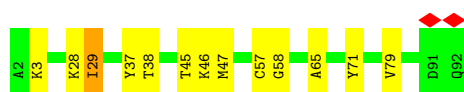
- Molecule 46: 60S ribosomal protein L36a

Chain o:  90% 10%



- Molecule 47: 60S ribosomal protein L37a

Chain p:  86% 13% .



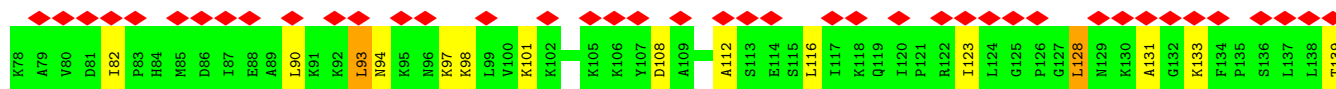
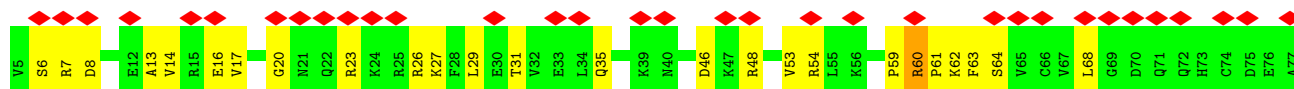
- Molecule 48: 60S ribosomal protein L28

Chain r:  79% 21%



- Molecule 49: 60S ribosomal protein L10a

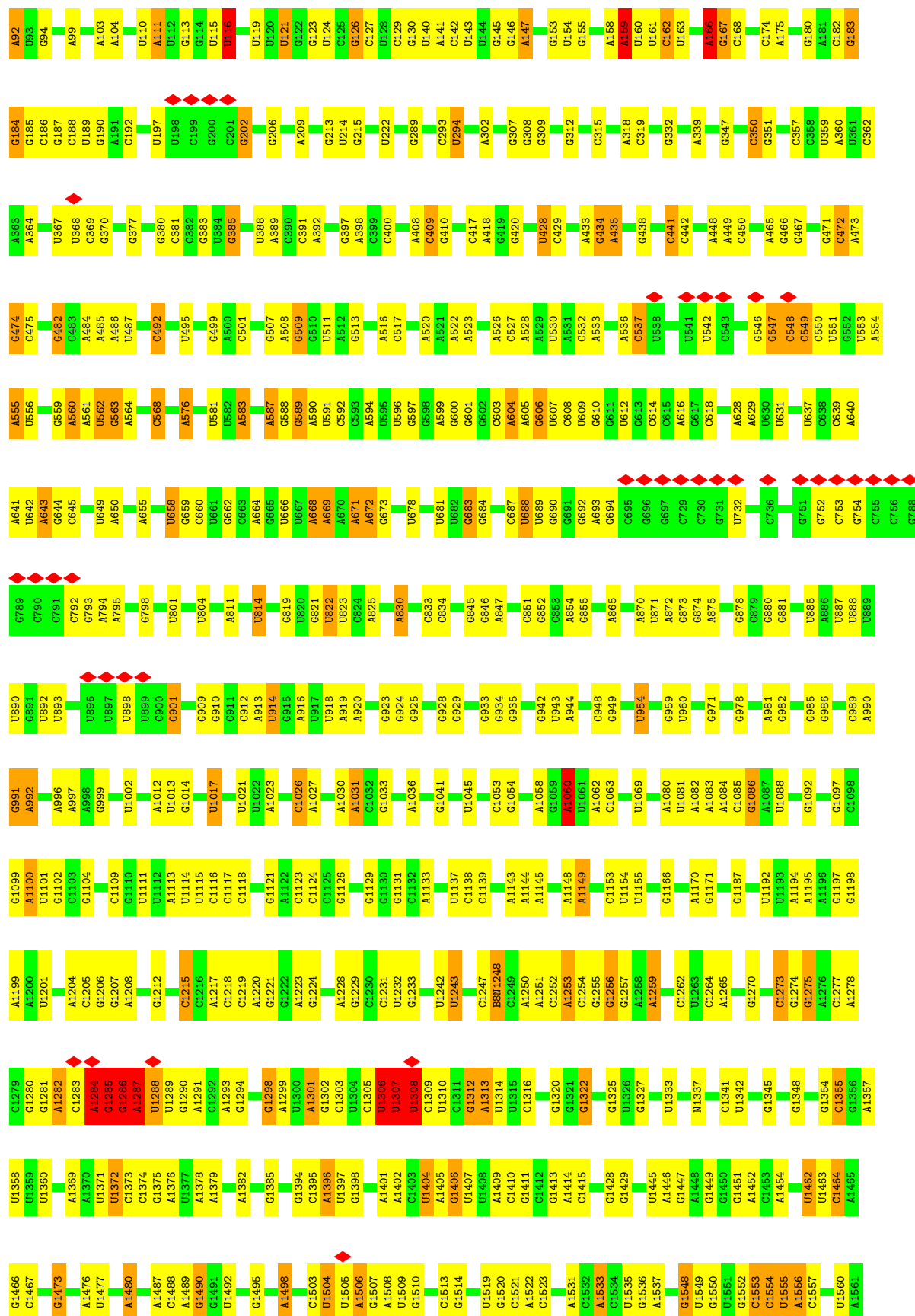
Chain u:  45% 70% 28% .

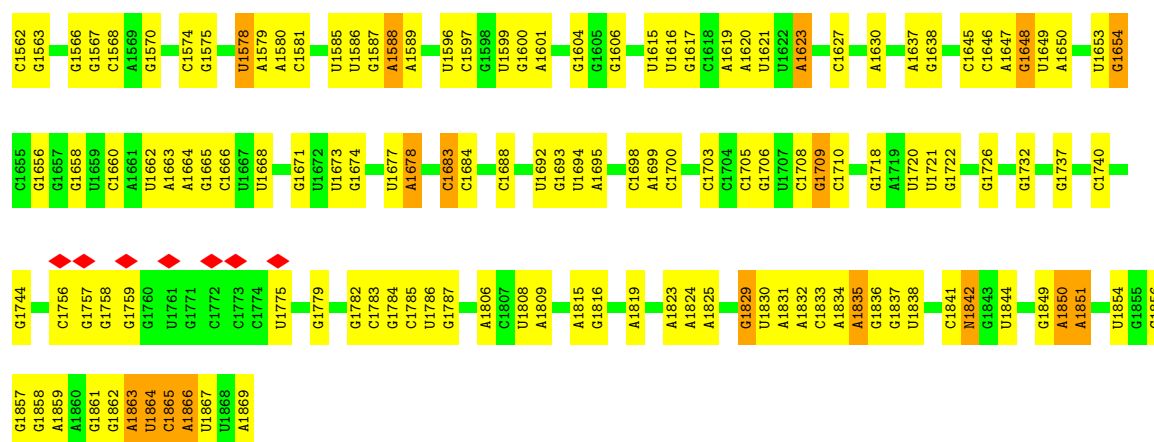


- Molecule 50: 18S rRNA

Chain 9:  57% 35% 7% .

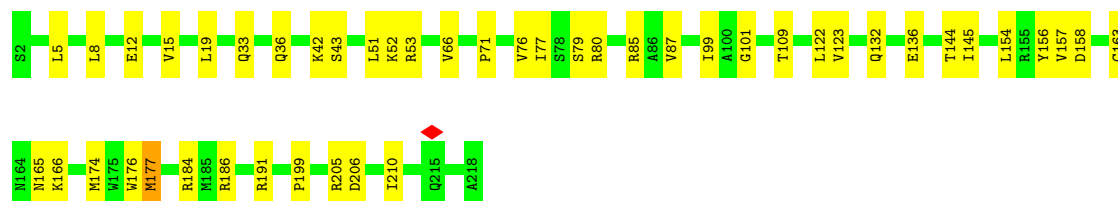






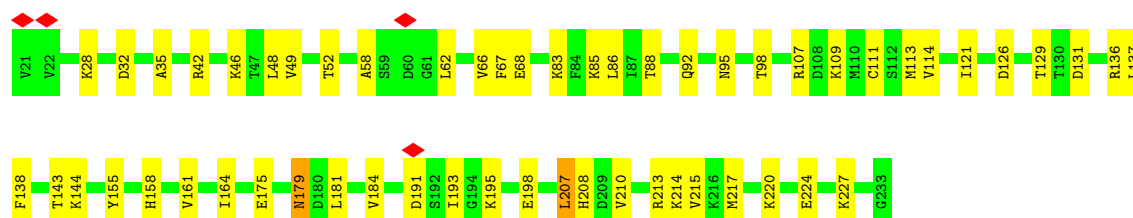
• Molecule 51: 40S ribosomal protein SA

Chain AA: 79% 21%



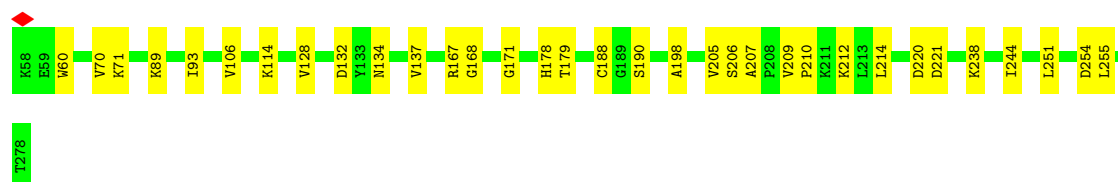
• Molecule 52: 40S ribosomal protein S3a

Chain BB: 74% 25%



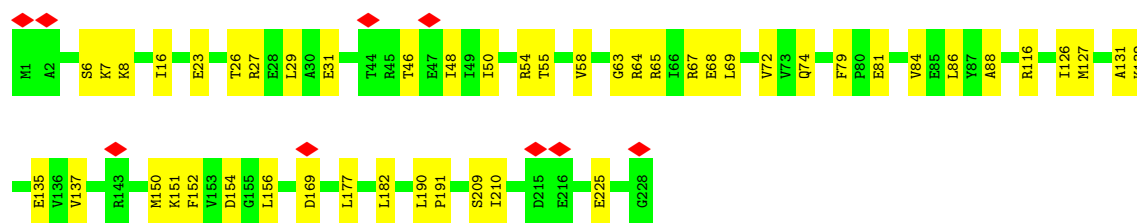
• Molecule 53: 40S ribosomal protein S2

Chain CC: 85% 15%

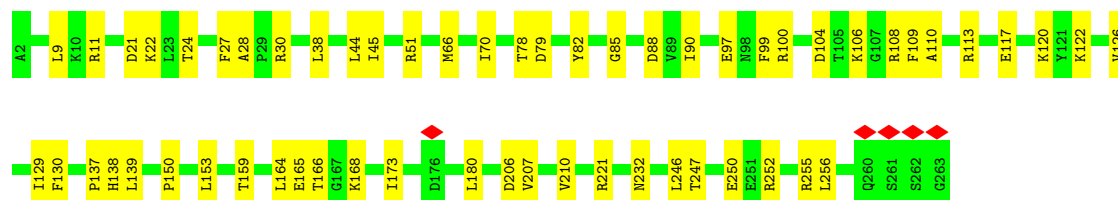
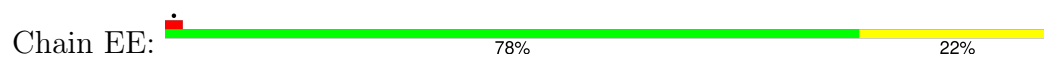


• Molecule 54: 40S ribosomal protein S3

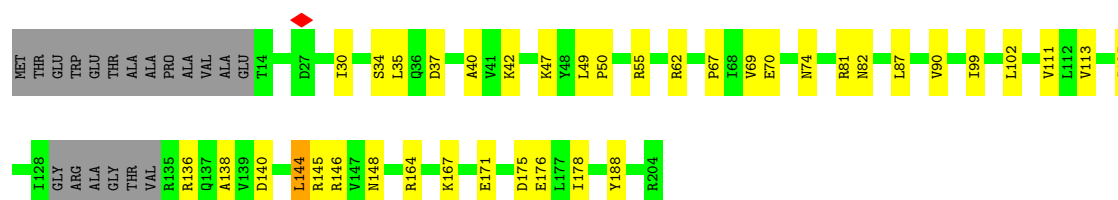
Chain DD: 79% 21%



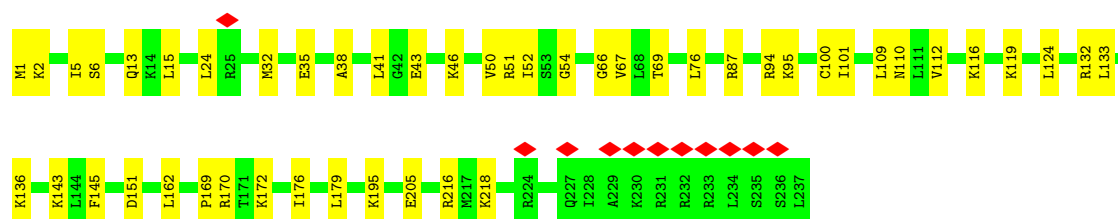
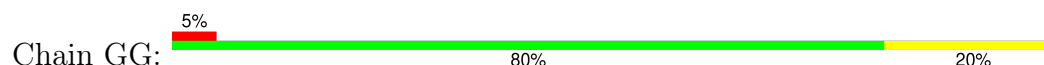
- Molecule 55: 40S ribosomal protein S4, X isoform



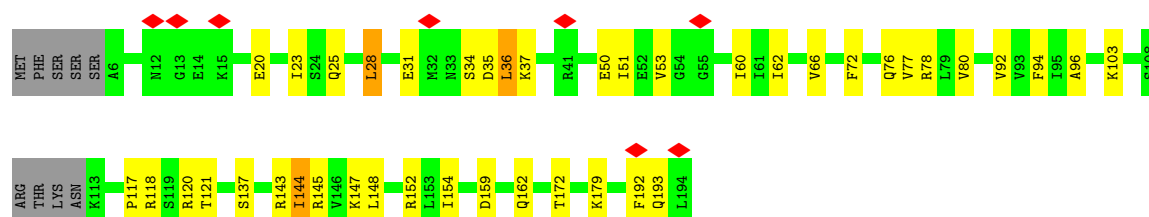
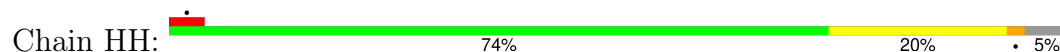
- Molecule 56: 40S ribosomal protein S5



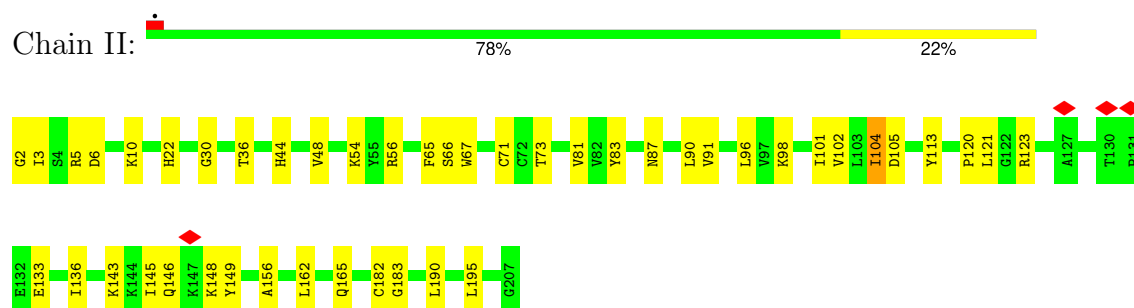
- Molecule 57: 40S ribosomal protein S6



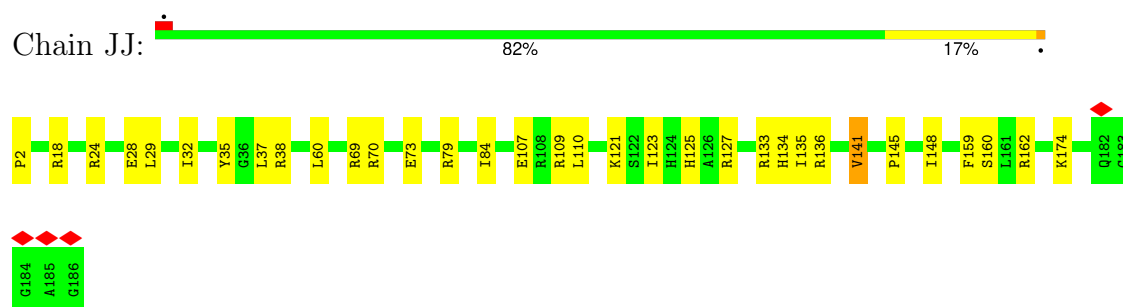
- Molecule 58: 40S ribosomal protein S7



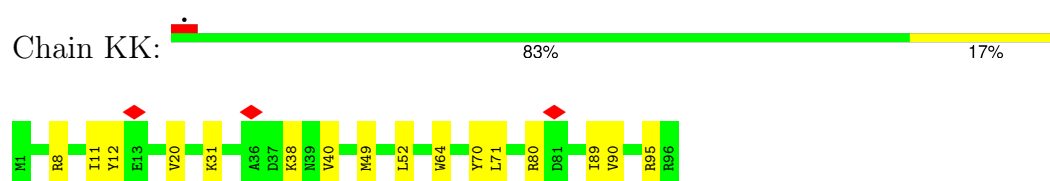
- Molecule 59: 40S ribosomal protein S8



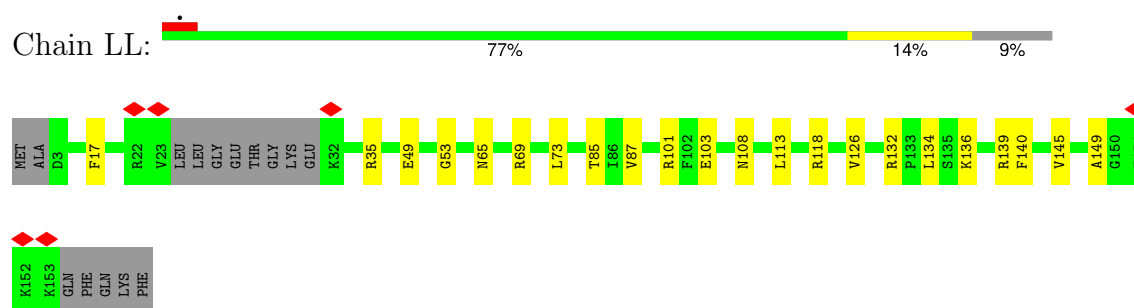
- Molecule 60: 40S ribosomal protein S9



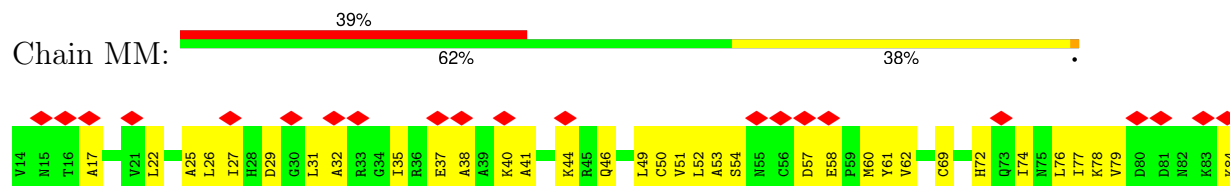
- Molecule 61: 40S ribosomal protein S10

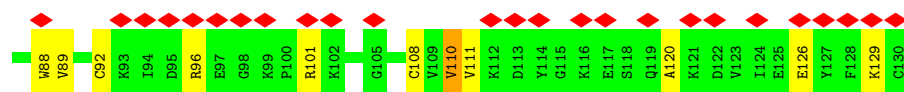


- Molecule 62: 40S ribosomal protein S11

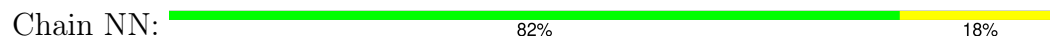


- Molecule 63: 40S ribosomal protein S12

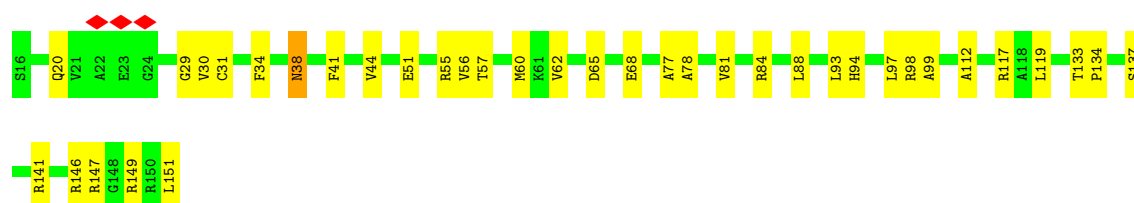
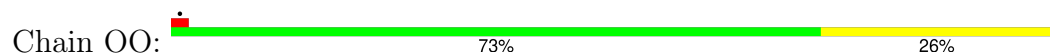




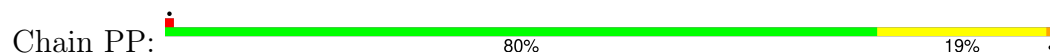
- Molecule 64: 40S ribosomal protein S13



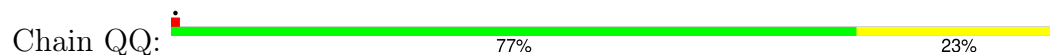
- Molecule 65: 40S ribosomal protein S14



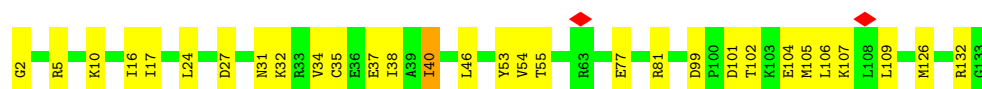
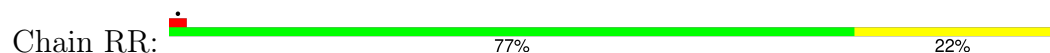
- Molecule 66: 40S ribosomal protein S15



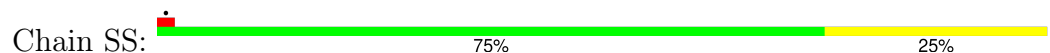
- Molecule 67: 40S ribosomal protein S16



- Molecule 68: 40S ribosomal protein S17

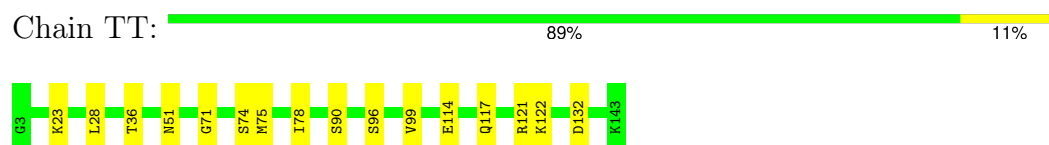


- Molecule 69: 40S ribosomal protein S18

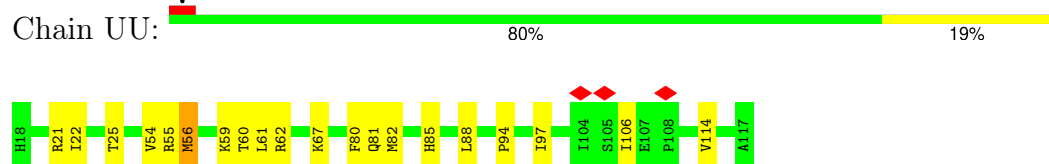




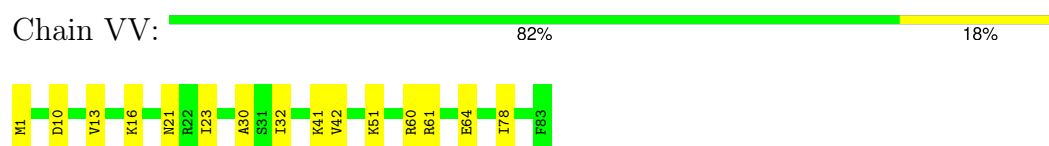
- Molecule 70: 40S ribosomal protein S19



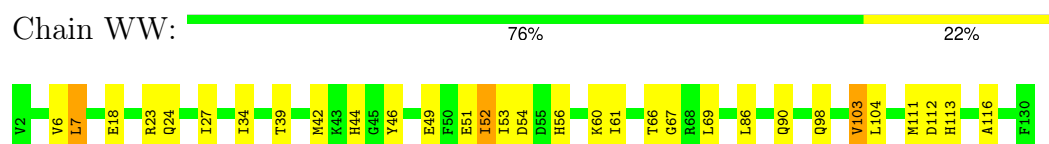
- Molecule 71: 40S ribosomal protein S20



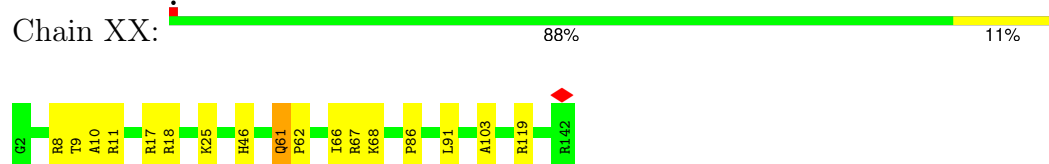
- Molecule 72: 40S ribosomal protein S21



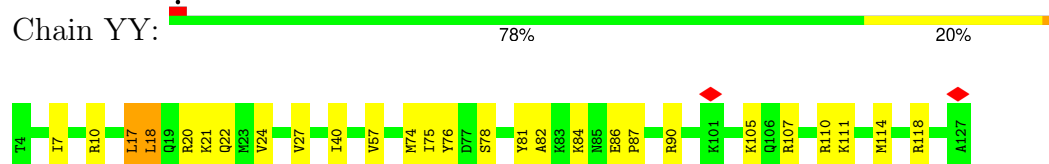
- Molecule 73: 40S ribosomal protein S15a



- Molecule 74: 40S ribosomal protein S23



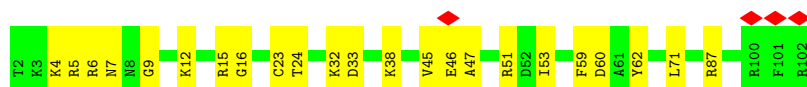
- Molecule 75: 40S ribosomal protein S24



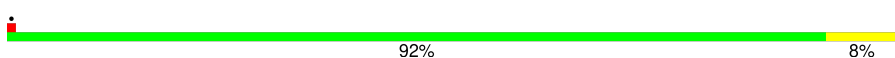
• Molecule 76: 40S ribosomal protein S25

Chain ZZ:  75% 23%

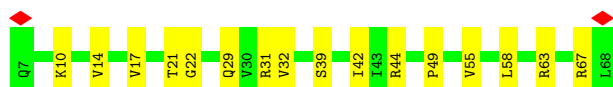
• Molecule 77: 40S ribosomal protein S26

Chain aa:  77% 23%

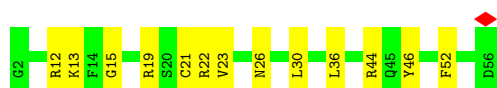
• Molecule 78: 40S ribosomal protein S27

Chain bb:  92% 8%

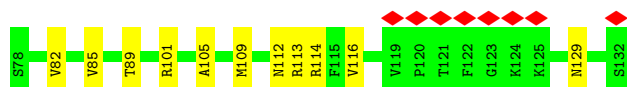
• Molecule 79: 40S ribosomal protein S28

Chain cc:  74% 26%

• Molecule 80: 40S ribosomal protein S29

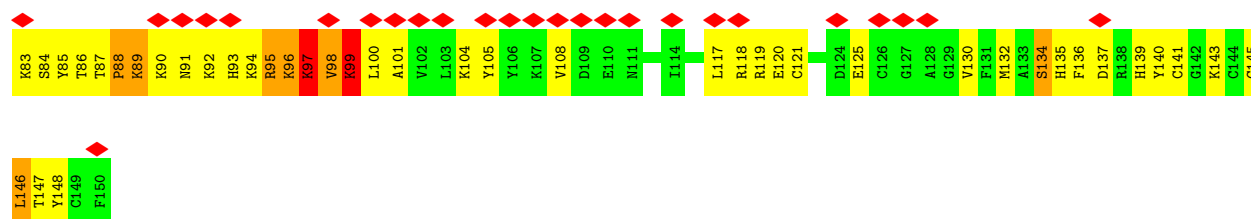
Chain dd:  76% 24%

• Molecule 81: 40S ribosomal protein S30

Chain ee:  15% 80% 20%

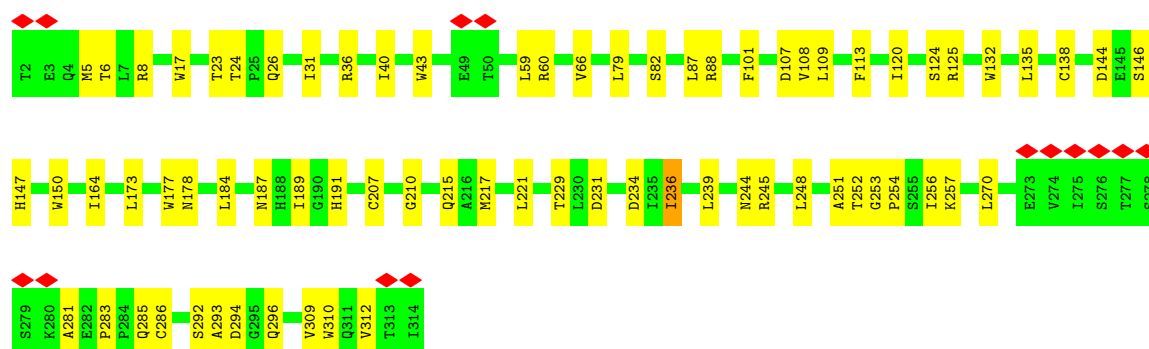
• Molecule 82: 40S ribosomal protein S27a

Chain ff:  38% 38% 49% 10%



- Molecule 83: Receptor of activated protein C kinase 1

Chain gg: 77% 23%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62560	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	0.797	Depositor
Minimum map value	-0.567	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.08	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: P7G, MA6, MHG, B8W, I4U, B8H, UR3, 1MA, B8Q, B8T, B9B, MG, OMG, OMC, 6MZ, PSU, 5MC, P4U, 7MG, 4AC, 2MG, OMU, B9H, E6G, BGH, 5MU, M7A, E3C, MLZ, B8K, E7G, ZN, B8N, A2M

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	1	0.32	0/166	0.42	0/256
2	2	0.29	0/1805	0.44	0/2809
3	4	0.22	0/1779	0.44	0/2771
4	5	0.51	2/83825 (0.0%)	0.51	10/130614 (0.0%)
5	7	0.50	0/2858	0.45	0/4455
6	8	0.50	0/3559	0.47	0/5543
7	A	0.57	0/1936	0.80	1/2596 (0.0%)
8	B	0.60	0/3240	0.75	0/4339
9	C	0.54	0/2927	0.70	0/3932
10	D	0.48	0/2437	0.66	0/3264
11	E	0.48	0/1762	0.75	2/2362 (0.1%)
12	F	0.56	0/1911	0.76	2/2549 (0.1%)
13	G	0.44	0/1910	0.69	0/2569
14	H	0.52	0/1535	0.75	0/2063
15	I	0.49	0/1702	0.65	0/2272
16	J	0.47	0/1385	0.81	0/1852
17	L	0.44	0/1733	0.71	0/2316
18	M	0.51	0/1158	0.78	0/1547
19	N	0.55	0/1746	0.74	0/2338
20	O	0.58	0/1662	0.79	0/2222
21	P	0.58	0/1268	0.75	0/1700
22	Q	0.54	0/1539	0.78	0/2054
23	R	0.46	0/1524	0.75	1/2013 (0.0%)
24	S	0.54	0/1501	0.72	2/2012 (0.1%)
25	T	0.52	0/1326	0.67	0/1770
26	U	0.39	0/823	0.72	0/1104
27	V	0.58	0/993	0.71	0/1332
28	W	0.51	1/873 (0.1%)	0.72	0/1158
29	X	0.48	0/984	0.65	0/1323
30	Y	0.52	0/1132	0.72	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Z	0.49	0/1130	0.65	0/1507
32	a	0.57	0/1191	0.71	0/1590
33	b	0.39	0/861	0.67	0/1138
34	c	0.47	0/771	0.69	0/1034
35	d	0.50	0/903	0.77	0/1216
36	e	0.57	0/1071	0.69	0/1429
37	f	0.62	0/895	0.80	1/1198 (0.1%)
38	g	0.48	0/916	0.74	0/1220
39	h	0.44	0/1021	0.75	0/1348
40	i	0.39	0/841	0.65	0/1112
41	j	0.53	0/720	0.75	0/952
42	k	0.41	0/575	0.68	0/761
43	l	0.55	0/459	0.75	0/608
44	m	0.52	0/425	0.85	0/561
45	n	0.48	0/240	0.83	0/305
46	o	0.46	0/855	0.62	0/1128
47	p	0.53	0/718	0.73	0/953
48	r	0.55	0/1010	0.79	0/1354
49	u	0.32	0/1680	0.86	1/2255 (0.0%)
50	9	0.48	7/39723 (0.0%)	0.53	17/61870 (0.0%)
51	AA	0.51	0/1747	0.71	1/2374 (0.0%)
52	BB	0.43	0/1756	0.72	0/2350
53	CC	0.53	0/1753	0.76	0/2369
54	DD	0.41	0/1796	0.77	2/2417 (0.1%)
55	EE	0.47	0/2118	0.75	0/2849
56	FF	0.44	0/1492	0.74	0/2005
57	GG	0.38	0/1946	0.68	0/2590
58	HH	0.39	0/1510	0.73	0/2022
59	II	0.48	0/1715	0.75	0/2287
60	JJ	0.43	0/1550	0.71	0/2069
61	KK	0.39	0/834	0.76	0/1125
62	LL	0.51	0/1195	0.71	0/1597
63	MM	0.33	0/918	0.83	2/1233 (0.2%)
64	NN	0.47	0/1226	0.75	0/1649
65	OO	0.47	0/1029	0.76	0/1380
66	PP	0.42	1/1017 (0.1%)	0.70	0/1358
67	QQ	0.42	0/1146	0.73	0/1534
68	RR	0.40	0/1082	0.72	0/1452
69	SS	0.41	0/1208	0.79	0/1618
70	TT	0.37	0/1115	0.64	0/1493
71	UU	0.37	0/805	0.69	0/1081
72	VV	0.53	0/643	0.69	0/860
73	WW	0.56	0/1051	0.76	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	XX	0.48	0/1116	0.69	0/1490
75	YY	0.39	0/1028	0.69	0/1366
76	ZZ	0.38	0/604	0.72	0/810
77	aa	0.49	0/828	0.70	0/1109
78	bb	0.43	0/665	0.78	0/891
79	cc	0.42	0/490	0.65	0/656
80	dd	0.43	0/470	0.69	0/623
81	ee	0.39	0/447	0.67	0/587
82	ff	1.10	7/567 (1.2%)	1.71	19/753 (2.5%)
83	gg	0.35	0/2493	0.73	2/3394 (0.1%)
All	All	0.49	18/228364 (0.0%)	0.61	63/334975 (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
8	B	0	1
9	C	0	2
10	D	0	1
13	G	0	1
14	H	0	1
19	N	0	3
25	T	0	1
30	Y	0	1
33	b	0	1
35	d	0	1
46	o	0	1
49	u	0	3
51	AA	0	2
63	MM	0	1
65	OO	0	1
69	SS	0	1
70	TT	0	1
71	UU	0	1
72	VV	0	1
73	WW	0	1
74	XX	0	1
82	ff	0	6
All	All	0	33

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	ff	98	VAL	C-N	10.56	1.44	1.33
50	9	1286	G	C5'-C4'	7.71	1.62	1.51
82	ff	97	LYS	CA-C	7.53	1.62	1.53
50	9	1286	G	C3'-O3'	7.35	1.54	1.43
50	9	1287	A	C5'-C4'	6.86	1.61	1.51
66	PP	85	ILE	C-N	-6.65	1.23	1.33
50	9	1286	G	O3'-P	6.60	1.71	1.61
82	ff	97	LYS	CD-CE	-6.57	1.32	1.52
82	ff	97	LYS	CB-CG	-6.47	1.33	1.52
50	9	1286	G	C4'-C3'	6.16	1.62	1.53
50	9	1287	A	P-O5'	5.79	1.68	1.59
82	ff	97	LYS	C-N	5.50	1.41	1.33
4	5	3785	A2M	O3'-P	5.39	1.61	1.56
82	ff	98	VAL	CA-C	5.36	1.59	1.52
50	9	1285	G	O3'-P	5.20	1.69	1.61
28	W	13	ILE	C-N	-5.20	1.18	1.33
82	ff	99	LYS	CB-CG	5.18	1.68	1.52
4	5	4523	A2M	O3'-P	5.11	1.61	1.56

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	ff	120	GLU	CA-C-N	10.22	134.55	120.65
82	ff	120	GLU	C-N-CA	10.22	134.55	120.65
82	ff	99	LYS	CB-CA-C	-9.95	101.96	114.40
50	9	1286	G	C5'-C4'-C3'	9.80	129.89	115.20
50	9	1287	A	P-O5'-C5'	9.78	135.56	120.90
4	5	4056	A	OP1-P-O3'	-9.46	79.61	108.00
50	9	1287	A	C4-N9-C1'	9.01	153.32	126.30
82	ff	99	LYS	CA-CB-CG	8.31	130.72	114.10
82	ff	97	LYS	CB-CG-CD	-8.15	92.55	111.30
82	ff	99	LYS	CA-C-N	7.99	134.17	122.82
82	ff	99	LYS	C-N-CA	7.99	134.17	122.82
82	ff	99	LYS	N-CA-C	7.97	120.53	109.29
50	9	1286	G	P-O3'-C3'	7.70	131.75	120.20
82	ff	88	PRO	CA-C-N	7.67	132.74	121.31
82	ff	88	PRO	C-N-CA	7.67	132.74	121.31
83	gg	281	ALA	CA-C-N	7.62	135.41	120.94
83	gg	281	ALA	C-N-CA	7.62	135.41	120.94
50	9	1308	U	O4'-C1'-N1	7.48	119.72	108.50
50	9	1286	G	P-O5'-C5'	7.36	131.94	120.90
82	ff	97	LYS	CA-C-N	7.34	135.18	121.97
82	ff	97	LYS	C-N-CA	7.34	135.18	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	u	123	ILE	N-CA-C	-7.31	106.77	113.71
82	ff	99	LYS	N-CA-CB	7.17	117.78	108.96
50	9	1307	U	O5'-C5'-C4'	6.50	121.25	111.50
50	9	1287	A	N7-C8-N9	6.39	132.99	113.80
82	ff	99	LYS	CG-CD-CE	6.39	126.01	111.30
50	9	1286	G	O5'-C5'-C4'	6.36	121.25	111.70
4	5	4056	A	OP2-P-O3'	-6.17	89.48	108.00
50	9	1286	G	C4'-C3'-O3'	6.16	118.63	109.40
63	MM	54	SER	CA-C-N	6.03	130.69	122.07
63	MM	54	SER	C-N-CA	6.03	130.69	122.07
82	ff	97	LYS	N-CA-C	6.01	119.81	107.37
24	S	170	LYS	CA-C-N	-5.90	112.77	120.67
24	S	170	LYS	C-N-CA	-5.90	112.77	120.67
4	5	2046	G	P-O3'-C3'	5.66	128.69	120.20
50	9	1307	U	O4'-C1'-N1	5.62	116.93	108.50
23	R	99	MET	CA-CB-CG	-5.60	102.90	114.10
82	ff	100	LEU	CA-CB-CG	5.57	135.78	116.30
4	5	3876	A	P-O3'-C3'	5.48	128.43	120.20
4	5	1406(B)	C	C2'-C3'-O3'	5.46	117.69	109.50
50	9	1307	U	C5-C6-N1	5.42	138.95	122.70
12	F	235	ARG	CA-C-N	-5.36	114.25	121.71
12	F	235	ARG	C-N-CA	-5.36	114.25	121.71
4	5	1406(B)	C	OP1-P-O3'	5.35	116.97	105.20
82	ff	97	LYS	CA-CB-CG	5.29	124.68	114.10
4	5	2695	A	P-O3'-C3'	5.25	128.07	120.20
4	5	4925	U	P-O3'-C3'	5.23	128.04	120.20
7	A	15	VAL	N-CA-C	-5.20	105.75	113.39
4	5	1406(B)	C	P-O3'-C3'	5.18	125.92	119.70
50	9	1306	U	O3'-P-O5'	5.17	111.75	104.00
82	ff	89	LYS	N-CA-C	5.14	117.54	110.35
50	9	1307	U	C2-N1-C1'	5.13	133.10	117.70
50	9	1284	A	O3'-P-O5'	5.13	111.69	104.00
50	9	501	C	C2-N1-C1'	5.12	134.15	118.80
82	ff	96	LYS	N-CA-C	5.11	116.92	108.13
54	DD	126	ILE	CA-C-N	-5.08	114.22	122.65
54	DD	126	ILE	C-N-CA	-5.08	114.22	122.65
50	9	1060	A	O4'-C1'-N9	5.07	115.81	108.20
11	E	156	LEU	CA-C-N	-5.06	112.71	121.52
11	E	156	LEU	C-N-CA	-5.06	112.71	121.52
51	AA	177	MET	CB-CG-SD	-5.06	97.53	112.70
4	5	3888	G	C2'-C3'-O3'	5.03	121.25	113.70
37	f	106	TYR	N-CA-C	5.01	120.88	109.81

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	AA	42	LYS	Peptide
51	AA	43	SER	Peptide
8	B	16	PHE	Peptide
9	C	69	THR	Peptide
9	C	73	VAL	Peptide
10	D	235	MET	Peptide
13	G	215	ASP	Peptide
14	H	50	LYS	Peptide
63	MM	72	HIS	Peptide
19	N	184	ILE	Peptide
19	N	76	PRO	Peptide
19	N	78	GLY	Peptide
65	OO	38	ASN	Peptide
69	SS	99	LEU	Peptide
25	T	80	VAL	Peptide
70	TT	117	GLN	Peptide
71	UU	56	MET	Peptide
72	VV	32	ILE	Peptide
73	WW	54	ASP	Peptide
74	XX	61	GLN	Peptide
30	Y	82	ILE	Peptide
33	b	101	HIS	Peptide
35	d	95	ASP	Peptide
82	ff	134	SER	Mainchain
82	ff	146	LEU	Peptide
82	ff	91	ASN	Peptide
82	ff	95	ARG	Peptide
82	ff	97	LYS	Peptide
82	ff	99	LYS	Peptide
46	o	74	GLU	Peptide
49	u	128	LEU	Peptide
49	u	20	GLY	Peptide
49	u	60	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	149	0	76	0	0
2	2	1616	0	824	7	0
3	4	1593	0	809	18	0
4	5	77254	0	38799	637	0
5	7	2558	0	1296	16	0
6	8	3209	0	1631	24	0
7	A	1898	0	1993	43	0
8	B	3172	0	3310	64	0
9	C	2884	0	3054	51	0
10	D	2391	0	2424	32	0
11	E	1729	0	1887	24	0
12	F	1875	0	1995	24	0
13	G	1879	0	2027	16	0
14	H	1516	0	1596	26	0
15	I	1664	0	1712	18	0
16	J	1362	0	1399	18	0
17	L	1702	0	1820	20	0
18	M	1137	0	1209	14	0
19	N	1701	0	1749	37	0
20	O	1630	0	1778	18	0
21	P	1242	0	1274	23	0
22	Q	1515	0	1634	25	0
23	R	1508	0	1664	22	0
24	S	1462	0	1508	27	0
25	T	1298	0	1366	17	0
26	U	809	0	833	8	0
27	V	979	0	1039	18	0
28	W	860	0	903	13	0
29	X	967	0	1040	15	0
30	Y	1115	0	1205	22	0
31	Z	1107	0	1182	16	0
32	a	1162	0	1209	21	0
33	b	848	0	920	6	0
34	c	761	0	794	10	0
35	d	888	0	930	5	0
36	e	1053	0	1147	13	0
37	f	876	0	912	16	0
38	g	906	0	998	16	0
39	h	1013	0	1147	11	0
40	i	830	0	916	8	0
41	j	705	0	737	11	0
42	k	569	0	637	7	0
43	l	447	0	480	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	m	430	0	466	11	0
45	n	239	0	289	5	0
46	o	842	0	913	8	0
47	p	708	0	756	12	0
48	r	994	0	1051	20	0
49	u	1654	0	1760	35	0
50	9	36291	0	18320	366	0
51	AA	1710	0	1708	30	0
52	BB	1729	0	1803	39	0
53	CC	1716	0	1806	22	0
54	DD	1768	0	1866	35	0
55	EE	2076	0	2177	33	0
56	FF	1471	0	1522	30	0
57	GG	1923	0	2089	39	0
58	HH	1488	0	1582	28	0
59	II	1686	0	1772	32	0
60	JJ	1525	0	1640	24	0
61	KK	810	0	836	9	0
62	LL	1175	0	1249	15	0
63	MM	908	0	939	25	0
64	NN	1202	0	1289	20	0
65	OO	1016	0	1039	27	0
66	PP	997	0	1045	18	0
67	QQ	1128	0	1195	23	0
68	RR	1068	0	1121	25	0
69	SS	1190	0	1249	26	0
70	TT	1097	0	1132	10	0
71	UU	795	0	862	15	0
72	VV	636	0	637	10	0
73	WW	1034	0	1080	25	0
74	XX	1098	0	1167	12	0
75	YY	1011	0	1083	21	0
76	ZZ	598	0	656	12	0
77	aa	814	0	863	18	0
78	bb	651	0	672	5	0
79	cc	488	0	514	12	0
80	dd	459	0	448	12	0
81	ee	443	0	492	7	0
82	ff	555	0	565	68	0
83	gg	2436	0	2393	44	0
84	5	198	0	0	0	0
84	7	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	8	8	0	0	0	0
84	9	78	0	0	0	0
84	A	1	0	0	0	0
84	P	1	0	0	0	0
84	TT	1	0	0	0	0
84	V	1	0	0	0	0
84	a	1	0	0	0	0
84	j	1	0	0	0	0
85	aa	1	0	0	0	0
85	dd	1	0	0	0	0
85	ff	1	0	0	0	0
85	g	1	0	0	0	0
85	j	1	0	0	0	0
85	m	1	0	0	0	0
85	o	1	0	0	0	0
85	p	1	0	0	0	0
All	All	216003	0	159909	2090	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 (2090) 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)
4:5:3762:B8H:C4	4:5:3762:B8H:C5	1.82	1.57
4:5:4296:B8H:C5	4:5:4296:B8H:C4	1.82	1.57
4:5:1860:B8H:C4	4:5:1860:B8H:C5	1.82	1.53
4:5:4296:B8H:N1	4:5:4296:B8H:C6	1.68	1.52
4:5:1860:B8H:C6	4:5:1860:B8H:N1	1.69	1.52
4:5:3762:B8H:C6	4:5:3762:B8H:N1	1.69	1.51
4:5:3718:A2M:C1'	4:5:3718:A2M:O4'	1.63	1.23
50:9:1031:A2M:C1'	50:9:1031:A2M:O4'	1.63	1.22
4:5:2754:B9B:C1'	4:5:2754:B9B:O4'	1.63	1.21
4:5:3723:A2M:C1'	4:5:3723:A2M:O4'	1.63	1.18
4:5:1574:B9B:C1'	4:5:1574:B9B:O4'	1.64	1.18
50:9:166:A2M:C1'	50:9:166:A2M:O4'	1.64	1.15
4:5:237:B9B:C1'	4:5:237:B9B:O4'	1.65	1.14
4:5:3899:BGH:C4'	4:5:3899:BGH:O4'	1.65	1.08
9:C:218:VAL:O	9:C:222:ARG:HB2	1.61	0.98
82:ff:139:HIS:HB2	82:ff:148:TYR:O	1.66	0.95
49:u:53:VAL:O	49:u:154:THR:HA	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:1286:G:H4'	82:ff:97:LYS:HA	1.48	0.95
4:5:3951:G:H1	4:5:4062:A:H2	1.11	0.92
2:2:50:U:H3	2:2:64:G:H1	0.92	0.89
4:5:3952:A:H2	4:5:4061:G:H1	1.07	0.89
82:ff:141:CYS:O	82:ff:145:CYS:HA	1.74	0.86
50:9:1452:A:H61	50:9:1473:G:H21	1.24	0.85
4:5:3946:G:H1	4:5:4067:U:H3	1.24	0.82
50:9:1287:A:H8	82:ff:97:LYS:HB3	1.43	0.81
3:4:6:G:H1	3:4:67:U:H3	1.27	0.80
4:5:3762:B8H:C5	4:5:3762:B8H:N1	2.36	0.78
4:5:4887:C:H42	4:5:4932:U:H3	1.32	0.78
4:5:3951:G:N1	4:5:4062:A:C2	2.47	0.77
50:9:1452:A:N6	50:9:1473:G:H21	1.85	0.74
4:5:3951:G:N1	4:5:4062:A:H2	1.85	0.73
4:5:3952:A:H2	4:5:4061:G:N1	1.85	0.73
79:cc:10:LYS:O	79:cc:58:LEU:HB2	1.87	0.73
57:GG:76:LEU:HG	57:GG:94:ARG:HE	1.54	0.73
10:D:232:THR:HG22	10:D:235:MET:HG2	1.71	0.73
4:5:1860:B8H:C6	4:5:1860:B8H:C2	2.65	0.72
4:5:758:G:H5''	14:H:54:ARG:HH22	1.55	0.72
4:5:3952:A:C2	4:5:4061:G:N1	2.49	0.71
73:WW:86:LEU:HD21	73:WW:113:HIS:HB2	1.72	0.71
4:5:4296:B8H:C6	4:5:4296:B8H:C2	2.65	0.70
4:5:1210:C:H42	12:F:65:ARG:HH12	1.38	0.70
4:5:3762:B8H:C6	4:5:3762:B8H:C2	2.66	0.70
4:5:1459:A:OP1	22:Q:65:ARG:NH2	2.25	0.70
50:9:1307:U:H2'	82:ff:134:SER:HA	1.74	0.69
41:j:19:CYS:SG	41:j:20:ARG:N	2.66	0.69
47:p:46:LYS:O	47:p:57:CYS:HA	1.92	0.69
4:5:4895:C:H1'	18:M:132:ARG:HH12	1.57	0.69
50:9:1286:G:O5'	82:ff:99:LYS:N	2.26	0.69
50:9:1452:A:H61	50:9:1473:G:N2	1.91	0.69
50:9:694:G:H1	50:9:732:U:H3	1.41	0.68
4:5:1870:C:H2'	4:5:1871:A2M:H8	1.75	0.68
63:MM:84:LYS:O	63:MM:88:TRP:HB2	1.92	0.68
50:9:1289:U:H5''	82:ff:93:HIS:HB3	1.75	0.68
50:9:1396:A:O2'	50:9:1398:G:N7	2.26	0.68
4:5:914:U:N3	4:5:918:G:N7	2.42	0.68
50:9:1285:G:H4'	82:ff:99:LYS:HG2	1.76	0.68
82:ff:132:MET:HG2	82:ff:141:CYS:HB3	1.77	0.67
63:MM:126:GLU:HA	63:MM:129:LYS:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SS:13:LEU:HB2	69:SS:20:ILE:HB	1.75	0.67
4:5:3692:A:H62	4:5:3823:G:H21	1.43	0.67
4:5:1661:C:OP1	36:e:36:ARG:NH2	2.29	0.66
7:A:97:ASN:OD1	7:A:100:ASN:ND2	2.29	0.66
50:9:111:A:O2'	62:LL:69:ARG:NH1	2.28	0.66
54:DD:46:THR:HB	54:DD:84:VAL:HG12	1.76	0.66
58:HH:144:ILE:HD11	58:HH:152:ARG:HD3	1.76	0.66
4:5:3722:G:H2'	4:5:3723:A2M:H8	1.78	0.66
11:E:115:MET:O	48:r:87:ARG:NH1	2.28	0.66
12:F:151:GLU:O	12:F:155:LYS:HB3	1.95	0.66
50:9:190:G:O2'	50:9:209:A:N6	2.29	0.66
50:9:197:U:H3	50:9:202:G:H1	1.41	0.66
36:e:7:LEU:HB2	36:e:93:LYS:HB3	1.77	0.65
50:9:1656:G:H1	50:9:1668:U:H3	1.44	0.65
65:OO:30:VAL:HG12	65:OO:94:HIS:HB2	1.78	0.65
44:m:77:LEU:HD21	44:m:84:CYS:HA	1.77	0.65
75:YY:20:ARG:HH21	75:YY:74:MET:HG2	1.61	0.65
4:5:2306:G:HO2'	4:5:2331:G:H1	1.43	0.65
6:8:75:G:OP2	30:Y:74:TYR:OH	2.14	0.65
6:8:49:G:H5'	39:h:47:ILE:HD11	1.79	0.65
83:gg:217:MET:HG2	83:gg:229:THR:HG22	1.79	0.65
4:5:4054:C:OP1	49:u:23:ARG:NH2	2.30	0.65
62:LL:101:ARG:HB2	74:XX:10:ALA:HB2	1.77	0.65
30:Y:59:ARG:HB2	30:Y:103:LYS:HG2	1.77	0.65
3:4:27:U:H3	3:4:43:A:H61	1.46	0.64
4:5:4558:U:OP2	8:B:246:ARG:NH2	2.30	0.64
8:B:10:ARG:NH1	8:B:265:SER:O	2.30	0.64
50:9:1307:U:H6	82:ff:137:ASP:H	1.44	0.64
44:m:69:ILE:HD11	44:m:96:ARG:HH21	1.63	0.64
4:5:4212:A:N1	25:T:3:ASN:ND2	2.41	0.64
51:AA:52:LYS:HB2	68:RR:109:LEU:HD21	1.79	0.64
67:QQ:85:ARG:NH2	67:QQ:116:ASP:OD2	2.29	0.64
9:C:153:VAL:HG12	9:C:252:TRP:HB2	1.79	0.64
50:9:1504:U:O4	82:ff:84:SER:OG	2.14	0.64
65:OO:34:PHE:HB3	65:OO:41:PHE:HB2	1.79	0.64
21:P:23:ARG:NH1	21:P:125:MET:SD	2.71	0.64
4:5:4621:C:OP1	27:V:48:ARG:NH2	2.31	0.64
50:9:1287:A:O4'	82:ff:97:LYS:N	2.29	0.64
4:5:482:G:H1	4:5:672:C:H42	1.45	0.63
4:5:200:U:O4	30:Y:103:LYS:NZ	2.31	0.63
82:ff:140:TYR:HA	82:ff:147:THR:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:68:C:H2'	3:4:69:G:H8	1.63	0.63
53:CC:206:SER:HB3	53:CC:210:PRO:HG2	1.81	0.63
50:9:819:G:OP1	60:JJ:79:ARG:NH2	2.32	0.63
50:9:1206:G:N2	50:9:1835:A:OP1	2.32	0.63
4:5:2007:G:H21	4:5:2012:A:H62	1.47	0.63
47:p:38:THR:HA	47:p:45:THR:HA	1.81	0.63
4:5:1090:G:OP1	25:T:142:ARG:NH1	2.32	0.63
21:P:91:LEU:HA	21:P:94:MET:HG2	1.80	0.63
50:9:925:G:H1	50:9:1017:U:H3	1.47	0.63
50:9:1677:U:OP1	56:FF:148:ASN:ND2	2.32	0.62
77:aa:12:LYS:HD3	77:aa:16:GLY:H	1.64	0.62
4:5:2528:G:H4'	4:5:2783:A:H4'	1.82	0.62
57:GG:54:GLY:O	57:GG:110:ASN:ND2	2.32	0.62
8:B:283:LYS:HD3	8:B:363:ILE:HD11	1.81	0.62
13:G:108:VAL:HG12	29:X:44:PRO:HA	1.80	0.62
28:W:4:GLU:OE2	28:W:20:ARG:NH2	2.33	0.62
50:9:1503:C:H2'	50:9:1504:U:C2	2.34	0.62
50:9:1284:A:H4'	82:ff:99:LYS:HD2	1.82	0.62
50:9:1287:A:O5'	82:ff:97:LYS:N	2.31	0.62
60:JJ:60:LEU:HD11	60:JJ:70:ARG:HA	1.81	0.62
4:5:4525:C:OP1	8:B:246:ARG:NH1	2.32	0.62
34:c:20:LEU:HD11	64:NN:44:GLY:HA3	1.81	0.62
4:5:1406:G:N3	4:5:1411(A):G:N2	2.47	0.62
5:7:6:C:H4'	10:D:52:ILE:HD13	1.82	0.62
19:N:68:ARG:NH1	19:N:124:ASP:O	2.32	0.62
24:S:34:ALA:HB1	24:S:39:VAL:HG13	1.82	0.62
27:V:82:ILE:HG22	27:V:83:ARG:HG3	1.82	0.62
83:gg:66:VAL:HA	83:gg:82:SER:HA	1.81	0.62
4:5:1882:U:OP2	36:e:46:ARG:NH1	2.32	0.62
11:E:141:ARG:NH1	11:E:172:SER:O	2.33	0.62
4:5:979:G:OP1	11:E:49:ASN:ND2	2.33	0.61
9:C:4:ALA:O	9:C:29:LYS:NZ	2.32	0.61
50:9:1354:G:N2	50:9:1357:A:OP2	2.33	0.61
81:ee:109:MET:SD	81:ee:113:ARG:NH1	2.73	0.61
4:5:3688:U:OP2	7:A:198:ARG:NH2	2.32	0.61
4:5:3972:A:N3	4:5:3973:G:N2	2.46	0.61
50:9:1192:U:OP2	74:XX:119:ARG:NH2	2.33	0.61
5:7:98:G:OP2	24:S:55:LYS:NZ	2.32	0.61
76:ZZ:100:VAL:HB	76:ZZ:108:ILE:HD12	1.82	0.61
49:u:68:LEU:O	49:u:112:ALA:HA	2.00	0.61
50:9:1285:G:H3'	82:ff:99:LYS:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:1597:C:OP2	76:ZZ:85:ARG:NH1	2.32	0.61
72:VV:21:ASN:HB3	73:WW:67:GLY:HA3	1.82	0.61
4:5:2089:G:H1	4:5:2099:C:H41	1.47	0.61
4:5:3953:G:H1	4:5:4060:U:H3	1.48	0.61
14:H:94:SER:HB3	14:H:142:ASP:HB3	1.81	0.61
16:J:51:SER:HB3	16:J:69:ALA:HB3	1.81	0.61
4:5:262:G:H2'	4:5:263:G:H8	1.65	0.61
4:5:4523:A2M:H5''	4:5:4524:G:H5'	1.81	0.61
7:A:45:VAL:HG12	7:A:61:VAL:HG22	1.81	0.61
4:5:1573:G:OP1	23:R:92:LYS:NZ	2.33	0.61
4:5:990:U:H3	4:5:1064:G:H1	1.49	0.61
4:5:3762:B8H:C6	4:5:3762:B8H:CN1	2.75	0.61
4:5:2583:C:OP2	38:g:76:ARG:NH1	2.35	0.60
4:5:4761:G:H2'	4:5:4762:A:H8	1.64	0.60
50:9:587:A:H5'	50:9:592:C:H41	1.66	0.60
53:CC:134:ASN:OD1	53:CC:167:ARG:NH1	2.34	0.60
56:FF:102:LEU:HD11	76:ZZ:67:LEU:HD23	1.81	0.60
77:aa:45:VAL:HG11	77:aa:53:ILE:HG13	1.83	0.60
30:Y:8:THR:HB	30:Y:10:ASP:H	1.66	0.60
50:9:1092:G:OP1	64:NN:2:GLY:N	2.33	0.60
57:GG:162:LEU:O	57:GG:169:PRO:HA	2.00	0.60
63:MM:26:LEU:HD12	63:MM:31:LEU:HD21	1.83	0.60
4:5:4933:C:OP2	11:E:265:LYS:NZ	2.35	0.60
24:S:80:ILE:HG12	24:S:129:VAL:HG22	1.82	0.60
6:8:94:G:OP2	41:j:72:ARG:NH2	2.34	0.60
50:9:1014:G:N2	78:bb:51:GLN:OE1	2.35	0.60
8:B:85:VAL:HG12	8:B:204:GLN:HG2	1.82	0.60
63:MM:53:ALA:HA	63:MM:79:VAL:O	2.01	0.60
4:5:973:C:O2	4:5:1282:G:N2	2.34	0.60
4:5:4594:U:H2'	4:5:4595:G:H8	1.65	0.60
50:9:639:C:H5''	81:ee:114:ARG:HH22	1.66	0.60
4:5:3952:A:N1	4:5:4061:G:O6	2.34	0.60
50:9:1286:G:C5'	82:ff:99:LYS:HD3	2.31	0.60
64:NN:45:LEU:HG	64:NN:49:GLN:HG3	1.83	0.60
68:RR:77:GLU:OE1	68:RR:81:ARG:NH1	2.35	0.60
76:ZZ:48:VAL:HG23	76:ZZ:80:ARG:HG3	1.84	0.60
4:5:931:C:OP2	9:C:350:ARG:NH2	2.35	0.60
4:5:3796:U:HO2'	50:9:1720:U:HO2'	1.49	0.60
9:C:5:ARG:HH22	9:C:26:ALA:HB2	1.66	0.60
24:S:13:VAL:HG23	24:S:62:VAL:HB	1.84	0.60
47:p:38:THR:HG22	47:p:45:THR:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:gg:79:LEU:HD21	83:gg:87:LEU:HD23	1.83	0.60
4:5:1867:A:OP1	15:I:13:LYS:NZ	2.34	0.60
28:W:80:ARG:NH2	50:9:167:G:O2'	2.34	0.60
4:5:2811:G:N1	4:5:2814:C:OP2	2.32	0.60
4:5:1351:G:OP1	9:C:33:ARG:NH1	2.32	0.59
4:5:1604:G:H2'	4:5:1605:7MG:H82	1.84	0.59
60:JJ:136:ARG:NH1	60:JJ:159:PHE:O	2.35	0.59
23:R:102:LEU:HD22	23:R:138:LEU:HD13	1.83	0.59
50:9:678:U:OP2	50:9:1026:C:N4	2.32	0.59
4:5:62:A:OP1	19:N:172:ARG:NH2	2.35	0.59
50:9:846:G:OP2	55:EE:108:ARG:NH1	2.36	0.59
51:AA:19:LEU:HD21	68:RR:106:LEU:HD11	1.85	0.59
83:gg:31:ILE:HG22	83:gg:43:TRP:HB2	1.84	0.59
7:A:245:ARG:HD3	7:A:247:ARG:HH12	1.68	0.59
50:9:1834:A:H2	50:9:1837:G:H1	1.49	0.59
4:5:705:G:OP2	36:e:5:ARG:NH2	2.35	0.59
16:J:94:LEU:O	16:J:174:ILE:HA	2.02	0.59
4:5:1390:G:N2	4:5:1393:G:OP2	2.34	0.59
23:R:173:ARG:O	23:R:176:ARG:NH2	2.36	0.59
83:gg:23:THR:HG22	83:gg:31:ILE:HD11	1.84	0.59
4:5:1080:C:H42	4:5:1219:G:H1	1.50	0.59
4:5:2836:A:H4'	8:B:229:LYS:HA	1.84	0.59
6:8:29:G:H5''	17:L:27:ASN:HB3	1.85	0.59
22:Q:97:LYS:NZ	22:Q:117:GLY:O	2.36	0.59
50:9:74:G:N2	50:9:77:A:OP1	2.35	0.59
23:R:139:MET:O	23:R:143:HIS:ND1	2.35	0.59
50:9:1616:U:OP2	66:PP:43:ARG:NH2	2.35	0.59
55:EE:137:PRO:HB2	55:EE:150:PRO:HD2	1.85	0.59
55:EE:159:THR:HG22	55:EE:173:ILE:HB	1.85	0.59
4:5:1860:B8H:C6	4:5:1860:B8H:CN1	2.76	0.59
4:5:4296:B8H:C5	4:5:4296:B8H:N1	2.34	0.59
50:9:159:A2M:H2	50:9:467:G:H21	1.66	0.59
57:GG:43:GLU:O	57:GG:46:LYS:NZ	2.35	0.59
64:NN:4:MET:SD	64:NN:124:ARG:NH1	2.76	0.59
4:5:2696:A:H5'	42:k:26:LYS:HE2	1.85	0.58
6:8:85:U:O4	30:Y:50:ARG:NH2	2.36	0.58
4:5:4677:U:O2'	4:5:4713:G:N2	2.36	0.58
19:N:181:HIS:O	19:N:195:ARG:NH2	2.35	0.58
23:R:176:ARG:NH1	50:9:910:G:OP1	2.29	0.58
83:gg:87:LEU:HB2	83:gg:101:PHE:HB2	1.84	0.58
56:FF:175:ASP:HA	56:FF:178:ILE:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:KK:20:VAL:HG12	61:KK:70:TYR:HA	1.84	0.58
4:5:2090:U:OP2	9:C:307:LYS:NZ	2.37	0.58
75:YY:20:ARG:NH2	75:YY:22:GLN:OE1	2.34	0.58
3:4:58:A:O2'	3:4:61:C:N4	2.37	0.58
4:5:27:C:O2'	4:5:60:A:N3	2.36	0.58
8:B:41:VAL:HA	8:B:187:GLY:HA3	1.84	0.58
27:V:69:LYS:NZ	27:V:71:GLU:OE2	2.37	0.58
50:9:15:U:O2'	50:9:669:A:N6	2.36	0.58
50:9:992:A:N7	77:aa:15:ARG:NH2	2.50	0.58
50:9:1252:C:N4	67:QQ:145:TYR:O	2.36	0.58
50:9:1617:G:O6	66:PP:43:ARG:NH1	2.37	0.58
52:BB:137:LEU:HG	52:BB:215:VAL:HG22	1.85	0.58
9:C:303:ARG:HH12	9:C:306:ARG:HG2	1.67	0.58
50:9:1287:A:C8	82:ff:97:LYS:HB3	2.32	0.58
55:EE:104:ASP:HB3	55:EE:110:ALA:HB2	1.85	0.58
10:D:32:ALA:O	10:D:36:LEU:HB2	2.04	0.58
43:l:20:ASN:O	43:l:41:ARG:NH1	2.37	0.58
55:EE:153:LEU:HD23	57:GG:216:ARG:HD3	1.85	0.58
50:9:1617:G:N1	50:9:1620:A:OP2	2.36	0.58
4:5:2322:G:OP1	36:e:36:ARG:NH1	2.37	0.58
5:7:120:U:OP1	10:D:259:ARG:NH1	2.37	0.58
34:c:11:LEU:HA	34:c:14:ILE:HG22	1.85	0.58
50:9:1148:A:OP1	77:aa:6:ARG:NH2	2.37	0.58
56:FF:125:SER:HB3	56:FF:136:ARG:HD3	1.86	0.58
4:5:942:G:OP1	12:F:244:ARG:NH1	2.37	0.58
4:5:2422:OMC:OP1	21:P:127:ARG:NH2	2.37	0.58
8:B:384:GLU:OE2	28:W:14:TYR:OH	2.22	0.58
17:L:21:ARG:HB3	19:N:197:THR:HG22	1.84	0.58
50:9:1488:C:O2'	50:9:1490:G:OP2	2.21	0.58
3:4:15:G:H2'	3:4:59:G:H1	1.69	0.57
4:5:1552:G:O2'	4:5:1574:B9B:N2	2.37	0.57
4:5:4296:B8H:C6	4:5:4296:B8H:CN1	2.75	0.57
7:A:116:LEU:HB3	7:A:126:LEU:HB2	1.85	0.57
51:AA:12:GLU:HA	51:AA:15:VAL:HG12	1.86	0.57
60:JJ:32:ILE:HG13	60:JJ:37:LEU:HB2	1.86	0.57
82:ff:139:HIS:CB	82:ff:148:TYR:O	2.47	0.57
4:5:2837:U:OP1	8:B:249:ARG:NH1	2.37	0.57
4:5:4887:C:N4	4:5:4932:U:H3	2.00	0.57
7:A:64:ARG:NH2	13:G:95:GLY:O	2.38	0.57
10:D:50:ARG:O	10:D:64:ILE:HA	2.04	0.57
28:W:23:ARG:HE	28:W:29:PHE:HE2	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:380:G:H1'	59:II:5:ARG:HH11	1.68	0.57
50:9:508:A:H3'	50:9:509:OMG:H8	1.70	0.57
50:9:616:A:OP1	74:XX:68:LYS:NZ	2.36	0.57
50:9:1205:C:O2'	50:9:1834:A:N6	2.33	0.57
83:gg:207:CYS:HB2	83:gg:221:LEU:HD11	1.85	0.57
4:5:1468:C:OP1	32:a:132:ARG:NH2	2.38	0.57
4:5:2793:G:H5'	4:5:2794:C:H5''	1.85	0.57
50:9:1677:U:H2'	50:9:1678:A2M:H8	1.86	0.57
4:5:976:C:O2	9:C:323:ARG:NH1	2.38	0.57
4:5:3877:A:O2'	4:5:4400:G:N2	2.38	0.57
4:5:3969:G:H1	4:5:4054:C:H42	1.52	0.57
8:B:287:ILE:HG12	8:B:331:VAL:HG12	1.87	0.57
50:9:1286:G:H5'	82:ff:99:LYS:HD3	1.87	0.57
50:9:1312:G:H1'	82:ff:95:ARG:HH21	1.69	0.57
66:PP:18:ARG:HE	69:SS:88:LYS:HG2	1.69	0.57
66:PP:81:ARG:NH1	66:PP:120:SER:OG	2.37	0.57
4:5:230:G:OP1	30:Y:15:ARG:NH1	2.37	0.57
4:5:1850:A:N3	4:5:2283:G:O2'	2.38	0.57
4:5:2411:C:H2'	4:5:2412:A:H8	1.69	0.57
4:5:3969:G:H1'	49:u:166:ALA:HB3	1.86	0.57
50:9:659:G:HO2'	50:9:662:G:HO2'	1.48	0.57
3:4:29:A:H2'	3:4:30:G:H8	1.69	0.57
4:5:2397:G:O6	38:g:4:ARG:NH2	2.38	0.57
50:9:162:C:O3'	57:GG:95:LYS:NZ	2.37	0.57
50:9:1017:U:H5'	64:NN:55:ARG:HG2	1.87	0.57
59:II:120:PRO:HB2	59:II:123:ARG:HG3	1.87	0.57
4:5:300:A:H2'	4:5:301:G:H8	1.69	0.57
4:5:4296:B8H:C5	4:5:4296:B8H:C2	2.82	0.57
53:CC:179:THR:HG21	53:CC:198:ALA:H	1.69	0.57
54:DD:8:LYS:HE3	71:UU:59:LYS:HD2	1.85	0.57
54:DD:135:GLU:HA	54:DD:152:PHE:O	2.05	0.57
4:5:2262:G:OP2	48:r:98:ARG:NH2	2.36	0.57
15:I:79:SER:OG	15:I:147:HIS:ND1	2.37	0.57
38:g:61:PRO:HA	38:g:64:LEU:HD13	1.85	0.57
49:u:131:ALA:HB3	49:u:133:LYS:HB2	1.87	0.57
50:9:925:G:OP1	64:NN:121:ARG:NH2	2.38	0.57
50:9:989:C:O2	77:aa:32:LYS:NZ	2.38	0.57
4:5:1830:G:O2'	33:b:68:ARG:NH1	2.37	0.57
19:N:47:LYS:HA	19:N:50:ARG:HG2	1.87	0.57
50:9:1228:A:H2'	50:9:1229:G:H8	1.70	0.57
50:9:1273:C:N3	50:9:1506:A:N6	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:1533:A:OP2	56:FF:164:ARG:NH2	2.37	0.57
70:TT:23:LYS:HE3	70:TT:51:ASN:HD22	1.69	0.57
4:5:303:C:OP2	19:N:68:ARG:NH2	2.38	0.56
4:5:4327:C:OP1	25:T:70:HIS:NE2	2.38	0.56
14:H:18:ILE:HG13	14:H:27:VAL:HG22	1.87	0.56
50:9:161:U:O2'	57:GG:87:ARG:NH1	2.33	0.56
4:5:4080:C:H2'	4:5:4081:G:H8	1.69	0.56
30:Y:1:MET:SD	30:Y:1:MET:N	2.72	0.56
59:II:143:LYS:HA	59:II:146:GLN:HB3	1.87	0.56
4:5:2093:G:OP1	48:r:101:LYS:NZ	2.39	0.56
4:5:4613:C:N3	14:H:121:LYS:NZ	2.54	0.56
4:5:4729:A:H5''	4:5:4965:U:H1'	1.88	0.56
24:S:95:ARG:NH2	24:S:112:ASP:OD2	2.38	0.56
50:9:526:A:O2'	60:JJ:125:HIS:ND1	2.38	0.56
50:9:1599:U:OP2	76:ZZ:46:ASN:ND2	2.37	0.56
69:SS:138:THR:HG23	69:SS:139:THR:HG23	1.87	0.56
83:gg:254:PRO:HA	83:gg:285:GLN:HA	1.87	0.56
4:5:2782:U:OP2	43:l:10:LYS:NZ	2.37	0.56
4:5:2891:U:OP2	23:R:74:ARG:NH2	2.39	0.56
4:5:4391:G:OP1	9:C:75:ARG:NH1	2.38	0.56
8:B:234:ARG:NH2	8:B:268:ARG:O	2.33	0.56
31:Z:21:ARG:NH1	31:Z:47:ASP:O	2.38	0.56
50:9:944:A:H5''	65:OO:134:PRO:HB2	1.87	0.56
50:9:1398:G:H4'	83:gg:88:ARG:HH22	1.68	0.56
54:DD:55:THR:HA	54:DD:58:VAL:HG12	1.87	0.56
4:5:2457:G:HO2'	4:5:3672:G:HO2'	1.53	0.56
7:A:10:LYS:HA	7:A:16:PHE:HD2	1.69	0.56
41:j:20:ARG:NH2	41:j:39:TYR:OH	2.38	0.56
58:HH:144:ILE:HG23	73:WW:52:ILE:HG12	1.88	0.56
4:5:1654:G:N2	4:5:1678:C:OP1	2.38	0.56
4:5:4220:6MZ:OP1	25:T:2:THR:N	2.39	0.56
32:a:81:LEU:HD21	32:a:103:VAL:HG23	1.88	0.56
49:u:48:ARG:NH2	49:u:159:MET:O	2.30	0.56
50:9:1737:G:OP1	57:GG:94:ARG:NH2	2.37	0.56
50:9:1854:U:OP2	65:OO:147:ARG:NH2	2.38	0.56
70:TT:114:GLU:OE2	70:TT:122:LYS:NZ	2.37	0.56
71:UU:94:PRO:HD2	71:UU:97:ILE:HD12	1.88	0.56
4:5:2276:A:OP1	12:F:165:ARG:NH1	2.37	0.56
17:L:186:ARG:HH21	40:i:9:VAL:HG11	1.71	0.56
23:R:172:ARG:NH2	50:9:909:G:OP2	2.39	0.56
50:9:1033:G:N1	50:9:1080:A:O2'	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:1228:A:H2'	50:9:1229:G:C8	2.41	0.56
50:9:1398:G:O2'	83:gg:88:ARG:NH2	2.39	0.56
83:gg:177:TRP:HA	83:gg:184:LEU:HA	1.87	0.56
4:5:4415:1MA:O2'	15:I:74:LYS:NZ	2.38	0.56
50:9:1060:A:O2'	50:9:1062:A:N7	2.37	0.56
50:9:1467:C:OP1	68:RR:2:GLY:N	2.39	0.56
57:GG:132:ARG:HG2	57:GG:133:LEU:HD12	1.87	0.56
83:gg:113:PHE:HA	83:gg:120:ILE:HG22	1.86	0.56
2:2:76:A:H1'	4:5:3909:OMC:HM21	1.86	0.56
4:5:2403:A:OP1	38:g:10:ARG:NH1	2.38	0.56
11:E:189:LEU:HD21	11:E:256:VAL:HG11	1.88	0.56
14:H:107:GLU:OE2	14:H:127:ARG:NH2	2.38	0.56
50:9:846:G:OP1	55:EE:106:LYS:NZ	2.38	0.56
50:9:1864:U:O2'	50:9:1866:A:N7	2.37	0.56
4:5:2848:G:O2'	4:5:3838:U:O4	2.23	0.56
4:5:4711:C:O2'	20:O:145:VAL:O	2.24	0.56
5:7:23:A:N3	5:7:118:C:O2'	2.34	0.56
28:W:86:SER:OG	28:W:87:LEU:N	2.39	0.56
4:5:1645:C:OP1	9:C:80:ARG:NH2	2.40	0.55
4:5:2429:A:H5''	43:l:43:HIS:HE2	1.71	0.55
4:5:2489:C:O2'	4:5:2491:C:N4	2.39	0.55
4:5:4583:C:O2'	4:5:4718:G:N2	2.38	0.55
19:N:165:THR:O	19:N:169:ARG:HB2	2.06	0.55
52:BB:109:LYS:HG3	52:BB:113:MET:HE2	1.88	0.55
58:HH:137:SER:OG	58:HH:162:GLN:O	2.24	0.55
4:5:3879:G:O2'	4:5:3881:G:OP2	2.21	0.55
12:F:231:ASP:OD1	12:F:235:ARG:NH1	2.39	0.55
30:Y:88:GLU:HA	30:Y:94:THR:HA	1.88	0.55
50:9:10:G:H21	53:CC:114:LYS:HA	1.70	0.55
52:BB:68:GLU:OE2	52:BB:83:LYS:NZ	2.35	0.55
58:HH:117:PRO:HG2	58:HH:120:ARG:HD3	1.88	0.55
63:MM:40:LYS:HG3	63:MM:44:LYS:HE3	1.88	0.55
4:5:1316:OMG:OP1	36:e:43:ASN:ND2	2.39	0.55
4:5:2062:C:O2'	24:S:111:ARG:NH1	2.38	0.55
4:5:4467:A:O2'	4:5:4510:A:N3	2.35	0.55
9:C:146:GLU:HG3	9:C:175:LYS:HB3	1.88	0.55
50:9:1658:G:OP2	50:9:1660:C:N4	2.39	0.55
4:5:4765:G:OP1	14:H:23:ARG:NE	2.38	0.55
4:5:4862:G:H2'	4:5:4863:G:H8	1.72	0.55
11:E:153:LEU:HD13	11:E:197:VAL:HG11	1.88	0.55
19:N:174:LEU:HA	19:N:183:THR:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:h:68:ASN:OD1	39:h:71:LYS:NZ	2.37	0.55
50:9:1262:C:O2'	80:dd:12:ARG:NH1	2.40	0.55
68:RR:104:GLU:HA	68:RR:107:LYS:HG2	1.88	0.55
4:5:1823:G:O2'	10:D:44:TYR:O	2.25	0.55
4:5:3619:G:H22	4:5:3624:A:H1'	1.72	0.55
7:A:95:GLN:O	7:A:100:ASN:ND2	2.39	0.55
49:u:54:ARG:NH2	49:u:150:GLU:OE2	2.40	0.55
50:9:94:G:HO2'	50:9:508:A:HO2'	1.54	0.55
50:9:1287:A:P	82:ff:98:VAL:H	2.29	0.55
59:II:105:ASP:N	59:II:105:ASP:OD1	2.38	0.55
6:8:26:C:O2'	9:C:53:ALA:O	2.25	0.55
8:B:216:MET:HE3	8:B:281:ASN:HB3	1.88	0.55
30:Y:80:ILE:HD11	30:Y:104:VAL:HG21	1.88	0.55
44:m:84:CYS:SG	44:m:85:ARG:N	2.80	0.55
50:9:383:G:H4'	62:LL:132:ARG:HD2	1.89	0.55
50:9:522:A:H5''	60:JJ:145:PRO:HD2	1.89	0.55
50:9:1654:G:OP1	70:TT:90:SER:OG	2.25	0.55
51:AA:33:GLN:NE2	72:VV:64:GLU:OE2	2.33	0.55
82:ff:105:TYR:O	82:ff:117:LEU:N	2.38	0.55
4:5:1081:C:N4	4:5:1219:G:O6	2.40	0.55
4:5:2520:C:H2'	4:5:2521:G:H8	1.72	0.55
14:H:126:VAL:HG11	14:H:161:ILE:HG22	1.89	0.55
47:p:37:TYR:HB2	47:p:47:MET:HB2	1.88	0.55
52:BB:52:THR:HG22	52:BB:58:ALA:H	1.71	0.55
54:DD:209:SER:HB3	68:RR:40:ILE:HD11	1.89	0.55
56:FF:30:ILE:HG12	56:FF:113:VAL:HG11	1.88	0.55
57:GG:66:GLY:N	57:GG:100:CYS:SG	2.74	0.55
4:5:2740:U:O2'	4:5:2742:G:N2	2.38	0.55
4:5:3762:B8H:C5	4:5:3762:B8H:C2	2.83	0.55
7:A:177:LYS:HB2	47:p:29:ILE:HG21	1.89	0.55
7:A:200:ARG:NH2	7:A:217:GLN:OE1	2.40	0.55
29:X:129:ARG:HD3	29:X:135:LYS:HE3	1.88	0.55
31:Z:54:THR:H	31:Z:57:MET:HE2	1.72	0.55
32:a:127:LYS:NZ	32:a:148:ALA:O	2.39	0.55
50:9:126:G:OP2	57:GG:195:LYS:NZ	2.36	0.55
50:9:583:A:OP1	60:JJ:162:ARG:NH1	2.40	0.55
50:9:1288:U:H1'	82:ff:96:LYS:HD2	1.89	0.55
62:LL:85:THR:HA	62:LL:113:LEU:H	1.70	0.55
73:WW:44:HIS:NE2	73:WW:112:ASP:OD2	2.40	0.55
12:F:93:ARG:NH2	12:F:95:ARG:O	2.40	0.55
24:S:82:LEU:HG	24:S:93:MET:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:CC:214:LEU:HD12	53:CC:244:ILE:HD11	1.89	0.55
61:KK:90:VAL:O	61:KK:95:ARG:NH2	2.39	0.55
71:UU:54:VAL:HG22	71:UU:88:LEU:HB2	1.88	0.55
4:5:1326:A2M:OP2	4:5:4445:U:O2'	2.26	0.54
4:5:4944:C:N4	37:f:58:VAL:O	2.38	0.54
21:P:4:TYR:HE2	21:P:16:LYS:HB3	1.71	0.54
55:EE:126:VAL:HG12	55:EE:139:LEU:HD13	1.89	0.54
4:5:1353:G:N7	22:Q:104:ARG:NH2	2.49	0.54
4:5:1895:G:OP1	12:F:95:ARG:NH2	2.40	0.54
12:F:227:VAL:HG13	24:S:39:VAL:HG23	1.89	0.54
50:9:1857:G:OP2	65:OO:141:ARG:NH1	2.35	0.54
55:EE:11:ARG:NH2	55:EE:24:THR:OG1	2.39	0.54
74:XX:91:LEU:HB3	81:ee:82:VAL:HG21	1.88	0.54
83:gg:173:LEU:HD22	83:gg:189:ILE:HG12	1.88	0.54
6:8:155:C:OP2	13:G:142:ARG:NH2	2.38	0.54
18:M:104:MET:HE2	20:O:199:HIS:HB3	1.89	0.54
32:a:89:ASN:O	32:a:93:ASN:HB2	2.08	0.54
42:k:24:LYS:HA	42:k:67:LYS:O	2.07	0.54
50:9:1579:A:H4'	50:9:1581:C:H5	1.72	0.54
56:FF:70:GLU:OE1	56:FF:74:ASN:ND2	2.39	0.54
75:YY:78:SER:HB2	75:YY:81:TYR:HD2	1.71	0.54
4:5:1435:G:N2	4:5:1450:C:N3	2.55	0.54
4:5:2457:G:OP1	19:N:65:ARG:NH1	2.39	0.54
4:5:4429:C:N3	15:I:158:LYS:NZ	2.49	0.54
8:B:218:ASP:OD2	8:B:348:ARG:NH1	2.40	0.54
50:9:548:C:H5'	50:9:549:C:H5''	1.90	0.54
50:9:1288:U:H1'	82:ff:96:LYS:HB3	1.89	0.54
54:DD:48:ILE:O	54:DD:86:LEU:HA	2.07	0.54
78:bb:33:MET:HE1	78:bb:73:LEU:HD11	1.89	0.54
83:gg:132:TRP:CD1	83:gg:138:CYS:HA	2.43	0.54
3:4:72:C:N4	3:4:73:G:O6	2.41	0.54
4:5:1479:G:H21	17:L:184:MET:HE2	1.72	0.54
11:E:286:PRO:HA	11:E:289:LEU:HG	1.90	0.54
14:H:23:ARG:HH21	14:H:39:ASN:HA	1.73	0.54
30:Y:30:MET:HB3	30:Y:101:PRO:HG2	1.88	0.54
50:9:641:A:O2'	50:9:645:C:OP1	2.26	0.54
52:BB:32:ASP:OD1	52:BB:46:LYS:NZ	2.37	0.54
55:EE:30:ARG:HE	55:EE:38:LEU:HD11	1.72	0.54
67:QQ:113:ILE:HG13	67:QQ:120:LEU:HD12	1.88	0.54
75:YY:82:ALA:O	75:YY:86:GLU:HB2	2.07	0.54
4:5:935:A:H5'	4:5:935(A):G:H4'	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:1645:C:H2'	4:5:1646:A:C8	2.43	0.54
4:5:2396:A:N6	4:5:2814:C:O2	2.40	0.54
5:7:17:C:OP1	16:J:156:ARG:NH2	2.40	0.54
9:C:10:VAL:HA	9:C:153:VAL:HG23	1.89	0.54
13:G:139:VAL:HG11	13:G:238:LYS:HE3	1.88	0.54
34:c:102:SER:O	34:c:106:ARG:NH2	2.41	0.54
44:m:68:MET:HG2	44:m:79:PRO:HA	1.90	0.54
50:9:57:U:O2'	50:9:499:G:N3	2.38	0.54
50:9:492:C:OP2	75:YY:107:ARG:NH2	2.41	0.54
50:9:1092:G:OP2	64:NN:9:LYS:NZ	2.40	0.54
52:BB:35:ALA:O	52:BB:42:ARG:NH1	2.40	0.54
52:BB:107:ARG:NH2	65:OO:133:THR:O	2.41	0.54
55:EE:85:GLY:N	55:EE:88:ASP:OD2	2.38	0.54
4:5:456:C:H2'	4:5:457:G:H8	1.73	0.54
4:5:1503:A:H4'	4:5:1504:G:H5'	1.89	0.54
4:5:4522:G:O2'	4:5:4525:C:OP2	2.24	0.54
23:R:35:ALA:O	23:R:40:GLN:NE2	2.29	0.54
4:5:923:C:H5'	4:5:924:C:H5''	1.89	0.54
4:5:2083:C:OP2	22:Q:14:ARG:NH2	2.40	0.54
4:5:4228:G:HO2'	4:5:4373:G:H1	1.54	0.54
4:5:4250:G:O2'	16:J:129:ASP:OD1	2.20	0.54
35:d:23:ARG:HG3	35:d:121:ASN:HA	1.89	0.54
50:9:56:G:OP1	75:YY:111:LYS:NZ	2.36	0.54
50:9:1086:G:OP2	77:aa:12:LYS:NZ	2.41	0.54
63:MM:60:MET:HE2	82:ff:108:VAL:HG22	1.90	0.54
77:aa:46:GLU:HG2	77:aa:47:ALA:H	1.72	0.54
4:5:4448:G:H5''	4:5:4449:A:H5'	1.89	0.54
4:5:4587:G:N2	8:B:15:GLY:O	2.35	0.54
8:B:154:LYS:HG3	8:B:194:LEU:HD22	1.90	0.54
19:N:5:LYS:HG3	40:i:40:VAL:HG11	1.90	0.54
50:9:185:G:O6	50:9:214:U:O2	2.26	0.54
50:9:688:U:H5	58:HH:103:LYS:H	1.55	0.54
83:gg:256:ILE:HD11	83:gg:270:LEU:HD23	1.90	0.54
4:5:67:C:OP2	4:5:312:G:N2	2.40	0.54
4:5:85:G:O2'	4:5:97:G:O6	2.26	0.54
4:5:1500:A:H5''	4:5:1501:C:H5'	1.90	0.54
4:5:2353:U:H5''	9:C:89:GLN:HG2	1.89	0.54
66:PP:22:LEU:HA	66:PP:25:LEU:HB2	1.89	0.54
4:5:1456:B8Q:O2	22:Q:75:ARG:NH2	2.42	0.53
4:5:2521:G:H2'	4:5:2522:7MG:H82	1.90	0.53
4:5:2847:G:OP1	27:V:85:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:3888:G:O6	20:O:96:GLN:NE2	2.41	0.53
4:5:4753:U:OP1	37:f:100:ARG:NH1	2.40	0.53
8:B:307:TYR:HD2	8:B:366:LYS:HG2	1.73	0.53
11:E:156:LEU:HD11	11:E:198:ILE:HG13	1.90	0.53
13:G:111:PRO:HD2	13:G:114:ILE:HD12	1.90	0.53
49:u:60:ARG:HG2	49:u:63:PHE:HD1	1.74	0.53
50:9:91:A:H5''	50:9:92:A:H5''	1.90	0.53
50:9:1280:G:OP2	63:MM:101:ARG:NH1	2.41	0.53
58:HH:34:SER:OG	58:HH:35:ASP:N	2.41	0.53
71:UU:80:PHE:HB3	80:dd:52:PHE:HB3	1.89	0.53
4:5:966:A:O4'	4:5:968:C:N4	2.41	0.53
4:5:4087:G:N7	7:A:67:TYR:OH	2.39	0.53
4:5:4454:G:O2'	4:5:4500:PSU:O2'	2.26	0.53
56:FF:35:LEU:HD11	56:FF:146:ARG:HD3	1.90	0.53
66:PP:18:ARG:NH1	69:SS:88:LYS:O	2.34	0.53
4:5:907:C:H2'	4:5:908:G:H8	1.73	0.53
4:5:1970:A:N6	4:5:2016:C:OP2	2.35	0.53
4:5:3759:A:OP2	4:5:3765:G:N1	2.38	0.53
7:A:137:ILE:HD11	7:A:149:LYS:HB2	1.89	0.53
51:AA:210:ILE:HG21	68:RR:81:ARG:HD3	1.89	0.53
54:DD:131:ALA:HA	54:DD:191:PRO:HD3	1.89	0.53
60:JJ:69:ARG:NH2	60:JJ:73:GLU:OE2	2.41	0.53
4:5:3604:A:H5''	23:R:71:ARG:HH12	1.73	0.53
4:5:4661:G:N2	4:5:5004:C:O3'	2.42	0.53
15:I:38:ARG:HB2	15:I:83:ASP:HB2	1.89	0.53
48:r:7:TRP:O	48:r:11:ARG:HB2	2.08	0.53
50:9:380:G:N3	59:II:5:ARG:NH1	2.55	0.53
50:9:649:U:H2'	50:9:650:A:H8	1.73	0.53
50:9:681:U:H5''	74:XX:8:ARG:HG3	1.91	0.53
61:KK:80:ARG:NH2	61:KK:89:ILE:O	2.42	0.53
4:5:337:U:H2'	4:5:338:A:H8	1.74	0.53
4:5:729:2MG:N2	24:S:66:GLN:O	2.42	0.53
4:5:1947:U:O2	4:5:4693:C:N4	2.41	0.53
4:5:4476:C:O2'	4:5:4478:G:OP2	2.22	0.53
7:A:225:ILE:HD11	7:A:235:VAL:H	1.74	0.53
15:I:66:GLU:OE2	15:I:69:ARG:NH1	2.40	0.53
17:L:21:ARG:NH1	19:N:196:ASN:O	2.42	0.53
21:P:18:ARG:NH1	21:P:20:SER:OG	2.41	0.53
22:Q:78:LYS:HG2	22:Q:137:VAL:HG23	1.90	0.53
31:Z:36:ARG:NH1	31:Z:38:TYR:OH	2.35	0.53
49:u:6:SER:OG	49:u:8:ASP:OD1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:359:U:OP2	74:XX:18:ARG:NH2	2.41	0.53
52:BB:121:ILE:HG12	52:BB:161:VAL:HG23	1.89	0.53
83:gg:210:GLY:HA3	83:gg:236:ILE:HD11	1.90	0.53
4:5:1077:C:OP1	4:5:1215:C:O2'	2.26	0.53
23:R:99:MET:HE1	23:R:128:LYS:HA	1.89	0.53
24:S:15:ARG:HH12	24:S:18:PRO:HG3	1.74	0.53
52:BB:191:ASP:OD1	52:BB:195:LYS:NZ	2.39	0.53
78:bb:36:LYS:HB3	78:bb:43:ILE:HG22	1.91	0.53
82:ff:85:TYR:HE2	82:ff:88:PRO:HB3	1.74	0.53
2:2:18:G:H21	2:2:58:A:H5'	1.73	0.53
4:5:1558:A:H2'	4:5:1559:G:H8	1.73	0.53
4:5:1931:C:N4	4:5:2040:A:O2'	2.42	0.53
4:5:4122:G:N2	38:g:98:GLU:OE2	2.39	0.53
12:F:70:MET:HA	12:F:73:MET:HG2	1.90	0.53
38:g:11:LEU:HD23	38:g:13:TYR:H	1.74	0.53
50:9:1535:U:O2'	56:FF:81:ARG:NH2	2.42	0.53
3:4:8:U:O2'	3:4:21:A:N1	2.35	0.53
4:5:280:G:N2	4:5:306:A:OP2	2.35	0.53
50:9:600:G:H2'	50:9:601:G:H8	1.73	0.53
50:9:1568:C:O2	50:9:1627:C:O2'	2.25	0.53
52:BB:129:THR:OG1	52:BB:131:ASP:O	2.26	0.53
56:FF:50:PRO:HB3	56:FF:69:VAL:HG12	1.90	0.53
62:LL:126:VAL:HG12	62:LL:145:VAL:HG22	1.91	0.53
4:5:375:G:N7	41:j:56:ARG:NH1	2.57	0.53
4:5:1466:G:OP1	33:b:44:ARG:NH2	2.41	0.53
4:5:2784:C:H41	43:l:3:SER:HB2	1.74	0.53
8:B:119:TYR:OH	8:B:129:ALA:N	2.42	0.53
14:H:59:LYS:HE2	14:H:66:GLU:HB3	1.90	0.53
16:J:18:ARG:HG3	16:J:135:GLY:HA3	1.89	0.53
50:9:1322:G:O6	82:ff:89:LYS:NZ	2.34	0.53
62:LL:49:GLU:OE2	62:LL:118:ARG:NH2	2.42	0.53
6:8:37:A:OP2	39:h:89:ARG:NH1	2.37	0.53
22:Q:59:PRO:HG3	22:Q:143:ARG:HA	1.91	0.53
50:9:1287:A:P	82:ff:96:LYS:HB2	2.49	0.53
50:9:1568:C:OP1	70:TT:96:SER:OG	2.27	0.53
55:EE:11:ARG:HA	55:EE:28:ALA:HB2	1.90	0.53
4:5:1914:C:H4'	20:O:89:PRO:HD3	1.91	0.52
4:5:4163:U:H5'	4:5:4164:C:H5''	1.90	0.52
50:9:1373:C:O2'	68:RR:10:LYS:NZ	2.32	0.52
57:GG:116:LYS:NZ	57:GG:119:LYS:O	2.42	0.52
66:PP:75:VAL:HG22	66:PP:93:MET:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:YY:74:MET:HE1	75:YY:90:ARG:HH12	1.73	0.52
4:5:440:U:O2'	37:f:91:ASN:O	2.27	0.52
4:5:442:G:OP1	37:f:68:ARG:NH1	2.42	0.52
4:5:1942:A:OP2	4:5:2040:A:N6	2.42	0.52
4:5:4280:A:OP2	10:D:23:ARG:NH2	2.42	0.52
39:h:105:LYS:HA	39:h:108:GLN:HG2	1.90	0.52
50:9:26:U:H2'	50:9:27:A2M:H8	1.91	0.52
50:9:472:C:O2	50:9:475:C:N4	2.42	0.52
50:9:609:U:H2'	50:9:610:G:H8	1.75	0.52
50:9:1307:U:H5''	82:ff:136:PHE:HA	1.92	0.52
58:HH:145:ARG:NH1	73:WW:51:GLU:OE1	2.40	0.52
4:5:1860:B8H:C5	4:5:1860:B8H:C2	2.84	0.52
4:5:2341:A:OP1	9:C:46:LYS:NZ	2.37	0.52
4:5:3807:A:OP1	45:n:23:ARG:NH2	2.43	0.52
4:5:3839:G:N2	4:5:3843:C:O2'	2.42	0.52
4:5:4895:C:O2	18:M:132:ARG:NH2	2.42	0.52
15:I:189:ARG:NH2	15:I:199:TYR:OH	2.43	0.52
18:M:4:ARG:HG3	18:M:5:ARG:HD2	1.90	0.52
27:V:31:ASN:ND2	27:V:115:SER:OG	2.39	0.52
54:DD:64:ARG:HA	54:DD:67:ARG:HH11	1.73	0.52
54:DD:67:ARG:NH2	61:KK:95:ARG:O	2.43	0.52
4:5:945:U:OP2	9:C:342:ARG:NH2	2.43	0.52
4:5:1429:C:O2'	22:Q:136:THR:O	2.27	0.52
4:5:2299:G:OP2	9:C:204:ARG:NH1	2.43	0.52
4:5:2521:G:O3'	38:g:25:THR:OG1	2.27	0.52
7:A:117:GLU:HB3	7:A:162:ASN:HB2	1.90	0.52
19:N:116:LEU:HD22	19:N:135:ILE:HD11	1.92	0.52
30:Y:50:ARG:HB2	30:Y:115:ARG:HH22	1.75	0.52
51:AA:71:PRO:HB3	51:AA:186:ARG:HH12	1.75	0.52
4:5:1869:G:N2	4:5:3876:A:OP2	2.43	0.52
8:B:189:THR:N	8:B:192:GLU:OE2	2.42	0.52
50:9:851:C:O2'	50:9:852:G:N2	2.40	0.52
50:9:1404:U:OP1	71:UU:21:ARG:NH2	2.43	0.52
51:AA:80:ARG:NH2	51:AA:165:ASN:O	2.38	0.52
65:OO:65:ASP:HA	65:OO:68:GLU:HG3	1.92	0.52
4:5:467:U:O2	4:5:686:A:N6	2.43	0.52
4:5:2297:E7G:O3'	9:C:140:LYS:NZ	2.43	0.52
7:A:36:GLU:HG3	7:A:91:GLY:HA2	1.92	0.52
8:B:150:PHE:HD1	8:B:194:LEU:HD23	1.75	0.52
49:u:31:THR:HA	49:u:171:HIS:HA	1.92	0.52
50:9:1273:C:O2'	82:ff:92:LYS:NZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:1286:G:P	82:ff:99:LYS:H	2.32	0.52
83:gg:5:MET:HE1	83:gg:312:VAL:HG22	1.92	0.52
4:5:4943:A:OP1	11:E:157:THR:OG1	2.21	0.52
27:V:87:SER:HA	27:V:97:TYR:HB3	1.92	0.52
50:9:929:G:N2	50:9:1104:G:O2'	2.42	0.52
50:9:996:A:H2'	50:9:997:A:C8	2.44	0.52
50:9:1308:U:H1'	82:ff:135:HIS:HA	1.92	0.52
54:DD:31:GLU:O	54:DD:54:ARG:NH2	2.38	0.52
56:FF:37:ASP:OD1	56:FF:37:ASP:N	2.40	0.52
66:PP:25:LEU:HA	66:PP:28:MET:HE3	1.90	0.52
4:5:1176:C:O3'	10:D:268:ARG:NH2	2.43	0.52
4:5:1320:U:O2'	4:5:1891:A:N1	2.32	0.52
4:5:2847:G:H1'	27:V:21:PRO:HD2	1.92	0.52
4:5:4748:U:H5''	37:f:54:LYS:HE2	1.91	0.52
5:7:38:U:N3	5:7:41:G:OP2	2.40	0.52
10:D:55:VAL:HG12	10:D:60:ILE:HG12	1.90	0.52
50:9:72:C:O2'	50:9:74:G:OP2	2.28	0.52
4:5:121:A:OP1	13:G:163:LYS:NZ	2.35	0.52
13:G:191:ALA:O	13:G:195:THR:OG1	2.28	0.52
41:j:34:CYS:SG	41:j:35:GLY:N	2.82	0.52
44:m:71:ARG:HE	44:m:96:ARG:HB2	1.75	0.52
50:9:1286:G:H3'	82:ff:98:VAL:C	2.35	0.52
59:II:190:LEU:HD23	59:II:195:LEU:HA	1.91	0.52
4:5:4586:G:OP1	20:O:72:HIS:N	2.42	0.52
17:L:64:VAL:HA	17:L:67:HIS:HD2	1.75	0.52
37:f:7:CYS:HB2	37:f:103:VAL:HG13	1.91	0.52
38:g:11:LEU:O	38:g:18:ASN:ND2	2.43	0.52
50:9:1562:C:H2'	50:9:1563:G:H8	1.75	0.52
53:CC:221:ASP:N	53:CC:221:ASP:OD1	2.41	0.52
73:WW:27:ILE:HB	73:WW:61:ILE:HG23	1.92	0.52
77:aa:59:PHE:HB2	77:aa:62:TYR:HB2	1.92	0.52
3:4:18:U:H4'	3:4:19:G:H5'	1.92	0.51
4:5:153:G:OP2	19:N:54:LYS:NZ	2.41	0.51
4:5:1427:A:OP2	4:5:1457:G:N2	2.37	0.51
4:5:1631:A:C8	7:A:199:VAL:HG21	2.45	0.51
9:C:79:VAL:HG21	9:C:86:ARG:HD2	1.91	0.51
50:9:520:A:O2'	50:9:825:A:N3	2.34	0.51
52:BB:175:GLU:HG2	52:BB:193:ILE:HG12	1.91	0.51
63:MM:41:ALA:HB1	63:MM:46:GLN:HB2	1.92	0.51
4:5:1802:A:O2'	4:5:1837:A:OP1	2.28	0.51
4:5:2543:A:H2	4:5:2773:OMG:HN21	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:2743:A:H1'	7:A:21:LYS:HE3	1.92	0.51
6:8:40:A:OP2	6:8:102:G:N1	2.36	0.51
22:Q:119:LYS:HE3	22:Q:121:LEU:HD11	1.92	0.51
82:ff:95:ARG:HD3	82:ff:96:LYS:H	1.75	0.51
4:5:666:G:OP2	48:r:67:ARG:NE	2.41	0.51
4:5:1502:G:OP2	22:Q:62:SER:OG	2.28	0.51
4:5:2607:C:H5''	23:R:96:MET:HE1	1.91	0.51
4:5:4398:C:H41	4:5:4446:U:H3	1.55	0.51
4:5:4949:G:H4'	4:5:4950:U:H5'	1.91	0.51
7:A:242:ARG:NH1	7:A:245:ARG:O	2.36	0.51
50:9:1566:G:O3'	50:9:1567:G:N2	2.42	0.51
55:EE:122:LYS:HG2	55:EE:164:LEU:HD21	1.92	0.51
59:II:6:ASP:OD1	59:II:6:ASP:N	2.41	0.51
73:WW:111:MET:HE3	73:WW:116:ALA:HA	1.92	0.51
3:4:49:C:H2'	3:4:50:A:H8	1.76	0.51
4:5:924:C:OP1	4:5:926:G:O2'	2.27	0.51
11:E:152:ILE:HG21	11:E:273:TYR:HE2	1.75	0.51
49:u:29:LEU:HD13	49:u:62:LYS:HD2	1.91	0.51
2:2:24:A:O2'	4:5:3770:U:OP1	2.29	0.51
4:5:114:G:N2	4:5:276:C:O2'	2.44	0.51
4:5:235:A:OP1	9:C:201:ARG:NH2	2.43	0.51
4:5:1736:A:N3	5:7:78:C:O2'	2.44	0.51
4:5:2263:A:OP1	48:r:107:ARG:NH1	2.32	0.51
4:5:3896:C:O2'	8:B:268:ARG:NH1	2.39	0.51
31:Z:14:LEU:HA	38:g:91:ILE:HD11	1.92	0.51
37:f:41:PHE:HE1	37:f:110:ILE:HD11	1.76	0.51
50:9:377:G:OP1	59:II:98:LYS:NZ	2.42	0.51
50:9:637:U:O2	81:ee:129:ASN:ND2	2.42	0.51
50:9:1273:C:H3'	82:ff:92:LYS:HD3	1.92	0.51
50:9:1718:G:O2'	50:9:1815:A:N6	2.43	0.51
57:GG:32:MET:HE2	57:GG:54:GLY:HA3	1.91	0.51
58:HH:20:GLU:HA	58:HH:23:ILE:HG22	1.92	0.51
4:5:3717:A:OP2	4:5:3735:G:N2	2.42	0.51
4:5:1481:C:O2'	4:5:1482:G:N3	2.39	0.51
4:5:1895:G:O2'	4:5:1907:A:N3	2.40	0.51
4:5:3946:G:O6	4:5:4067:U:O4	2.29	0.51
8:B:58:ARG:NH1	8:B:361:GLU:OE2	2.36	0.51
19:N:54:LYS:H	19:N:59:TYR:HE2	1.59	0.51
20:O:77:SER:HB2	20:O:104:VAL:HG12	1.92	0.51
24:S:19:THR:HG23	24:S:22:CYS:H	1.76	0.51
57:GG:2:LYS:HB3	57:GG:15:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:RR:101:ASP:OD1	68:RR:101:ASP:N	2.44	0.51
73:WW:53:ILE:HD11	73:WW:60:LYS:HB2	1.93	0.51
4:5:2465:C:H1'	4:5:3672:G:H22	1.75	0.51
4:5:4627:U:H4'	8:B:373:LYS:HD2	1.91	0.51
7:A:133:TYR:HB3	7:A:168:VAL:HG12	1.92	0.51
22:Q:16:LYS:O	22:Q:33:ARG:NH2	2.44	0.51
48:r:85:ASN:N	48:r:85:ASN:OD1	2.43	0.51
52:BB:126:ASP:OD1	52:BB:136:ARG:NH2	2.43	0.51
60:JJ:110:LEU:HD21	60:JJ:135:ILE:HD11	1.93	0.51
69:SS:65:GLU:HA	69:SS:68:ILE:HG22	1.91	0.51
4:5:1666:C:O2'	4:5:1688:G:OP1	2.23	0.51
4:5:3641:U:OP2	4:5:3646:A:N6	2.44	0.51
19:N:155:VAL:O	19:N:162:ARG:NH2	2.44	0.51
31:Z:22:LYS:NZ	31:Z:129:TRP:O	2.39	0.51
37:f:77:ALA:HA	37:f:84:VAL:HG23	1.93	0.51
47:p:46:LYS:HB3	47:p:58:GLY:H	1.76	0.51
50:9:1144:A:H5'	50:9:1355:C:H41	1.75	0.51
53:CC:255:LEU:O	72:VV:16:LYS:NZ	2.35	0.51
71:UU:67:LYS:O	80:dd:44:ARG:NH1	2.44	0.51
75:YY:87:PRO:HG2	75:YY:90:ARG:HH21	1.74	0.51
4:5:70:A:OP2	32:a:64:LYS:NZ	2.39	0.51
4:5:4764:A:O2'	14:H:43:VAL:O	2.25	0.51
5:7:92:C:H2'	5:7:93:G:H8	1.75	0.51
8:B:62:ARG:HH12	8:B:358:ARG:HH21	1.59	0.51
23:R:168:GLU:OE1	23:R:171:LYS:NZ	2.44	0.51
24:S:3:ALA:O	24:S:111:ARG:NH1	2.43	0.51
36:e:22:ARG:HB2	36:e:35:TRP:HA	1.92	0.51
50:9:919:A:OP2	64:NN:64:ARG:NH2	2.37	0.51
58:HH:144:ILE:HB	58:HH:154:ILE:HG22	1.93	0.51
4:5:3897:B8K:O2'	4:5:3898:G:OP2	2.28	0.50
4:5:4101:C:O2	4:5:4107:G:N2	2.40	0.50
11:E:291:PHE:HZ	37:f:110:ILE:HD13	1.76	0.50
37:f:50:VAL:HG22	37:f:69:VAL:HG12	1.94	0.50
50:9:1285:G:O6	63:MM:57:ASP:N	2.44	0.50
4:5:1332:C:H2'	4:5:1333:A:H8	1.76	0.50
4:5:1340:C:OP2	32:a:6:ARG:NH1	2.41	0.50
4:5:1358:G:H1	4:5:1381:U:H3	1.57	0.50
4:5:1526:G:N1	4:5:1649:U:O4	2.44	0.50
4:5:2647:A:H62	4:5:2686:G:H8	1.60	0.50
4:5:3937:C:H1'	19:N:125:SER:HB3	1.92	0.50
4:5:5038:A:OP1	28:W:61:LYS:NZ	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:u:46:ASP:OD1	49:u:46:ASP:N	2.44	0.50
64:NN:99:ARG:NH2	64:NN:119:GLU:OE2	2.42	0.50
68:RR:99:ASP:OD1	68:RR:102:THR:OG1	2.28	0.50
4:5:20:U:OP2	6:8:36:G:N1	2.44	0.50
4:5:243:A:H5''	30:Y:3:PHE:HD2	1.76	0.50
4:5:4537:C:H2'	4:5:4538:G:C8	2.46	0.50
10:D:37:VAL:HG12	10:D:50:ARG:HD3	1.92	0.50
30:Y:55:VAL:HG12	30:Y:106:ILE:HA	1.94	0.50
49:u:155:ILE:HG21	49:u:167:VAL:HG13	1.93	0.50
50:9:599:A:H2'	50:9:606:G:H21	1.77	0.50
50:9:1270:G:O2'	50:9:1301:A:N7	2.44	0.50
50:9:1313:A:N7	82:ff:95:ARG:NH2	2.59	0.50
50:9:1563:G:OP1	70:TT:121:ARG:NH2	2.39	0.50
59:II:81:VAL:HG22	59:II:102:VAL:HG12	1.94	0.50
48:r:2:SER:OG	48:r:3:ALA:N	2.44	0.50
50:9:1498:A:OP2	54:DD:27:ARG:NH1	2.44	0.50
56:FF:50:PRO:HG2	56:FF:90:VAL:HG22	1.93	0.50
58:HH:51:ILE:HG21	58:HH:179:LYS:HG2	1.93	0.50
4:5:229:G:H5''	30:Y:11:ARG:HG3	1.93	0.50
20:O:55:LEU:HD23	20:O:58:LEU:HD12	1.94	0.50
50:9:527:C:H4'	60:JJ:121:LYS:HD3	1.94	0.50
50:9:581:U:OP1	60:JJ:133:ARG:NH2	2.45	0.50
69:SS:35:GLY:O	69:SS:97:GLN:NE2	2.42	0.50
82:ff:118:ARG:HE	82:ff:119:ARG:H	1.60	0.50
83:gg:234:ASP:OD1	83:gg:252:THR:OG1	2.28	0.50
4:5:3680:U:OP1	7:A:54:ARG:NH2	2.43	0.50
15:I:6:ALA:O	15:I:10:ARG:HB2	2.11	0.50
15:I:28:ASP:HB3	15:I:32:ARG:HH22	1.76	0.50
21:P:86:LYS:HA	21:P:89:GLU:HG2	1.93	0.50
51:AA:132:GLN:NE2	51:AA:136:GLU:OE2	2.44	0.50
61:KK:8:ARG:NH2	61:KK:12:TYR:OH	2.36	0.50
4:5:4537:C:H2'	4:5:4538:G:H8	1.77	0.50
4:5:5001:U:H4'	8:B:317:LEU:HB3	1.93	0.50
7:A:112:ILE:HG13	47:p:79:VAL:HG22	1.94	0.50
12:F:189:LEU:HD21	12:F:207:LEU:HD21	1.93	0.50
13:G:214:VAL:HG23	13:G:217:ILE:HA	1.94	0.50
50:9:94:G:O2'	50:9:508:A:O2'	2.27	0.50
50:9:604:A:N3	50:9:639:C:O2'	2.36	0.50
50:9:942:G:N2	65:OO:137:SER:OG	2.42	0.50
50:9:948:C:H2'	50:9:949:G:H8	1.76	0.50
50:9:1451:G:OP1	68:RR:32:LYS:NZ	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:KK:31:LYS:NZ	61:KK:38:LYS:O	2.44	0.50
4:5:1306:C:H2'	4:5:1307:A:H8	1.77	0.50
4:5:1631:A:O2'	7:A:203:ALA:O	2.28	0.50
4:5:4232:U:O4	46:o:8:ARG:NH1	2.44	0.50
4:5:1591:U:OP2	4:5:2856:C:O2'	2.27	0.50
4:5:2533:C:OP1	29:X:139:ARG:NH2	2.45	0.50
4:5:4967:A:H2'	4:5:4968:A:H8	1.77	0.50
9:C:170:LEU:HD23	9:C:221:PHE:HZ	1.77	0.50
22:Q:82:VAL:HG12	22:Q:84:GLY:H	1.75	0.50
50:9:523:A:OP2	60:JJ:38:ARG:NH2	2.44	0.50
50:9:1232:U:H2'	50:9:1233:G:C8	2.47	0.50
52:BB:144:LYS:HD3	52:BB:208:HIS:HB3	1.94	0.50
81:ee:101:ARG:HH21	81:ee:105:ALA:HB1	1.76	0.50
4:5:4135:G:H2'	4:5:4136:G:H8	1.76	0.49
8:B:10:ARG:HH22	8:B:265:SER:HB2	1.77	0.49
26:U:40:GLU:HB2	26:U:63:LEU:HD11	1.93	0.49
50:9:1550:G:H3'	50:9:1579:A:H61	1.77	0.49
50:9:1615:U:O4	66:PP:40:ARG:NH1	2.45	0.49
50:9:1694:U:HO2'	50:9:1833:C:HO2'	1.53	0.49
63:MM:92:CYS:O	63:MM:96:ARG:NH2	2.45	0.49
77:aa:38:LYS:HB2	77:aa:71:LEU:HB2	1.93	0.49
4:5:1481:C:O2'	4:5:1482:G:O4'	2.30	0.49
4:5:1837:A:O2'	25:T:130:ARG:O	2.26	0.49
4:5:1933:G:H2'	4:5:1934:A:C8	2.47	0.49
4:5:2537:A:OP1	42:k:42:LEU:N	2.45	0.49
4:5:3697:U:H5''	4:5:3698:G:H5'	1.94	0.49
17:L:169:ILE:HG12	32:a:123:ILE:HD11	1.94	0.49
34:c:54:ALA:HA	34:c:57:LYS:HG2	1.93	0.49
54:DD:7:LYS:HD3	71:UU:25:THR:HG21	1.93	0.49
55:EE:66:MET:HG3	55:EE:78:THR:HB	1.93	0.49
60:JJ:109:ARG:HH22	60:JJ:127:ARG:HH12	1.60	0.49
69:SS:39:ARG:NH1	70:TT:36:THR:O	2.44	0.49
4:5:667:A:H5''	4:5:668:C:H5	1.76	0.49
4:5:1866:UR3:H3U2	4:5:4405:G:H8	1.76	0.49
4:5:2514:G:O2'	4:5:2743:A:N6	2.44	0.49
10:D:41:LYS:NZ	25:T:32:ARG:O	2.38	0.49
19:N:62:TYR:O	19:N:131:GLU:HA	2.12	0.49
50:9:397:G:OP2	62:LL:108:ASN:ND2	2.41	0.49
50:9:916:A:C5	64:NN:73:ARG:HD3	2.47	0.49
50:9:1556:A:H2'	80:dd:13:LYS:HE2	1.94	0.49
51:AA:156:TYR:OH	72:VV:61:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DD:132:LYS:O	54:DD:156:LEU:N	2.45	0.49
67:QQ:16:LYS:HG3	67:QQ:17:LYS:H	1.78	0.49
67:QQ:41:MET:N	67:QQ:41:MET:SD	2.85	0.49
70:TT:71:GLY:H	70:TT:74:SER:HB2	1.77	0.49
72:VV:51:LYS:HD2	72:VV:78:ILE:HD11	1.92	0.49
4:5:4622:A:H4'	8:B:13:SER:HB2	1.94	0.49
19:N:146:PRO:HG3	39:h:102:LEU:HD12	1.94	0.49
50:9:350:C:O2'	50:9:383:G:N1	2.43	0.49
50:9:1506:A:C2	82:ff:90:LYS:HG2	2.48	0.49
58:HH:53:VAL:HG21	58:HH:172:THR:HA	1.92	0.49
59:II:36:THR:OG1	59:II:96:LEU:O	2.29	0.49
63:MM:40:LYS:HE2	82:ff:130:VAL:HA	1.94	0.49
68:RR:37:GLU:OE1	83:gg:150:TRP:NE1	2.45	0.49
4:5:362:A:N6	43:l:37:TYR:O	2.42	0.49
4:5:3717:A:H2'	4:5:3718:A2M:H8	1.93	0.49
4:5:4318:C:H4'	46:o:17:LYS:HA	1.94	0.49
4:5:4693:C:OP1	14:H:64:ARG:NH2	2.42	0.49
50:9:561:A:HO2'	60:JJ:134:HIS:HE2	1.60	0.49
50:9:639:C:H2'	50:9:640:A:H8	1.76	0.49
50:9:830:A:OP2	50:9:846:G:N2	2.45	0.49
50:9:1549:U:OP2	54:DD:8:LYS:NZ	2.34	0.49
50:9:1692:U:H2'	50:9:1693:G:H8	1.77	0.49
50:9:1808:U:H2'	50:9:1809:A:H8	1.78	0.49
51:AA:76:VAL:HG12	51:AA:87:VAL:HG23	1.95	0.49
52:BB:131:ASP:OD1	52:BB:131:ASP:N	2.46	0.49
55:EE:97:GLU:OE2	55:EE:113:ARG:NE	2.39	0.49
2:2:52:G:H2'	2:2:53:G:H8	1.77	0.49
4:5:1088:C:H2'	4:5:1089:G:H8	1.76	0.49
11:E:76:ALA:HB2	33:b:117:ARG:HB2	1.94	0.49
19:N:182:HIS:HA	19:N:195:ARG:HH12	1.78	0.49
26:U:106:THR:HG1	26:U:109:SER:HG	1.59	0.49
28:W:90:ILE:HG23	57:GG:145:PHE:HE1	1.77	0.49
28:W:97:LYS:HD3	28:W:99:GLU:H	1.77	0.49
50:9:943:U:OP1	52:BB:214:LYS:NZ	2.45	0.49
54:DD:132:LYS:HE3	54:DD:191:PRO:HA	1.93	0.49
63:MM:32:ALA:HB1	63:MM:37:GLU:HG3	1.94	0.49
4:5:1598:C:H2'	4:5:1599:G:H8	1.78	0.49
4:5:4251:A:H5''	16:J:108:GLY:HA3	1.94	0.49
39:h:31:LEU:HB3	39:h:47:ILE:HG22	1.95	0.49
50:9:350:C:HO2'	50:9:383:G:H1	1.58	0.49
50:9:687:C:N3	58:HH:118:ARG:NH2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BB:224:GLU:OE1	52:BB:227:LYS:N	2.43	0.49
4:5:1236:C:O2'	4:5:1238:A:OP1	2.29	0.49
4:5:4146:G:H2'	4:5:4147:G:H8	1.78	0.49
8:B:140:ASP:OD2	8:B:144:ARG:NH2	2.45	0.49
11:E:163:LYS:HG2	11:E:277:VAL:HG12	1.95	0.49
22:Q:67:ILE:HD11	22:Q:95:VAL:HG13	1.94	0.49
63:MM:17:ALA:HA	63:MM:120:ALA:HB1	1.95	0.49
68:RR:35:CYS:HA	68:RR:38:ILE:HG22	1.95	0.49
69:SS:121:ARG:HG3	69:SS:131:VAL:HB	1.93	0.49
77:aa:33:ASP:OD1	77:aa:33:ASP:N	2.46	0.49
4:5:410:A:O2'	4:5:414:C:O2'	2.26	0.49
4:5:3870:C:O3'	8:B:261:ARG:NH1	2.45	0.49
48:r:64:MET:HB2	48:r:78:VAL:HG23	1.94	0.49
50:9:991:G:N7	77:aa:7:ASN:ND2	2.60	0.49
50:9:1286:G:H21	82:ff:95:ARG:HH22	1.59	0.49
50:9:1288:U:O2'	82:ff:94:LYS:O	2.24	0.49
50:9:1858:G:OP2	65:OO:146:ARG:NH2	2.39	0.49
83:gg:107:ASP:O	83:gg:124:SER:OG	2.28	0.49
4:5:1757:U:OP1	4:5:1768:C:N4	2.45	0.49
4:5:4195:G:N2	4:5:4222:G:OP1	2.36	0.49
26:U:84:LYS:HB2	26:U:110:TYR:CZ	2.47	0.49
50:9:1208:A:O2'	50:9:1835:A:N7	2.42	0.49
50:9:1683:C:H2'	50:9:1684:C:H6	1.77	0.49
71:UU:56:MET:HE2	71:UU:56:MET:HB3	1.69	0.49
81:ee:85:VAL:O	81:ee:89:THR:HB	2.13	0.49
4:5:364:G:O6	41:j:52:LYS:NZ	2.42	0.48
4:5:2758:G:O2'	4:5:2765:A:N3	2.45	0.48
4:5:2812:A:OP1	23:R:83:GLY:N	2.45	0.48
4:5:4688:C:O2'	14:H:155:SER:OG	2.26	0.48
8:B:322:HIS:O	8:B:342:LYS:NZ	2.40	0.48
50:9:1030:A:H2'	50:9:1031:A2M:H8	1.95	0.48
50:9:1265:A:O2'	50:9:1327:G:OP2	2.25	0.48
51:AA:36:GLN:O	51:AA:53:ARG:NH1	2.46	0.48
55:EE:130:PHE:HB3	55:EE:138:HIS:HB2	1.93	0.48
59:II:66:SER:HA	59:II:73:THR:HG22	1.93	0.48
69:SS:84:LEU:HD22	69:SS:97:GLN:HB2	1.95	0.48
77:aa:23:CYS:SG	77:aa:24:THR:N	2.87	0.48
4:5:1354:A:O2'	32:a:77:LYS:NZ	2.41	0.48
4:5:4662:C:O2'	4:5:5004:C:OP1	2.28	0.48
32:a:103:VAL:HG22	32:a:108:TYR:HB2	1.94	0.48
50:9:639:C:H2'	50:9:640:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:1325:G:O6	82:ff:83:LYS:N	2.46	0.48
51:AA:77:ILE:HG12	51:AA:99:ILE:HD12	1.94	0.48
4:5:1620:U:HO2'	4:5:2450:G:HO2'	1.61	0.48
4:5:2848:G:N2	4:5:3839:G:OP2	2.37	0.48
4:5:4045:G:OP2	49:u:98:LYS:NZ	2.36	0.48
45:n:11:ARG:NH2	50:9:1844:U:OP1	2.46	0.48
49:u:90:LEU:HA	49:u:93:LEU:HB2	1.94	0.48
63:MM:52:LEU:HD22	63:MM:78:LYS:HE2	1.95	0.48
73:WW:39:THR:HA	73:WW:42:MET:HG2	1.93	0.48
4:5:438:G:N2	37:f:23:GLU:OE2	2.29	0.48
6:8:110:U:OP2	43:l:8:ARG:NH1	2.41	0.48
55:EE:11:ARG:NH2	55:EE:21:ASP:OD1	2.46	0.48
4:5:232:G:O6	30:Y:61:HIS:N	2.42	0.48
4:5:382:G:N1	4:5:385:A:OP2	2.44	0.48
4:5:2049:G:HO2'	4:5:3884:U:HO2'	1.60	0.48
4:5:3663:A:N6	4:5:4168:G:O2'	2.46	0.48
4:5:4215:C:O2	25:T:60:LYS:NZ	2.43	0.48
6:8:8:U:H2'	6:8:9:A:H8	1.79	0.48
8:B:56:ILE:HD12	8:B:365:LEU:HD22	1.95	0.48
31:Z:21:ARG:NH1	31:Z:47:ASP:OD1	2.45	0.48
50:9:65:C:H41	57:GG:136:LYS:HB2	1.77	0.48
50:9:65:C:H4'	57:GG:172:LYS:HE2	1.95	0.48
51:AA:5:LEU:HD11	72:VV:41:LYS:HA	1.96	0.48
66:PP:13:ARG:HE	66:PP:14:LYS:H	1.61	0.48
66:PP:41:GLN:NE2	66:PP:113:GLY:O	2.46	0.48
75:YY:7:ILE:HG22	75:YY:27:VAL:HG13	1.95	0.48
4:5:958:G:O2'	11:E:126:ARG:O	2.31	0.48
4:5:1199:G:H2'	4:5:1200:G:H8	1.79	0.48
4:5:1942:A:H2'	4:5:1943:A:C8	2.49	0.48
4:5:4274:A:H2'	4:5:4275:G:C8	2.49	0.48
4:5:4458:C:OP1	8:B:11:HIS:NE2	2.46	0.48
11:E:144:ARG:NE	37:f:110:ILE:OXT	2.44	0.48
14:H:58:ASP:OD1	14:H:58:ASP:N	2.46	0.48
15:I:54:SER:HB2	15:I:135:ILE:HD11	1.95	0.48
28:W:102:LYS:HA	28:W:105:ARG:HG2	1.95	0.48
50:9:687:C:O3'	58:HH:121:THR:OG1	2.30	0.48
50:9:851:C:H5''	50:9:852:G:H5'	1.95	0.48
50:9:1841:C:H2'	50:9:1842:4AC:H6	1.96	0.48
53:CC:168:GLY:N	53:CC:179:THR:O	2.41	0.48
63:MM:35:ILE:HG12	63:MM:108:CYS:HB2	1.94	0.48
83:gg:244:ASN:ND2	83:gg:294:ASP:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:365:U:O2'	43:l:40:LYS:NZ	2.30	0.48
4:5:2459:G:N2	4:5:2462:C:OP2	2.43	0.48
41:j:2:THR:O	41:j:7:SER:OG	2.31	0.48
45:n:1:MET:HB2	50:9:1706:G:H5'	1.96	0.48
50:9:555:A:H61	50:9:589:G:H21	1.62	0.48
50:9:1012:A:H5''	64:NN:10:GLY:HA3	1.95	0.48
50:9:1144:A:H2'	50:9:1145:A:C8	2.49	0.48
63:MM:69:CYS:HA	63:MM:74:ILE:HD11	1.94	0.48
83:gg:231:ASP:OD1	83:gg:231:ASP:N	2.47	0.48
4:5:690:C:H4'	48:r:85:ASN:HD22	1.78	0.48
4:5:1502:G:H22	32:a:77:LYS:HE3	1.78	0.48
4:5:2337:C:H4'	48:r:19:LYS:HB2	1.96	0.48
19:N:184:ILE:O	19:N:194:ARG:NH1	2.38	0.48
23:R:42:ARG:HA	23:R:45:ILE:HD12	1.95	0.48
50:9:1204:A:O2'	50:9:1700:C:OP2	2.28	0.48
50:9:1277:C:H2'	50:9:1278:A:H8	1.78	0.48
50:9:1740:C:OP1	59:II:44:HIS:ND1	2.43	0.48
52:BB:46:LYS:HE3	65:OO:20:GLN:HB2	1.95	0.48
52:BB:66:VAL:HA	52:BB:86:LEU:O	2.14	0.48
57:GG:151:ASP:OD1	57:GG:151:ASP:N	2.46	0.48
66:PP:38:SER:OG	66:PP:41:GLN:OE1	2.32	0.48
4:5:407:A:O2'	4:5:410:A:OP1	2.31	0.48
4:5:1332:C:H2'	4:5:1333:A:C8	2.49	0.48
4:5:2344:U:H2'	32:a:9:ARG:HH22	1.78	0.48
4:5:4088:C:N3	13:G:106:ARG:NH1	2.62	0.48
4:5:4699:U:H1'	4:5:4700:A:H5''	1.96	0.48
4:5:4918:C:H2'	4:5:4919:G:C8	2.49	0.48
31:Z:90:PRO:HB2	31:Z:117:LYS:HZ3	1.79	0.48
34:c:101:ASP:N	34:c:101:ASP:OD1	2.42	0.48
48:r:17:LEU:HD21	48:r:19:LYS:HE3	1.96	0.48
50:9:31:U:O2'	50:9:643:A:N1	2.40	0.48
50:9:1309:C:H5'	82:ff:105:TYR:HE1	1.78	0.48
50:9:1325:G:N7	82:ff:83:LYS:N	2.62	0.48
50:9:1345:G:OP1	50:9:1688:C:O2'	2.31	0.48
50:9:1536:G:H2'	50:9:1537:A:C8	2.49	0.48
54:DD:154:ASP:N	54:DD:154:ASP:OD1	2.45	0.48
4:5:419:A:N3	4:5:1332:C:O2'	2.40	0.48
4:5:1360:G:OP2	17:L:28:GLN:NE2	2.36	0.48
4:5:4594:U:H2'	4:5:4595:G:C8	2.47	0.48
4:5:4754:G:OP1	37:f:4:ARG:NH1	2.47	0.48
7:A:158:ILE:HG23	7:A:162:ASN:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:53:VAL:HG11	10:D:159:VAL:HA	1.95	0.48
11:E:144:ARG:HG3	11:E:194:GLN:HE21	1.79	0.48
11:E:264:ILE:HB	11:E:270:LEU:HD23	1.95	0.48
15:I:93:PRO:HB2	15:I:125:THR:HG22	1.95	0.48
36:e:30:LYS:HG3	36:e:31:ILE:HG13	1.95	0.48
47:p:47:MET:HE2	47:p:71:TYR:HE1	1.79	0.48
48:r:65:LYS:O	48:r:102:TYR:OH	2.24	0.48
50:9:28:U:H2'	50:9:29:G:H8	1.79	0.48
50:9:516:A:N1	50:9:643:A:O2'	2.42	0.48
50:9:1281:G:H3'	50:9:1282:A:H8	1.79	0.48
52:BB:88:THR:HA	52:BB:98:THR:HA	1.96	0.48
54:DD:169:ASP:HB2	54:DD:190:LEU:HD11	1.96	0.48
63:MM:22:LEU:HD22	63:MM:89:VAL:HG23	1.96	0.48
83:gg:292:SER:OG	83:gg:293:ALA:N	2.47	0.48
4:5:365:U:H2'	4:5:366:A:H8	1.79	0.47
4:5:1761:G:O6	4:5:1772:C:N4	2.47	0.47
4:5:3777:G:O2'	4:5:3815:G:O6	2.29	0.47
4:5:3951:G:O6	4:5:4062:A:N1	2.46	0.47
4:5:4348:A:O2'	4:5:4350:C:OP2	2.30	0.47
4:5:4354:U:O4	32:a:61:TYR:N	2.36	0.47
4:5:4875:G:H2'	24:S:169:THR:HG22	1.96	0.47
14:H:103:VAL:HG21	14:H:144:LEU:HD11	1.96	0.47
28:W:94:ARG:HG2	57:GG:145:PHE:HA	1.96	0.47
49:u:14:VAL:HA	49:u:17:VAL:HG22	1.95	0.47
50:9:5:U:H2'	50:9:6:G:H8	1.78	0.47
50:9:472:C:O2'	50:9:474:G:OP1	2.25	0.47
50:9:885:U:O2	50:9:901:G:O6	2.32	0.47
50:9:1673:U:H5''	67:QQ:78:VAL:HG22	1.95	0.47
51:AA:80:ARG:HH22	51:AA:166:LYS:HA	1.79	0.47
59:II:81:VAL:HG12	59:II:91:VAL:HG23	1.96	0.47
4:5:1346:C:H2'	4:5:1347:G:H8	1.79	0.47
4:5:2055:G:OP2	20:O:133:ARG:NH1	2.44	0.47
4:5:4646:U:OP1	23:R:59:SER:N	2.39	0.47
44:m:73:CYS:HB3	44:m:89:CYS:HB3	1.96	0.47
50:9:391:C:H2'	50:9:392:A:H8	1.79	0.47
50:9:1277:C:H2'	50:9:1278:A:C8	2.49	0.47
53:CC:70:VAL:HG21	53:CC:93:ILE:HG12	1.96	0.47
55:EE:11:ARG:HH22	55:EE:24:THR:HG1	1.62	0.47
58:HH:80:VAL:HG23	58:HH:92:VAL:HG13	1.95	0.47
60:JJ:84:ILE:HD11	60:JJ:148:ILE:HG12	1.96	0.47
4:5:2267:U:OP1	48:r:37:SER:OG	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:2735:G:H2'	4:5:2736:G:H8	1.79	0.47
4:5:4645:C:OP2	23:R:62:ARG:NH2	2.46	0.47
5:7:29:C:H4'	16:J:12:MET:HE1	1.96	0.47
8:B:92:TYR:HB2	8:B:159:VAL:HG13	1.96	0.47
34:c:46:VAL:HB	34:c:71:VAL:HG22	1.96	0.47
46:o:2:VAL:N	46:o:90:HIS:O	2.47	0.47
50:9:1166:G:N7	74:XX:25:LYS:NZ	2.50	0.47
50:9:1620:A:N3	66:PP:40:ARG:NH2	2.61	0.47
50:9:1865:C:OP1	77:aa:87:ARG:NH1	2.46	0.47
54:DD:29:LEU:HD21	54:DD:50:ILE:HD11	1.96	0.47
65:OO:99:ALA:H	65:OO:133:THR:HG22	1.79	0.47
69:SS:86:ARG:HG3	69:SS:89:ASP:HB3	1.96	0.47
4:5:668:C:H4'	9:C:6:PRO:HB3	1.95	0.47
4:5:1436:C:H5''	4:5:1437:C:H5'	1.96	0.47
4:5:4134:C:H2'	4:5:4135:G:H8	1.79	0.47
50:9:64:A:H2	50:9:83:A:H62	1.63	0.47
50:9:380:G:OP1	59:II:56:ARG:NH2	2.47	0.47
50:9:1308:U:O5'	82:ff:134:SER:OG	2.30	0.47
55:EE:100:ARG:HH22	55:EE:122:LYS:HA	1.78	0.47
62:LL:103:GLU:HG3	74:XX:11:ARG:HB2	1.95	0.47
65:OO:117:ARG:HH12	79:cc:42:ILE:HD11	1.80	0.47
68:RR:99:ASP:O	68:RR:102:THR:OG1	2.31	0.47
4:5:983:U:OP1	11:E:75:TYR:OH	2.31	0.47
4:5:1567:U:OP1	47:p:3:LYS:NZ	2.36	0.47
4:5:4966:A:OP2	8:B:126:LYS:NZ	2.40	0.47
6:8:152:U:O2'	13:G:213:ASP:OD2	2.31	0.47
9:C:218:VAL:HG12	9:C:229:LEU:HG	1.97	0.47
48:r:63:VAL:HG22	48:r:79:ARG:HD3	1.95	0.47
50:9:814:5MU:OP1	55:EE:22:LYS:NZ	2.47	0.47
50:9:1255:G:OP1	50:9:1256:G:O2'	2.29	0.47
4:5:68:U:OP1	19:N:178:HIS:ND1	2.39	0.47
4:5:1073:G:H1	4:5:1238:A:H2	1.62	0.47
4:5:1202:C:H2'	4:5:1203:G:C8	2.49	0.47
4:5:3970:G:H4'	49:u:168:ALA:HB2	1.96	0.47
5:7:57:C:H2'	5:7:58:A:H8	1.79	0.47
9:C:333:MLZ:HCM3	9:C:337:ARG:HH11	1.79	0.47
16:J:90:ARG:NH2	16:J:108:GLY:O	2.47	0.47
29:X:87:MET:HA	29:X:90:ILE:HG12	1.96	0.47
50:9:70:G:N2	50:9:71:G:O6	2.48	0.47
54:DD:69:LEU:HA	54:DD:72:VAL:HB	1.97	0.47
66:PP:57:LEU:HD21	66:PP:86:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:YY:18:LEU:HD23	75:YY:20:ARG:HE	1.79	0.47
83:gg:108:VAL:HA	83:gg:124:SER:HA	1.96	0.47
4:5:1645:C:H2'	4:5:1646:A:H8	1.80	0.47
4:5:2589:C:HO2'	4:5:2767:U:HO2'	1.58	0.47
4:5:3919:C:OP1	7:A:2:GLY:N	2.48	0.47
4:5:4929:C:OP1	18:M:114:LYS:NZ	2.41	0.47
8:B:57:VAL:HB	8:B:367:PHE:HB3	1.96	0.47
10:D:77:ALA:O	10:D:108:ARG:NH2	2.47	0.47
14:H:86:LEU:HD23	14:H:186:THR:HG21	1.97	0.47
50:9:30:C:O2'	50:9:596:U:OP1	2.32	0.47
50:9:85:A:H5''	75:YY:118:ARG:HE	1.77	0.47
50:9:1139:C:H41	50:9:1149:A:H62	1.61	0.47
50:9:1284:A:O4'	50:9:1313:A:N6	2.48	0.47
50:9:1623:A:N7	69:SS:132:ARG:NH2	2.63	0.47
51:AA:109:THR:O	53:CC:89:LYS:NZ	2.41	0.47
52:BB:49:VAL:HG21	52:BB:62:LEU:HD22	1.97	0.47
58:HH:143:ARG:HG3	73:WW:53:ILE:HG22	1.96	0.47
71:UU:22:ILE:HG22	71:UU:114:VAL:HG22	1.97	0.47
82:ff:125:GLU:OE1	82:ff:143:LYS:NZ	2.39	0.47
4:5:2361:G:O2'	4:5:3859:G:O6	2.31	0.47
4:5:2557:G:H1	4:5:2570:U:H3	1.61	0.47
4:5:4617:G:O2'	27:V:13:LYS:O	2.33	0.47
28:W:101:ARG:HB3	28:W:105:ARG:HH21	1.80	0.47
49:u:68:LEU:HB3	49:u:116:LEU:HD23	1.96	0.47
50:9:1287:A:OP2	82:ff:96:LYS:HB2	2.15	0.47
50:9:1553:C:O2'	50:9:1554:C:O4'	2.33	0.47
56:FF:167:LYS:HA	76:ZZ:71:ALA:HB1	1.97	0.47
60:JJ:136:ARG:HH11	60:JJ:160:SER:HA	1.80	0.47
62:LL:136:LYS:O	62:LL:139:ARG:NH1	2.48	0.47
73:WW:18:GLU:HG2	73:WW:69:LEU:HB3	1.95	0.47
4:5:1382:G:H2'	4:5:1383:G:H8	1.80	0.47
4:5:1812:C:H5'	33:b:56:LYS:HE2	1.97	0.47
4:5:4485:C:H4'	44:m:88:LYS:HE3	1.96	0.47
8:B:213:GLN:NE2	8:B:285:TYR:O	2.35	0.47
9:C:336:ARG:HA	9:C:339:THR:HG22	1.97	0.47
12:F:91:VAL:O	12:F:119:GLY:HA2	2.15	0.47
16:J:160:GLU:HA	16:J:163:MET:HG2	1.97	0.47
18:M:9:VAL:HG11	18:M:66:HIS:HA	1.97	0.47
50:9:383:G:O3'	62:LL:132:ARG:NH1	2.48	0.47
50:9:1036:A:N3	50:9:1844:U:O2'	2.48	0.47
50:9:1415:C:O2'	70:TT:132:ASP:OD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:1503:C:C5	82:ff:84:SER:HB3	2.50	0.47
50:9:1808:U:H2'	50:9:1809:A:C8	2.49	0.47
57:GG:67:VAL:HG12	57:GG:69:THR:HG22	1.97	0.47
4:5:679:C:H2'	4:5:680:G:H8	1.79	0.47
4:5:4274:A:H2'	4:5:4275:G:H8	1.79	0.47
4:5:5047:C:O2'	4:5:5050:C:OP2	2.33	0.47
9:C:167:ALA:HB2	9:C:220:ALA:HB1	1.96	0.47
19:N:160:GLU:HG2	19:N:161:MET:HG3	1.95	0.47
47:p:28:LYS:HG3	47:p:29:ILE:HD12	1.97	0.47
55:EE:168:LYS:NZ	57:GG:205:GLU:OE2	2.36	0.47
59:II:162:LEU:HD23	59:II:165:GLN:HE21	1.80	0.47
62:LL:73:LEU:HD12	62:LL:140:PHE:HE2	1.79	0.47
4:5:93:G:OP2	32:a:54:GLY:N	2.48	0.46
14:H:128:MET:HG3	14:H:157:SER:HB3	1.97	0.46
21:P:64:ASN:HB2	21:P:80:GLN:NE2	2.30	0.46
24:S:76:LYS:HD2	24:S:131:GLU:HG3	1.97	0.46
50:9:537:C:N3	50:9:547:G:N2	2.60	0.46
57:GG:5:ILE:HG22	57:GG:124:LEU:HD21	1.97	0.46
67:QQ:97:GLN:OE1	83:gg:60:ARG:NH2	2.47	0.46
4:5:295:A:OP2	46:o:39:ARG:NE	2.48	0.46
4:5:358:C:H2'	4:5:359:A:H8	1.81	0.46
4:5:1352:C:O2'	4:5:1356:U:OP1	2.30	0.46
4:5:2778:G:N1	6:8:113:C:OP1	2.46	0.46
4:5:4981:G:O6	8:B:21:ARG:NH2	2.47	0.46
4:5:4991:U:H2'	4:5:4992:G:H8	1.80	0.46
24:S:161:ARG:HG3	24:S:164:LYS:HE3	1.97	0.46
50:9:294:U:C4	62:LL:65:ASN:HB3	2.51	0.46
50:9:1013:U:OP1	50:9:1129:G:O2'	2.34	0.46
50:9:1220:A:N3	50:9:1677:U:O2'	2.39	0.46
50:9:1588:A:H2'	50:9:1589:A:C8	2.50	0.46
53:CC:220:ASP:OD1	53:CC:220:ASP:N	2.47	0.46
55:EE:207:VAL:HA	55:EE:221:ARG:HA	1.97	0.46
3:4:6:G:H2'	3:4:7:A:C8	2.50	0.46
4:5:2406:G:N7	43:l:2:SER:N	2.64	0.46
4:5:2791:C:OP1	43:l:48:LYS:NZ	2.42	0.46
4:5:4992:G:H2'	4:5:4993:G:C8	2.51	0.46
9:C:78:ARG:HB3	9:C:88:GLY:HA2	1.96	0.46
26:U:23:LEU:HD11	26:U:83:LEU:HD21	1.98	0.46
50:9:161:U:HO2'	57:GG:87:ARG:HH12	1.60	0.46
50:9:482:G:N1	50:9:485:A:OP2	2.48	0.46
63:MM:49:LEU:HB3	63:MM:111:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:VV:1:MET:SD	72:VV:1:MET:N	2.88	0.46
73:WW:42:MET:HE3	73:WW:42:MET:HB2	1.83	0.46
4:5:1636:U:H5''	4:5:1637:A:H5'	1.97	0.46
4:5:2695:A:OP2	42:k:33:LYS:NZ	2.43	0.46
4:5:3952:A:N1	4:5:4061:G:C6	2.84	0.46
6:8:30:U:OP1	17:L:34:ARG:NH2	2.49	0.46
10:D:232:THR:HG23	10:D:234:ASP:H	1.81	0.46
11:E:152:ILE:HA	11:E:165:VAL:O	2.15	0.46
50:9:1285:G:C3'	82:ff:99:LYS:HE2	2.45	0.46
52:BB:121:ILE:HD13	52:BB:164:ILE:HG21	1.96	0.46
53:CC:251:LEU:HD23	72:VV:23:ILE:HG13	1.97	0.46
63:MM:52:LEU:HD11	63:MM:62:VAL:HG23	1.98	0.46
4:5:8:U:OP1	19:N:41:ARG:NH1	2.48	0.46
4:5:3651:A:OP2	7:A:200:ARG:NH1	2.49	0.46
7:A:33:ASP:N	7:A:33:ASP:OD1	2.44	0.46
10:D:178:LYS:HG2	10:D:179:ARG:HH11	1.81	0.46
50:9:1306:U:O2	82:ff:137:ASP:HB3	2.15	0.46
52:BB:111:CYS:HA	52:BB:114:VAL:HG12	1.98	0.46
54:DD:74:GLN:HA	54:DD:79:PHE:HB2	1.98	0.46
73:WW:6:VAL:HG22	73:WW:34:ILE:HD11	1.96	0.46
73:WW:24:GLN:HG3	78:bb:7:LEU:HD13	1.97	0.46
73:WW:103:VAL:HA	73:WW:112:ASP:HA	1.97	0.46
83:gg:253:GLY:O	83:gg:286:CYS:N	2.39	0.46
4:5:951:G:H2'	4:5:952:G:H8	1.81	0.46
4:5:1538:U:H2'	4:5:1539:G:H8	1.80	0.46
4:5:1813:U:H5'	33:b:53:GLY:HA3	1.98	0.46
4:5:2778:G:N2	6:8:113:C:OP2	2.40	0.46
4:5:4319:C:H2'	4:5:4320:G:H8	1.80	0.46
8:B:224:LYS:HG3	8:B:340:THR:HB	1.98	0.46
29:X:77:ILE:HG22	29:X:100:VAL:HG12	1.97	0.46
50:9:385:G:O2'	59:II:10:LYS:NZ	2.48	0.46
50:9:1462:U:O2	50:9:1464:C:N4	2.49	0.46
50:9:1504:U:O2'	82:ff:86:THR:O	2.29	0.46
51:AA:33:GLN:HB3	51:AA:154:LEU:HD12	1.98	0.46
56:FF:144:LEU:HB3	79:cc:49:PRO:HG2	1.97	0.46
63:MM:51:VAL:HA	63:MM:77:ILE:O	2.16	0.46
76:ZZ:92:LEU:HD11	76:ZZ:99:LEU:HB2	1.97	0.46
81:ee:112:ASN:HA	81:ee:116:VAL:HG12	1.98	0.46
4:5:2621:A:H2'	4:5:2622:G:C8	2.51	0.46
4:5:4174:U:H2'	4:5:4175:G:H8	1.80	0.46
8:B:50:LYS:HB2	8:B:345:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:317:LEU:HB2	8:B:372:SER:HB2	1.97	0.46
10:D:215:ASP:OD1	10:D:215:ASP:N	2.49	0.46
18:M:101:LYS:HA	18:M:104:MET:HE3	1.98	0.46
31:Z:5:MET:O	31:Z:28:ASN:ND2	2.44	0.46
50:9:1410:C:H2'	50:9:1411:G:C8	2.51	0.46
53:CC:178:HIS:ND1	53:CC:179:THR:HG23	2.31	0.46
54:DD:16:ILE:HD13	80:dd:22:ARG:HH11	1.81	0.46
62:LL:35:ARG:NH1	62:LL:53:GLY:O	2.48	0.46
67:QQ:25:CYS:HB3	67:QQ:68:ILE:HG12	1.98	0.46
67:QQ:34:VAL:HG22	67:QQ:70:VAL:HB	1.97	0.46
4:5:3870:C:H2'	4:5:3871:A:H8	1.80	0.46
4:5:4424:A:H4'	44:m:96:ARG:HH22	1.79	0.46
6:8:14:OMU:HM23	6:8:14:OMU:H1'	1.61	0.46
11:E:217:ASP:N	11:E:217:ASP:OD1	2.46	0.46
18:M:41:PRO:HG3	18:M:73:VAL:HG13	1.97	0.46
36:e:26:ASP:N	36:e:26:ASP:OD1	2.44	0.46
50:9:681:U:H4'	74:XX:9:THR:HG22	1.98	0.46
50:9:923:G:H2'	50:9:924:G:H8	1.80	0.46
56:FF:138:ALA:O	79:cc:63:ARG:NH2	2.49	0.46
75:YY:20:ARG:NH2	75:YY:74:MET:HG2	2.30	0.46
76:ZZ:102:LYS:HD2	76:ZZ:107:VAL:HG12	1.98	0.46
79:cc:29:GLN:HE22	79:cc:67:ARG:HA	1.80	0.46
83:gg:6:THR:O	83:gg:310:TRP:HA	2.16	0.46
83:gg:17:TRP:O	83:gg:36:ARG:N	2.49	0.46
4:5:158:A:H5''	4:5:159:C:H2'	1.98	0.46
4:5:1548:G:O2'	4:5:2812:A:N3	2.44	0.46
4:5:1985:G:O2'	4:5:2003:G:OP2	2.34	0.46
4:5:3617:G:O2'	4:5:3620:G:N7	2.48	0.46
12:F:178:LEU:HD22	12:F:183:ILE:HD11	1.98	0.46
17:L:179:PHE:N	32:a:134:GLU:OE1	2.43	0.46
28:W:79:GLN:HG2	28:W:80:ARG:H	1.81	0.46
35:d:27:ILE:O	35:d:83:ARG:HA	2.16	0.46
50:9:954:U:O2	65:OO:55:ARG:NH2	2.38	0.46
56:FF:82:ASN:OD1	56:FF:82:ASN:N	2.47	0.46
56:FF:99:ILE:HA	56:FF:102:LEU:HG	1.98	0.46
58:HH:66:VAL:HG22	58:HH:96:ALA:HB1	1.98	0.46
58:HH:159:ASP:OD1	58:HH:159:ASP:N	2.47	0.46
75:YY:40:ILE:HD11	75:YY:57:VAL:HG11	1.98	0.46
4:5:947:C:OP1	9:C:336:ARG:NH2	2.42	0.46
4:5:1352:C:H41	22:Q:55:ARG:HH12	1.61	0.46
6:8:27:U:H4'	9:C:53:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:287:THR:HG21	48:r:5:LEU:HD12	1.98	0.46
25:T:41:ASP:OD1	25:T:61:THR:OG1	2.33	0.46
27:V:18:LEU:HD13	27:V:54:ALA:HB3	1.98	0.46
37:f:59:THR:OG1	37:f:65:ASN:OD1	2.31	0.46
50:9:1850:MA6:H8	50:9:1850:MA6:O5'	2.16	0.46
54:DD:116:ARG:HE	54:DD:150:MET:HE2	1.81	0.46
57:GG:52:ILE:HD11	57:GG:109:LEU:HD22	1.96	0.46
57:GG:162:LEU:HD22	57:GG:170:ARG:HB2	1.98	0.46
58:HH:25:GLN:HA	58:HH:28:LEU:HD23	1.98	0.46
58:HH:50:GLU:HB3	58:HH:60:ILE:HG22	1.97	0.46
4:5:478:G:H2'	4:5:479:G:H8	1.81	0.45
4:5:658:C:H2'	4:5:659:G:H8	1.81	0.45
4:5:1198:G:H2'	4:5:1199:G:C8	2.51	0.45
4:5:1461:C:H2'	4:5:1462:A:C8	2.51	0.45
4:5:2411:C:O2'	4:5:2526:C:O2'	2.21	0.45
20:O:43:ILE:HD11	20:O:138:LEU:HD13	1.97	0.45
22:Q:124:ASP:OD1	22:Q:124:ASP:N	2.49	0.45
24:S:71:SER:O	24:S:76:LYS:NZ	2.49	0.45
50:9:409:C:H2'	50:9:410:G:H8	1.80	0.45
4:5:423:G:OP1	21:P:62:ARG:NH2	2.41	0.45
4:5:4056:A:H1'	49:u:164:CYS:HB3	1.98	0.45
7:A:247:ARG:HD2	50:9:1069:U:H4'	1.97	0.45
35:d:36:VAL:HG11	35:d:44:ARG:HD3	1.98	0.45
50:9:153:G:N3	57:GG:13:GLN:NE2	2.62	0.45
80:dd:15:GLY:O	80:dd:19:ARG:NE	2.46	0.45
4:5:469:C:H42	11:E:108:ARG:HH21	1.63	0.45
4:5:1869:G:O2'	4:5:3877:A:N1	2.47	0.45
4:5:4153:C:H2'	4:5:4154:G:C8	2.52	0.45
4:5:4700:A:H2	14:H:69:THR:HG22	1.80	0.45
5:7:75:G:N2	5:7:100:A:OP2	2.43	0.45
6:8:13:G:O2'	21:P:121:LYS:O	2.34	0.45
15:I:150:GLU:OE2	15:I:153:ARG:NH1	2.50	0.45
30:Y:36:LYS:HA	30:Y:39:ARG:HG2	1.98	0.45
31:Z:50:PRO:HD3	31:Z:68:ILE:HG12	1.98	0.45
42:k:49:ASP:HB3	42:k:52:LYS:HE2	1.99	0.45
50:9:918:U:O2'	73:WW:56:HIS:O	2.34	0.45
51:AA:206:ASP:N	51:AA:206:ASP:OD1	2.49	0.45
69:SS:47:LYS:NZ	69:SS:78:LYS:O	2.50	0.45
80:dd:21:CYS:HB3	80:dd:26:ASN:H	1.80	0.45
3:4:5:G:H2'	3:4:6:G:H8	1.82	0.45
13:G:226:LEU:HD12	40:i:43:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:59:ARG:NH1	32:a:61:TYR:OH	2.48	0.45
50:9:77:A:H1'	57:GG:176:ILE:HG12	1.98	0.45
50:9:928:G:H2'	50:9:929:G:C8	2.51	0.45
54:DD:23:GLU:OE1	80:dd:46:TYR:OH	2.22	0.45
76:ZZ:100:VAL:HG21	76:ZZ:110:THR:HG23	1.98	0.45
4:5:1450:C:H2'	4:5:1451:G:C8	2.51	0.45
4:5:3974:G:N7	4:5:4039:G:N2	2.64	0.45
4:5:4457:U:OP1	27:V:50:ASN:ND2	2.49	0.45
31:Z:14:LEU:HD12	38:g:91:ILE:HD11	1.99	0.45
50:9:5:U:H2'	50:9:6:G:C8	2.51	0.45
61:KK:49:MET:HA	61:KK:52:LEU:HB2	1.99	0.45
62:LL:149:ALA:O	64:NN:133:ARG:NH1	2.44	0.45
70:TT:75:MET:HA	70:TT:78:ILE:HG22	1.98	0.45
73:WW:90:GLN:OE1	73:WW:113:HIS:CD2	2.69	0.45
4:5:679:C:H2'	4:5:680:G:C8	2.51	0.45
4:5:1170:G:H2'	4:5:1171:G:H8	1.81	0.45
4:5:4080:C:H2'	4:5:4081:G:C8	2.50	0.45
4:5:4492:U:O2'	4:5:4512:U:O2	2.28	0.45
5:7:15:C:H2'	5:7:16:A:H8	1.82	0.45
17:L:184:MET:HE3	17:L:184:MET:HB2	1.82	0.45
18:M:16:SER:OG	18:M:56:GLN:OE1	2.29	0.45
46:o:63:THR:HB	46:o:87:ARG:HH11	1.80	0.45
50:9:441:C:OP2	59:II:2:GLY:N	2.50	0.45
50:9:1513:C:H2'	50:9:1514:G:H8	1.82	0.45
50:9:1548:G:OP1	71:UU:60:THR:OG1	2.34	0.45
52:BB:198:GLU:HB2	52:BB:210:VAL:HG21	1.97	0.45
63:MM:38:ALA:HB2	63:MM:110:VAL:HG11	1.99	0.45
64:NN:57:SER:OG	64:NN:58:HIS:ND1	2.50	0.45
65:OO:57:THR:HG23	65:OO:60:MET:HE3	1.97	0.45
69:SS:114:LEU:HD11	69:SS:121:ARG:HH11	1.82	0.45
75:YY:81:TYR:HA	75:YY:84:LYS:HG2	1.97	0.45
83:gg:40:ILE:HB	83:gg:59:LEU:HB2	1.99	0.45
4:5:151:G:N7	13:G:194:ASN:ND2	2.64	0.45
4:5:956:A:H1'	4:5:2076:G:H5''	1.99	0.45
4:5:2483:G:H2'	4:5:2484:A:C8	2.52	0.45
4:5:3974:G:H4'	49:u:27:LYS:HD2	1.99	0.45
4:5:4280:A:N6	10:D:28:THR:O	2.45	0.45
4:5:4431:U:OP2	15:I:3:ARG:NH2	2.37	0.45
16:J:146:ARG:HD3	16:J:147:ARG:HG3	1.98	0.45
20:O:157:GLU:HA	20:O:160:ARG:HG2	1.99	0.45
24:S:36:ASN:N	24:S:36:ASN:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:56:LEU:HD12	26:U:61:VAL:HB	1.99	0.45
44:m:69:ILE:HD11	44:m:96:ARG:HE	1.81	0.45
49:u:171:HIS:CE1	49:u:174:MET:HE2	2.52	0.45
77:aa:51:ARG:NH1	79:cc:39:SER:O	2.40	0.45
4:5:268:G:H2'	4:5:269:G:H8	1.81	0.45
4:5:1338:G:OP2	32:a:12:ARG:NH2	2.50	0.45
4:5:1512:G:OP1	32:a:7:LYS:NZ	2.44	0.45
4:5:2352:U:H1'	9:C:96:CYS:HA	1.99	0.45
7:A:113:VAL:HG13	7:A:164:ALA:HB1	1.98	0.45
7:A:116:LEU:N	7:A:126:LEU:O	2.50	0.45
14:H:41:ILE:HD11	14:H:69:THR:HB	1.99	0.45
14:H:80:MET:HE3	14:H:80:MET:HB2	1.64	0.45
20:O:15:LEU:HB2	20:O:18:ARG:HB3	1.99	0.45
27:V:18:LEU:H	27:V:18:LEU:HG	1.59	0.45
50:9:671:A:H4'	50:9:672:A:H5''	1.99	0.45
50:9:1232:U:H2'	50:9:1233:G:H8	1.80	0.45
50:9:1286:G:C4'	82:ff:97:LYS:HA	2.33	0.45
50:9:1579:A:O2'	50:9:1581:C:OP2	2.27	0.45
51:AA:184:ARG:HG2	51:AA:191:ARG:HG2	1.99	0.45
52:BB:143:THR:HA	52:BB:207:LEU:HA	1.98	0.45
57:GG:6:SER:HB3	57:GG:112:VAL:HG12	1.97	0.45
4:5:238:C:OP2	30:Y:45:ARG:NH2	2.49	0.45
4:5:327:U:O2'	40:i:30:ARG:NH1	2.45	0.45
4:5:1440:U:OP2	12:F:33:ARG:NH1	2.50	0.45
4:5:2838:G:OP1	8:B:248:LEU:N	2.50	0.45
4:5:4452:U:OP2	4:5:4522:G:N2	2.39	0.45
4:5:4572:U:O2'	4:5:4573:G:O4'	2.34	0.45
6:8:141:C:H5''	19:N:60:VAL:HG11	1.98	0.45
19:N:5:LYS:HD3	19:N:8:GLN:HE21	1.82	0.45
19:N:9:GLU:OE2	19:N:12:ARG:NH2	2.46	0.45
23:R:99:MET:HE2	23:R:127:VAL:HG12	1.98	0.45
35:d:64:ILE:HG23	35:d:68:LEU:HD23	1.99	0.45
50:9:4:C:H4'	53:CC:207:ALA:HB2	1.99	0.45
51:AA:79:SER:HA	51:AA:101:GLY:HA2	1.99	0.45
59:II:83:TYR:HB3	59:II:101:ILE:HD12	1.99	0.45
69:SS:36:VAL:HG23	69:SS:40:TYR:HD2	1.81	0.45
69:SS:48:ALA:HB2	69:SS:70:ILE:HD12	1.98	0.45
69:SS:92:ASP:OD1	69:SS:92:ASP:N	2.49	0.45
73:WW:23:ARG:HD3	78:bb:4:ALA:HB2	1.99	0.45
76:ZZ:51:ASP:OD1	76:ZZ:54:THR:OG1	2.29	0.45
76:ZZ:73:VAL:HG12	76:ZZ:79:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:1351:G:P	9:C:33:ARG:HH12	2.38	0.45
4:5:2335:C:H2'	4:5:2336:G:H8	1.81	0.45
4:5:4078:C:O2'	4:5:4172:A:N6	2.50	0.45
8:B:55:HIS:HB2	8:B:369:ASP:HB3	1.99	0.45
19:N:96:ARG:NH1	19:N:104:GLU:OE1	2.50	0.45
49:u:59:PRO:HB2	49:u:170:GLY:H	1.82	0.45
50:9:618:C:H41	74:XX:67:ARG:NH1	2.15	0.45
53:CC:254:ASP:OD1	53:CC:254:ASP:N	2.50	0.45
54:DD:50:ILE:HG23	54:DD:88:ALA:HA	1.98	0.45
55:EE:206:ASP:OD1	55:EE:206:ASP:N	2.49	0.45
60:JJ:136:ARG:HA	60:JJ:141:VAL:HA	1.99	0.45
4:5:4980:C:N3	21:P:69:ARG:NH1	2.64	0.44
8:B:44:THR:HG21	8:B:186:ASN:HD22	1.82	0.44
9:C:292:ILE:HG21	22:Q:31:LEU:HD11	1.99	0.44
45:n:7:LYS:NZ	45:n:11:ARG:HH21	2.15	0.44
50:9:116:OMU:H1'	50:9:116:OMU:HM23	1.64	0.44
50:9:1053:C:H2'	50:9:1054:G:H8	1.82	0.44
50:9:1307:U:C2	82:ff:139:HIS:HA	2.51	0.44
56:FF:87:LEU:HD21	67:QQ:78:VAL:HG11	1.98	0.44
68:RR:31:ASN:HD21	68:RR:55:THR:HG22	1.81	0.44
77:aa:7:ASN:O	77:aa:9:GLY:N	2.51	0.44
4:5:32:G:OP1	19:N:73:ARG:NH1	2.51	0.44
4:5:724:C:H1'	9:C:343:GLN:HG2	1.98	0.44
4:5:728:U:OP1	12:F:75:ARG:NH2	2.50	0.44
4:5:1081:C:H42	4:5:1218:G:H1	1.64	0.44
4:5:1420:A:N7	32:a:116:LYS:NZ	2.54	0.44
4:5:2441:C:H4'	38:g:9:ARG:HE	1.82	0.44
4:5:4626:A:H4'	8:B:53:MET:HG3	1.98	0.44
8:B:56:ILE:HD13	8:B:56:ILE:HA	1.81	0.44
10:D:17:GLN:OE1	25:T:20:ARG:O	2.35	0.44
11:E:217:ASP:O	11:E:221:LYS:HB2	2.16	0.44
34:c:78:ASN:N	34:c:78:ASN:OD1	2.48	0.44
50:9:1445:U:O2'	71:UU:55:ARG:O	2.30	0.44
50:9:1786:U:H2'	50:9:1787:G:H8	1.83	0.44
54:DD:137:VAL:HG22	54:DD:151:LYS:HD2	1.98	0.44
63:MM:50:CYS:O	63:MM:76:LEU:HA	2.17	0.44
64:NN:4:MET:HE3	64:NN:121:ARG:HG2	1.98	0.44
72:VV:30:ALA:O	72:VV:60:ARG:NH1	2.46	0.44
73:WW:46:TYR:O	73:WW:66:THR:OG1	2.35	0.44
2:2:23:C:H2'	2:2:24:A:C8	2.52	0.44
4:5:2411:C:H2'	4:5:2412:A:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:12:LEU:HB2	31:Z:81:MET:HB3	1.99	0.44
50:9:1648:G:O2'	50:9:1674:G:O6	2.29	0.44
54:DD:16:ILE:HD12	80:dd:36:LEU:HD23	1.98	0.44
59:II:48:VAL:HG11	59:II:54:LYS:HD3	1.98	0.44
83:gg:254:PRO:HB3	83:gg:283:PRO:HG2	1.99	0.44
3:4:18:U:O2'	3:4:57:A:N1	2.51	0.44
4:5:86:U:H2'	4:5:87:A:H8	1.82	0.44
4:5:318:A:H2'	4:5:319:A:H8	1.83	0.44
4:5:2835:A:O2'	8:B:228:TYR:O	2.31	0.44
4:5:4301:U:OP1	25:T:78:LYS:NZ	2.47	0.44
15:I:98:ARG:HB3	15:I:120:GLY:HA3	1.98	0.44
16:J:150:CYS:SG	16:J:151:ILE:N	2.89	0.44
23:R:96:MET:HE3	23:R:100:ARG:HH12	1.82	0.44
50:9:146:G:O2'	50:9:147:A:O5'	2.35	0.44
50:9:854:A:H2'	50:9:855:G:H8	1.82	0.44
50:9:1124:C:O2'	68:RR:126:MET:O	2.34	0.44
50:9:1201:U:O2'	50:9:1358:U:O2'	2.31	0.44
58:HH:36:LEU:HD21	58:HH:78:ARG:HG2	1.98	0.44
68:RR:5:ARG:HH11	68:RR:53:TYR:HD1	1.66	0.44
4:5:1558:A:H2'	4:5:1559:G:C8	2.52	0.44
4:5:4135:G:H2'	4:5:4136:G:C8	2.53	0.44
4:5:4260:U:H2'	4:5:4261:C:C6	2.52	0.44
18:M:70:GLN:HA	18:M:73:VAL:HG12	1.99	0.44
21:P:124:LYS:HD3	21:P:140:MET:HG2	2.00	0.44
38:g:60:ARG:HD3	38:g:61:PRO:HD2	1.98	0.44
49:u:94:ASN:OD1	49:u:97:LYS:NZ	2.37	0.44
76:ZZ:88:LEU:HB3	76:ZZ:109:TYR:HE2	1.83	0.44
83:gg:8:ARG:HB2	83:gg:309:VAL:HG23	1.99	0.44
4:5:1605:7MG:H2'	4:5:1606:U:O4'	2.18	0.44
4:5:1962:A:OP2	4:5:2024:G:N2	2.39	0.44
4:5:1984:A:N7	4:5:2010:A:O2'	2.51	0.44
4:5:2444:U:HO2'	6:8:112:G:HO2'	1.46	0.44
4:5:3722:G:OP1	40:i:68:ARG:NH2	2.51	0.44
4:5:3870:C:H2'	4:5:3871:A:C8	2.53	0.44
4:5:3944:G:H1	4:5:4069:U:H3	1.65	0.44
4:5:4174:U:H2'	4:5:4175:G:C8	2.53	0.44
4:5:4403:PSU:HN1	4:5:4440:G:H1	1.66	0.44
4:5:4424:A:O5'	44:m:96:ARG:NH1	2.51	0.44
4:5:5002:U:H2'	4:5:5003:U:C6	2.52	0.44
19:N:46:ASP:OD1	19:N:47:LYS:N	2.51	0.44
26:U:28:PRO:HB2	26:U:34:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:80:PRO:HA	29:X:98:PHE:HA	1.99	0.44
50:9:1281:G:H3'	50:9:1282:A:C8	2.53	0.44
51:AA:154:LEU:HD22	51:AA:157:VAL:HG21	2.00	0.44
52:BB:179:ASN:H	52:BB:179:ASN:HD22	1.65	0.44
52:BB:181:LEU:HA	52:BB:184:VAL:HG12	1.99	0.44
52:BB:217:MET:HE1	52:BB:220:LYS:HB3	2.00	0.44
57:GG:6:SER:O	57:GG:112:VAL:HA	2.18	0.44
60:JJ:29:LEU:HA	60:JJ:32:ILE:HG22	1.99	0.44
64:NN:32:ASP:HA	64:NN:35:GLU:HG3	2.00	0.44
64:NN:64:ARG:HD3	64:NN:70:LYS:HE2	2.00	0.44
83:gg:245:ARG:NH1	83:gg:296:GLN:OE1	2.49	0.44
3:4:49:C:H2'	3:4:50:A:C8	2.53	0.44
4:5:43:U:H1'	46:o:52:THR:HG23	2.00	0.44
4:5:1906:U:H2'	4:5:1907:A:H8	1.83	0.44
4:5:4322:G:N2	4:5:4325:A:OP2	2.49	0.44
4:5:4745:G:H1	4:5:4955:A:H61	1.65	0.44
5:7:92:C:H2'	5:7:93:G:C8	2.53	0.44
7:A:40:TYR:HA	7:A:90:CYS:O	2.17	0.44
34:c:47:ILE:HD12	34:c:94:LEU:HD11	1.99	0.44
35:d:26:THR:HB	35:d:85:ARG:HH11	1.82	0.44
48:r:96:MET:O	48:r:100:ASN:ND2	2.51	0.44
49:u:7:ARG:HH12	49:u:184:HIS:HB2	1.82	0.44
50:9:495:U:O2'	55:EE:27:PHE:O	2.36	0.44
50:9:640:A:H2'	50:9:641:A:C8	2.51	0.44
52:BB:207:LEU:H	52:BB:207:LEU:HG	1.65	0.44
67:QQ:58:LEU:HD11	67:QQ:112:LEU:HD11	1.99	0.44
67:QQ:60:LYS:H	67:QQ:60:LYS:HD2	1.82	0.44
4:5:287:U:H2'	4:5:288:G:C8	2.52	0.44
4:5:478:G:H2'	4:5:479:G:C8	2.52	0.44
4:5:517:C:H2'	4:5:518:G:H8	1.83	0.44
4:5:2394:G:O2'	4:5:2819:U:O4	2.27	0.44
4:5:3860:A:H61	4:5:4560:C:H5	1.65	0.44
17:L:143:GLU:HA	17:L:146:LEU:HG	1.98	0.44
50:9:434:G:H2'	50:9:435:A:C8	2.53	0.44
50:9:692:G:H2'	50:9:693:A:H8	1.83	0.44
50:9:1492:U:O2'	50:9:1495:G:OP1	2.32	0.44
50:9:1504:U:H3	82:ff:84:SER:C	2.26	0.44
52:BB:179:ASN:N	52:BB:179:ASN:ND2	2.64	0.44
55:EE:51:ARG:NH1	55:EE:109:PHE:O	2.50	0.44
59:II:87:ASN:HB3	59:II:90:LEU:HD23	1.98	0.44
69:SS:61:GLU:HA	69:SS:64:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:YY:17:LEU:H	75:YY:17:LEU:HG	1.58	0.44
4:5:279:A:C5	19:N:12:ARG:HD2	2.52	0.44
4:5:1577:G:OP2	7:A:181:LYS:NZ	2.43	0.44
4:5:1866:UR3:O5'	4:5:1866:UR3:H6	2.18	0.44
4:5:2566:G:H2'	4:5:2567:G:H8	1.83	0.44
4:5:2588:C:OP2	4:5:2769:U:O2'	2.35	0.44
4:5:4323:A:H2	10:D:146:LEU:HD12	1.83	0.44
37:f:40:GLU:O	37:f:109:ARG:NH2	2.51	0.44
40:i:71:LYS:HA	40:i:74:LYS:HG2	2.00	0.44
45:n:2:ARG:NH1	50:9:1841:C:OP2	2.41	0.44
53:CC:60:TRP:CZ3	53:CC:71:LYS:HB3	2.53	0.44
56:FF:34:SER:HA	79:cc:55:VAL:HG23	1.99	0.44
59:II:3:ILE:O	59:II:30:GLY:N	2.37	0.44
59:II:67:TRP:O	59:II:71:CYS:N	2.51	0.44
60:JJ:18:ARG:O	60:JJ:24:ARG:NH2	2.50	0.44
82:ff:94:LYS:HE2	82:ff:94:LYS:HB3	1.77	0.44
4:5:162:A:H2'	4:5:163:A:C8	2.53	0.43
4:5:1316:OMG:HM23	4:5:1316:OMG:H1'	1.77	0.43
4:5:3651:A:H5'	7:A:199:VAL:HG22	1.99	0.43
4:5:4680:G:H2'	4:5:4681:A:C8	2.53	0.43
8:B:83:PRO:O	8:B:167:GLN:NE2	2.51	0.43
24:S:113:MET:HB3	24:S:119:ALA:HB3	2.00	0.43
27:V:13:LYS:HB2	27:V:128:LEU:HD11	1.99	0.43
49:u:13:ALA:HA	49:u:16:GLU:HG2	2.00	0.43
50:9:1623:A:H62	69:SS:132:ARG:HH21	1.65	0.43
51:AA:210:ILE:HD13	68:RR:81:ARG:HD3	2.00	0.43
52:BB:67:PHE:O	52:BB:85:LYS:HA	2.18	0.43
54:DD:127:MET:HE2	54:DD:127:MET:HB3	1.75	0.43
83:gg:146:SER:OG	83:gg:147:HIS:N	2.51	0.43
4:5:1327:C:H2'	4:5:1328:G:H8	1.83	0.43
4:5:2399:G:N3	38:g:4:ARG:NH2	2.67	0.43
4:5:2527:A:N6	29:X:85:SER:OG	2.52	0.43
4:5:2878:G:H4'	4:5:3825:A2M:H5''	2.00	0.43
4:5:2893:U:H2'	4:5:2894:A:H8	1.81	0.43
4:5:3610:A:H2'	4:5:3611:A:H8	1.81	0.43
7:A:82:ILE:HG22	47:p:65:ALA:HB3	1.98	0.43
13:G:189:LEU:HD21	13:G:246:LEU:HD23	2.01	0.43
15:I:31:ILE:HB	15:I:66:GLU:HB2	2.00	0.43
49:u:139:THR:OG1	49:u:140:HIS:N	2.51	0.43
50:9:1360:U:O2'	50:9:1379:A:OP2	2.35	0.43
52:BB:28:LYS:NZ	65:OO:51:GLU:OE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DD:210:ILE:HD13	68:RR:16:ILE:HG12	2.01	0.43
3:4:6:G:N2	3:4:67:U:O2	2.39	0.43
4:5:2385:U:OP1	23:R:5:ARG:NH2	2.48	0.43
4:5:2599:G:O2'	4:5:2746:A:N6	2.51	0.43
4:5:4518:A:OP1	4:5:4520:G:O2'	2.24	0.43
4:5:4860:G:H5'	20:O:169:ARG:HD3	2.00	0.43
6:8:67:U:H2'	6:8:68:G:H8	1.84	0.43
8:B:99:LEU:HD11	8:B:159:VAL:HG11	1.99	0.43
8:B:232:THR:HG21	8:B:249:ARG:HB3	2.00	0.43
9:C:279:LEU:HD23	9:C:279:LEU:HA	1.86	0.43
10:D:277:LYS:HA	10:D:280:VAL:HG22	2.00	0.43
12:F:192:GLU:O	12:F:195:THR:O	2.36	0.43
21:P:48:LEU:HA	21:P:51:VAL:HG12	1.99	0.43
23:R:77:GLY:O	23:R:81:ARG:NE	2.49	0.43
50:9:190:G:OP1	59:II:149:TYR:OH	2.32	0.43
50:9:1101:U:H2'	50:9:1102:G:C8	2.54	0.43
50:9:1596:U:O3'	69:SS:25:LYS:NZ	2.51	0.43
57:GG:143:LYS:HD2	57:GG:143:LYS:HA	1.85	0.43
64:NN:119:GLU:HA	64:NN:122:ILE:HG12	1.99	0.43
65:OO:78:ALA:HB1	65:OO:119:LEU:HD12	1.98	0.43
4:5:4054:C:O2	49:u:35:GLN:NE2	2.40	0.43
4:5:4313:A:OP1	25:T:92:ARG:NH2	2.40	0.43
10:D:41:LYS:NZ	25:T:30:TYR:O	2.50	0.43
17:L:64:VAL:HA	17:L:67:HIS:CD2	2.54	0.43
21:P:64:ASN:HB2	21:P:80:GLN:HE22	1.82	0.43
50:9:1275:G:H8	82:ff:92:LYS:HZ1	1.67	0.43
50:9:1578:U:H1'	54:DD:6:SER:HB3	2.00	0.43
53:CC:132:ASP:N	53:CC:132:ASP:OD1	2.52	0.43
56:FF:67:PRO:HG2	56:FF:70:GLU:HB2	2.01	0.43
4:5:62:A:N3	4:5:77:U:O2'	2.39	0.43
4:5:2502:A:O2'	4:5:2503:G:O5'	2.33	0.43
4:5:3723:A2M:HM'3	4:5:3723:A2M:H1'	1.91	0.43
4:5:3811:G:O2'	4:5:3814:U:OP2	2.36	0.43
4:5:3848:U:H2'	4:5:3849:A:H8	1.83	0.43
4:5:4134:C:H2'	4:5:4135:G:C8	2.54	0.43
6:8:8:U:H2'	6:8:9:A:C8	2.53	0.43
19:N:103:GLU:OE2	19:N:165:THR:OG1	2.35	0.43
41:j:67:LEU:HA	41:j:70:VAL:HG12	2.00	0.43
48:r:52:GLU:HB2	48:r:61:VAL:HG23	2.01	0.43
50:9:183:G:O2'	50:9:184:G:O4'	2.35	0.43
50:9:658:U:H1'	74:XX:17:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:912:C:O2'	50:9:914:U:O2'	2.29	0.43
50:9:1856:C:N4	50:9:1857:G:O6	2.51	0.43
52:BB:179:ASN:HD22	52:BB:179:ASN:N	2.15	0.43
54:DD:177:LEU:HD23	54:DD:182:LEU:HD13	2.00	0.43
55:EE:9:LEU:HB2	55:EE:30:ARG:HD3	2.00	0.43
4:5:1313:C:O2	4:5:3881:G:O2'	2.29	0.43
4:5:2573:A:H62	4:5:2761:U:H3	1.65	0.43
4:5:3687:A:O2'	7:A:236:GLY:N	2.51	0.43
4:5:3930:U:H3	4:5:4180:G:H1	1.65	0.43
4:5:4238:G:H2'	4:5:4239:A:C8	2.54	0.43
4:5:4474:A:H2'	4:5:4476:C:H5''	2.01	0.43
11:E:122:GLU:HG3	36:e:7:LEU:HD22	1.99	0.43
20:O:12:ARG:HH21	24:S:171:ARG:CZ	2.31	0.43
22:Q:44:ASN:HA	22:Q:47:VAL:HG12	2.01	0.43
50:9:159:A2M:H8	50:9:159:A2M:OP2	2.19	0.43
50:9:1198:G:H2'	50:9:1199:A:C8	2.53	0.43
50:9:1619:A:OP2	66:PP:47:ARG:NH2	2.51	0.43
50:9:1705:C:H2'	50:9:1706:G:C8	2.53	0.43
51:AA:163:CYS:HB3	51:AA:174:MET:HE2	2.01	0.43
55:EE:165:GLU:HG3	55:EE:166:THR:HG23	1.99	0.43
56:FF:140:ASP:CG	79:cc:44:ARG:HH22	2.26	0.43
65:OO:29:GLY:O	65:OO:93:LEU:HA	2.18	0.43
4:5:2607:C:H2'	4:5:2608:G:H8	1.84	0.43
4:5:3889:G:O2'	4:5:4571:A2M:H2	2.18	0.43
9:C:150:LEU:O	9:C:152:LEU:N	2.52	0.43
9:C:287:THR:HG21	48:r:5:LEU:HB2	2.01	0.43
21:P:131:ARG:HG3	21:P:137:ASN:ND2	2.34	0.43
29:X:80:PRO:HD2	39:h:33:VAL:HG22	2.00	0.43
30:Y:50:ARG:HG2	30:Y:51:LYS:H	1.83	0.43
50:9:486:A:H1'	50:9:513:G:H22	1.84	0.43
50:9:528:A:OP1	60:JJ:121:LYS:NZ	2.52	0.43
50:9:1143:A:H5'	53:CC:190:SER:HB3	2.00	0.43
50:9:1298:G:N7	66:PP:79:HIS:ND1	2.67	0.43
50:9:1307:U:H6	82:ff:137:ASP:N	2.14	0.43
54:DD:65:ARG:HA	54:DD:68:GLU:HB3	2.01	0.43
55:EE:90:ILE:HB	55:EE:99:PHE:HB2	2.01	0.43
56:FF:49:LEU:HG	67:QQ:49:TYR:HB2	2.01	0.43
77:aa:60:ASP:OD1	77:aa:60:ASP:N	2.48	0.43
79:cc:14:VAL:HG22	79:cc:32:VAL:HG12	2.01	0.43
83:gg:191:HIS:NE2	83:gg:215:GLN:O	2.52	0.43
4:5:1480:C:O2'	4:5:1482:G:OP2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:3672:G:C6	4:5:3674:G:H1'	2.54	0.43
4:5:3717:A:H2'	4:5:3718:A2M:C8	2.48	0.43
4:5:3773:U:H2'	4:5:3775:A:H2	1.84	0.43
4:5:4354:U:H3	32:a:60:HIS:CE1	2.36	0.43
4:5:4716:C:OP2	8:B:30:LYS:NZ	2.38	0.43
9:C:210:ILE:HG22	9:C:232:VAL:HG22	1.99	0.43
21:P:16:LYS:O	21:P:101:ASN:ND2	2.52	0.43
21:P:135:ARG:HH12	21:P:137:ASN:HD21	1.65	0.43
29:X:100:VAL:HG21	29:X:109:ILE:HD11	1.99	0.43
50:9:1536:G:H2'	50:9:1537:A:H8	1.83	0.43
55:EE:252:ARG:HA	55:EE:255:ARG:HG2	1.99	0.43
59:II:65:PHE:HD2	59:II:104:ILE:HG12	1.83	0.43
65:OO:62:VAL:HG11	65:OO:68:GLU:HA	2.01	0.43
71:UU:61:LEU:HB2	71:UU:82:MET:HB3	2.00	0.43
75:YY:110:ARG:NH2	75:YY:114:MET:SD	2.92	0.43
4:5:36:U:O4	19:N:83:LYS:NZ	2.51	0.43
4:5:1524:A2M:N6	4:5:3915:U:O2'	2.40	0.43
4:5:2809:G:O2'	4:5:4644:G:OP1	2.29	0.43
8:B:55:HIS:CE1	28:W:16:GLY:HA3	2.54	0.43
10:D:152:ARG:HG3	10:D:154:THR:HG23	2.01	0.43
16:J:17:ILE:HA	16:J:134:LEU:HA	2.01	0.43
27:V:112:MET:HE2	27:V:112:MET:HB3	1.88	0.43
31:Z:84:ARG:NH2	31:Z:85:TYR:OH	2.52	0.43
53:CC:106:VAL:HG22	53:CC:128:VAL:HG22	2.01	0.43
57:GG:218:LYS:HE2	57:GG:218:LYS:HB3	1.86	0.43
58:HH:148:LEU:HA	73:WW:42:MET:HE2	2.01	0.43
69:SS:104:ASP:OD1	69:SS:104:ASP:N	2.45	0.43
83:gg:24:THR:HG22	83:gg:26:GLN:H	1.83	0.43
4:5:1282:G:OP2	9:C:316:LYS:NZ	2.40	0.43
4:5:1784:U:H1'	15:I:92:HIS:HD2	1.84	0.43
4:5:4619:U:H2'	4:5:4620:OMU:H6	1.99	0.43
4:5:5053:U:OP1	4:5:5054:C:N4	2.52	0.43
5:7:87:G:OP1	24:S:87:ARG:NH2	2.52	0.43
21:P:47:TYR:OH	21:P:57:CYS:O	2.31	0.43
27:V:13:LYS:HD3	27:V:128:LEU:HD11	2.01	0.43
50:9:65:C:C4	57:GG:133:LEU:HD23	2.54	0.43
50:9:560:A:H5'	60:JJ:174:LYS:HD3	2.01	0.43
50:9:1758:G:H2'	50:9:1759:G:C8	2.53	0.43
51:AA:122:LEU:HB2	51:AA:144:THR:HG22	2.00	0.43
51:AA:123:VAL:HA	51:AA:145:ILE:HB	2.01	0.43
63:MM:52:LEU:HD22	63:MM:78:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:OO:56:VAL:HG13	65:OO:77:ALA:HB1	2.01	0.43
4:5:163:A:H2'	4:5:164:G:H8	1.83	0.42
4:5:1471:U:H2'	4:5:1472:C:C6	2.54	0.42
4:5:1940:G:N2	4:5:4434:C:OP1	2.47	0.42
4:5:2326:G:H5''	36:e:127:ALA:HB1	2.01	0.42
4:5:2492:C:H2'	4:5:2493:G:C8	2.54	0.42
4:5:3720:G:OP2	40:i:75:LYS:NZ	2.49	0.42
4:5:4472:B8W:O2'	44:m:74:TYR:O	2.37	0.42
14:H:103:VAL:HG11	14:H:144:LEU:HD21	2.01	0.42
49:u:64:SER:HB3	49:u:108:ASP:H	1.84	0.42
50:9:1217:A:H2'	50:9:1218:C:C6	2.53	0.42
50:9:1259:A:N6	50:9:1519:U:O5'	2.52	0.42
67:QQ:97:GLN:HB3	67:QQ:105:LYS:HE2	2.01	0.42
4:5:51:A:N3	4:5:1528:U:O2'	2.52	0.42
4:5:456:C:H2'	4:5:457:G:C8	2.52	0.42
4:5:725:G:N3	4:5:944:A:O2'	2.45	0.42
4:5:1444:G:H2'	4:5:1445:U:H6	1.84	0.42
4:5:2759:G:H1'	4:5:2764:A:H2	1.84	0.42
4:5:3932:U:H2'	4:5:3933:G:H8	1.84	0.42
10:D:156:GLY:HA2	10:D:181:PRO:HD3	1.99	0.42
19:N:165:THR:O	19:N:169:ARG:CB	2.67	0.42
21:P:148:MET:HE2	21:P:150:LEU:HD11	1.99	0.42
22:Q:33:ARG:HE	22:Q:52:PHE:HZ	1.66	0.42
22:Q:61:LEU:HD22	22:Q:82:VAL:HG21	2.01	0.42
27:V:42:VAL:HG13	27:V:61:VAL:HG12	2.00	0.42
31:Z:66:SER:O	31:Z:66:SER:OG	2.36	0.42
50:9:880:G:H2'	50:9:881:G:H8	1.84	0.42
50:9:1286:G:H5''	82:ff:97:LYS:HA	1.99	0.42
50:9:1287:A:C4'	82:ff:97:LYS:H	2.32	0.42
55:EE:247:THR:OG1	55:EE:250:GLU:OE1	2.28	0.42
67:QQ:25:CYS:HA	67:QQ:67:ASP:O	2.19	0.42
69:SS:26:ILE:H	69:SS:26:ILE:HG13	1.69	0.42
4:5:469:C:H2'	4:5:470:A:H8	1.84	0.42
4:5:1949:U:OP1	14:H:64:ARG:NH1	2.53	0.42
4:5:4578:G:H2'	4:5:4579:U:C6	2.54	0.42
8:B:234:ARG:NH1	8:B:271:GLN:O	2.39	0.42
9:C:207:PRO:HB3	9:C:249:PHE:CD2	2.54	0.42
12:F:170:ASP:N	12:F:170:ASP:OD1	2.51	0.42
13:G:119:GLN:HA	13:G:122:ILE:HB	2.01	0.42
16:J:37:ALA:HA	16:J:70:VAL:HG11	2.00	0.42
38:g:63:VAL:HG22	38:g:66:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:441:C:H2'	50:9:442:C:C6	2.54	0.42
50:9:981:A:H2'	50:9:982:G:C8	2.54	0.42
50:9:1708:C:H2'	50:9:1709:G:H8	1.83	0.42
52:BB:68:GLU:HG2	52:BB:83:LYS:HD2	2.02	0.42
53:CC:188:CYS:SG	53:CC:238:LYS:HG3	2.59	0.42
58:HH:77:VAL:HA	58:HH:80:VAL:HG12	2.01	0.42
83:gg:239:LEU:HD22	83:gg:248:LEU:HD11	2.02	0.42
4:5:163:A:H2'	4:5:164:G:C8	2.55	0.42
4:5:1338:G:H4'	4:5:1339:U:C6	2.55	0.42
4:5:2333:G:H5''	9:C:195:LYS:HE3	2.00	0.42
4:5:2491:C:H2'	4:5:2492:C:C6	2.54	0.42
4:5:3612:C:H1'	4:5:5016:A:C8	2.54	0.42
4:5:3848:U:H2'	4:5:3849:A:C8	2.55	0.42
4:5:3970:G:H21	49:u:209:THR:HG22	1.84	0.42
4:5:4060:U:H2'	4:5:4061:G:C8	2.54	0.42
8:B:217:ILE:HD11	8:B:333:LEU:HD21	2.01	0.42
9:C:284:MET:HE3	22:Q:124:ASP:HB3	2.02	0.42
21:P:122:ALA:HB3	21:P:143:PRO:HG2	2.01	0.42
24:S:92:ASN:ND2	25:T:156:TYR:O	2.43	0.42
30:Y:21:ALA:O	30:Y:26:ARG:NE	2.45	0.42
33:b:101:HIS:NE2	33:b:104:LEU:HB2	2.33	0.42
40:i:44:ILE:HD13	40:i:44:ILE:HA	1.91	0.42
50:9:433:A:H5''	59:II:22:HIS:HB3	2.01	0.42
50:9:1021:U:OP1	64:NN:132:LYS:NZ	2.36	0.42
50:9:1215:C:O2'	50:9:1645:C:OP2	2.33	0.42
50:9:1589:A:N3	50:9:1653:U:O2'	2.48	0.42
50:9:1650:A:H5''	67:QQ:139:ALA:HB2	2.00	0.42
54:DD:63:GLY:O	54:DD:67:ARG:NE	2.45	0.42
57:GG:1:MET:HE2	57:GG:24:LEU:HD23	2.01	0.42
57:GG:109:LEU:HD23	57:GG:109:LEU:HA	1.83	0.42
59:II:133:GLU:HA	59:II:136:ILE:HG12	2.01	0.42
61:KK:64:TRP:CD2	80:dd:23:VAL:HG12	2.54	0.42
69:SS:132:ARG:HB2	69:SS:134:GLN:HE22	1.84	0.42
4:5:74:G:H1'	17:L:62:PRO:HG3	2.01	0.42
4:5:162:A:H2'	4:5:163:A:H8	1.84	0.42
4:5:2485:U:N3	4:5:2493:G:N1	2.67	0.42
4:5:2738:C:O2'	4:5:2740:U:O2	2.33	0.42
4:5:3932:U:H2'	4:5:3933:G:C8	2.54	0.42
10:D:40:ASP:HB2	10:D:43:LYS:HG2	2.00	0.42
20:O:32:LYS:HG2	20:O:101:ARG:HB2	2.02	0.42
23:R:136:ARG:HA	23:R:139:MET:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:17:ARG:HD3	25:T:45:MET:HG3	2.00	0.42
50:9:1309:C:H5'	82:ff:105:TYR:CE1	2.55	0.42
51:AA:144:THR:N	51:AA:158:ASP:OD2	2.41	0.42
52:BB:92:GLN:HB2	52:BB:95:ASN:HB2	2.01	0.42
54:DD:225:GLU:HG3	83:gg:187:ASN:HD22	1.84	0.42
66:PP:35:GLN:HE21	66:PP:35:GLN:HB2	1.67	0.42
67:QQ:120:LEU:HD23	67:QQ:120:LEU:HA	1.87	0.42
83:gg:144:ASP:OD1	83:gg:144:ASP:N	2.48	0.42
4:5:517:C:H2'	4:5:518:G:C8	2.55	0.42
4:5:2581:A:H2'	4:5:2582:A:C8	2.55	0.42
4:5:4929:C:OP1	18:M:117:LYS:NZ	2.49	0.42
6:8:19:C:H2'	6:8:20:A:C8	2.55	0.42
7:A:58:LEU:HD23	7:A:58:LEU:HA	1.87	0.42
8:B:81:THR:HA	8:B:82:PRO:HD2	1.92	0.42
10:D:29:ASP:HB2	10:D:150:LEU:HD21	2.01	0.42
16:J:93:GLU:HA	16:J:173:ILE:O	2.19	0.42
17:L:28:GLN:HB3	19:N:202:ARG:HE	1.84	0.42
24:S:47:PHE:HE1	24:S:125:GLN:HG3	1.83	0.42
49:u:101:LYS:HB3	49:u:128:LEU:HD21	2.00	0.42
50:9:377:G:H5'	59:II:98:LYS:HB3	2.01	0.42
50:9:428:U:H4'	60:JJ:2:PRO:HG3	2.02	0.42
50:9:672:A:N6	50:9:1027:A:OP1	2.50	0.42
50:9:1286:G:OP1	82:ff:99:LYS:NZ	2.41	0.42
50:9:1413:G:H2'	50:9:1414:A:H8	1.85	0.42
51:AA:51:LEU:H	68:RR:105:MET:HE1	1.85	0.42
56:FF:42:LYS:HD3	56:FF:42:LYS:HA	1.95	0.42
58:HH:62:ILE:HD12	58:HH:94:PHE:HE1	1.84	0.42
68:RR:17:ILE:HD11	68:RR:54:VAL:HA	2.01	0.42
82:ff:101:ALA:HA	82:ff:104:LYS:NZ	2.35	0.42
4:5:2400:G:H21	38:g:6:THR:HG22	1.84	0.42
4:5:2793:G:H4'	41:j:8:PHE:HD2	1.85	0.42
4:5:3747:A:N7	7:A:245:ARG:HD2	2.34	0.42
4:5:4985:U:H4'	8:B:175:GLN:HE21	1.85	0.42
50:9:1372:U:OP1	50:9:1385:G:N2	2.43	0.42
56:FF:40:ALA:HB3	56:FF:67:PRO:HA	2.01	0.42
57:GG:51:ARG:HB3	57:GG:112:VAL:HG23	2.01	0.42
73:WW:112:ASP:OD1	73:WW:112:ASP:N	2.52	0.42
4:5:423:G:N3	21:P:118:GLN:NE2	2.68	0.42
4:5:952:G:H5''	37:f:73:LYS:HD3	2.01	0.42
4:5:1306:C:H2'	4:5:1307:A:C8	2.54	0.42
4:5:1790:U:OP2	25:T:13:TYR:OH	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:3807:A:O2'	50:9:1816:G:O2'	2.25	0.42
4:5:4635:A:H8	4:5:5048:A:H61	1.67	0.42
10:D:106:ALA:HB2	10:D:166:ALA:HA	2.01	0.42
12:F:89:ALA:HB2	12:F:124:LEU:HD21	2.02	0.42
17:L:48:PRO:HB2	39:h:120:ALA:HB2	2.02	0.42
25:T:64:VAL:HG22	25:T:74:ILE:HG22	2.00	0.42
50:9:1445:U:O4	50:9:1446:A:N6	2.52	0.42
51:AA:177:MET:HE2	51:AA:177:MET:HB3	1.71	0.42
52:BB:158:HIS:HA	52:BB:161:VAL:HG12	2.02	0.42
59:II:113:TYR:OH	59:II:156:ALA:O	2.38	0.42
67:QQ:31:LEU:HD11	67:QQ:33:LYS:HE3	2.02	0.42
4:5:99:A:H4'	19:N:181:HIS:CD2	2.55	0.42
4:5:975:C:H41	4:5:1281:G:H21	1.66	0.42
4:5:1094:G:H2'	4:5:1095:A:H8	1.85	0.42
4:5:1346:C:H2'	4:5:1347:G:C8	2.55	0.42
4:5:1989:G:H2'	4:5:1990:A:H8	1.85	0.42
4:5:2288:G:O6	32:a:10:LYS:NZ	2.52	0.42
4:5:2364:OMG:HM23	4:5:2364:OMG:H1'	1.89	0.42
4:5:2540:C:H2'	4:5:2541:G:H8	1.85	0.42
4:5:2893:U:H2'	4:5:2894:A:C8	2.55	0.42
4:5:4862:G:H2'	4:5:4863:G:C8	2.52	0.42
4:5:4915:G:H2'	4:5:4916:G:C8	2.55	0.42
29:X:145:ASP:N	29:X:145:ASP:OD1	2.50	0.42
50:9:507:G:O6	75:YY:105:LYS:NZ	2.38	0.42
50:9:1100:A:O5'	68:RR:132:ARG:NH2	2.53	0.42
50:9:1829:G:H1'	50:9:1850:MA6:H2	2.01	0.42
53:CC:171:GLY:O	73:WW:98:GLN:NE2	2.43	0.42
56:FF:47:LYS:NZ	67:QQ:115:TYR:O	2.52	0.42
58:HH:192:PHE:HD2	58:HH:193:GLN:HG2	1.85	0.42
72:VV:1:MET:HB2	72:VV:10:ASP:HB2	2.02	0.42
83:gg:109:LEU:HD13	83:gg:125:ARG:HG3	2.02	0.42
83:gg:164:ILE:HG22	83:gg:178:ASN:HA	2.01	0.42
4:5:3599:A:H2'	4:5:3600:G:C8	2.55	0.42
9:C:95:MET:HE3	9:C:95:MET:HB2	1.95	0.42
18:M:12:VAL:HG22	18:M:60:PHE:HB2	2.02	0.42
50:9:923:G:H2'	50:9:924:G:C8	2.55	0.42
51:AA:85:ARG:HH12	51:AA:205:ARG:HE	1.68	0.42
56:FF:55:ARG:O	56:FF:62:ARG:NH1	2.44	0.42
64:NN:29:THR:N	64:NN:32:ASP:OD1	2.53	0.42
82:ff:95:ARG:CD	82:ff:96:LYS:H	2.33	0.42
4:5:307:A:N3	4:5:310:G:O2'	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:398:A2M:O5'	4:5:398:A2M:H8	2.20	0.41
4:5:651:C:H2'	4:5:652:G:H8	1.85	0.41
4:5:3892:U:O2'	21:P:80:GLN:OE1	2.32	0.41
7:A:51:ASP:OD1	7:A:51:ASP:N	2.50	0.41
8:B:340:THR:OG1	8:B:341:LYS:N	2.53	0.41
9:C:305:PRO:HD3	22:Q:38:ARG:HH21	1.85	0.41
12:F:94:ILE:HD13	12:F:94:ILE:HA	1.87	0.41
26:U:40:GLU:OE1	26:U:65:ARG:NH2	2.53	0.41
30:Y:34:LEU:HD23	30:Y:38:LEU:HB3	2.01	0.41
32:a:34:ASN:HB2	32:a:45:PHE:HZ	1.84	0.41
50:9:146:G:O2'	50:9:147:A:O4'	2.36	0.41
50:9:186:C:H2'	50:9:187:G:H8	1.85	0.41
50:9:1662:U:O4	50:9:1663:A:N6	2.53	0.41
50:9:1737:G:H5''	57:GG:76:LEU:HD11	2.02	0.41
55:EE:180:LEU:HG	55:EE:232:ASN:HA	2.02	0.41
63:MM:25:ALA:O	63:MM:29:ASP:HA	2.20	0.41
68:RR:31:ASN:HA	68:RR:34:VAL:HB	2.02	0.41
79:cc:21:THR:OG1	79:cc:22:GLY:N	2.52	0.41
4:5:311:G:H2'	4:5:312:G:H8	1.85	0.41
4:5:3607:U:H2'	4:5:3608:A:C8	2.55	0.41
4:5:3810:C:H6	4:5:3810:C:H2'	1.67	0.41
4:5:4041:C:OP2	4:5:4042:G:N2	2.53	0.41
4:5:4229:U:OP1	46:o:63:THR:OG1	2.31	0.41
7:A:20:VAL:HG12	7:A:23:ARG:HD2	2.02	0.41
12:F:82:VAL:HG22	24:S:62:VAL:HA	2.02	0.41
19:N:22:LEU:HA	19:N:22:LEU:HD23	1.81	0.41
24:S:107:THR:OG1	24:S:111:ARG:NH2	2.53	0.41
27:V:82:ILE:HG23	27:V:121:VAL:HA	2.02	0.41
41:j:13:ASN:OD1	41:j:13:ASN:N	2.52	0.41
59:II:113:TYR:CD2	59:II:121:LEU:HD22	2.54	0.41
75:YY:76:TYR:OH	75:YY:86:GLU:OE1	2.23	0.41
2:2:35:A:OP1	67:QQ:146:ARG:NH2	2.53	0.41
4:5:1497:A:OP1	22:Q:180:ARG:NH2	2.53	0.41
4:5:2458:C:O2'	4:5:3671:G:N3	2.51	0.41
4:5:2520:C:H2'	4:5:2521:G:C8	2.54	0.41
7:A:206:PRO:HD3	7:A:213:GLY:HA3	2.02	0.41
8:B:36:ASP:HA	8:B:37:PRO:HD3	1.94	0.41
11:E:181:PRO:HB3	11:E:257:ASP:HB2	2.02	0.41
27:V:60:MET:HE2	27:V:78:PRO:HB2	2.02	0.41
29:X:79:PHE:CD2	39:h:36:VAL:HG21	2.55	0.41
50:9:1447:G:OP1	71:UU:85:HIS:ND1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:1555:U:H5'	50:9:1556:A:C8	2.55	0.41
56:FF:145:ARG:HB2	79:cc:49:PRO:HD2	2.02	0.41
65:OO:98:ARG:HH21	65:OO:134:PRO:HG3	1.86	0.41
73:WW:7:LEU:HD23	73:WW:34:ILE:HG12	2.01	0.41
75:YY:21:LYS:HG3	75:YY:75:ILE:HB	2.02	0.41
79:cc:42:ILE:HG22	79:cc:44:ARG:HG3	2.01	0.41
3:4:28:C:H2'	3:4:29:A:C8	2.56	0.41
3:4:30:G:H2'	3:4:31:A:H8	1.85	0.41
4:5:1333:A:H2'	4:5:1334:A:C8	2.55	0.41
4:5:4188:U:H2'	4:5:4189:U:C6	2.55	0.41
9:C:232:VAL:HG12	9:C:263:LEU:HD11	2.03	0.41
15:I:46:PHE:HB3	15:I:139:ARG:HG2	2.02	0.41
50:9:792:C:H2'	50:9:793:G:C8	2.55	0.41
50:9:959:G:OP2	65:OO:38:ASN:ND2	2.50	0.41
50:9:1256:G:N2	80:dd:30:LEU:O	2.49	0.41
51:AA:66:VAL:HG22	51:AA:186:ARG:HG3	2.03	0.41
55:EE:44:LEU:HD21	55:EE:70:ILE:HG21	2.03	0.41
63:MM:58:GLU:HG3	63:MM:61:TYR:CZ	2.55	0.41
65:OO:97:LEU:HD11	65:OO:112:ALA:HB1	2.02	0.41
4:5:295:A:H5''	4:5:296:A:H5'	2.03	0.41
4:5:971:U:H2'	4:5:971(A):G:C8	2.56	0.41
4:5:3942:A:H2'	4:5:3943:A:C8	2.55	0.41
4:5:4620:OMU:HM23	4:5:4620:OMU:H1'	1.73	0.41
12:F:165:ARG:HD2	12:F:208:TRP:CE2	2.56	0.41
14:H:7:ASN:HB3	14:H:58:ASP:HB3	2.02	0.41
39:h:4:ILE:O	39:h:56:ARG:NH1	2.53	0.41
50:9:1:U:H6	53:CC:205:VAL:HG12	1.86	0.41
50:9:1062:A:H2'	50:9:1063:C:C6	2.55	0.41
50:9:1307:U:C5	82:ff:135:HIS:HB3	2.55	0.41
55:EE:117:GLU:HA	55:EE:120:LYS:HE2	2.02	0.41
65:OO:38:ASN:OD1	65:OO:38:ASN:N	2.52	0.41
68:RR:16:ILE:HG22	68:RR:24:LEU:HD11	2.01	0.41
73:WW:52:ILE:HA	73:WW:61:ILE:HA	2.02	0.41
4:5:1406:G:OP2	4:5:1406(B):C:O2'	2.38	0.41
4:5:2869:U:O2'	4:5:2881:A:N7	2.50	0.41
15:I:38:ARG:HD3	15:I:83:ASP:HB2	2.02	0.41
30:Y:100:HIS:HA	30:Y:101:PRO:HD3	1.96	0.41
67:QQ:130:LYS:HG3	67:QQ:136:GLY:O	2.21	0.41
69:SS:14:ARG:HA	69:SS:14:ARG:HD2	1.73	0.41
83:gg:252:THR:HG21	83:gg:257:LYS:HZ3	1.85	0.41
4:5:87:A:OP2	22:Q:173:LYS:NZ	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:1088:C:H2'	4:5:1089:G:C8	2.54	0.41
4:5:1402:C:H2'	4:5:1403:G:H8	1.85	0.41
4:5:1444:G:H2'	4:5:1445:U:C6	2.56	0.41
4:5:2568:C:H2'	4:5:2569:G:H8	1.86	0.41
4:5:4976:U:O3'	8:B:343:ARG:NH2	2.54	0.41
10:D:61:ILE:HG23	10:D:79:TYR:HE1	1.85	0.41
36:e:22:ARG:HG3	36:e:36:ARG:H	1.85	0.41
50:9:511:U:O2'	50:9:576:A:N6	2.53	0.41
50:9:935:G:O2'	64:NN:108:ASP:OD1	2.33	0.41
50:9:1312:G:N3	82:ff:95:ARG:NH2	2.68	0.41
50:9:1647:A:H5'	67:QQ:138:ARG:NH2	2.36	0.41
50:9:1693:G:N2	50:9:1834:A:H8	2.19	0.41
56:FF:50:PRO:O	56:FF:70:GLU:HG2	2.21	0.41
58:HH:72:PHE:O	58:HH:76:GLN:HB2	2.21	0.41
69:SS:47:LYS:NZ	69:SS:77:TYR:O	2.36	0.41
4:5:17:A:OP2	29:X:60:TYR:OH	2.30	0.41
4:5:245:C:O2'	4:5:246:G:OP2	2.33	0.41
4:5:483:G:H5''	4:5:484:U:H2'	2.02	0.41
4:5:1086:C:H2'	4:5:1087:A:C8	2.55	0.41
4:5:1837:A:OP1	25:T:108:ARG:NH2	2.53	0.41
4:5:3940:U:H5''	13:G:128:LYS:HD2	2.01	0.41
4:5:4091:G:H2'	4:5:4092:G:H8	1.85	0.41
7:A:192:LYS:HB3	7:A:193:ARG:HE	1.86	0.41
8:B:85:VAL:HA	8:B:204:GLN:HA	2.02	0.41
8:B:254:ILE:HD13	8:B:254:ILE:HA	1.86	0.41
8:B:276:HIS:O	8:B:277:ARG:NH1	2.52	0.41
9:C:327:LYS:HE2	12:F:170:ASP:HB3	2.01	0.41
17:L:72:ALA:HB2	17:L:157:ILE:HG21	2.03	0.41
26:U:33:ILE:H	26:U:33:ILE:HG13	1.56	0.41
34:c:46:VAL:O	34:c:71:VAL:HA	2.20	0.41
49:u:26:ARG:HH22	49:u:209:THR:H	1.68	0.41
49:u:26:ARG:NH1	49:u:31:THR:H	2.19	0.41
50:9:28:U:H2'	50:9:29:G:C8	2.56	0.41
50:9:989:C:OP2	52:BB:155:TYR:OH	2.32	0.41
50:9:1290:G:H2'	50:9:1291:A:O4'	2.20	0.41
51:AA:176:TRP:CD2	51:AA:199:PRO:HB3	2.56	0.41
57:GG:38:ALA:HB1	57:GG:41:LEU:HD12	2.02	0.41
74:XX:46:HIS:CD2	74:XX:103:ALA:HB2	2.56	0.41
4:5:32:G:N1	4:5:49:U:OP2	2.52	0.41
4:5:72:C:N3	17:L:60:ARG:NH2	2.69	0.41
4:5:287:U:H2'	4:5:288:G:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:318:A:H2'	4:5:319:A:C8	2.56	0.41
4:5:347:A:H2'	4:5:348:G:C8	2.55	0.41
4:5:674:G:H2'	4:5:675:C:C6	2.56	0.41
4:5:713:C:H2'	4:5:714:G:H8	1.85	0.41
4:5:1170:G:H2'	4:5:1171:G:C8	2.55	0.41
4:5:1202:C:H2'	4:5:1203:G:H8	1.85	0.41
4:5:1298:C:H2'	4:5:1299:G:H8	1.86	0.41
4:5:1444:G:N2	4:5:2111:U:O4	2.54	0.41
4:5:1481:C:O2'	4:5:1482:G:O5'	2.38	0.41
4:5:1824:G:H2'	4:5:1825:A:C8	2.56	0.41
4:5:1983:A:C4	4:5:2010:A:H5''	2.56	0.41
4:5:3709:U:H2'	4:5:3710:G:C8	2.56	0.41
4:5:3904:G:O2'	4:5:3905:A:O4'	2.39	0.41
4:5:4419:U:OP1	4:5:4421:C:N4	2.54	0.41
4:5:4630:G:H2'	4:5:4631:G:H8	1.86	0.41
5:7:11:A:O2'	5:7:13:A:OP2	2.35	0.41
7:A:58:LEU:HD13	7:A:75:LEU:HD23	2.03	0.41
8:B:331:VAL:HG21	8:B:347:LEU:HD21	2.03	0.41
10:D:64:ILE:HD11	10:D:75:VAL:HB	2.02	0.41
10:D:131:ASN:OD1	10:D:131:ASN:N	2.53	0.41
12:F:178:LEU:HD21	12:F:203:ALA:HA	2.02	0.41
17:L:70:VAL:HG12	17:L:157:ILE:HD11	2.02	0.41
21:P:94:MET:HB2	21:P:94:MET:HE3	1.78	0.41
23:R:2:SER:OG	23:R:3:MET:N	2.53	0.41
24:S:150:ILE:HD12	24:S:150:ILE:HA	1.92	0.41
31:Z:4:PHE:O	31:Z:9:LYS:NZ	2.44	0.41
31:Z:41:ALA:HB2	31:Z:77:TYR:HE1	1.86	0.41
49:u:82:ILE:HG13	49:u:144:MET:HE1	2.02	0.41
50:9:1284:A:O5'	82:ff:99:LYS:NZ	2.54	0.41
54:DD:23:GLU:HA	54:DD:26:THR:HG22	2.03	0.41
55:EE:79:ASP:HB3	55:EE:82:TYR:HB2	2.03	0.41
60:JJ:24:ARG:O	60:JJ:28:GLU:HG3	2.21	0.41
60:JJ:35:TYR:OH	60:JJ:107:GLU:OE2	2.35	0.41
61:KK:11:ILE:HD11	61:KK:40:VAL:HG11	2.03	0.41
65:OO:31:CYS:HB3	65:OO:44:VAL:HG22	2.02	0.41
68:RR:27:ASP:OD1	68:RR:27:ASP:N	2.49	0.41
69:SS:86:ARG:NH2	69:SS:110:ASP:OD2	2.53	0.41
83:gg:107:ASP:HB3	83:gg:125:ARG:HD2	2.03	0.41
83:gg:251:ALA:HA	83:gg:256:ILE:HG22	2.03	0.41
4:5:1403:G:H2'	4:5:1404:G:C8	2.56	0.41
4:5:1839:U:H2'	4:5:1840:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:2639:U:H1'	38:g:26:PRO:HB3	2.02	0.41
4:5:2699:C:H2'	4:5:2700:G:H8	1.86	0.41
4:5:4764:A:H3'	14:H:23:ARG:HH11	1.86	0.41
8:B:261:ARG:HB2	20:O:64:THR:HG21	2.03	0.41
8:B:317:LEU:HD21	8:B:381:THR:HA	2.02	0.41
9:C:27:VAL:HG22	9:C:264:TYR:HB2	2.02	0.41
12:F:188:ASP:OD1	12:F:188:ASP:N	2.47	0.41
14:H:170:LYS:HD2	14:H:175:PHE:HE2	1.85	0.41
16:J:26:VAL:HG23	16:J:28:GLU:H	1.86	0.41
20:O:12:ARG:HE	24:S:171:ARG:HH12	1.67	0.41
29:X:39:LYS:HB3	29:X:40:ILE:H	1.60	0.41
42:k:10:ASP:N	42:k:10:ASP:OD1	2.54	0.41
50:9:145:G:H2'	50:9:146:G:C8	2.56	0.41
50:9:1231:C:O2'	50:9:1253:A:N6	2.54	0.41
50:9:1630:A:H5''	69:SS:37:GLY:N	2.35	0.41
52:BB:144:LYS:HB2	52:BB:208:HIS:HB3	2.03	0.41
59:II:182:CYS:SG	59:II:183:GLY:N	2.93	0.41
75:YY:10:ARG:HB2	75:YY:24:VAL:HG23	2.03	0.41
82:ff:121:CYS:HA	82:ff:132:MET:HE3	2.02	0.41
4:5:164:G:H2'	4:5:165:A:H8	1.85	0.40
4:5:383:A:N6	4:5:405:U:O3'	2.54	0.40
4:5:1625:OMG:N2	4:5:4186:A:OP1	2.54	0.40
4:5:2540:C:H2'	4:5:2541:G:C8	2.56	0.40
4:5:2588:C:OP1	4:5:2768:C:O2'	2.33	0.40
4:5:2621:A:H2'	4:5:2622:G:H8	1.87	0.40
4:5:2845:A:H61	4:5:3843:C:H42	1.69	0.40
5:7:97:G:H4'	12:F:133:ARG:NH1	2.35	0.40
14:H:160:LEU:O	14:H:164:ALA:HB2	2.21	0.40
16:J:19:LYS:HG2	16:J:133:VAL:HG12	2.03	0.40
16:J:174:ILE:H	16:J:174:ILE:HG13	1.74	0.40
17:L:201:GLU:HA	17:L:204:GLU:HG2	2.03	0.40
18:M:12:VAL:HA	18:M:25:VAL:O	2.21	0.40
31:Z:46:ILE:HA	31:Z:70:SER:HA	2.02	0.40
41:j:14:LYS:HE2	41:j:14:LYS:HB3	1.92	0.40
50:9:794:A:H2'	50:9:795:A:H8	1.86	0.40
50:9:960:U:H5''	65:OO:149:ARG:HH22	1.86	0.40
50:9:1406:G:H2'	50:9:1407:U:C6	2.56	0.40
56:FF:99:ILE:HD11	56:FF:171:GLU:HA	2.03	0.40
58:HH:31:GLU:HA	58:HH:37:LYS:HE3	2.02	0.40
65:OO:20:GLN:HE21	65:OO:20:GLN:HB3	1.76	0.40
4:5:1086:C:H2'	4:5:1087:A:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:1180:C:OP2	10:D:286:SER:OG	2.34	0.40
4:5:1341:U:O3'	19:N:204:ARG:NH1	2.54	0.40
4:5:2654:C:H2'	4:5:2655:C:H6	1.86	0.40
4:5:4966:A:H2'	4:5:4967:A:O4'	2.21	0.40
7:A:48:ILE:HD13	47:p:65:ALA:HB2	2.02	0.40
7:A:111:THR:OG1	7:A:112:ILE:N	2.55	0.40
9:C:209:VAL:HB	9:C:229:LEU:HD13	2.02	0.40
16:J:31:ASP:HA	16:J:34:THR:HG22	2.03	0.40
27:V:69:LYS:HA	27:V:70:PRO:HD3	1.91	0.40
29:X:71:LEU:HD21	29:X:76:ILE:HD13	2.03	0.40
29:X:143:ASP:OD1	29:X:143:ASP:N	2.53	0.40
30:Y:80:ILE:HG23	30:Y:101:PRO:HG3	2.02	0.40
36:e:90:MET:HG3	48:r:33:LYS:HA	2.03	0.40
50:9:222:U:H5''	62:LL:17:PHE:CG	2.55	0.40
50:9:388:U:H2'	50:9:389:A:H8	1.86	0.40
50:9:562:U:H2'	50:9:563:G:C8	2.55	0.40
57:GG:35:GLU:HA	57:GG:50:VAL:O	2.21	0.40
58:HH:36:LEU:H	58:HH:36:LEU:HG	1.54	0.40
59:II:145:ILE:HG23	59:II:148:LYS:HE2	2.03	0.40
3:4:30:G:H2'	3:4:31:A:C8	2.57	0.40
4:5:86:U:H2'	4:5:87:A:C8	2.56	0.40
4:5:1802:A:H5''	4:5:1803:G:H5'	2.04	0.40
4:5:2075:G:H2'	4:5:2076:G:H8	1.86	0.40
4:5:2082:G:H5''	22:Q:12:LYS:HG2	2.03	0.40
10:D:184:ASP:OD1	10:D:184:ASP:N	2.54	0.40
13:G:247:VAL:HB	13:G:249:ARG:HE	1.86	0.40
14:H:66:GLU:OE2	20:O:132:THR:OG1	2.24	0.40
20:O:58:LEU:HD11	20:O:145:VAL:HG13	2.04	0.40
49:u:177:ASP:HA	49:u:180:VAL:HG22	2.03	0.40
50:9:1171:G:O2'	50:9:1187:G:O6	2.32	0.40
56:FF:176:GLU:OE2	56:FF:188:TYR:N	2.54	0.40
66:PP:41:GLN:HG3	66:PP:84:ILE:HD12	2.02	0.40
75:YY:18:LEU:HD12	75:YY:18:LEU:HA	1.92	0.40
83:gg:124:SER:OG	83:gg:125:ARG:N	2.54	0.40
4:5:1556:C:O2'	4:5:2669:C:OP1	2.30	0.40
4:5:2385:U:H2'	4:5:2386:U:H6	1.87	0.40
4:5:4870:OMG:C6	18:M:56:GLN:HG3	2.57	0.40
8:B:307:TYR:CD2	8:B:366:LYS:HG2	2.54	0.40
34:c:38:ILE:HG21	34:c:63:TYR:HB3	2.02	0.40
50:9:51:U:H2'	50:9:52:G:C8	2.57	0.40
50:9:1863:A:OP2	77:aa:4:LYS:NZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BB:48:LEU:O	65:OO:51:GLU:HG3	2.22	0.40
54:DD:74:GLN:HE22	54:DD:81:GLU:HA	1.86	0.40
57:GG:176:ILE:HG13	57:GG:179:LEU:HD23	2.02	0.40
59:II:65:PHE:CD2	59:II:104:ILE:HG12	2.55	0.40
71:UU:62:ARG:NH1	71:UU:81:GLN:HE21	2.19	0.40
77:aa:4:LYS:HG2	77:aa:5:ARG:HD3	2.03	0.40
4:5:2352:U:OP1	9:C:78:ARG:NH2	2.55	0.40
4:5:3661:G:N2	4:5:3681:G:O2'	2.52	0.40
4:5:4285:U:OP2	46:o:100:LYS:NZ	2.46	0.40
4:5:4991:U:H2'	4:5:4992:G:C8	2.57	0.40
9:C:12:SER:HA	9:C:155:GLU:HG2	2.04	0.40
10:D:50:ARG:NH2	10:D:147:ASP:OD2	2.48	0.40
21:P:4:TYR:HD1	21:P:4:TYR:HA	1.77	0.40
22:Q:68:ARG:HH11	22:Q:68:ARG:HD3	1.78	0.40
24:S:112:ASP:OD1	24:S:116:ARG:NH1	2.54	0.40
39:h:12:LYS:HE3	39:h:12:LYS:HB2	1.87	0.40
42:k:33:LYS:HG2	42:k:46:VAL:HB	2.04	0.40
49:u:35:GLN:N	49:u:205:TYR:O	2.49	0.40
50:9:1480:A:H5'	67:QQ:131:LYS:HE3	2.04	0.40
52:BB:138:PHE:O	52:BB:213:ARG:N	2.54	0.40
58:HH:147:LYS:HA	73:WW:49:GLU:HG3	2.02	0.40
70:TT:96:SER:HB3	70:TT:99:VAL:HG22	2.04	0.40
71:UU:67:LYS:HA	80:dd:44:ARG:HH12	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	A	246/248 (99%)	225 (92%)	21 (8%)	0	100	100
8	B	392/394 (100%)	366 (93%)	26 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	C	359/362 (99%)	340 (95%)	19 (5%)	0	100	100
10	D	291/293 (99%)	275 (94%)	16 (6%)	0	100	100
11	E	208/291 (72%)	198 (95%)	10 (5%)	0	100	100
12	F	223/247 (90%)	212 (95%)	11 (5%)	0	100	100
13	G	229/319 (72%)	221 (96%)	8 (4%)	0	100	100
14	H	188/190 (99%)	175 (93%)	13 (7%)	0	100	100
15	I	201/214 (94%)	186 (92%)	15 (8%)	0	100	100
16	J	168/178 (94%)	160 (95%)	8 (5%)	0	100	100
17	L	208/210 (99%)	198 (95%)	9 (4%)	1 (0%)	24	57
18	M	136/138 (99%)	122 (90%)	14 (10%)	0	100	100
19	N	201/203 (99%)	187 (93%)	14 (7%)	0	100	100
20	O	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
21	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
22	Q	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
23	R	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
24	S	174/176 (99%)	159 (91%)	14 (8%)	1 (1%)	21	54
25	T	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
26	U	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
27	V	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
28	W	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
29	X	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
30	Y	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
31	Z	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	16	49
32	a	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
33	b	100/245 (41%)	93 (93%)	7 (7%)	0	100	100
34	c	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	d	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
36	e	126/128 (98%)	114 (90%)	12 (10%)	0	100	100
37	f	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
38	g	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
39	h	120/122 (98%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	i	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
41	j	84/86 (98%)	77 (92%)	7 (8%)	0	100	100
42	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
43	l	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
44	m	49/52 (94%)	44 (90%)	4 (8%)	1 (2%)	6	32
45	n	23/25 (92%)	23 (100%)	0	0	100	100
46	o	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
47	p	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
48	r	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
49	u	204/206 (99%)	171 (84%)	32 (16%)	1 (0%)	24	57
51	AA	215/217 (99%)	203 (94%)	12 (6%)	0	100	100
52	BB	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
53	CC	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
54	DD	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
55	EE	260/262 (99%)	241 (93%)	19 (7%)	0	100	100
56	FF	181/204 (89%)	169 (93%)	12 (7%)	0	100	100
57	GG	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
58	HH	181/194 (93%)	169 (93%)	12 (7%)	0	100	100
59	II	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
60	JJ	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
61	KK	94/96 (98%)	86 (92%)	8 (8%)	0	100	100
62	LL	139/158 (88%)	128 (92%)	11 (8%)	0	100	100
63	MM	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
64	NN	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
65	OO	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
66	PP	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
67	QQ	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
68	RR	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
69	SS	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
70	TT	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
71	UU	98/100 (98%)	95 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	VV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
73	WW	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
74	XX	139/141 (99%)	128 (92%)	8 (6%)	3 (2%)	5	30
75	YY	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
76	ZZ	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
77	aa	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
78	bb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
79	cc	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
80	dd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
81	ee	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
82	ff	66/68 (97%)	49 (74%)	17 (26%)	0	100	100
83	gg	311/313 (99%)	279 (90%)	32 (10%)	0	100	100
All	All	11375/11984 (95%)	10695 (94%)	672 (6%)	8 (0%)	49	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	m	73	CYS
24	S	166	ARG
49	u	61	PRO
74	XX	62	PRO
31	Z	90	PRO
74	XX	86	PRO
74	XX	61	GLN
17	L	62	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	A	190/190 (100%)	188 (99%)	2 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	B	342/342 (100%)	333 (97%)	9 (3%)	40	62
9	C	301/301 (100%)	300 (100%)	1 (0%)	86	83
10	D	247/247 (100%)	244 (99%)	3 (1%)	63	73
11	E	190/251 (76%)	189 (100%)	1 (0%)	81	80
12	F	196/215 (91%)	196 (100%)	0	100	100
13	G	200/272 (74%)	198 (99%)	2 (1%)	68	75
14	H	169/169 (100%)	167 (99%)	2 (1%)	63	73
15	I	175/181 (97%)	173 (99%)	2 (1%)	65	74
16	J	143/149 (96%)	139 (97%)	4 (3%)	38	60
17	L	175/175 (100%)	174 (99%)	1 (1%)	78	79
18	M	117/117 (100%)	114 (97%)	3 (3%)	40	62
19	N	171/171 (100%)	168 (98%)	3 (2%)	51	68
20	O	171/171 (100%)	170 (99%)	1 (1%)	78	79
21	P	134/134 (100%)	134 (100%)	0	100	100
22	Q	164/164 (100%)	163 (99%)	1 (1%)	78	79
23	R	159/159 (100%)	157 (99%)	2 (1%)	61	72
24	S	157/157 (100%)	155 (99%)	2 (1%)	61	72
25	T	139/139 (100%)	137 (99%)	2 (1%)	59	71
26	U	89/89 (100%)	86 (97%)	3 (3%)	32	57
27	V	101/101 (100%)	100 (99%)	1 (1%)	68	75
28	W	86/126 (68%)	83 (96%)	3 (4%)	32	57
29	X	106/106 (100%)	106 (100%)	0	100	100
30	Y	124/124 (100%)	124 (100%)	0	100	100
31	Z	117/117 (100%)	117 (100%)	0	100	100
32	a	119/119 (100%)	119 (100%)	0	100	100
33	b	84/184 (46%)	84 (100%)	0	100	100
34	c	84/84 (100%)	83 (99%)	1 (1%)	63	73
35	d	98/98 (100%)	98 (100%)	0	100	100
36	e	114/114 (100%)	114 (100%)	0	100	100
37	f	88/88 (100%)	88 (100%)	0	100	100
38	g	98/98 (100%)	95 (97%)	3 (3%)	35	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	h	109/109 (100%)	109 (100%)	0	100	100
40	i	86/86 (100%)	86 (100%)	0	100	100
41	j	73/73 (100%)	72 (99%)	1 (1%)	59	71
42	k	64/64 (100%)	62 (97%)	2 (3%)	35	59
43	l	47/47 (100%)	46 (98%)	1 (2%)	47	65
44	m	47/47 (100%)	46 (98%)	1 (2%)	47	65
45	n	24/24 (100%)	24 (100%)	0	100	100
46	o	91/91 (100%)	91 (100%)	0	100	100
47	p	74/74 (100%)	73 (99%)	1 (1%)	59	71
48	r	108/108 (100%)	107 (99%)	1 (1%)	70	76
49	u	186/186 (100%)	182 (98%)	4 (2%)	45	65
51	AA	180/181 (99%)	179 (99%)	1 (1%)	78	79
52	BB	194/194 (100%)	192 (99%)	2 (1%)	68	75
53	CC	187/187 (100%)	184 (98%)	3 (2%)	55	69
54	DD	190/190 (100%)	190 (100%)	0	100	100
55	EE	224/224 (100%)	219 (98%)	5 (2%)	45	65
56	FF	158/170 (93%)	156 (99%)	2 (1%)	61	72
57	GG	207/207 (100%)	206 (100%)	1 (0%)	81	80
58	HH	165/174 (95%)	162 (98%)	3 (2%)	51	68
59	II	178/178 (100%)	177 (99%)	1 (1%)	78	79
60	JJ	161/161 (100%)	159 (99%)	2 (1%)	63	73
61	KK	87/87 (100%)	86 (99%)	1 (1%)	65	74
62	LL	130/142 (92%)	128 (98%)	2 (2%)	57	70
63	MM	99/99 (100%)	97 (98%)	2 (2%)	48	66
64	NN	130/130 (100%)	127 (98%)	3 (2%)	44	64
65	OO	106/106 (100%)	102 (96%)	4 (4%)	29	55
66	PP	109/109 (100%)	106 (97%)	3 (3%)	38	60
67	QQ	117/117 (100%)	113 (97%)	4 (3%)	32	57
68	RR	119/119 (100%)	117 (98%)	2 (2%)	53	69
69	SS	125/125 (100%)	124 (99%)	1 (1%)	73	77
70	TT	111/111 (100%)	110 (99%)	1 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	UU	92/92 (100%)	91 (99%)	1 (1%)	65	74
72	VV	67/67 (100%)	65 (97%)	2 (3%)	36	59
73	WW	112/112 (100%)	108 (96%)	4 (4%)	31	56
74	XX	113/113 (100%)	112 (99%)	1 (1%)	70	76
75	YY	107/107 (100%)	105 (98%)	2 (2%)	50	67
76	ZZ	66/66 (100%)	64 (97%)	2 (3%)	36	59
77	aa	88/88 (100%)	88 (100%)	0	100	100
78	bb	75/75 (100%)	75 (100%)	0	100	100
79	cc	55/55 (100%)	53 (96%)	2 (4%)	31	56
80	dd	48/48 (100%)	48 (100%)	0	100	100
81	ee	46/46 (100%)	46 (100%)	0	100	100
82	ff	61/61 (100%)	57 (93%)	4 (7%)	15	43
83	gg	272/272 (100%)	270 (99%)	2 (1%)	76	78
All	All	9936/10274 (97%)	9810 (99%)	126 (1%)	59	72

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	4	VAL
7	A	113	VAL
8	B	17	LEU
8	B	56	ILE
8	B	81	THR
8	B	85	VAL
8	B	159	VAL
8	B	251	VAL
8	B	262	VAL
8	B	278	THR
8	B	300	LYS
9	C	57	LEU
10	D	36	LEU
10	D	56	THR
10	D	64	ILE
11	E	51	VAL
13	G	122	ILE
13	G	215	ASP
14	H	57	VAL

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Mol	Chain	Res	Type
14	H	161	ILE
15	I	48	LEU
15	I	99	ILE
16	J	57	VAL
16	J	132	VAL
16	J	151	ILE
16	J	174	ILE
17	L	22	VAL
18	M	38	VAL
18	M	58	THR
18	M	96	GLU
19	N	7	ILE
19	N	23	LEU
19	N	64	ILE
20	O	22	ILE
22	Q	67	ILE
23	R	123	LEU
23	R	177	LEU
24	S	75	VAL
24	S	90	THR
25	T	68	THR
25	T	154	ILE
26	U	33	ILE
26	U	40	GLU
26	U	47	ILE
27	V	18	LEU
28	W	3	VAL
28	W	28	VAL
28	W	109	ILE
34	c	20	LEU
38	g	5	LEU
38	g	59	VAL
38	g	107	LEU
41	j	67	LEU
42	k	9	LYS
42	k	47	ILE
43	l	33	ASN
44	m	51	ILE
47	p	29	ILE
48	r	106	LEU
49	u	93	LEU
49	u	183	ILE

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Mol	Chain	Res	Type
49	u	199	GLN
49	u	206	ILE
51	AA	8	LEU
52	BB	179	ASN
52	BB	207	LEU
53	CC	137	VAL
53	CC	209	VAL
53	CC	212	LYS
55	EE	45	ILE
55	EE	129	ILE
55	EE	210	VAL
55	EE	246	LEU
55	EE	256	LEU
56	FF	111	VAL
56	FF	144	LEU
57	GG	101	ILE
58	HH	28	LEU
58	HH	36	LEU
58	HH	144	ILE
59	II	104	ILE
60	JJ	123	ILE
60	JJ	141	VAL
61	KK	71	LEU
62	LL	87	VAL
62	LL	134	LEU
63	MM	27	ILE
63	MM	110	VAL
64	NN	28	LEU
64	NN	37	ILE
64	NN	50	ILE
65	OO	81	VAL
65	OO	84	ARG
65	OO	88	LEU
65	OO	151	LEU
66	PP	35	GLN
66	PP	76	VAL
66	PP	121	ILE
67	QQ	22	VAL
67	QQ	53	GLU
67	QQ	81	ILE
67	QQ	92	LEU
68	RR	40	ILE

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Mol	Chain	Res	Type
68	RR	46	LEU
69	SS	45	LEU
70	TT	28	LEU
71	UU	106	ILE
72	VV	13	VAL
72	VV	42	VAL
73	WW	7	LEU
73	WW	52	ILE
73	WW	103	VAL
73	WW	104	LEU
74	XX	66	ILE
75	YY	17	LEU
75	YY	18	LEU
76	ZZ	67	LEU
76	ZZ	108	ILE
79	cc	17	VAL
79	cc	31	ARG
82	ff	87	THR
82	ff	97	LYS
82	ff	99	LYS
82	ff	146	LEU
83	gg	135	LEU
83	gg	236	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
7	A	8	GLN
7	A	205	ASN
8	B	109	HIS
8	B	145	GLN
8	B	175	GLN
8	B	236	HIS
8	B	245	HIS
8	B	258	HIS
8	B	322	HIS
9	C	61	GLN
9	C	142	HIS
10	D	122	GLN
10	D	282	GLN
11	E	253	GLN
12	F	199	HIS

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Mol	Chain	Res	Type
13	G	259	GLN
13	G	261	ASN
15	I	123	GLN
15	I	163	GLN
16	J	71	HIS
17	L	67	HIS
18	M	20	HIS
18	M	48	GLN
18	M	70	GLN
18	M	120	ASN
19	N	32	GLN
19	N	86	HIS
19	N	117	ASN
19	N	182	HIS
19	N	196	ASN
20	O	42	ASN
20	O	50	ASN
20	O	72	HIS
20	O	184	ASN
21	P	10	ASN
21	P	75	GLN
22	Q	7	HIS
23	R	121	HIS
23	R	141	HIS
24	S	91	HIS
24	S	117	HIS
27	V	27	ASN
28	W	50	ASN
29	X	57	GLN
29	X	69	ASN
29	X	107	HIS
30	Y	18	HIS
30	Y	96	HIS
30	Y	100	HIS
32	a	14	HIS
32	a	60	HIS
33	b	27	GLN
34	c	19	GLN
34	c	72	HIS
35	d	79	ASN
37	f	56	ASN
39	h	98	HIS

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Mol	Chain	Res	Type
41	j	76	HIS
44	m	91	HIS
46	o	3	ASN
46	o	45	GLN
47	p	92	GLN
49	u	44	GLN
51	AA	141	ASN
52	BB	92	GLN
52	BB	179	ASN
53	CC	267	GLN
54	DD	57	ASN
54	DD	101	GLN
54	DD	179	GLN
55	EE	188	ASN
56	FF	36	GLN
56	FF	79	HIS
57	GG	177	GLN
58	HH	68	GLN
58	HH	165	ASN
58	HH	193	GLN
59	II	146	GLN
59	II	168	GLN
64	NN	5	HIS
66	PP	53	GLN
66	PP	104	GLN
66	PP	114	HIS
67	QQ	24	HIS
68	RR	83	ASN
69	SS	105	ASN
73	WW	24	GLN
73	WW	82	GLN
74	XX	77	ASN
79	cc	29	GLN
83	gg	119	GLN
83	gg	187	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	6/7 (85%)	3 (50%)	0
2	2	74/76 (97%)	21 (28%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	4	74/75 (98%)	37 (50%)	1 (1%)
4	5	3559/3597 (98%)	875 (24%)	67 (1%)
5	7	119/120 (99%)	16 (13%)	0
50	9	1683/1698 (99%)	415 (24%)	26 (1%)
6	8	149/151 (98%)	30 (20%)	1 (0%)
All	All	5664/5724 (98%)	1397 (24%)	95 (1%)

All (1397) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	43	A
1	1	46	G
1	1	47	U
2	2	7	G
2	2	8	U
2	2	9	A
2	2	13	U
2	2	16	C
2	2	20	U
2	2	20(A)	U
2	2	21	A
2	2	34	A
2	2	35	A
2	2	42	A
2	2	48	C
2	2	49	C
2	2	56	C
2	2	58	A
2	2	63	G
2	2	65	G
2	2	67	G
2	2	72	C
2	2	75	C
2	2	76	A
3	4	2	C
3	4	3	C
3	4	4	C
3	4	7	A
3	4	8	U
3	4	10	G
3	4	13	C
3	4	14	A

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Mol	Chain	Res	Type
3	4	15	G
3	4	16	C
3	4	18	U
3	4	19	G
3	4	20	U
3	4	21	A
3	4	26	A
3	4	27	U
3	4	33	U
3	4	34	U
3	4	35	U
3	4	36	U
3	4	37	A
3	4	38	A
3	4	39	U
3	4	46	G
3	4	47	U
3	4	48	C
3	4	49	C
3	4	56	C
3	4	57	A
3	4	58	A
3	4	59	G
3	4	60	U
3	4	61	C
3	4	70	G
3	4	71	G
3	4	72	C
3	4	73	G
4	5	5	A
4	5	12	A
4	5	13	U
4	5	17	A
4	5	21	G
4	5	25	A
4	5	39	A
4	5	42	A
4	5	43	U
4	5	47	A
4	5	48	G
4	5	49	U
4	5	56	A

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Mol	Chain	Res	Type
4	5	58	G
4	5	59	A
4	5	64	A
4	5	65	A
4	5	71	C
4	5	72	C
4	5	73	A
4	5	76	A
4	5	84	A
4	5	91	G
4	5	93	G
4	5	104	G
4	5	108	A
4	5	109	G
4	5	110	C
4	5	116	G
4	5	119	G
4	5	120	A
4	5	122	U
4	5	126	C
4	5	134	G
4	5	135	G
4	5	136	C
4	5	137	G
4	5	142	G
4	5	146	G
4	5	151	G
4	5	157	U
4	5	159	C
4	5	167	C
4	5	170	C
4	5	172	C
4	5	173	C
4	5	182	G
4	5	195	C
4	5	200	U
4	5	201	C
4	5	203	U
4	5	205	C
4	5	209	U
4	5	216	C
4	5	218	A

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Mol	Chain	Res	Type
4	5	220	C
4	5	224	U
4	5	225	G
4	5	233	U
4	5	234	G
4	5	237	B9B
4	5	245	C
4	5	246	G
4	5	256	G
4	5	265	C
4	5	266	C
4	5	267	G
4	5	275	C
4	5	276	C
4	5	280	G
4	5	297	U
4	5	306	A
4	5	309	C
4	5	310	G
4	5	315	G
4	5	316	U
4	5	334	A
4	5	340	C
4	5	345	C
4	5	349	A
4	5	350	C
4	5	357	U
4	5	362	A
4	5	363	A
4	5	379	G
4	5	386	A
4	5	387	G
4	5	398	A2M
4	5	401	G
4	5	407	A
4	5	409	G
4	5	412	G
4	5	413	G
4	5	414	C
4	5	431	G
4	5	433	A
4	5	440	U

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Mol	Chain	Res	Type
4	5	446	C
4	5	449	C
4	5	450	G
4	5	452	A
4	5	453	G
4	5	454	U
4	5	455	C
4	5	463	A
4	5	464	G
4	5	467	U
4	5	468	U
4	5	482	G
4	5	483	G
4	5	486	C
4	5	489	C
4	5	492	U
4	5	493	G
4	5	496	G
4	5	497	G
4	5	498	C
4	5	499	G
4	5	505	G
4	5	506	C
4	5	510	U
4	5	522	C
4	5	641	G
4	5	667	A
4	5	669	C
4	5	684	G
4	5	685	C
4	5	686	A
4	5	687	U
4	5	688	U
4	5	692	A
4	5	696	C
4	5	697	G
4	5	704	C
4	5	705	G
4	5	708	G
4	5	719	C
4	5	722	G
4	5	729	2MG

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Mol	Chain	Res	Type
4	5	730	G
4	5	731	G
4	5	742	G
4	5	746	A
4	5	747	A
4	5	748	G
4	5	749	G
4	5	758	G
4	5	759	G
4	5	914	U
4	5	917	A
4	5	918	G
4	5	925	C
4	5	926	G
4	5	929	A
4	5	931	C
4	5	932	A
4	5	933	G
4	5	934	C
4	5	938	C
4	5	939	G
4	5	943	A
4	5	944	A
4	5	945	U
4	5	956	A
4	5	959	G
4	5	960	A
4	5	961	G
4	5	964	A
4	5	965	G
4	5	966	A
4	5	967	C
4	5	968	C
4	5	969	C
4	5	970	G
4	5	972	C
4	5	978	C
4	5	980	C
4	5	983	U
4	5	1072	C
4	5	1073	G
4	5	1078	A

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Mol	Chain	Res	Type
4	5	1079	C
4	5	1080	C
4	5	1081	C
4	5	1084	C
4	5	1098	G
4	5	1175	A
4	5	1179	U
4	5	1180	C
4	5	1187	G
4	5	1193	C
4	5	1195	G
4	5	1211	G
4	5	1212	G
4	5	1214	C
4	5	1215	C
4	5	1234	G
4	5	1235	G
4	5	1236	C
4	5	1237	C
4	5	1238	A
4	5	1239	C
4	5	1272	C
4	5	1273	G
4	5	1275	G
4	5	1276	C
4	5	1279	A
4	5	1281	G
4	5	1284	G
4	5	1287	G
4	5	1292	C
4	5	1293	G
4	5	1294	A
4	5	1295	U
4	5	1296	G
4	5	1301	C
4	5	1303	A
4	5	1304	C
4	5	1314	C
4	5	1319	U
4	5	1321	G
4	5	1322	1MA
4	5	1326	A2M

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Mol	Chain	Res	Type
4	5	1330	A
4	5	1337	A
4	5	1348	P4U
4	5	1353	G
4	5	1354	A
4	5	1358	G
4	5	1359	G
4	5	1371	A
4	5	1372	A
4	5	1377	G
4	5	1381	U
4	5	1382	G
4	5	1387	A
4	5	1394	G
4	5	1397	A
4	5	1398	A
4	5	1406(C)	G
4	5	1411(C)	C
4	5	1412	G
4	5	1415	G
4	5	1419	G
4	5	1420	A
4	5	1421	G
4	5	1429	C
4	5	1436	C
4	5	1437	C
4	5	1438	U
4	5	1440	U
4	5	1441	C
4	5	1443	A
4	5	1445	U
4	5	1446	C
4	5	1448	G
4	5	1456	B8Q
4	5	1457	G
4	5	1458	C
4	5	1465	G
4	5	1475	G
4	5	1476	C
4	5	1477	C
4	5	1482	G
4	5	1483	C

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Mol	Chain	Res	Type
4	5	1497	A
4	5	1498	G
4	5	1502	G
4	5	1514	U
4	5	1518	A
4	5	1523	A
4	5	1534	A2M
4	5	1535	C
4	5	1547	A
4	5	1563	A
4	5	1566	C
4	5	1574	B9B
4	5	1578	U
4	5	1582	PSU
4	5	1591	U
4	5	1596	U
4	5	1602	U
4	5	1612	G
4	5	1613	A
4	5	1624	G
4	5	1625	OMG
4	5	1626	G
4	5	1627	G
4	5	1631	A
4	5	1633	G
4	5	1634	A
4	5	1638	A
4	5	1640	C
4	5	1649	U
4	5	1650	A
4	5	1654	G
4	5	1661	C
4	5	1671	U
4	5	1676	C
4	5	1677	PSU
4	5	1678	C
4	5	1679	A
4	5	1691	G
4	5	1724	G
4	5	1726	U
4	5	1731	C
4	5	1741	G

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Mol	Chain	Res	Type
4	5	1742	A
4	5	1751	A
4	5	1755	C
4	5	1756	U
4	5	1757	U
4	5	1764	G
4	5	1768	C
4	5	1772	C
4	5	1773	U
4	5	1774	C
4	5	1775	A
4	5	1776	A
4	5	1781	U
4	5	1787	A
4	5	1797	E7G
4	5	1804	A
4	5	1805	A
4	5	1806	G
4	5	1808	C
4	5	1812	C
4	5	1815	G
4	5	1819	G
4	5	1821	G
4	5	1828	C
4	5	1833	G
4	5	1834	U
4	5	1835	G
4	5	1836	G
4	5	1837	A
4	5	1842	G
4	5	1843	A
4	5	1855	G
4	5	1866	UR3
4	5	1869	G
4	5	1881	C
4	5	1888	A
4	5	1897	A
4	5	1917	A
4	5	1918	U
4	5	1920	C
4	5	1921	C
4	5	1922	G

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Mol	Chain	Res	Type
4	5	1930	U
4	5	1931	C
4	5	1938	C
4	5	1940	G
4	5	1945	G
4	5	1948	G
4	5	1957	U
4	5	1958	A
4	5	1960	A
4	5	1961	G
4	5	1962	A
4	5	1969	G
4	5	1971	U
4	5	1972	G
4	5	1974	U
4	5	1975	G
4	5	1976	G
4	5	1977	C
4	5	1978	C
4	5	1980	U
4	5	1983	A
4	5	1984	A
4	5	1987	C
4	5	1991	A
4	5	1992	U
4	5	1997	U
4	5	2001	G
4	5	2002	A
4	5	2003	G
4	5	2004	U
4	5	2010	A
4	5	2011	C
4	5	2025	A
4	5	2026	A
4	5	2029	A
4	5	2030	A
4	5	2033	A
4	5	2034	G
4	5	2046	G
4	5	2047	A
4	5	2048	U
4	5	2052	G

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Mol	Chain	Res	Type
4	5	2055	G
4	5	2056	G
4	5	2058	G
4	5	2062	C
4	5	2069	A
4	5	2070	U
4	5	2072	C
4	5	2084	U
4	5	2085	G
4	5	2089	G
4	5	2090	U
4	5	2092	G
4	5	2093	G
4	5	2094	C
4	5	2095	A
4	5	2097	A
4	5	2098	G
4	5	2100	G
4	5	2102	G
4	5	2104	A
4	5	2106	G
4	5	2107	A
4	5	2108	G
4	5	2109	A
4	5	2259	G
4	5	2260	C
4	5	2267	U
4	5	2268	A
4	5	2269	C
4	5	2270	G
4	5	2275	G
4	5	2289	C
4	5	2300	A
4	5	2301	G
4	5	2304	U
4	5	2307	A
4	5	2313	A
4	5	2314	G
4	5	2316	G
4	5	2319	C
4	5	2332	A
4	5	2333	G

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Mol	Chain	Res	Type
4	5	2335	C
4	5	2347	A
4	5	2348	G
4	5	2351	C
4	5	2355	G
4	5	2357	G
4	5	2360	A
4	5	2364	OMG
4	5	2380	B8W
4	5	2395	A
4	5	2396	A
4	5	2398	U
4	5	2408	U
4	5	2410	C
4	5	2416	G
4	5	2417	A
4	5	2422	OMC
4	5	2424	OMG
4	5	2425	U
4	5	2433	G
4	5	2441	C
4	5	2442	G
4	5	2447	U
4	5	2450	G
4	5	2453	A
4	5	2467	U
4	5	2471	G
4	5	2474	G
4	5	2475	G
4	5	2488	C
4	5	2489	C
4	5	2490	U
4	5	2491	C
4	5	2495	U
4	5	2503	G
4	5	2504	C
4	5	2505	C
4	5	2506	G
4	5	2513	A
4	5	2529	A
4	5	2530	U
4	5	2537	A

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Mol	Chain	Res	Type
4	5	2544	G
4	5	2546	G
4	5	2547	G
4	5	2553	A
4	5	2554	U
4	5	2566	G
4	5	2568	C
4	5	2571	C
4	5	2575	U
4	5	2583	C
4	5	2586	G
4	5	2587	A
4	5	2588	C
4	5	2589	C
4	5	2600	A
4	5	2601	A
4	5	2611	A
4	5	2618	G
4	5	2620	G
4	5	2623	A
4	5	2627	C
4	5	2638	G
4	5	2639	U
4	5	2649	G
4	5	2653	C
4	5	2659	A
4	5	2661	U
4	5	2662	G
4	5	2663	G
4	5	2668	G
4	5	2669	C
4	5	2670	C
4	5	2673	G
4	5	2676	A
4	5	2679	G
4	5	2681	G
4	5	2686	G
4	5	2687	U
4	5	2694	G
4	5	2695	A
4	5	2696	A
4	5	2708	U

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Mol	Chain	Res	Type
4	5	2710	C
4	5	2711	G
4	5	2714	G
4	5	2715	G
4	5	2723	U
4	5	2724	G
4	5	2725	A
4	5	2726	G
4	5	2740	U
4	5	2743	A
4	5	2744	A
4	5	2752	G
4	5	2753	G
4	5	2754	B9B
4	5	2755	A
4	5	2763	U
4	5	2764	A
4	5	2769	U
4	5	2787	A
4	5	2788	U
4	5	2790	U
4	5	2794	C
4	5	2798	A
4	5	2803	U
4	5	2814	C
4	5	2826	U
4	5	2827	G
4	5	2828	U
4	5	2829	U
4	5	2837	U
4	5	2838	G
4	5	2842	G
4	5	2849	A
4	5	2855	G
4	5	2856	C
4	5	2869	U
4	5	2875	C
4	5	2879	A
4	5	2884	G
4	5	2898	G
4	5	3598	C
4	5	3604	A

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Mol	Chain	Res	Type
4	5	3605	C
4	5	3606	U
4	5	3615	G
4	5	3616	U
4	5	3625	G
4	5	3626	G
4	5	3630	A
4	5	3635	A
4	5	3643	A
4	5	3646	A
4	5	3650	C
4	5	3662	A
4	5	3664	G
4	5	3673	C
4	5	3674	G
4	5	3679	U
4	5	3680	U
4	5	3691	G
4	5	3692	A
4	5	3696	C
4	5	3698	G
4	5	3705	G
4	5	3712	A
4	5	3714	G
4	5	3729	PSU
4	5	3740	G
4	5	3753	G
4	5	3759	A
4	5	3760	A
4	5	3762	B8H
4	5	3763	A
4	5	3765	G
4	5	3773	U
4	5	3774	A
4	5	3776	G
4	5	3777	G
4	5	3783	A
4	5	3784	A
4	5	3785	A2M
4	5	3786	U
4	5	3787	G
4	5	3789	C

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Mol	Chain	Res	Type
4	5	3792	OMG
4	5	3799	A
4	5	3810	C
4	5	3811	G
4	5	3812	C
4	5	3814	U
4	5	3817	A
4	5	3819	G
4	5	3822	U
4	5	3838	U
4	5	3839	G
4	5	3840	U
4	5	3851	U
4	5	3865	A
4	5	3867	A2M
4	5	3868	G
4	5	3876	A
4	5	3877	A
4	5	3878	C
4	5	3879	G
4	5	3889	G
4	5	3892	U
4	5	3897	B8K
4	5	3898	G
4	5	3899	BGH
4	5	3901	A
4	5	3904	G
4	5	3905	A
4	5	3906	A
4	5	3907	G
4	5	3908	A
4	5	3915	U
4	5	3916	G
4	5	3926	C
4	5	3927	U
4	5	3938	G
4	5	3939	G
4	5	3946	G
4	5	3947	A
4	5	3948	C
4	5	3956	G
4	5	3957	U

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Mol	Chain	Res	Type
4	5	3965	A
4	5	3971	G
4	5	3972	A
4	5	3973	G
4	5	3974	G
4	5	3975	C
4	5	3976	C
4	5	4043	G
4	5	4047	A
4	5	4050	A
4	5	4051	C
4	5	4053	A
4	5	4054	C
4	5	4055	U
4	5	4056	A
4	5	4061	G
4	5	4066	U
4	5	4073	A
4	5	4076	G
4	5	4084	G
4	5	4085	A
4	5	4086	G
4	5	4097	G
4	5	4116	C
4	5	4119	C
4	5	4120	U
4	5	4121	G
4	5	4125	C
4	5	4127	A
4	5	4158	C
4	5	4162	C
4	5	4166	G
4	5	4170	A
4	5	4171	C
4	5	4172	A
4	5	4173	G
4	5	4183	G
4	5	4184	G
4	5	4191	G
4	5	4194	I4U
4	5	4197	G
4	5	4212	A

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Mol	Chain	Res	Type
4	5	4213	A
4	5	4229	U
4	5	4232	U
4	5	4233	A
4	5	4241	C
4	5	4251	A
4	5	4254	G
4	5	4255	A
4	5	4265	U
4	5	4266	G
4	5	4268	A
4	5	4271	A
4	5	4273	A
4	5	4281	A
4	5	4282	A
4	5	4287	G
4	5	4291	G
4	5	4293	PSU
4	5	4304	A
4	5	4305	G
4	5	4306	OMU
4	5	4308	C
4	5	4314	C
4	5	4317	A
4	5	4318	C
4	5	4319	C
4	5	4326	G
4	5	4330	G
4	5	4332	C
4	5	4348	A
4	5	4349	C
4	5	4354	U
4	5	4355	E6G
4	5	4364	G
4	5	4371	MHG
4	5	4373	G
4	5	4376	A
4	5	4377	G
4	5	4378	A
4	5	4379	A
4	5	4380	A
4	5	4387	C

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Mol	Chain	Res	Type
4	5	4391	G
4	5	4393	G
4	5	4394	A
4	5	4395	U
4	5	4396	A
4	5	4398	C
4	5	4415	1MA
4	5	4419	U
4	5	4422	A
4	5	4424	A
4	5	4438	U
4	5	4440	G
4	5	4448	G
4	5	4449	A
4	5	4450	PSU
4	5	4464	A
4	5	4475	G
4	5	4476	C
4	5	4482	U
4	5	4495	G
4	5	4500	PSU
4	5	4502	C
4	5	4510	A
4	5	4512	U
4	5	4513	A
4	5	4515	G
4	5	4518	A
4	5	4519	C
4	5	4520	G
4	5	4522	G
4	5	4523	A2M
4	5	4524	G
4	5	4530	UR3
4	5	4548	A
4	5	4549	G
4	5	4560	C
4	5	4567	G
4	5	4572	U
4	5	4573	G
4	5	4574	U
4	5	4575	G
4	5	4584	A

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Mol	Chain	Res	Type
4	5	4586	G
4	5	4587	G
4	5	4589	A
4	5	4590	A
4	5	4599	A
4	5	4627	U
4	5	4629	U
4	5	4633	G
4	5	4635	A
4	5	4636	PSU
4	5	4637	OMG
4	5	4639	G
4	5	4656	A
4	5	4657	U
4	5	4661	G
4	5	4664	A
4	5	4670	C
4	5	4672	A
4	5	4677	U
4	5	4693	C
4	5	4694	G
4	5	4695	C
4	5	4700	A
4	5	4702	G
4	5	4709	U
4	5	4718	G
4	5	4719	G
4	5	4720	C
4	5	4745	G
4	5	4750	G
4	5	4754	G
4	5	4756	C
4	5	4757	C
4	5	4759	C
4	5	4761	G
4	5	4765	G
4	5	4771	C
4	5	4772	C
4	5	4860	G
4	5	4868	G
4	5	4870	OMG
4	5	4872	2MG

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Mol	Chain	Res	Type
4	5	4873	G
4	5	4875	G
4	5	4877	G
4	5	4882	U
4	5	4883	C
4	5	4885	U
4	5	4887	C
4	5	4895	C
4	5	4896	G
4	5	4903	G
4	5	4904	G
4	5	4906	C
4	5	4910	A
4	5	4912	G
4	5	4914	G
4	5	4915	G
4	5	4920	C
4	5	4921	C
4	5	4924	C
4	5	4925	U
4	5	4926	C
4	5	4927	G
4	5	4928	C
4	5	4931	G
4	5	4937	C
4	5	4938	A
4	5	4940	C
4	5	4943	A
4	5	4944	C
4	5	4947	U
4	5	4948	C
4	5	4949	G
4	5	4950	U
4	5	4951	G
4	5	4956	A
4	5	4957	C
4	5	4959	U
4	5	4964	C
4	5	4965	U
4	5	4966	A
4	5	4975	G
4	5	4976	U

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Mol	Chain	Res	Type
4	5	4982	A
4	5	4985	U
4	5	4988	U
4	5	4990	C
4	5	4991	U
4	5	4993	G
4	5	4999	G
4	5	5006	U
4	5	5014	A
4	5	5017	G
4	5	5022	U
4	5	5034	A
4	5	5040	U
4	5	5041	G
4	5	5047	C
4	5	5050	C
4	5	5053	U
4	5	5054	C
4	5	5058	A
4	5	5061	A
4	5	5062	G
4	5	5064	G
5	7	7	G
5	7	13	A
5	7	22	A
5	7	25	G
5	7	33	U
5	7	41	G
5	7	53	U
5	7	54	A
5	7	63	C
5	7	64	G
5	7	97	G
5	7	100	A
5	7	102	U
5	7	110	G
5	7	111	C
5	7	120	U
6	8	2	G
6	8	3	A
6	8	23	C
6	8	34	U

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Mol	Chain	Res	Type
6	8	35	C
6	8	39	G
6	8	49	G
6	8	51	U
6	8	59	A
6	8	62	A
6	8	63	U
6	8	64	U
6	8	75	G
6	8	77	A
6	8	78	G
6	8	79	G
6	8	87	G
6	8	99	U
6	8	103	A
6	8	105	C
6	8	109	C
6	8	110	U
6	8	111	U
6	8	114	G
6	8	124	U
6	8	125	C
6	8	126	C
6	8	127	U
6	8	137	A
6	8	147	G
50	9	2	A
50	9	3	C
50	9	17	C
50	9	25	A
50	9	26	U
50	9	33	G
50	9	41	G
50	9	44	U
50	9	45	A
50	9	46	A
50	9	56	G
50	9	58	C
50	9	62	G
50	9	67	C
50	9	68	A
50	9	70	G

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Mol	Chain	Res	Type
50	9	71	G
50	9	73	C
50	9	74	G
50	9	77	A
50	9	79	A
50	9	92	A
50	9	99	A
50	9	103	A
50	9	104	A
50	9	110	U
50	9	111	A
50	9	113	G
50	9	115	U
50	9	116	OMU
50	9	121	OMU
50	9	123	G
50	9	124	U
50	9	126	G
50	9	127	C
50	9	129	C
50	9	130	G
50	9	141	A
50	9	142	C
50	9	143	U
50	9	147	A
50	9	154	U
50	9	155	G
50	9	158	A
50	9	159	A2M
50	9	160	U
50	9	162	C
50	9	163	U
50	9	166	A2M
50	9	167	G
50	9	168	C
50	9	175	A
50	9	180	G
50	9	182	C
50	9	183	G
50	9	184	G
50	9	188	C
50	9	189	U

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Mol	Chain	Res	Type
50	9	192	C
50	9	202	G
50	9	206	G
50	9	213	G
50	9	215	G
50	9	289	G
50	9	293	C
50	9	294	U
50	9	302	A
50	9	307	G
50	9	308	G
50	9	309	G
50	9	312	G
50	9	315	C
50	9	318	A
50	9	319	C
50	9	332	G
50	9	339	A
50	9	347	G
50	9	350	C
50	9	351	G
50	9	357	C
50	9	360	A
50	9	362	C
50	9	364	A
50	9	367	U
50	9	368	U
50	9	369	C
50	9	370	G
50	9	381	C
50	9	385	G
50	9	398	A
50	9	400	C
50	9	408	A
50	9	409	C
50	9	417	C
50	9	418	A
50	9	420	G
50	9	428	U
50	9	429	C
50	9	435	A
50	9	438	G

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Mol	Chain	Res	Type
50	9	441	C
50	9	448	A
50	9	449	A
50	9	450	C
50	9	465	A
50	9	466	G
50	9	471	G
50	9	472	C
50	9	473	A
50	9	474	G
50	9	482	G
50	9	487	U
50	9	492	C
50	9	530	U
50	9	532	C
50	9	533	A
50	9	536	A
50	9	537	C
50	9	542	U
50	9	546	G
50	9	547	G
50	9	548	C
50	9	549	C
50	9	550	C
50	9	551	U
50	9	554	A
50	9	555	A
50	9	556	U
50	9	559	G
50	9	560	A
50	9	562	U
50	9	563	G
50	9	564	A
50	9	568	E3C
50	9	576	A
50	9	583	A
50	9	587	A
50	9	588	G
50	9	589	G
50	9	590	A
50	9	591	U
50	9	594	A

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Mol	Chain	Res	Type
50	9	597	G
50	9	603	C
50	9	604	A
50	9	605	A
50	9	606	G
50	9	607	U
50	9	608	C
50	9	614	C
50	9	628	A
50	9	629	A
50	9	631	U
50	9	643	A
50	9	655	A
50	9	658	U
50	9	660	C
50	9	664	A
50	9	666	U
50	9	668	A2M
50	9	669	A
50	9	671	A
50	9	672	A
50	9	673	G
50	9	683	OMG
50	9	684	G
50	9	688	U
50	9	689	U
50	9	690	G
50	9	752	G
50	9	753	C
50	9	754	G
50	9	798	G
50	9	801	U
50	9	804	U
50	9	811	A
50	9	821	G
50	9	822	PSU
50	9	830	A
50	9	833	C
50	9	834	C
50	9	845	G
50	9	847	A
50	9	865	A

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Mol	Chain	Res	Type
50	9	870	A
50	9	871	U
50	9	872	A
50	9	873	G
50	9	875	A
50	9	878	G
50	9	887	U
50	9	888	U
50	9	890	U
50	9	892	U
50	9	893	U
50	9	898	U
50	9	901	G
50	9	913	A
50	9	914	U
50	9	920	A
50	9	933	G
50	9	934	G
50	9	954	U
50	9	971	G
50	9	978	G
50	9	985	G
50	9	986	G
50	9	990	A
50	9	991	G
50	9	992	A
50	9	999	G
50	9	1002	U
50	9	1017	U
50	9	1023	A
50	9	1026	C
50	9	1041	G
50	9	1045	U
50	9	1058	A
50	9	1060	A
50	9	1082	A
50	9	1083	A
50	9	1084	A
50	9	1085	C
50	9	1086	G
50	9	1088	U
50	9	1097	G

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Mol	Chain	Res	Type
50	9	1099	G
50	9	1100	A
50	9	1109	C
50	9	1111	U
50	9	1113	A
50	9	1114	U
50	9	1115	U
50	9	1116	C
50	9	1117	C
50	9	1118	C
50	9	1121	G
50	9	1123	C
50	9	1126	G
50	9	1131	G
50	9	1133	A
50	9	1138	C
50	9	1149	A
50	9	1153	C
50	9	1154	U
50	9	1155	U
50	9	1170	A
50	9	1194	A
50	9	1195	A
50	9	1197	G
50	9	1207	G
50	9	1212	G
50	9	1215	C
50	9	1221	G
50	9	1223	A
50	9	1224	G
50	9	1242	U
50	9	1243	PSU
50	9	1247	C
50	9	1248	B8N
50	9	1250	A
50	9	1251	A
50	9	1253	A
50	9	1254	C
50	9	1256	G
50	9	1257	G
50	9	1259	A
50	9	1264	C

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Mol	Chain	Res	Type
50	9	1273	C
50	9	1274	G
50	9	1275	G
50	9	1282	A
50	9	1283	C
50	9	1284	A
50	9	1285	G
50	9	1286	G
50	9	1287	A
50	9	1288	U
50	9	1293	A
50	9	1294	G
50	9	1298	G
50	9	1299	A
50	9	1301	A
50	9	1302	G
50	9	1303	C
50	9	1305	C
50	9	1306	U
50	9	1307	U
50	9	1308	U
50	9	1310	U
50	9	1312	G
50	9	1313	A
50	9	1314	U
50	9	1316	C
50	9	1320	G
50	9	1322	G
50	9	1333	U
50	9	1341	C
50	9	1342	U
50	9	1348	G
50	9	1355	C
50	9	1369	A
50	9	1371	U
50	9	1372	U
50	9	1375	G
50	9	1376	A
50	9	1378	A
50	9	1382	A
50	9	1395	C
50	9	1396	A

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Mol	Chain	Res	Type
50	9	1397	U
50	9	1401	A
50	9	1402	A
50	9	1404	U
50	9	1405	A
50	9	1406	G
50	9	1409	A
50	9	1428	G
50	9	1429	G
50	9	1449	G
50	9	1454	A
50	9	1462	U
50	9	1463	U
50	9	1464	C
50	9	1466	G
50	9	1473	G
50	9	1476	A
50	9	1477	U
50	9	1480	A
50	9	1487	A
50	9	1489	A
50	9	1490	G
50	9	1498	A
50	9	1504	U
50	9	1506	A
50	9	1507	G
50	9	1508	A
50	9	1509	U
50	9	1510	G
50	9	1521	C
50	9	1522	A
50	9	1523	C
50	9	1531	A
50	9	1533	A
50	9	1548	G
50	9	1552	G
50	9	1553	C
50	9	1554	C
50	9	1555	U
50	9	1556	A
50	9	1557	C
50	9	1560	U

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Mol	Chain	Res	Type
50	9	1570	G
50	9	1574	C
50	9	1575	G
50	9	1578	U
50	9	1580	A
50	9	1585	U
50	9	1586	U
50	9	1587	G
50	9	1588	A
50	9	1600	G
50	9	1601	A
50	9	1604	G
50	9	1606	G
50	9	1621	U
50	9	1623	A
50	9	1637	A
50	9	1638	G
50	9	1646	C
50	9	1648	G
50	9	1649	U
50	9	1654	G
50	9	1664	A
50	9	1665	G
50	9	1666	C
50	9	1671	G
50	9	1683	C
50	9	1695	A
50	9	1698	C
50	9	1699	A
50	9	1709	G
50	9	1721	U
50	9	1722	G
50	9	1726	G
50	9	1732	G
50	9	1744	G
50	9	1756	C
50	9	1757	G
50	9	1775	U
50	9	1779	G
50	9	1782	G
50	9	1783	C
50	9	1784	G

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Mol	Chain	Res	Type
50	9	1785	C
50	9	1819	A
50	9	1823	A
50	9	1824	A
50	9	1825	A
50	9	1829	G
50	9	1831	A
50	9	1835	A
50	9	1836	G
50	9	1838	U
50	9	1849	G
50	9	1851	MA6
50	9	1859	A
50	9	1861	G
50	9	1862	G
50	9	1863	A
50	9	1864	U
50	9	1865	C
50	9	1866	A
50	9	1867	U
50	9	1869	A

All (95) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	4	72	C
4	5	12	A
4	5	47	A
4	5	48	G
4	5	125	C
4	5	134	G
4	5	217	C
4	5	245	C
4	5	265	C
4	5	266	C
4	5	275	C
4	5	385	A
4	5	406	C
4	5	449	C
4	5	485	C
4	5	492	U
4	5	504	G

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Mol	Chain	Res	Type
4	5	684	G
4	5	696	C
4	5	930	G
4	5	959	G
4	5	1072	C
4	5	1174	G
4	5	1211	G
4	5	1236	C
4	5	1238	A
4	5	1291	G
4	5	1329	G
4	5	1370	G
4	5	1406(B)	C
4	5	1440	U
4	5	1445	U
4	5	1633	G
4	5	1804	A
4	5	1818	G
4	5	1979	A
4	5	1983	A
4	5	2046	G
4	5	2089	G
4	5	2266	C
4	5	2474	G
4	5	2502	A
4	5	2546	G
4	5	2587	A
4	5	2661	U
4	5	2695	A
4	5	3603	G
4	5	3625	G
4	5	3697	U
4	5	3876	A
4	5	3888	G
4	5	3904	G
4	5	3973	G
4	5	4053	A
4	5	4065	G
4	5	4075	U
4	5	4119	C
4	5	4232	U
4	5	4254	G

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Mol	Chain	Res	Type
4	5	4447	5MC
4	5	4448	G
4	5	4559	A
4	5	4699	U
4	5	4719	G
4	5	4884	G
4	5	4925	U
4	5	4936	G
4	5	4947	U
6	8	124	U
50	9	110	U
50	9	140	U
50	9	369	C
50	9	434	G
50	9	465	A
50	9	532	C
50	9	553	U
50	9	642	U
50	9	688	U
50	9	752	G
50	9	870	A
50	9	874	G
50	9	1137	U
50	9	1253	A
50	9	1285	G
50	9	1286	G
50	9	1394	G
50	9	1395	C
50	9	1489	A
50	9	1505	U
50	9	1508	A
50	9	1520	G
50	9	1637	A
50	9	1664	A
50	9	1665	G
50	9	1824	A

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

137 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
4	5MU	5	4083	4	19,22,23	4.69	7 (36%)	27,32,35	3.62	11 (40%)
4	5MC	5	3782	4	19,22,23	3.51	8 (42%)	26,32,35	1.44	5 (19%)
4	MHG	5	4371	4	29,32,33	3.63	11 (37%)	34,46,49	2.35	12 (35%)
50	A2M	9	1678	50	22,25,26	3.97	12 (54%)	30,36,39	2.53	12 (40%)
4	B8T	5	4483	4	19,22,23	3.02	8 (42%)	25,31,34	1.11	2 (8%)
4	OMC	5	2861	4	19,22,23	2.85	7 (36%)	25,31,34	1.08	2 (8%)
50	PSU	9	612	50	18,21,22	1.04	3 (16%)	21,30,33	1.71	4 (19%)
4	B8T	5	4671	4	19,22,23	2.93	8 (42%)	25,31,34	0.92	1 (4%)
4	A2M	5	1871	4,84	22,25,26	3.91	12 (54%)	30,36,39	2.46	12 (40%)
4	A2M	5	398	4	22,25,26	3.89	10 (45%)	30,36,39	2.29	9 (30%)
4	B8K	5	3897	4	24,28,29	4.72	17 (70%)	29,42,45	2.70	12 (41%)
4	PSU	5	4500	4	18,21,22	1.08	3 (16%)	21,30,33	2.21	5 (23%)
4	B9B	5	1574	4	25,28,29	3.74	9 (36%)	35,40,43	2.45	13 (37%)
4	A2M	5	3718	4	22,25,26	3.97	13 (59%)	30,36,39	2.06	9 (30%)
4	OMC	5	3701	4,84	19,22,23	2.74	7 (36%)	25,31,34	0.82	0
4	A2M	5	1326	4	22,25,26	4.01	11 (50%)	30,36,39	2.33	9 (30%)
4	OMC	5	3869	4	19,22,23	2.69	7 (36%)	25,31,34	0.92	0
4	A2M	5	4571	4	22,25,26	3.94	12 (54%)	30,36,39	2.38	12 (40%)
50	A2M	9	166	50	22,25,26	3.92	10 (45%)	30,36,39	2.63	12 (40%)
50	OMC	9	517	50	19,22,23	2.83	7 (36%)	25,31,34	1.05	1 (4%)
50	OMC	9	1703	50	19,22,23	2.88	7 (36%)	25,31,34	0.71	0
4	I4U	5	4194	4	20,24,25	4.99	13 (65%)	27,34,37	2.04	5 (18%)
4	E7G	5	1797	4	24,27,28	3.09	11 (45%)	28,40,43	2.31	10 (35%)
4	A2M	5	4523	4,84	22,25,26	3.90	12 (54%)	30,36,39	2.54	13 (43%)
4	OMC	5	2422	4,84	19,22,23	2.84	7 (36%)	25,31,34	0.83	1 (4%)
4	PSU	5	4403	4	18,21,22	1.08	2 (11%)	21,30,33	1.97	6 (28%)
50	E3C	9	568	50	19,23,24	3.38	6 (31%)	21,33,36	2.72	7 (33%)
50	5MC	9	1374	50	19,22,23	3.81	8 (42%)	26,32,35	1.12	2 (7%)
4	PSU	5	4636	4	18,21,22	1.10	3 (16%)	21,30,33	2.21	6 (28%)
4	6MZ	5	4220	4	22,25,26	2.89	6 (27%)	29,36,39	4.22	12 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	MA6	9	1850	50	23,26,27	1.60	5 (21%)	33,38,41	2.75	11 (33%)
4	OMG	5	4196	2,4	23,26,27	2.37	9 (39%)	32,38,41	1.88	7 (21%)
50	B8N	9	1248	50	25,29,30	3.07	8 (32%)	28,42,45	2.15	8 (28%)
4	OMG	5	4637	4	23,26,27	2.31	7 (30%)	32,38,41	1.94	8 (25%)
50	OMG	9	644	50	23,26,27	2.40	7 (30%)	32,38,41	1.94	8 (25%)
4	OMG	5	1625	4,84	23,26,27	2.38	7 (30%)	32,38,41	2.06	9 (28%)
50	A2M	9	668	50,84	22,25,26	3.95	11 (50%)	30,36,39	2.42	13 (43%)
50	A2M	9	159	50	22,25,26	4.00	12 (54%)	30,36,39	2.42	13 (43%)
4	M7A	5	4564	4	19,25,26	1.58	3 (15%)	25,37,40	3.99	7 (28%)
4	PSU	5	4531	4	18,21,22	1.12	3 (16%)	21,30,33	1.82	4 (19%)
4	OMG	5	3792	4	23,26,27	2.42	8 (34%)	32,38,41	2.11	8 (25%)
50	OMU	9	121	50	19,22,23	2.87	7 (36%)	25,31,34	1.94	5 (20%)
4	B9H	5	2786	4	21,25,26	2.96	3 (14%)	22,35,38	2.11	4 (18%)
4	E7G	5	2297	4	24,27,28	3.00	11 (45%)	28,40,43	2.27	9 (32%)
4	B8H	5	4296	4	19,22,23	6.93	8 (42%)	21,32,35	2.76	6 (28%)
50	PSU	9	1243	50	18,21,22	1.31	1 (5%)	21,30,33	1.60	4 (19%)
4	UR3	5	4530	4	19,22,23	2.54	7 (36%)	26,32,35	1.74	4 (15%)
50	OMC	9	1710	50	19,22,23	2.89	7 (36%)	25,31,34	1.05	1 (4%)
4	PSU	5	4628	4	18,21,22	1.11	3 (16%)	21,30,33	2.13	4 (19%)
4	PSU	5	1677	4	18,21,22	1.15	3 (16%)	21,30,33	2.01	6 (28%)
4	E6G	5	4355	4	24,27,28	3.60	12 (50%)	34,39,42	2.54	13 (38%)
4	OMG	5	4494	4	23,26,27	2.43	7 (30%)	32,38,41	1.98	10 (31%)
50	PSU	9	822	50	18,21,22	1.10	2 (11%)	21,30,33	2.18	6 (28%)
4	OMC	5	3887	4	19,22,23	2.85	7 (36%)	25,31,34	0.90	1 (4%)
4	OMC	5	4536	4	19,22,23	2.70	7 (36%)	25,31,34	1.10	2 (8%)
4	P7G	5	1909	4	24,28,29	3.54	10 (41%)	25,41,44	1.59	2 (8%)
4	1MA	5	1322	4,84	21,25,26	2.54	7 (33%)	30,37,40	2.02	8 (26%)
4	OMG	5	1316	4	23,26,27	2.42	8 (34%)	32,38,41	1.81	9 (28%)
4	P4U	5	1348	4,84	21,24,25	3.36	7 (33%)	28,33,36	2.00	5 (17%)
50	4AC	9	1842	50	21,24,25	3.03	10 (47%)	28,34,37	1.56	7 (25%)
4	B8H	5	3762	4	19,22,23	6.86	6 (31%)	21,32,35	2.61	5 (23%)
4	A2M	5	3723	4	22,25,26	3.92	12 (54%)	30,36,39	2.24	8 (26%)
4	B9B	5	237	4	25,28,29	3.77	11 (44%)	35,40,43	2.62	15 (42%)
4	PSU	5	3715	4	18,21,22	0.97	1 (5%)	21,30,33	1.82	4 (19%)
4	PSU	5	2508	4	18,21,22	1.00	1 (5%)	21,30,33	1.77	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMC	5	2365	4	19,22,23	2.79	7 (36%)	25,31,34	0.76	0
4	5MC	5	4447	4	19,22,23	3.69	8 (42%)	26,32,35	1.17	2 (7%)
9	MLZ	C	333	9	8,9,10	0.93	0	4,9,11	0.93	0
4	5MC	5	4335	4	19,22,23	3.78	8 (42%)	26,32,35	1.32	3 (11%)
50	PSU	9	119	50	18,21,22	0.88	1 (5%)	21,30,33	1.78	4 (19%)
4	B8K	5	4690	4	24,28,29	4.85	17 (70%)	29,42,45	2.94	12 (41%)
4	UR3	5	4597	4	19,22,23	2.61	6 (31%)	26,32,35	1.50	5 (19%)
4	7MG	5	1605	4	23,26,27	3.14	10 (43%)	27,39,42	2.22	10 (37%)
4	B8W	5	2380	4	23,26,27	3.39	12 (52%)	33,38,41	5.65	18 (54%)
4	OMG	5	1522	4	23,26,27	2.35	8 (34%)	32,38,41	1.99	8 (25%)
4	7MG	5	2522	4	23,26,27	3.18	10 (43%)	27,39,42	2.22	8 (29%)
4	PSU	5	4442	4	18,21,22	1.10	3 (16%)	21,30,33	2.24	6 (28%)
4	A2M	5	2363	4,84	22,25,26	3.99	12 (54%)	30,36,39	2.47	12 (40%)
4	B8W	5	4129	4	23,26,27	3.38	11 (47%)	33,38,41	5.77	20 (60%)
4	A2M	5	3825	4	22,25,26	4.01	11 (50%)	30,36,39	2.37	9 (30%)
4	P7G	5	3880	4	24,28,29	3.40	10 (41%)	25,41,44	1.44	3 (12%)
50	A2M	9	1031	50	22,25,26	3.96	12 (54%)	30,36,39	2.42	11 (36%)
50	A2M	9	27	50,84	22,25,26	3.94	12 (54%)	30,36,39	2.34	9 (30%)
4	OMG	5	2424	4	23,26,27	2.43	9 (39%)	32,38,41	1.92	7 (21%)
50	UR3	9	1830	50	19,22,23	2.54	6 (31%)	26,32,35	1.96	5 (19%)
50	A2M	9	484	50	22,25,26	3.87	12 (54%)	30,36,39	2.35	12 (40%)
4	2MG	5	1517	4	23,26,27	2.86	7 (30%)	33,38,41	2.70	10 (30%)
50	OMG	9	683	50	23,26,27	2.42	9 (39%)	32,38,41	1.98	7 (21%)
50	PSU	9	823	50	18,21,22	1.11	3 (16%)	21,30,33	1.81	4 (19%)
50	4AC	9	1337	50	21,24,25	3.12	10 (47%)	28,34,37	1.21	4 (14%)
4	OMG	5	4870	4	23,26,27	2.43	8 (34%)	32,38,41	1.96	8 (25%)
50	MA6	9	1851	50	23,26,27	1.61	4 (17%)	33,38,41	2.74	12 (36%)
4	B8W	5	4529	4,84	23,26,27	3.41	12 (52%)	33,38,41	5.91	20 (60%)
4	OMU	5	4620	4	19,22,23	2.64	6 (31%)	25,31,34	1.87	5 (20%)
50	OMG	9	509	50,84	23,26,27	2.36	8 (34%)	32,38,41	1.87	7 (21%)
4	2MG	5	4872	4	23,26,27	2.89	9 (39%)	33,38,41	2.93	16 (48%)
4	A2M	5	1524	4	22,25,26	3.92	11 (50%)	30,36,39	2.59	11 (36%)
50	OMC	9	174	50	19,22,23	2.89	7 (36%)	25,31,34	0.85	0
50	M7A	9	1806	50	19,25,26	1.59	3 (15%)	25,37,40	3.91	8 (32%)
4	OMG	5	2773	4	23,26,27	2.39	9 (39%)	32,38,41	1.81	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2M	5	3785	4	22,25,26	3.85	13 (59%)	30,36,39	2.52	13 (43%)
4	7MG	5	4550	4	23,26,27	3.09	10 (43%)	27,39,42	2.06	10 (37%)
50	6MZ	9	1832	50,84	22,25,26	3.03	5 (22%)	29,36,39	4.16	12 (41%)
4	1MA	5	4415	4	21,25,26	2.72	5 (23%)	30,37,40	1.85	5 (16%)
4	UR3	5	1866	4	19,22,23	2.39	6 (31%)	26,32,35	1.39	4 (15%)
4	PSU	5	3729	4	18,21,22	1.11	2 (11%)	21,30,33	2.00	4 (19%)
44	MLZ	m	72	44	8,9,10	0.80	0	4,9,11	1.04	0
50	B8Q	9	1219	50,84	18,22,23	2.88	5 (27%)	21,32,35	2.64	7 (33%)
4	OMC	5	2804	4	19,22,23	2.83	7 (36%)	25,31,34	0.90	0
4	PSU	5	1582	4	18,21,22	1.14	3 (16%)	21,30,33	1.92	4 (19%)
4	OMU	5	4306	4	19,22,23	2.75	8 (42%)	25,31,34	1.86	5 (20%)
4	OMG	5	1883	4	23,26,27	2.41	8 (34%)	32,38,41	2.18	8 (25%)
4	B8W	5	4472	4	23,26,27	3.44	12 (52%)	33,38,41	5.29	17 (51%)
4	OMG	5	2050	4	23,26,27	2.36	8 (34%)	32,38,41	1.94	7 (21%)
4	A2M	5	3867	4	22,25,26	3.95	11 (50%)	30,36,39	2.49	14 (46%)
4	OMG	5	2364	4	23,26,27	2.33	7 (30%)	32,38,41	1.79	7 (21%)
4	B8W	5	4185	4	23,26,27	3.38	11 (47%)	33,38,41	5.56	23 (69%)
4	OMG	5	4623	4	23,26,27	2.38	7 (30%)	32,38,41	1.90	7 (21%)
50	PSU	9	1081	50	18,21,22	1.14	3 (16%)	21,30,33	1.91	5 (23%)
4	OMC	5	3909	4	19,22,23	2.69	7 (36%)	25,31,34	0.97	1 (4%)
50	OMU	9	116	50	19,22,23	2.78	7 (36%)	25,31,34	1.95	5 (20%)
4	B8Q	5	1456	4	18,22,23	2.65	5 (27%)	21,32,35	1.89	5 (23%)
6	OMU	8	14	4,6	19,22,23	2.67	6 (31%)	25,31,34	1.97	5 (20%)
4	A2M	5	1534	4,84	22,25,26	3.98	10 (45%)	30,36,39	2.54	11 (36%)
4	OMG	5	373	4	23,26,27	2.39	8 (34%)	32,38,41	1.85	8 (25%)
4	BGH	5	3899	4,84	25,29,30	4.08	15 (60%)	30,43,46	2.77	14 (46%)
4	PSU	5	4293	4	18,21,22	1.11	3 (16%)	21,30,33	1.94	4 (19%)
4	A2M	5	2401	4,84	22,25,26	3.91	12 (54%)	30,36,39	2.35	8 (26%)
4	2MG	5	729	4	23,26,27	2.94	7 (30%)	33,38,41	2.37	9 (27%)
4	B8H	5	1860	4	19,22,23	6.85	6 (31%)	21,32,35	2.51	5 (23%)
50	5MU	9	814	50	19,22,23	4.82	7 (36%)	27,32,35	3.39	13 (48%)
4	PSU	5	3764	4	18,21,22	1.02	1 (5%)	21,30,33	1.73	4 (19%)
4	B9B	5	2754	4,84	25,28,29	3.78	8 (32%)	35,40,43	2.39	12 (34%)
4	PSU	5	1683	4	18,21,22	1.20	2 (11%)	21,30,33	2.00	4 (19%)
4	OMG	5	4370	4	23,26,27	2.36	8 (34%)	32,38,41	1.85	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	5	4450	4,84	18,21,22	1.14	3 (16%)	21,30,33	2.16	5 (23%)
4	I4U	5	1659	4	20,24,25	4.92	13 (65%)	27,34,37	2.13	3 (11%)

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
4	5MU	5	4083	4	-	0/7/25/26	0/2/2/2
4	5MC	5	3782	4	-	0/7/25/26	0/2/2/2
4	MHG	5	4371	4	-	6/16/46/47	0/3/3/3
50	A2M	9	1678	50	-	0/9/27/28	0/3/3/3
4	B8T	5	4483	4	-	0/7/27/28	0/2/2/2
4	OMC	5	2861	4	-	1/9/27/28	0/2/2/2
50	PSU	9	612	50	-	0/7/25/26	0/2/2/2
4	B8T	5	4671	4	-	0/7/27/28	0/2/2/2
4	A2M	5	1871	4,84	-	0/9/27/28	0/3/3/3
4	A2M	5	398	4	-	2/9/27/28	0/3/3/3
4	B8K	5	3897	4	-	3/11/41/42	0/3/3/3
4	PSU	5	4500	4	-	3/7/25/26	0/2/2/2
4	B9B	5	1574	4	-	3/11/29/30	0/3/3/3
4	A2M	5	3718	4	-	0/9/27/28	0/3/3/3
4	OMC	5	3701	4,84	-	6/9/27/28	0/2/2/2
4	A2M	5	1326	4	-	1/9/27/28	0/3/3/3
4	OMC	5	3869	4	-	0/9/27/28	0/2/2/2
4	A2M	5	4571	4	-	0/9/27/28	0/3/3/3
50	A2M	9	166	50	-	2/9/27/28	0/3/3/3
50	OMC	9	517	50	-	0/9/27/28	0/2/2/2
50	OMC	9	1703	50	-	2/9/27/28	0/2/2/2
4	I4U	5	4194	4	-	4/9/29/30	0/2/2/2
4	E7G	5	1797	4	-	2/9/39/40	0/3/3/3
4	A2M	5	4523	4,84	-	3/9/27/28	0/3/3/3
4	OMC	5	2422	4,84	-	0/9/27/28	0/2/2/2
4	PSU	5	4403	4	-	3/7/25/26	0/2/2/2
50	E3C	9	568	50	-	4/9/44/45	0/2/2/2
50	5MC	9	1374	50	-	0/7/25/26	0/2/2/2
4	PSU	5	4636	4	-	3/7/25/26	0/2/2/2
4	6MZ	5	4220	4	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	MA6	9	1850	50	-	1/11/29/30	0/3/3/3
4	OMG	5	4196	2,4	-	0/9/27/28	0/3/3/3
50	B8N	9	1248	50	-	2/16/34/35	0/2/2/2
4	OMG	5	4637	4	-	2/9/27/28	0/3/3/3
50	OMG	9	644	50	-	2/9/27/28	0/3/3/3
4	OMG	5	1625	4,84	-	1/9/27/28	0/3/3/3
50	A2M	9	668	50,84	-	4/9/27/28	0/3/3/3
50	A2M	9	159	50	-	3/9/27/28	0/3/3/3
4	M7A	5	4564	4	-	0/7/37/38	0/3/3/3
4	PSU	5	4531	4	-	0/7/25/26	0/2/2/2
4	OMG	5	3792	4	-	2/9/27/28	0/3/3/3
50	OMU	9	121	50	-	2/9/27/28	0/2/2/2
4	B9H	5	2786	4	-	2/12/47/48	0/2/2/2
4	E7G	5	2297	4	-	1/9/39/40	0/3/3/3
4	B8H	5	4296	4	-	0/7/25/26	0/2/2/2
50	PSU	9	1243	50	-	2/7/25/26	0/2/2/2
4	UR3	5	4530	4	-	1/7/25/26	0/2/2/2
50	OMC	9	1710	50	-	1/9/27/28	0/2/2/2
4	PSU	5	4628	4	-	0/7/25/26	0/2/2/2
4	PSU	5	1677	4	-	1/7/25/26	0/2/2/2
4	E6G	5	4355	4	-	5/10/28/29	0/3/3/3
4	OMG	5	4494	4	-	0/9/27/28	0/3/3/3
50	PSU	9	822	50	-	0/7/25/26	0/2/2/2
4	OMC	5	3887	4	-	1/9/27/28	0/2/2/2
4	OMC	5	4536	4	-	0/9/27/28	0/2/2/2
4	P7G	5	1909	4	-	3/10/40/41	0/3/3/3
4	1MA	5	1322	4,84	-	0/7/25/26	0/3/3/3
4	OMG	5	1316	4	-	1/9/27/28	0/3/3/3
4	P4U	5	1348	4,84	-	5/10/29/30	0/2/2/2
50	4AC	9	1842	50	-	0/11/29/30	0/2/2/2
4	B8H	5	3762	4	-	2/7/25/26	0/2/2/2
4	A2M	5	3723	4	-	0/9/27/28	0/3/3/3
4	B9B	5	237	4	-	4/11/29/30	0/3/3/3
4	PSU	5	3715	4	-	0/7/25/26	0/2/2/2
4	PSU	5	2508	4	-	0/7/25/26	0/2/2/2
4	OMC	5	2365	4	-	0/9/27/28	0/2/2/2
4	5MC	5	4447	4	-	4/7/25/26	0/2/2/2
9	MLZ	C	333	9	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5MC	5	4335	4	-	0/7/25/26	0/2/2/2
50	PSU	9	119	50	-	0/7/25/26	0/2/2/2
4	B8K	5	4690	4	-	0/11/41/42	0/3/3/3
4	UR3	5	4597	4	-	0/7/25/26	0/2/2/2
4	7MG	5	1605	4	-	0/7/37/38	0/3/3/3
4	B8W	5	2380	4	-	4/9/27/28	0/3/3/3
4	OMG	5	1522	4	-	0/9/27/28	0/3/3/3
4	7MG	5	2522	4	-	0/7/37/38	0/3/3/3
4	PSU	5	4442	4	-	0/7/25/26	0/2/2/2
4	A2M	5	2363	4,84	-	1/9/27/28	0/3/3/3
4	B8W	5	4129	4	-	3/9/27/28	0/3/3/3
4	A2M	5	3825	4	-	0/9/27/28	0/3/3/3
4	P7G	5	3880	4	-	2/10/40/41	0/3/3/3
50	A2M	9	1031	50	-	0/9/27/28	0/3/3/3
50	A2M	9	27	50,84	-	0/9/27/28	0/3/3/3
4	OMG	5	2424	4	-	2/9/27/28	0/3/3/3
50	UR3	9	1830	50	-	2/7/25/26	0/2/2/2
50	A2M	9	484	50	-	0/9/27/28	0/3/3/3
4	2MG	5	1517	4	-	0/9/27/28	0/3/3/3
50	OMG	9	683	50	-	2/9/27/28	0/3/3/3
50	PSU	9	823	50	-	0/7/25/26	0/2/2/2
50	4AC	9	1337	50	-	2/11/29/30	0/2/2/2
4	OMG	5	4870	4	-	4/9/27/28	0/3/3/3
50	MA6	9	1851	50	-	4/11/29/30	0/3/3/3
4	B8W	5	4529	4,84	-	4/9/27/28	0/3/3/3
4	OMU	5	4620	4	-	1/9/27/28	0/2/2/2
50	OMG	9	509	50,84	-	0/9/27/28	0/3/3/3
4	2MG	5	4872	4	-	2/9/27/28	0/3/3/3
4	A2M	5	1524	4	-	0/9/27/28	0/3/3/3
50	OMC	9	174	50	-	0/9/27/28	0/2/2/2
50	M7A	9	1806	50	-	0/7/37/38	0/3/3/3
4	OMG	5	2773	4	-	0/9/27/28	0/3/3/3
4	A2M	5	3785	4	-	4/9/27/28	0/3/3/3
4	7MG	5	4550	4	-	0/7/37/38	0/3/3/3
50	6MZ	9	1832	50,84	-	2/9/27/28	0/3/3/3
4	1MA	5	4415	4	-	2/7/25/26	0/3/3/3
4	UR3	5	1866	4	-	2/7/25/26	0/2/2/2
4	PSU	5	3729	4	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	MLZ	m	72	44	-	1/7/8/10	-
50	B8Q	9	1219	50,84	-	1/7/42/43	0/2/2/2
4	OMC	5	2804	4	-	0/9/27/28	0/2/2/2
4	PSU	5	1582	4	-	2/7/25/26	0/2/2/2
4	OMU	5	4306	4	-	1/9/27/28	0/2/2/2
4	OMG	5	1883	4	-	2/9/27/28	0/3/3/3
4	B8W	5	4472	4	-	3/9/27/28	0/3/3/3
4	OMG	5	2050	4	-	0/9/27/28	0/3/3/3
4	A2M	5	3867	4	-	2/9/27/28	0/3/3/3
4	OMG	5	2364	4	-	2/9/27/28	0/3/3/3
4	B8W	5	4185	4	-	3/9/27/28	0/3/3/3
4	OMG	5	4623	4	-	0/9/27/28	0/3/3/3
50	PSU	9	1081	50	-	1/7/25/26	0/2/2/2
4	OMC	5	3909	4	-	0/9/27/28	0/2/2/2
50	OMU	9	116	50	-	3/9/27/28	0/2/2/2
4	B8Q	5	1456	4	-	0/7/42/43	0/2/2/2
6	OMU	8	14	4,6	-	1/9/27/28	0/2/2/2
4	A2M	5	1534	4,84	-	2/9/27/28	0/3/3/3
4	OMG	5	373	4	-	0/9/27/28	0/3/3/3
4	BGH	5	3899	4,84	-	3/13/43/44	0/3/3/3
4	PSU	5	4293	4	-	2/7/25/26	0/2/2/2
4	A2M	5	2401	4,84	-	1/9/27/28	0/3/3/3
4	2MG	5	729	4	-	2/9/27/28	0/3/3/3
4	B8H	5	1860	4	-	0/7/25/26	0/2/2/2
50	5MU	9	814	50	-	1/7/25/26	0/2/2/2
4	PSU	5	3764	4	-	0/7/25/26	0/2/2/2
4	B9B	5	2754	4,84	-	4/11/29/30	0/3/3/3
4	PSU	5	1683	4	-	0/7/25/26	0/2/2/2
4	OMG	5	4370	4	-	0/9/27/28	0/3/3/3
4	PSU	5	4450	4,84	-	4/7/25/26	0/2/2/2
4	I4U	5	1659	4	-	1/9/29/30	0/2/2/2

All (1045) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4296	B8H	C6-C5	-16.32	1.11	1.35
4	5	1860	B8H	C6-C5	-15.78	1.12	1.35
4	5	3762	B8H	C6-C5	-15.68	1.12	1.35
4	5	4296	B8H	C4-N3	-15.18	1.10	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	1860	B8H	C4-N3	-14.96	1.10	1.38
4	5	3762	B8H	C4-N3	-14.90	1.11	1.38
4	5	3762	B8H	C4-C5	13.83	1.82	1.44
4	5	4296	B8H	C4-C5	13.70	1.82	1.44
4	5	1860	B8H	C4-C5	13.65	1.82	1.44
4	5	3762	B8H	C6-N1	13.52	1.69	1.36
4	5	1860	B8H	C6-N1	13.47	1.69	1.36
4	5	4296	B8H	C6-N1	13.20	1.68	1.36
50	9	1832	6MZ	C6-N6	12.16	1.48	1.34
4	5	4690	B8K	C3'-C4'	-11.77	1.23	1.53
4	5	3897	B8K	C3'-C4'	-11.63	1.23	1.53
4	5	4194	I4U	C3'-C2'	-11.57	1.22	1.53
4	5	1659	I4U	C3'-C2'	-11.49	1.22	1.53
50	9	814	5MU	C2-N1	11.45	1.56	1.38
4	5	4220	6MZ	C6-N6	11.19	1.47	1.34
4	5	4083	5MU	C6-N1	10.52	1.55	1.38
4	5	3899	BGH	C3'-C4'	-10.46	1.26	1.53
4	5	1348	P4U	C4-N3	10.12	1.44	1.31
4	5	1659	I4U	C4-N3	10.08	1.44	1.31
4	5	4083	5MU	C2-N1	10.06	1.54	1.38
50	9	814	5MU	C6-N1	10.05	1.55	1.38
4	5	237	B9B	O4'-C1'	9.97	1.65	1.42
4	5	4194	I4U	C4-N3	9.88	1.44	1.31
4	5	1909	P7G	C8-N9	9.87	1.52	1.45
50	9	166	A2M	O4'-C1'	9.73	1.64	1.42
4	5	1574	B9B	O4'-C1'	9.55	1.64	1.42
4	5	2754	B9B	O4'-C1'	9.46	1.63	1.42
4	5	4447	5MC	C6-C5	9.44	1.50	1.34
50	9	1031	A2M	O4'-C1'	9.41	1.63	1.42
4	5	3718	A2M	O4'-C1'	9.32	1.63	1.42
4	5	3723	A2M	O4'-C1'	9.29	1.63	1.42
4	5	4083	5MU	C4-C5	9.27	1.59	1.44
50	9	814	5MU	C4-C5	9.25	1.59	1.44
50	9	1374	5MC	C6-C5	9.21	1.49	1.34
50	9	159	A2M	O4'-C1'	9.20	1.63	1.42
4	5	4523	A2M	O4'-C1'	9.20	1.63	1.42
4	5	398	A2M	O4'-C1'	9.18	1.63	1.42
4	5	1534	A2M	O4'-C1'	9.14	1.63	1.42
4	5	2401	A2M	O4'-C1'	9.13	1.63	1.42
4	5	2363	A2M	O4'-C1'	9.11	1.63	1.42
4	5	3899	BGH	O4'-C4'	9.11	1.65	1.45
4	5	3825	A2M	O4'-C1'	9.09	1.63	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	27	A2M	O4'-C1'	9.05	1.62	1.42
4	5	1524	A2M	O4'-C1'	9.04	1.62	1.42
50	9	1678	A2M	O4'-C1'	9.04	1.62	1.42
4	5	1326	A2M	O4'-C1'	9.00	1.62	1.42
4	5	3825	A2M	C2'-C1'	-8.98	1.31	1.53
4	5	2786	B9H	C2-N3	8.96	1.48	1.37
4	5	1871	A2M	O4'-C1'	8.91	1.62	1.42
4	5	3867	A2M	O4'-C1'	8.91	1.62	1.42
50	9	484	A2M	O4'-C1'	8.88	1.62	1.42
4	5	4415	1MA	C2-N3	8.84	1.46	1.30
4	5	3880	P7G	C8-N9	8.83	1.51	1.45
4	5	4355	E6G	O4'-C1'	8.76	1.62	1.42
4	5	4571	A2M	O4'-C1'	8.74	1.62	1.42
4	5	2754	B9B	C2'-C1'	-8.73	1.26	1.53
4	5	3897	B8K	C2'-C1'	-8.72	1.26	1.53
4	5	1456	B8Q	C6-C5	8.71	1.51	1.33
50	9	1219	B8Q	C6-C5	8.70	1.51	1.33
4	5	4335	5MC	C6-C5	8.70	1.48	1.34
4	5	4371	MHG	C8-N9	8.66	1.51	1.45
50	9	1248	B8N	C4-N3	-8.65	1.25	1.40
4	5	4194	I4U	O4'-C4'	-8.57	1.25	1.45
4	5	4690	B8K	C8-N9	8.55	1.51	1.45
50	9	568	E3C	C2-N1	8.54	1.50	1.38
50	9	668	A2M	O4'-C4'	-8.53	1.26	1.45
4	5	2363	A2M	C2'-C1'	-8.51	1.32	1.53
4	5	3867	A2M	C2'-C1'	-8.50	1.32	1.53
4	5	1574	B9B	C2'-C1'	-8.50	1.26	1.53
50	9	668	A2M	O4'-C1'	8.45	1.61	1.42
4	5	1534	A2M	C2'-C1'	-8.44	1.32	1.53
4	5	3785	A2M	O4'-C1'	8.44	1.61	1.42
4	5	1326	A2M	C2'-C1'	-8.44	1.32	1.53
4	5	237	B9B	C2'-C1'	-8.42	1.27	1.53
4	5	3785	A2M	C2'-C1'	-8.36	1.32	1.53
4	5	4571	A2M	C2'-C1'	-8.36	1.32	1.53
50	9	814	5MU	C4-N3	-8.36	1.23	1.38
50	9	1678	A2M	C2'-C1'	-8.35	1.32	1.53
4	5	4083	5MU	C4-N3	-8.31	1.23	1.38
50	9	159	A2M	C2'-C1'	-8.27	1.32	1.53
4	5	3718	A2M	C2'-C1'	-8.25	1.32	1.53
4	5	4371	MHG	C2-N3	8.23	1.47	1.32
50	9	568	E3C	C2-N3	8.22	1.47	1.37
4	5	1322	1MA	C2-N3	8.22	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	27	A2M	C2'-C1'	-8.20	1.32	1.53
4	5	2401	A2M	C2'-C1'	-8.19	1.32	1.53
4	5	4690	B8K	C2'-C1'	-8.18	1.27	1.53
4	5	3782	5MC	C6-C5	8.17	1.47	1.34
50	9	668	A2M	C2'-C1'	-8.14	1.33	1.53
4	5	1871	A2M	C2'-C1'	-8.09	1.33	1.53
4	5	398	A2M	C2'-C1'	-8.08	1.33	1.53
4	5	4523	A2M	C2'-C1'	-8.04	1.33	1.53
50	9	1031	A2M	C2'-C1'	-8.04	1.33	1.53
4	5	3723	A2M	C2'-C1'	-8.03	1.33	1.53
4	5	1524	A2M	C2'-C1'	-8.01	1.33	1.53
50	9	159	A2M	O4'-C4'	-7.90	1.27	1.45
4	5	1659	I4U	O4'-C4'	-7.90	1.27	1.45
4	5	1326	A2M	O4'-C4'	-7.90	1.27	1.45
50	9	166	A2M	C2'-C1'	-7.89	1.33	1.53
4	5	2363	A2M	O4'-C4'	-7.88	1.27	1.45
50	9	484	A2M	C2'-C1'	-7.85	1.33	1.53
4	5	4355	E6G	O4'-C4'	-7.83	1.27	1.45
50	9	484	A2M	O4'-C4'	-7.83	1.27	1.45
4	5	4571	A2M	O4'-C4'	-7.81	1.27	1.45
4	5	3867	A2M	O4'-C4'	-7.80	1.27	1.45
4	5	1909	P7G	C5-N7	7.80	1.45	1.35
4	5	4371	MHG	C5-N7	7.80	1.45	1.35
4	5	3880	P7G	C5-N7	7.77	1.45	1.35
50	9	1678	A2M	O4'-C4'	-7.76	1.27	1.45
4	5	1534	A2M	O4'-C4'	-7.74	1.27	1.45
4	5	4129	B8W	O4'-C1'	7.72	1.59	1.42
4	5	1524	A2M	O4'-C4'	-7.70	1.27	1.45
4	5	4523	A2M	O4'-C4'	-7.65	1.28	1.45
4	5	2380	B8W	O4'-C1'	7.64	1.59	1.42
4	5	3825	A2M	O4'-C4'	-7.62	1.28	1.45
4	5	4355	E6G	C2'-C1'	-7.61	1.29	1.53
4	5	4472	B8W	O4'-C1'	7.57	1.59	1.42
50	9	1031	A2M	O4'-C4'	-7.57	1.28	1.45
4	5	1871	A2M	O4'-C4'	-7.55	1.28	1.45
4	5	3723	A2M	O4'-C4'	-7.53	1.28	1.45
50	9	27	A2M	O4'-C4'	-7.50	1.28	1.45
4	5	3785	A2M	O4'-C4'	-7.49	1.28	1.45
4	5	729	2MG	C2-N3	7.48	1.46	1.32
4	5	2401	A2M	O4'-C4'	-7.46	1.28	1.45
4	5	4529	B8W	O4'-C1'	7.44	1.59	1.42
4	5	2786	B9H	C6-C5	7.42	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	2754	B9B	O4'-C4'	-7.41	1.28	1.45
4	5	4185	B8W	O4'-C1'	7.38	1.59	1.42
4	5	3718	A2M	O4'-C4'	-7.35	1.28	1.45
4	5	398	A2M	O4'-C4'	-7.35	1.28	1.45
50	9	166	A2M	O4'-C4'	-7.29	1.28	1.45
4	5	2754	B9B	C2-N2	7.26	1.48	1.33
4	5	1574	B9B	O4'-C4'	-7.25	1.28	1.45
50	9	1374	5MC	C4-N3	7.24	1.45	1.34
4	5	3897	B8K	O4'-C4'	7.22	1.61	1.45
50	9	1248	B8N	C6-N1	7.19	1.54	1.36
4	5	3782	5MC	C4-N3	7.17	1.45	1.34
4	5	237	B9B	O4'-C4'	-7.17	1.29	1.45
4	5	1574	B9B	C2-N2	7.14	1.48	1.33
4	5	4529	B8W	C2'-C1'	-7.14	1.31	1.53
50	9	1337	4AC	C4-N3	7.13	1.44	1.32
4	5	4529	B8W	C3'-C4'	-7.13	1.34	1.53
50	9	568	E3C	C6-C5	7.05	1.47	1.33
4	5	237	B9B	C2-N2	7.05	1.47	1.33
4	5	4185	B8W	C3'-C4'	-7.04	1.35	1.53
4	5	1797	E7G	C5-N7	7.00	1.44	1.35
4	5	4690	B8K	O4'-C4'	6.99	1.60	1.45
4	5	4335	5MC	C4-N3	6.98	1.45	1.34
4	5	4129	B8W	C2'-C1'	-6.92	1.31	1.53
4	5	1517	2MG	C2-N3	6.88	1.45	1.32
4	5	4129	B8W	C3'-C4'	-6.82	1.35	1.53
4	5	2380	B8W	C3'-C4'	-6.77	1.35	1.53
4	5	4472	B8W	C2'-C1'	-6.74	1.32	1.53
4	5	729	2MG	C4-N3	6.73	1.49	1.34
4	5	4550	7MG	C8-N9	6.73	1.50	1.45
4	5	2297	E7G	C5-N7	6.73	1.44	1.35
4	5	4472	B8W	C3'-C4'	-6.72	1.35	1.53
4	5	4185	B8W	C2'-C1'	-6.70	1.32	1.53
4	5	4872	2MG	C2-N2	6.70	1.47	1.33
4	5	2380	B8W	C2'-C1'	-6.67	1.32	1.53
4	5	4447	5MC	C4-N3	6.66	1.44	1.34
4	5	2522	7MG	C5-N7	6.65	1.44	1.35
4	5	2522	7MG	C8-N9	6.62	1.50	1.45
50	9	121	OMU	C2-N3	6.61	1.49	1.38
4	5	4371	MHG	C2-N2	6.59	1.47	1.33
4	5	1605	7MG	C5-N7	6.58	1.44	1.35
4	5	4597	UR3	C2-N1	6.57	1.47	1.38
50	9	116	OMU	C2-N3	6.55	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	166	A2M	C6-N6	6.54	1.50	1.34
4	5	3897	B8K	C8-N9	6.51	1.50	1.45
4	5	4550	7MG	C5-N7	6.50	1.43	1.35
50	9	1374	5MC	C2-N3	6.50	1.49	1.36
4	5	4872	2MG	C2-N3	6.49	1.44	1.32
4	5	1517	2MG	C4-N3	6.48	1.49	1.34
4	5	3718	A2M	C6-N6	6.47	1.50	1.34
4	5	4870	OMG	C4-N3	6.47	1.49	1.34
4	5	4335	5MC	C5-C4	6.46	1.49	1.44
50	9	1248	B8N	C4-C5	6.45	1.62	1.47
50	9	1830	UR3	C2-N1	6.44	1.47	1.38
4	5	4483	B8T	C4-N3	6.43	1.43	1.32
4	5	1326	A2M	C6-N6	6.42	1.50	1.34
4	5	2424	OMG	C4-N3	6.42	1.48	1.34
4	5	3867	A2M	C6-N6	6.41	1.50	1.34
4	5	4671	B8T	C4-N3	6.41	1.43	1.32
4	5	4571	A2M	C6-N6	6.41	1.50	1.34
4	5	4530	UR3	C2-N1	6.39	1.47	1.38
6	8	14	OMU	C2-N3	6.39	1.49	1.38
50	9	1842	4AC	C4-N3	6.38	1.43	1.32
4	5	398	A2M	C6-N6	6.37	1.50	1.34
50	9	1031	A2M	C6-N6	6.37	1.50	1.34
4	5	1517	2MG	C2-N2	6.36	1.46	1.33
50	9	174	OMC	C2-N3	6.36	1.49	1.36
50	9	159	A2M	C6-N6	6.36	1.50	1.34
4	5	4523	A2M	C6-N6	6.36	1.50	1.34
50	9	683	OMG	C4-N3	6.35	1.48	1.34
50	9	27	A2M	C6-N6	6.35	1.50	1.34
4	5	1883	OMG	C4-N3	6.34	1.48	1.34
4	5	1871	A2M	C6-N6	6.34	1.50	1.34
4	5	4620	OMU	C2-N3	6.33	1.49	1.38
4	5	3723	A2M	C6-N6	6.33	1.50	1.34
50	9	1678	A2M	C6-N6	6.31	1.50	1.34
50	9	668	A2M	C6-N6	6.31	1.50	1.34
4	5	3792	OMG	C4-N3	6.31	1.48	1.34
4	5	3825	A2M	C6-N6	6.31	1.50	1.34
4	5	1625	OMG	C4-N3	6.30	1.48	1.34
4	5	729	2MG	C2-N2	6.29	1.46	1.33
4	5	2786	B9H	C2-N1	6.26	1.47	1.38
4	5	4371	MHG	C2-N1	6.25	1.46	1.36
4	5	4306	OMU	C2-N3	6.25	1.48	1.38
4	5	2422	OMC	C6-C5	6.24	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	484	A2M	C6-N6	6.22	1.50	1.34
4	5	3782	5MC	C2-N3	6.19	1.48	1.36
50	9	1710	OMC	C2-N3	6.19	1.48	1.36
50	9	1703	OMC	C6-C5	6.18	1.49	1.35
4	5	2363	A2M	C6-N6	6.18	1.50	1.34
4	5	2401	A2M	C6-N6	6.18	1.50	1.34
4	5	1524	A2M	C6-N6	6.16	1.49	1.34
4	5	1534	A2M	C6-N6	6.15	1.49	1.34
4	5	4483	B8T	C2-N3	6.14	1.48	1.36
4	5	1797	E7G	C8-N9	6.14	1.49	1.45
4	5	1659	I4U	C2-N3	6.14	1.48	1.36
4	5	2861	OMC	C2-N3	6.14	1.48	1.36
50	9	1710	OMC	C6-C5	6.13	1.49	1.35
50	9	644	OMG	C4-N3	6.11	1.48	1.34
4	5	373	OMG	C4-N3	6.09	1.48	1.34
50	9	174	OMC	C6-C5	6.09	1.49	1.35
50	9	517	OMC	C6-C5	6.09	1.49	1.35
4	5	4494	OMG	C4-N3	6.09	1.48	1.34
4	5	4196	OMG	C4-N3	6.08	1.48	1.34
4	5	2804	OMC	C6-C5	6.08	1.49	1.35
4	5	4335	5MC	C2-N3	6.08	1.48	1.36
4	5	2365	OMC	C6-C5	6.07	1.49	1.35
4	5	4194	I4U	C1'-N1	-6.07	1.30	1.47
4	5	4370	OMG	C4-N3	6.06	1.48	1.34
50	9	116	OMU	C2-N1	6.06	1.47	1.38
4	5	2861	OMC	C6-C5	6.05	1.49	1.35
4	5	2050	OMG	C4-N3	6.05	1.48	1.34
4	5	2804	OMC	C2-N3	6.04	1.48	1.36
4	5	2773	OMG	C4-N3	6.03	1.48	1.34
4	5	1348	P4U	C2-N3	6.03	1.48	1.36
4	5	3869	OMC	C6-C5	6.03	1.49	1.35
4	5	3887	OMC	C6-C5	6.03	1.49	1.35
50	9	1337	4AC	C2-N3	6.01	1.48	1.36
50	9	1219	B8Q	C2-N3	6.01	1.46	1.35
4	5	1348	P4U	C6-C5	6.00	1.49	1.35
4	5	3887	OMC	C2-N3	6.00	1.48	1.36
50	9	1842	4AC	C6-C5	6.00	1.49	1.35
4	5	4671	B8T	C2-N3	6.00	1.48	1.36
4	5	1605	7MG	C8-N9	5.98	1.49	1.45
50	9	1703	OMC	C2-N3	5.98	1.48	1.36
4	5	4536	OMC	C2-N3	5.97	1.48	1.36
4	5	4415	1MA	C4-N3	5.96	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	814	5MU	C6-C5	5.95	1.44	1.34
4	5	2422	OMC	C2-N3	5.95	1.48	1.36
4	5	4447	5MC	C2-N3	5.94	1.48	1.36
50	9	1337	4AC	C6-C5	5.93	1.48	1.35
4	5	4623	OMG	C4-N3	5.93	1.47	1.34
4	5	2365	OMC	C2-N3	5.92	1.48	1.36
50	9	509	OMG	C4-N3	5.92	1.47	1.34
50	9	1830	UR3	C6-C5	5.92	1.48	1.35
4	5	3909	OMC	C6-C5	5.91	1.48	1.35
4	5	1522	OMG	C4-N3	5.90	1.47	1.34
4	5	4637	OMG	C4-N3	5.90	1.47	1.34
50	9	1842	4AC	C2-N3	5.89	1.48	1.36
4	5	3701	OMC	C6-C5	5.88	1.48	1.35
4	5	4306	OMU	C2-N1	5.88	1.47	1.38
4	5	1316	OMG	C4-N3	5.87	1.47	1.34
50	9	517	OMC	C2-N3	5.86	1.48	1.36
4	5	4530	UR3	C6-C5	5.84	1.48	1.35
4	5	4597	UR3	C6-C5	5.84	1.48	1.35
4	5	3701	OMC	C2-N3	5.83	1.47	1.36
50	9	121	OMU	C2-N1	5.82	1.47	1.38
4	5	4536	OMC	C6-C5	5.81	1.48	1.35
4	5	4483	B8T	C6-C5	5.80	1.48	1.35
4	5	3785	A2M	C6-N6	5.79	1.49	1.34
4	5	1574	B9B	O6-C6	5.79	1.43	1.34
4	5	2364	OMG	C4-N3	5.76	1.47	1.34
50	9	174	OMC	C4-N3	5.76	1.45	1.34
4	5	4194	I4U	C2-N3	5.73	1.47	1.36
4	5	1866	UR3	C6-C5	5.71	1.48	1.35
4	5	2754	B9B	O6-C6	5.69	1.43	1.34
4	5	2380	B8W	C2-N2	5.67	1.45	1.33
4	5	4872	2MG	C4-N3	5.66	1.47	1.34
4	5	2522	7MG	C2-N3	5.64	1.46	1.33
4	5	2861	OMC	C4-N3	5.64	1.45	1.34
6	8	14	OMU	C2-N1	5.64	1.47	1.38
4	5	2297	E7G	C2-N3	5.63	1.46	1.33
4	5	3869	OMC	C2-N3	5.63	1.47	1.36
50	9	1703	OMC	C4-N3	5.62	1.45	1.34
4	5	3887	OMC	C4-N3	5.61	1.45	1.34
4	5	4371	MHG	C4-N3	5.61	1.47	1.34
4	5	2804	OMC	C4-N3	5.60	1.45	1.34
4	5	1909	P7G	C2-N1	5.59	1.46	1.33
4	5	4083	5MU	C6-C5	5.59	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4671	B8T	C6-C5	5.58	1.48	1.35
4	5	4194	I4U	C6-C5	5.58	1.48	1.35
50	9	1710	OMC	C4-N3	5.58	1.45	1.34
4	5	3701	OMC	C4-N3	5.58	1.45	1.34
4	5	2422	OMC	C4-N3	5.57	1.45	1.34
4	5	1659	I4U	C6-C5	5.56	1.48	1.35
4	5	1797	E7G	C2-N3	5.56	1.46	1.33
4	5	3762	B8H	C2-N3	5.54	1.47	1.38
4	5	1605	7MG	C2-N3	5.53	1.46	1.33
4	5	237	B9B	O6-C6	5.49	1.43	1.34
4	5	3880	P7G	C2-N1	5.49	1.46	1.33
50	9	121	OMU	C6-C5	5.48	1.47	1.35
4	5	2297	E7G	C8-N9	5.46	1.49	1.45
50	9	517	OMC	C4-N3	5.44	1.45	1.34
4	5	2365	OMC	C4-N3	5.44	1.45	1.34
4	5	2522	7MG	C4-N3	5.42	1.46	1.34
4	5	4355	E6G	C2-N2	5.42	1.44	1.33
4	5	1605	7MG	C4-N3	5.41	1.46	1.34
4	5	1866	UR3	C2-N1	5.41	1.46	1.38
4	5	4550	7MG	C2-N3	5.41	1.46	1.33
4	5	2424	OMG	C2-N3	5.40	1.46	1.33
4	5	3909	OMC	C2-N3	5.36	1.47	1.36
4	5	3880	P7G	C4-N3	5.35	1.46	1.37
4	5	4306	OMU	C6-C5	5.34	1.47	1.35
4	5	3897	B8K	C3'-C2'	5.33	1.67	1.53
4	5	4870	OMG	C2-N3	5.33	1.46	1.33
4	5	4690	B8K	C4-N3	5.31	1.46	1.34
4	5	1322	1MA	C4-N3	5.30	1.46	1.35
4	5	4129	B8W	C2-N2	5.29	1.44	1.33
50	9	644	OMG	C2-N3	5.28	1.46	1.33
4	5	4690	B8K	C2-N3	5.24	1.45	1.33
4	5	1883	OMG	C2-N3	5.24	1.45	1.33
4	5	4550	7MG	C4-N3	5.23	1.46	1.34
4	5	1909	P7G	C4-N3	5.22	1.46	1.37
4	5	3899	BGH	O4'-C1'	-5.20	1.30	1.42
50	9	116	OMU	C6-C5	5.20	1.47	1.35
4	5	3899	BGH	C2-N3	5.18	1.45	1.33
4	5	3792	OMG	C2-N3	5.16	1.45	1.33
4	5	1659	I4U	C1'-N1	-5.16	1.32	1.47
4	5	1625	OMG	C2-N3	5.15	1.45	1.33
4	5	4620	OMU	C2-N1	5.15	1.46	1.38
50	9	1248	B8N	C2-N1	5.12	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	509	OMG	C2-N3	5.12	1.45	1.33
4	5	3869	OMC	C4-N3	5.11	1.44	1.34
4	5	4620	OMU	C6-C5	5.10	1.46	1.35
4	5	1860	B8H	C2-N3	5.09	1.46	1.38
4	5	3897	B8K	C4-N3	5.09	1.45	1.34
4	5	4690	B8K	C3'-C2'	5.08	1.67	1.53
4	5	4185	B8W	C2-N2	5.08	1.44	1.33
4	5	4529	B8W	C2-N2	5.06	1.44	1.33
4	5	1797	E7G	C4-N9	5.04	1.44	1.37
50	9	683	OMG	C2-N3	5.04	1.45	1.33
4	5	4623	OMG	C2-N3	5.01	1.45	1.33
4	5	1522	OMG	C2-N3	5.01	1.45	1.33
4	5	3899	BGH	C8-N9	5.01	1.49	1.45
4	5	3897	B8K	C2-N3	5.00	1.45	1.33
4	5	3897	B8K	C4-N9	4.99	1.44	1.37
4	5	4472	B8W	C2-N2	4.99	1.43	1.33
4	5	4370	OMG	C2-N3	4.98	1.45	1.33
4	5	2773	OMG	C2-N3	4.98	1.45	1.33
4	5	3899	BGH	C4-N3	4.97	1.45	1.34
4	5	4296	B8H	C2-N3	4.97	1.46	1.38
4	5	4536	OMC	C4-N3	4.96	1.44	1.34
4	5	4196	OMG	C2-N3	4.96	1.45	1.33
50	9	1374	5MC	C5-C4	4.96	1.47	1.44
4	5	4597	UR3	C2-N3	4.95	1.48	1.39
4	5	373	OMG	C2-N3	4.95	1.45	1.33
4	5	2050	OMG	C2-N3	4.95	1.45	1.33
4	5	4194	I4U	C3'-C4'	4.94	1.65	1.53
4	5	3909	OMC	C4-N3	4.93	1.44	1.34
50	9	1374	5MC	C4-N4	4.92	1.46	1.34
50	9	27	A2M	O3'-C3'	-4.86	1.30	1.43
4	5	1456	B8Q	C2-N3	4.86	1.44	1.35
4	5	2297	E7G	C4-N9	4.82	1.43	1.37
4	5	4637	OMG	C2-N3	4.81	1.44	1.33
4	5	2364	OMG	C2-N3	4.80	1.44	1.33
50	9	159	A2M	O3'-C3'	-4.78	1.31	1.43
4	5	4335	5MC	C4-N4	4.78	1.46	1.34
4	5	1316	OMG	C2-N3	4.77	1.44	1.33
4	5	4494	OMG	C2-N3	4.77	1.44	1.33
4	5	3782	5MC	C4-N4	4.74	1.46	1.34
4	5	2522	7MG	C2-N2	4.73	1.45	1.34
4	5	3792	OMG	C2-N2	4.73	1.45	1.34
4	5	1909	P7G	C2-N2	4.71	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	1605	7MG	C2-N2	4.69	1.45	1.34
6	8	14	OMU	C6-C5	4.68	1.45	1.35
4	5	4870	OMG	C2-N2	4.67	1.45	1.34
50	9	1219	B8Q	C2-N1	4.66	1.45	1.38
50	9	683	OMG	C2-N2	4.66	1.45	1.34
4	5	3880	P7G	C2-N2	4.65	1.45	1.34
4	5	1797	E7G	C4-N3	4.65	1.44	1.34
4	5	4690	B8K	C4-N9	4.64	1.43	1.37
4	5	4571	A2M	O3'-C3'	-4.64	1.31	1.43
4	5	4550	7MG	C2-N2	4.63	1.45	1.34
4	5	3825	A2M	O3'-C3'	-4.63	1.31	1.43
4	5	4447	5MC	C6-N1	4.63	1.45	1.38
4	5	4690	B8K	C2-N2	4.62	1.45	1.34
4	5	1316	OMG	C2-N2	4.62	1.45	1.34
4	5	2424	OMG	C2-N2	4.62	1.45	1.34
4	5	4196	OMG	C2-N2	4.61	1.45	1.34
4	5	2364	OMG	C2-N2	4.59	1.44	1.34
4	5	373	OMG	C2-N2	4.57	1.44	1.34
4	5	2297	E7G	C4-N3	4.57	1.44	1.34
50	9	644	OMG	C2-N2	4.56	1.44	1.34
4	5	4370	OMG	C2-N2	4.56	1.44	1.34
4	5	2773	OMG	C2-N2	4.55	1.44	1.34
4	5	4447	5MC	C4-N4	4.55	1.45	1.34
4	5	1625	OMG	C2-N2	4.55	1.44	1.34
4	5	4494	OMG	C2-N2	4.55	1.44	1.34
50	9	1031	A2M	O3'-C3'	-4.55	1.31	1.43
4	5	1909	P7G	C4-N9	4.53	1.42	1.35
4	5	3899	BGH	C2-N2	4.53	1.44	1.34
4	5	1524	A2M	O3'-C3'	-4.53	1.31	1.43
4	5	1326	A2M	O3'-C3'	-4.52	1.31	1.43
4	5	4371	MHG	C4-N9	4.52	1.43	1.37
4	5	2401	A2M	O3'-C3'	-4.50	1.31	1.43
4	5	3899	BGH	O2'-C2'	-4.49	1.31	1.42
4	5	4690	B8K	C71-N7	4.49	1.49	1.39
4	5	3723	A2M	O3'-C3'	-4.49	1.31	1.43
4	5	1883	OMG	C2-N2	4.49	1.44	1.34
4	5	4623	OMG	C2-N2	4.47	1.44	1.34
4	5	398	A2M	O3'-C3'	-4.47	1.31	1.43
4	5	3880	P7G	C4-N9	4.45	1.42	1.35
4	5	1659	I4U	C3'-C4'	4.45	1.64	1.53
4	5	4690	B8K	O4'-C1'	4.44	1.52	1.42
4	5	1522	OMG	C2-N2	4.43	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	1337	4AC	C7-N4	4.43	1.46	1.37
50	9	166	A2M	O3'-C3'	-4.41	1.32	1.43
4	5	4872	2MG	C2-N1	4.41	1.43	1.36
50	9	668	A2M	O3'-C3'	-4.40	1.32	1.43
4	5	1605	7MG	C4-N9	4.39	1.43	1.37
50	9	1678	A2M	O3'-C3'	-4.39	1.32	1.43
50	9	509	OMG	C2-N2	4.38	1.44	1.34
4	5	3897	B8K	C2-N2	4.35	1.44	1.34
50	9	1830	UR3	C2-N3	4.33	1.47	1.39
50	9	484	A2M	O3'-C3'	-4.33	1.32	1.43
4	5	3718	A2M	O3'-C3'	-4.29	1.32	1.43
4	5	4637	OMG	C2-N2	4.27	1.44	1.34
4	5	1871	A2M	O3'-C3'	-4.27	1.32	1.43
50	9	1374	5MC	C2-N1	4.27	1.49	1.40
50	9	1806	M7A	C6-N6	4.27	1.45	1.34
4	5	1534	A2M	O3'-C3'	-4.26	1.32	1.43
4	5	4415	1MA	C2-N1	4.26	1.44	1.35
4	5	4483	B8T	C4-N4	4.25	1.44	1.36
4	5	2363	A2M	O3'-C3'	-4.25	1.32	1.43
4	5	1659	I4U	O4'-C1'	4.24	1.51	1.42
4	5	3897	B8K	C5-N7	4.22	1.48	1.39
50	9	1842	4AC	C7-N4	4.22	1.45	1.37
4	5	3867	A2M	O3'-C3'	-4.21	1.32	1.43
4	5	3909	OMC	O2-C2	-4.20	1.15	1.23
4	5	3782	5MC	C2-N1	4.20	1.48	1.40
4	5	4671	B8T	C4-N4	4.18	1.44	1.36
4	5	4564	M7A	C6-N6	4.18	1.44	1.34
4	5	1348	P4U	O4-C4	4.15	1.40	1.35
4	5	3897	B8K	C71-N7	4.13	1.48	1.39
4	5	1326	A2M	C5-N7	-4.13	1.31	1.39
4	5	4690	B8K	C5-N7	4.12	1.47	1.39
4	5	4129	B8W	O6-C6	4.11	1.41	1.35
4	5	4185	B8W	O6-C6	4.11	1.41	1.35
4	5	237	B9B	O3'-C3'	-4.10	1.32	1.43
4	5	3897	B8K	O4'-C1'	4.10	1.51	1.42
50	9	1842	4AC	C4-N4	4.10	1.46	1.39
50	9	1374	5MC	C6-N1	4.09	1.45	1.38
4	5	1348	P4U	C2-N1	4.09	1.48	1.40
4	5	2050	OMG	C2-N2	4.08	1.43	1.34
4	5	2297	E7G	C2-N2	4.08	1.43	1.34
4	5	3785	A2M	C5-C4	-4.07	1.31	1.39
4	5	4447	5MC	C5-C4	4.07	1.47	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	729	2MG	C5-N7	-4.04	1.31	1.39
50	9	1248	B8N	C6-C5	4.02	1.40	1.35
4	5	1517	2MG	C2-N1	4.01	1.43	1.36
4	5	2363	A2M	C5-N7	-3.99	1.31	1.39
50	9	1337	4AC	C4-N4	3.99	1.45	1.39
4	5	3782	5MC	C6-N1	3.98	1.44	1.38
4	5	4530	UR3	C2-N3	3.97	1.46	1.39
4	5	4523	A2M	O3'-C3'	-3.96	1.33	1.43
4	5	1866	UR3	C2-N3	3.95	1.46	1.39
4	5	4220	6MZ	C5-C4	-3.92	1.32	1.39
4	5	2522	7MG	C4-N9	3.92	1.42	1.37
50	9	1710	OMC	C2-N1	3.90	1.48	1.40
50	9	121	OMU	C4-N3	3.88	1.45	1.38
4	5	3718	A2M	C5-N7	-3.88	1.32	1.39
4	5	3887	OMC	C4-N4	3.88	1.43	1.33
4	5	4872	2MG	O6-C6	-3.85	1.16	1.23
4	5	4472	B8W	C5-C4	-3.84	1.32	1.39
50	9	484	A2M	C5-N7	-3.84	1.32	1.39
4	5	1797	E7G	C2-N2	3.84	1.43	1.34
4	5	4447	5MC	C2-N1	3.83	1.48	1.40
4	5	4335	5MC	C6-N1	3.83	1.44	1.38
4	5	4335	5MC	C2-N1	3.82	1.48	1.40
50	9	1243	PSU	C6-C5	3.82	1.39	1.35
50	9	517	OMC	C2-N1	3.81	1.48	1.40
4	5	4529	B8W	O6-C6	3.81	1.40	1.35
4	5	1871	A2M	C5-N7	-3.80	1.32	1.39
4	5	2422	OMC	C4-N4	3.79	1.43	1.33
50	9	1806	M7A	C5-N7	3.79	1.48	1.39
4	5	4690	B8K	O6-C6	-3.79	1.16	1.23
4	5	4623	OMG	C5-N7	-3.78	1.31	1.39
50	9	517	OMC	C4-N4	3.78	1.43	1.33
50	9	1703	OMC	C4-N4	3.78	1.43	1.33
50	9	1710	OMC	C4-N4	3.78	1.43	1.33
4	5	729	2MG	O6-C6	-3.77	1.16	1.23
4	5	2804	OMC	C4-N4	3.77	1.43	1.33
4	5	1524	A2M	C5-N7	-3.76	1.32	1.39
4	5	4523	A2M	C5-C4	-3.74	1.32	1.39
50	9	27	A2M	C5-N7	-3.74	1.32	1.39
50	9	174	OMC	C2-N1	3.72	1.47	1.40
4	5	1517	2MG	C5-N7	-3.71	1.31	1.39
50	9	116	OMU	C4-N3	3.70	1.45	1.38
4	5	1534	A2M	C8-N9	-3.70	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	668	A2M	C5-C4	-3.70	1.32	1.39
4	5	3869	OMC	C4-N4	3.69	1.42	1.33
4	5	1517	2MG	O6-C6	-3.69	1.16	1.23
50	9	1851	MA6	C6-N6	3.69	1.47	1.36
4	5	2050	OMG	C5-N7	-3.68	1.31	1.39
4	5	3880	P7G	C2-N3	3.67	1.46	1.37
4	5	4472	B8W	O4'-C4'	3.67	1.53	1.45
4	5	729	2MG	C2-N1	3.67	1.42	1.36
50	9	174	OMC	C4-N4	3.66	1.42	1.33
4	5	2365	OMC	C4-N4	3.66	1.42	1.33
4	5	3785	A2M	C5-N7	-3.66	1.32	1.39
4	5	1534	A2M	C5-N7	-3.66	1.32	1.39
50	9	1832	6MZ	C8-N9	-3.65	1.31	1.37
4	5	4472	B8W	O6-C6	3.65	1.40	1.35
4	5	2861	OMC	C4-N4	3.65	1.42	1.33
4	5	398	A2M	C5-N7	-3.65	1.32	1.39
50	9	1031	A2M	C5-C4	-3.64	1.32	1.39
50	9	166	A2M	C5-N7	-3.64	1.32	1.39
4	5	1574	B9B	O3'-C3'	-3.63	1.34	1.43
4	5	3899	BGH	C4-N9	3.63	1.42	1.37
4	5	4355	E6G	C5-C4	-3.62	1.32	1.39
4	5	4671	B8T	C2-N1	3.61	1.47	1.40
4	5	3723	A2M	O2'-C2'	3.61	1.51	1.42
4	5	4355	E6G	O6-C6	3.61	1.40	1.34
4	5	2380	B8W	C5-C4	-3.61	1.32	1.39
50	9	1031	A2M	C5-N7	-3.61	1.32	1.39
4	5	3701	OMC	C4-N4	3.61	1.42	1.33
50	9	1678	A2M	O2'-C2'	3.60	1.51	1.42
4	5	1524	A2M	C5-C4	-3.60	1.32	1.39
4	5	2380	B8W	O4'-C4'	3.59	1.53	1.45
4	5	2401	A2M	C5-N7	-3.59	1.32	1.39
4	5	3792	OMG	C5-N7	-3.58	1.31	1.39
50	9	1842	4AC	C2-N1	3.58	1.47	1.40
4	5	4571	A2M	C5-C4	-3.57	1.32	1.39
4	5	4523	A2M	C5-N7	-3.57	1.32	1.39
50	9	27	A2M	C5-C4	-3.56	1.32	1.39
4	5	1534	A2M	C5-C4	-3.55	1.32	1.39
4	5	2363	A2M	C5-C4	-3.55	1.32	1.39
6	8	14	OMU	O4-C4	-3.55	1.17	1.24
4	5	3825	A2M	C5-N7	-3.54	1.32	1.39
4	5	1625	OMG	C5-N7	-3.53	1.32	1.39
4	5	2754	B9B	O3'-C3'	-3.53	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	8	14	OMU	C4-N3	3.53	1.44	1.38
4	5	2773	OMG	C5-N7	-3.53	1.32	1.39
50	9	644	OMG	C5-N7	-3.53	1.32	1.39
4	5	4494	OMG	C5-N7	-3.52	1.32	1.39
4	5	4370	OMG	C5-N7	-3.52	1.32	1.39
4	5	2861	OMC	C2-N1	3.52	1.47	1.40
4	5	373	OMG	C5-N7	-3.51	1.32	1.39
4	5	2401	A2M	C5-C4	-3.51	1.32	1.39
50	9	1851	MA6	C5-N7	-3.51	1.32	1.39
50	9	1850	MA6	C6-N6	3.50	1.46	1.36
50	9	159	A2M	O2'-C2'	3.50	1.51	1.42
4	5	3867	A2M	O2'-C2'	3.50	1.51	1.42
4	5	1326	A2M	C5-C4	-3.50	1.32	1.39
50	9	509	OMG	C5-N7	-3.50	1.32	1.39
4	5	4536	OMC	C4-N4	3.50	1.42	1.33
4	5	4620	OMU	C4-N3	3.49	1.44	1.38
4	5	4529	B8W	C5-N7	-3.49	1.32	1.39
4	5	1797	E7G	C5-C6	3.49	1.52	1.43
4	5	4335	5MC	O2-C2	-3.48	1.17	1.23
4	5	4550	7MG	C4-N9	3.48	1.42	1.37
4	5	1871	A2M	C5-C4	-3.47	1.32	1.39
4	5	3897	B8K	C2-N1	3.47	1.46	1.37
4	5	4472	B8W	C5-N7	-3.47	1.32	1.39
4	5	4637	OMG	C5-N7	-3.47	1.32	1.39
4	5	3899	BGH	C5-C6	3.46	1.52	1.43
4	5	4129	B8W	O4'-C4'	3.46	1.52	1.45
4	5	4571	A2M	C5-N7	-3.46	1.32	1.39
4	5	2363	A2M	C8-N9	-3.45	1.31	1.37
4	5	4194	I4U	C2-N1	3.45	1.47	1.40
50	9	1703	OMC	O2-C2	-3.44	1.17	1.23
4	5	3718	A2M	O2'-C2'	3.44	1.51	1.42
4	5	4196	OMG	C5-N7	-3.44	1.32	1.39
4	5	3887	OMC	O2-C2	-3.43	1.17	1.23
4	5	1605	7MG	C2-N1	3.43	1.45	1.37
4	5	4483	B8T	C2-N1	3.42	1.47	1.40
50	9	1337	4AC	C5-C4	3.42	1.48	1.41
4	5	4185	B8W	C5-C4	-3.41	1.33	1.39
50	9	166	A2M	C5-C4	-3.41	1.33	1.39
4	5	4194	I4U	O4-C41	-3.41	1.39	1.47
4	5	4194	I4U	O4'-C1'	3.40	1.49	1.42
50	9	668	A2M	C5-N7	-3.40	1.32	1.39
4	5	2297	E7G	C5-C6	3.40	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	484	A2M	C5-C4	-3.39	1.33	1.39
4	5	3723	A2M	C5-N7	-3.39	1.32	1.39
50	9	1337	4AC	C2-N1	3.39	1.47	1.40
4	5	2522	7MG	C5-C6	3.38	1.52	1.43
50	9	1678	A2M	C5-C4	-3.38	1.33	1.39
4	5	3785	A2M	O3'-C3'	-3.38	1.34	1.43
50	9	1703	OMC	C6-N1	3.37	1.46	1.38
4	5	2522	7MG	C2-N1	3.37	1.45	1.37
4	5	4472	B8W	C5-C6	-3.36	1.35	1.41
4	5	4129	B8W	C3'-C2'	3.36	1.62	1.53
4	5	1316	OMG	C4-N9	-3.36	1.29	1.38
4	5	4472	B8W	C3'-C2'	3.35	1.62	1.53
4	5	1883	OMG	C5-N7	-3.35	1.32	1.39
4	5	4447	5MC	O2-C2	-3.35	1.17	1.23
50	9	1832	6MZ	C5-C4	-3.34	1.33	1.39
4	5	4185	B8W	O4'-C4'	3.34	1.52	1.45
4	5	4355	E6G	C5-N7	-3.34	1.33	1.39
4	5	4870	OMG	C5-N7	-3.34	1.32	1.39
4	5	2422	OMC	O2-C2	-3.34	1.17	1.23
4	5	2380	B8W	C3'-C2'	3.34	1.62	1.53
4	5	2365	OMC	C6-N1	3.33	1.46	1.38
4	5	4371	MHG	C8-N7	3.33	1.51	1.45
4	5	1659	I4U	O2-C2	-3.32	1.17	1.23
4	5	1316	OMG	C5-N7	-3.32	1.32	1.39
4	5	3825	A2M	C5-C4	-3.32	1.33	1.39
4	5	4536	OMC	O2-C2	-3.32	1.17	1.23
4	5	4306	OMU	C4-N3	3.31	1.44	1.38
50	9	568	E3C	C4-N3	3.31	1.53	1.48
50	9	1678	A2M	C5-N7	-3.31	1.33	1.39
4	5	398	A2M	C5-C4	-3.31	1.33	1.39
50	9	484	A2M	O2'-C2'	3.31	1.50	1.42
4	5	2297	E7G	C2-N1	3.31	1.45	1.37
50	9	159	A2M	C5-C4	-3.30	1.33	1.39
4	5	2364	OMG	C5-N7	-3.30	1.32	1.39
4	5	4355	E6G	O2'-C2'	3.30	1.51	1.43
50	9	683	OMG	C5-N7	-3.30	1.32	1.39
4	5	1909	P7G	C2-N3	3.29	1.45	1.37
50	9	1850	MA6	C8-N9	-3.29	1.31	1.37
4	5	1522	OMG	C5-N7	-3.29	1.32	1.39
4	5	4872	2MG	C5-N7	-3.28	1.32	1.39
4	5	4564	M7A	C5-N7	3.28	1.46	1.39
4	5	1871	A2M	C8-N9	-3.28	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	517	OMC	C6-N1	3.27	1.45	1.38
4	5	4690	B8K	C2-N1	3.27	1.45	1.37
4	5	1326	A2M	O2'-C2'	3.26	1.50	1.42
4	5	3867	A2M	C5-C4	-3.26	1.33	1.39
4	5	4620	OMU	O4-C4	-3.26	1.18	1.24
4	5	1322	1MA	C5-C6	3.25	1.52	1.43
4	5	398	A2M	O2'-C2'	3.25	1.50	1.42
4	5	3909	OMC	C4-N4	3.24	1.41	1.33
4	5	4296	B8H	O4-C4	-3.24	1.17	1.23
50	9	159	A2M	C5-N7	-3.24	1.33	1.39
4	5	4355	E6G	O3'-C3'	-3.24	1.34	1.43
4	5	4536	OMC	C2-N1	3.23	1.46	1.40
4	5	3897	B8K	O6-C6	-3.23	1.17	1.23
4	5	4529	B8W	C3'-C2'	3.23	1.62	1.53
4	5	1797	E7G	C2-N1	3.23	1.45	1.37
50	9	1703	OMC	C2-N1	3.23	1.46	1.40
50	9	1850	MA6	C5-N7	-3.23	1.33	1.39
4	5	3867	A2M	C5-N7	-3.22	1.33	1.39
4	5	1797	E7G	C8-N7	3.22	1.51	1.45
50	9	121	OMU	O4-C4	-3.21	1.18	1.24
4	5	4483	B8T	O2-C2	-3.21	1.17	1.23
50	9	166	A2M	O2'-C2'	3.21	1.50	1.42
50	9	1031	A2M	O2'-C2'	3.21	1.50	1.42
4	5	3887	OMC	C2-N1	3.20	1.46	1.40
50	9	116	OMU	O4-C4	-3.20	1.18	1.24
4	5	3899	BGH	O6-C6	-3.20	1.17	1.23
4	5	2804	OMC	O2-C2	-3.19	1.17	1.23
50	9	1851	MA6	C8-N9	-3.19	1.32	1.37
4	5	2401	A2M	O2'-C2'	3.19	1.50	1.42
4	5	2861	OMC	C6-N1	3.19	1.45	1.38
4	5	2804	OMC	C2-N1	3.19	1.46	1.40
4	5	1605	7MG	C5-C6	3.19	1.51	1.43
4	5	3701	OMC	C2-N1	3.18	1.46	1.40
4	5	4571	A2M	O2'-C2'	3.18	1.50	1.42
4	5	3723	A2M	C5-C4	-3.18	1.33	1.39
50	9	1842	4AC	C5-C4	3.17	1.48	1.41
4	5	1860	B8H	O4-C4	-3.17	1.17	1.23
4	5	4550	7MG	C5-C6	3.17	1.51	1.43
4	5	2297	E7G	C8-N7	3.17	1.51	1.45
4	5	4185	B8W	C3'-C2'	3.16	1.61	1.53
4	5	2422	OMC	C2-N1	3.16	1.46	1.40
4	5	1524	A2M	O2'-C2'	3.16	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4371	MHG	C5-C6	3.16	1.51	1.43
50	9	174	OMC	C6-N1	3.16	1.45	1.38
4	5	2365	OMC	O2-C2	-3.16	1.17	1.23
4	5	4306	OMU	O4-C4	-3.15	1.18	1.24
4	5	3785	A2M	C3'-C4'	3.15	1.61	1.53
4	5	3785	A2M	O2'-C2'	3.15	1.50	1.42
4	5	2422	OMC	C6-N1	3.15	1.45	1.38
4	5	3825	A2M	O2'-C2'	3.15	1.50	1.42
50	9	121	OMU	O2-C2	-3.14	1.17	1.23
50	9	1710	OMC	C6-N1	3.14	1.45	1.38
4	5	2424	OMG	C5-N7	-3.14	1.32	1.39
4	5	3869	OMC	O2-C2	-3.13	1.17	1.23
4	5	1348	P4U	O2-C2	-3.13	1.17	1.23
4	5	1322	1MA	C2-N1	3.13	1.42	1.35
4	5	1659	I4U	O4-C41	-3.13	1.40	1.47
4	5	4690	B8K	C5-C6	3.13	1.51	1.43
4	5	3718	A2M	C5-C4	-3.12	1.33	1.39
4	5	4185	B8W	C4-N9	-3.12	1.31	1.37
4	5	1871	A2M	O2'-C2'	3.11	1.50	1.42
4	5	3897	B8K	C5-C6	3.11	1.51	1.43
4	5	4529	B8W	O4'-C4'	3.11	1.51	1.45
4	5	3762	B8H	O4-C4	-3.11	1.17	1.23
4	5	1683	PSU	C6-C5	3.11	1.38	1.35
4	5	4529	B8W	C5-C4	-3.11	1.33	1.39
4	5	3825	A2M	C8-N9	-3.10	1.32	1.37
50	9	1851	MA6	C5-C4	-3.10	1.33	1.39
4	5	2861	OMC	O2-C2	-3.10	1.17	1.23
4	5	1456	B8Q	C2-N1	3.08	1.42	1.38
4	5	4083	5MU	O4-C4	-3.07	1.17	1.23
4	5	1909	P7G	C5-C4	3.07	1.44	1.36
4	5	2380	B8W	C5-N7	-3.07	1.33	1.39
4	5	4550	7MG	C2-N1	3.07	1.45	1.37
4	5	2804	OMC	C6-N1	3.07	1.45	1.38
4	5	4523	A2M	O2'-C2'	3.06	1.50	1.42
4	5	1524	A2M	C8-N9	-3.06	1.32	1.37
4	5	3718	A2M	C8-N9	-3.05	1.32	1.37
4	5	3701	OMC	C6-N1	3.05	1.45	1.38
4	5	4571	A2M	C8-N9	-3.05	1.32	1.37
4	5	3792	OMG	O6-C6	-3.05	1.17	1.23
50	9	668	A2M	O2'-C2'	3.04	1.50	1.42
50	9	1374	5MC	O2-C2	-3.04	1.18	1.23
4	5	4483	B8T	C5-C4	3.04	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	3782	5MC	C5-C4	3.04	1.46	1.44
4	5	3867	A2M	C8-N9	-3.04	1.32	1.37
4	5	1326	A2M	C8-N9	-3.03	1.32	1.37
4	5	4494	OMG	C4-N9	-3.03	1.30	1.38
4	5	4129	B8W	C5-C4	-3.03	1.33	1.39
4	5	3909	OMC	C6-N1	3.03	1.45	1.38
4	5	3869	OMC	C6-N1	3.03	1.45	1.38
4	5	3899	BGH	C2-N1	3.02	1.45	1.37
4	5	4194	I4U	O2'-C2'	3.02	1.50	1.43
4	5	3899	BGH	C5-N7	3.02	1.45	1.39
4	5	2363	A2M	O2'-C2'	3.01	1.50	1.42
50	9	1850	MA6	C5-C4	-3.01	1.33	1.39
4	5	3764	PSU	C6-C5	3.01	1.38	1.35
4	5	4494	OMG	O6-C6	-3.01	1.17	1.23
50	9	1710	OMC	O2-C2	-3.00	1.18	1.23
50	9	159	A2M	C8-N9	-3.00	1.32	1.37
50	9	668	A2M	C8-N9	-3.00	1.32	1.37
4	5	4472	B8W	C4-N9	-3.00	1.31	1.37
4	5	1582	PSU	C6-C5	3.00	1.38	1.35
4	5	1534	A2M	O2'-C2'	3.00	1.50	1.42
4	5	4415	1MA	C5-C6	2.99	1.51	1.43
4	5	2380	B8W	C5-C6	-2.99	1.36	1.41
4	5	4531	PSU	C6-C5	2.99	1.38	1.35
4	5	3729	PSU	C6-C5	2.99	1.38	1.35
4	5	1659	I4U	C2-N1	2.98	1.46	1.40
4	5	3782	5MC	O2-C2	-2.98	1.18	1.23
4	5	4371	MHG	C6-N1	2.98	1.44	1.38
50	9	1842	4AC	O2-C2	-2.98	1.18	1.23
50	9	27	A2M	O2'-C2'	2.98	1.50	1.42
50	9	1678	A2M	C8-N9	-2.98	1.32	1.37
50	9	822	PSU	C6-C5	2.98	1.38	1.35
4	5	1316	OMG	O6-C6	-2.98	1.17	1.23
4	5	3887	OMC	C6-N1	2.97	1.45	1.38
4	5	2365	OMC	C2-N1	2.97	1.46	1.40
50	9	517	OMC	O2-C2	-2.97	1.18	1.23
4	5	4671	B8T	O2-C2	-2.95	1.18	1.23
4	5	1522	OMG	O6-C6	-2.94	1.18	1.23
4	5	1605	7MG	O6-C6	-2.93	1.18	1.23
4	5	1659	I4U	O2'-C2'	2.93	1.50	1.43
50	9	1337	4AC	O2-C2	-2.93	1.18	1.23
4	5	4872	2MG	C4-N9	-2.91	1.30	1.38
4	5	1883	OMG	O6-C6	-2.91	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4194	I4U	O2-C2	-2.90	1.18	1.23
4	5	4306	OMU	O2-C2	-2.89	1.17	1.23
50	9	174	OMC	O2-C2	-2.88	1.18	1.23
4	5	2364	OMG	O6-C6	-2.87	1.18	1.23
4	5	4637	OMG	O6-C6	-2.87	1.18	1.23
4	5	4623	OMG	O6-C6	-2.87	1.18	1.23
4	5	4355	E6G	C5-C6	-2.87	1.36	1.41
4	5	3785	A2M	C8-N9	-2.87	1.32	1.37
50	9	683	OMG	O6-C6	-2.86	1.18	1.23
4	5	2050	OMG	O6-C6	-2.86	1.18	1.23
4	5	4185	B8W	C5-N7	-2.86	1.33	1.39
4	5	4220	6MZ	C5-C6	-2.85	1.35	1.41
50	9	1832	6MZ	C4-N9	-2.85	1.31	1.37
4	5	4220	6MZ	C6-N1	-2.85	1.30	1.35
50	9	1337	4AC	C6-N1	2.85	1.44	1.38
50	9	1031	A2M	C8-N9	-2.84	1.32	1.37
4	5	3880	P7G	C5-C4	2.84	1.43	1.36
4	5	4483	B8T	C6-N1	2.84	1.44	1.38
4	5	1625	OMG	O6-C6	-2.84	1.18	1.23
4	5	2380	B8W	O6-C6	2.84	1.39	1.35
4	5	4671	B8T	C5-C4	2.84	1.47	1.41
50	9	568	E3C	C6-N1	2.83	1.44	1.38
4	5	4870	OMG	O6-C6	-2.82	1.18	1.23
50	9	644	OMG	O6-C6	-2.82	1.18	1.23
4	5	3701	OMC	O2-C2	-2.82	1.18	1.23
4	5	3909	OMC	C2-N1	2.82	1.46	1.40
50	9	814	5MU	O4-C4	-2.81	1.18	1.23
4	5	2754	B9B	C5-C4	-2.81	1.34	1.39
4	5	398	A2M	C8-N9	-2.81	1.32	1.37
50	9	166	A2M	C8-N9	-2.81	1.32	1.37
4	5	2424	OMG	O6-C6	-2.80	1.18	1.23
4	5	4220	6MZ	C8-N9	-2.80	1.32	1.37
4	5	4620	OMU	O2-C2	-2.80	1.18	1.23
4	5	1909	P7G	O6-C6	-2.80	1.18	1.23
4	5	4293	PSU	C6-C5	2.80	1.38	1.35
4	5	4536	OMC	C6-N1	2.80	1.44	1.38
4	5	1456	B8Q	O2-C2	-2.80	1.17	1.22
4	5	4129	B8W	C5-N7	-2.79	1.34	1.39
50	9	1219	B8Q	O2-C2	-2.79	1.17	1.22
4	5	3869	OMC	C2-N1	2.79	1.45	1.40
50	9	823	PSU	C6-C5	2.79	1.38	1.35
4	5	237	B9B	C5-C4	-2.79	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	1677	PSU	C6-C5	2.79	1.38	1.35
4	5	2364	OMG	C4-N9	-2.79	1.31	1.38
4	5	1866	UR3	O4-C4	-2.78	1.17	1.23
4	5	4129	B8W	C8-N9	-2.78	1.32	1.37
4	5	2401	A2M	C8-N9	-2.78	1.32	1.37
4	5	4370	OMG	O6-C6	-2.78	1.18	1.23
4	5	4442	PSU	C6-C5	2.78	1.38	1.35
4	5	3899	BGH	C71-N7	2.77	1.45	1.39
4	5	3723	A2M	C8-N9	-2.76	1.32	1.37
4	5	4083	5MU	O2-C2	-2.76	1.18	1.23
4	5	4628	PSU	C6-C5	2.74	1.38	1.35
4	5	373	OMG	C4-N9	-2.74	1.31	1.38
4	5	3897	B8K	C6-N1	2.74	1.44	1.38
50	9	509	OMG	O6-C6	-2.73	1.18	1.23
4	5	3715	PSU	C6-C5	2.72	1.38	1.35
4	5	2773	OMG	O6-C6	-2.72	1.18	1.23
50	9	116	OMU	O2-C2	-2.72	1.18	1.23
4	5	4529	B8W	C8-N9	-2.72	1.32	1.37
4	5	2508	PSU	C6-C5	2.71	1.38	1.35
4	5	1605	7MG	C6-N1	2.71	1.43	1.38
4	5	2522	7MG	O6-C6	-2.70	1.18	1.23
50	9	27	A2M	C8-N9	-2.70	1.33	1.37
4	5	2050	OMG	C4-N9	-2.70	1.31	1.38
50	9	1830	UR3	O2-C2	-2.68	1.17	1.22
4	5	4623	OMG	C4-N9	-2.68	1.31	1.38
4	5	2773	OMG	C2-N1	2.68	1.44	1.37
50	9	1081	PSU	C6-C5	2.68	1.38	1.35
4	5	4220	6MZ	C4-N9	-2.68	1.32	1.37
4	5	1574	B9B	C5-C4	-2.67	1.34	1.39
4	5	4185	B8W	C8-N9	-2.66	1.33	1.37
4	5	4529	B8W	C5-C6	-2.65	1.36	1.41
4	5	1659	I4U	C6-N1	2.63	1.44	1.38
50	9	484	A2M	C8-N9	-2.62	1.33	1.37
4	5	2773	OMG	C4-N9	-2.62	1.31	1.38
4	5	4530	UR3	C6-N1	2.62	1.44	1.38
6	8	14	OMU	O2-C2	-2.61	1.18	1.23
50	9	814	5MU	O2-C2	-2.61	1.18	1.23
4	5	373	OMG	O6-C6	-2.61	1.18	1.23
4	5	2754	B9B	O2'-C2'	2.61	1.49	1.43
4	5	2522	7MG	C6-N1	2.61	1.43	1.38
4	5	3880	P7G	O6-C6	-2.59	1.19	1.23
4	5	4597	UR3	C6-N1	2.59	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4129	B8W	C4-N9	-2.59	1.32	1.37
4	5	4550	7MG	O6-C6	-2.58	1.18	1.23
4	5	4415	1MA	C5-N7	-2.58	1.33	1.39
50	9	1832	6MZ	C6-N1	-2.57	1.31	1.35
50	9	1081	PSU	O4'-C1'	-2.57	1.40	1.43
4	5	4403	PSU	C6-C5	2.56	1.38	1.35
4	5	4530	UR3	O4-C4	-2.56	1.18	1.23
4	5	1866	UR3	O2-C2	-2.56	1.17	1.22
50	9	668	A2M	C4-N9	-2.56	1.32	1.37
4	5	1683	PSU	C4-C5	-2.56	1.37	1.44
4	5	2380	B8W	C8-N9	-2.56	1.33	1.37
4	5	1522	OMG	C4-N9	-2.55	1.31	1.38
4	5	4371	MHG	O6-C6	-2.54	1.18	1.23
4	5	4636	PSU	C4-C5	-2.54	1.37	1.44
4	5	4196	OMG	O6-C6	-2.54	1.18	1.23
50	9	1248	B8N	O4-C4	-2.54	1.17	1.23
50	9	644	OMG	C4-N9	-2.54	1.31	1.38
4	5	4550	7MG	C6-N1	2.54	1.43	1.38
50	9	683	OMG	C2-N1	2.53	1.43	1.37
50	9	612	PSU	C6-C5	2.52	1.38	1.35
4	5	1677	PSU	O4'-C1'	-2.52	1.40	1.43
4	5	4637	OMG	C4-N9	-2.51	1.31	1.38
50	9	1830	UR3	C6-N1	2.51	1.44	1.38
4	5	4530	UR3	O2-C2	-2.51	1.17	1.22
4	5	4450	PSU	C4-C5	-2.51	1.37	1.44
4	5	4472	B8W	C8-N9	-2.51	1.33	1.37
50	9	1842	4AC	C6-N1	2.50	1.44	1.38
4	5	1866	UR3	C6-N1	2.50	1.44	1.38
50	9	509	OMG	C2-N1	2.50	1.43	1.37
50	9	509	OMG	C4-N9	-2.49	1.31	1.38
4	5	4523	A2M	C8-N9	-2.49	1.33	1.37
4	5	237	B9B	O2'-C2'	2.49	1.49	1.43
4	5	2364	OMG	C2-N1	2.48	1.43	1.37
4	5	1797	E7G	O6-C6	-2.47	1.18	1.23
4	5	4690	B8K	C6-N1	2.46	1.43	1.38
4	5	373	OMG	C2-N1	2.44	1.43	1.37
4	5	4196	OMG	C4-N9	-2.44	1.31	1.38
4	5	1574	B9B	O2'-C2'	2.43	1.49	1.43
4	5	4370	OMG	C2-N1	2.42	1.43	1.37
4	5	3899	BGH	C6-N1	2.42	1.43	1.38
4	5	4370	OMG	C4-N9	-2.42	1.31	1.38
4	5	1326	A2M	C6-N1	-2.42	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	1678	A2M	C4-N9	-2.42	1.32	1.37
4	5	2297	E7G	C6-N1	2.41	1.43	1.38
4	5	1322	1MA	C5-N7	-2.41	1.34	1.39
50	9	159	A2M	C5'-C4'	2.41	1.58	1.51
4	5	4293	PSU	C4-C5	-2.41	1.37	1.44
4	5	2380	B8W	C4-N9	-2.39	1.32	1.37
50	9	121	OMU	C6-N1	2.39	1.43	1.38
4	5	4597	UR3	O4-C4	-2.39	1.18	1.23
4	5	3718	A2M	C4-N9	-2.39	1.32	1.37
4	5	4523	A2M	C4-N9	-2.38	1.32	1.37
50	9	644	OMG	C2-N1	2.38	1.43	1.37
50	9	1248	B8N	O2-C2	-2.38	1.18	1.22
4	5	4196	OMG	C2-N1	2.37	1.43	1.37
4	5	2424	OMG	C5-C6	2.37	1.53	1.44
50	9	823	PSU	C4-C5	-2.37	1.37	1.44
4	5	4306	OMU	C6-N1	2.37	1.43	1.38
50	9	159	A2M	C4-N9	-2.37	1.32	1.37
4	5	4571	A2M	C5'-C4'	2.37	1.58	1.51
4	5	4500	PSU	C4-C5	-2.36	1.37	1.44
4	5	1348	P4U	C6-N1	2.36	1.43	1.38
50	9	1830	UR3	O4-C4	-2.35	1.18	1.23
50	9	27	A2M	C5'-C4'	2.35	1.58	1.51
4	5	1797	E7G	C6-N1	2.35	1.43	1.38
4	5	4194	I4U	C6-N1	2.34	1.43	1.38
4	5	1883	OMG	C5-C6	2.33	1.53	1.44
50	9	568	E3C	O2-C2	-2.33	1.18	1.22
4	5	3785	A2M	C4-N9	-2.33	1.32	1.37
4	5	4494	OMG	C2-N1	2.33	1.43	1.37
4	5	2424	OMG	C4-N9	-2.33	1.32	1.38
4	5	1677	PSU	C4-C5	-2.32	1.37	1.44
4	5	2424	OMG	C2-N1	2.31	1.43	1.37
4	5	4671	B8T	C6-N1	2.31	1.43	1.38
4	5	4597	UR3	O2-C2	-2.31	1.18	1.22
50	9	1842	4AC	O7-C7	-2.31	1.18	1.23
50	9	822	PSU	O4'-C1'	-2.30	1.40	1.43
50	9	683	OMG	C4-N9	-2.29	1.32	1.38
4	5	4623	OMG	C2-N1	2.28	1.43	1.37
50	9	1031	A2M	C5'-C4'	2.28	1.58	1.51
4	5	4529	B8W	C4-N9	-2.28	1.32	1.37
4	5	4872	2MG	C5-C6	2.28	1.52	1.44
4	5	3880	P7G	C8-N7	2.28	1.49	1.45
4	5	3867	A2M	C5'-C4'	2.26	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	1524	A2M	C6-N1	-2.25	1.29	1.35
4	5	4450	PSU	O4'-C1'	-2.25	1.40	1.43
50	9	27	A2M	C6-N1	-2.25	1.29	1.35
4	5	2297	E7G	O6-C6	-2.25	1.19	1.23
4	5	1574	B9B	C5'-C4'	2.24	1.58	1.51
4	5	1316	OMG	C2-N1	2.24	1.43	1.37
4	5	3897	B8K	C5-C4	2.24	1.44	1.37
4	5	3723	A2M	C5'-C4'	2.24	1.58	1.51
4	5	4355	E6G	C8-N9	-2.23	1.33	1.37
4	5	3718	A2M	C5'-C4'	2.23	1.58	1.51
4	5	1326	A2M	C4-N9	-2.23	1.33	1.37
4	5	3718	A2M	C3'-C4'	2.23	1.58	1.53
4	5	1625	OMG	C2-N1	2.23	1.43	1.37
4	5	4870	OMG	C2-N1	2.23	1.43	1.37
50	9	1081	PSU	C4-C5	-2.21	1.38	1.44
4	5	1522	OMG	C2-N1	2.21	1.43	1.37
4	5	1871	A2M	C6-N1	-2.21	1.29	1.35
4	5	4628	PSU	O4'-C1'	-2.21	1.40	1.43
4	5	4442	PSU	C4-C5	-2.20	1.38	1.44
4	5	3785	A2M	C5'-C4'	2.20	1.58	1.51
50	9	668	A2M	C6-N1	-2.20	1.29	1.35
4	5	1534	A2M	C6-N1	-2.20	1.29	1.35
50	9	612	PSU	O4'-C1'	-2.20	1.40	1.43
4	5	3792	OMG	C4-N9	-2.20	1.32	1.38
4	5	3718	A2M	C6-N1	-2.20	1.29	1.35
4	5	4500	PSU	O4'-C1'	-2.20	1.40	1.43
50	9	683	OMG	C5-C6	2.19	1.52	1.44
4	5	2363	A2M	C5'-C4'	2.19	1.58	1.51
4	5	4531	PSU	O4'-C1'	-2.19	1.40	1.43
4	5	1909	P7G	C8-N7	2.19	1.49	1.45
4	5	1582	PSU	O4'-C1'	-2.19	1.40	1.43
4	5	2363	A2M	C6-N1	-2.19	1.29	1.35
4	5	4870	OMG	C4-N9	-2.19	1.32	1.38
50	9	119	PSU	C6-C5	2.19	1.37	1.35
4	5	2050	OMG	C2-N1	2.18	1.42	1.37
4	5	4637	OMG	C2-N1	2.18	1.42	1.37
4	5	1871	A2M	C5'-C4'	2.17	1.58	1.51
4	5	4196	OMG	C6-N1	2.17	1.42	1.38
4	5	3785	A2M	C6-N1	-2.17	1.29	1.35
4	5	4564	M7A	C5-C6	-2.16	1.35	1.40
4	5	4571	A2M	C4-N9	-2.16	1.33	1.37
4	5	4500	PSU	C6-C5	2.16	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	1219	B8Q	C4-N3	-2.15	1.45	1.48
50	9	484	A2M	C4-N9	-2.15	1.33	1.37
4	5	1322	1MA	C4-N9	-2.15	1.32	1.38
50	9	27	A2M	C4-N9	-2.15	1.33	1.37
4	5	3792	OMG	C2-N1	2.14	1.42	1.37
4	5	1871	A2M	C4-N9	-2.14	1.33	1.37
4	5	1883	OMG	C2-N1	2.14	1.42	1.37
4	5	4530	UR3	C4-N3	2.14	1.44	1.40
50	9	612	PSU	C4-C5	-2.13	1.38	1.44
4	5	2363	A2M	C4-N9	-2.13	1.33	1.37
4	5	3723	A2M	C4-N9	-2.13	1.33	1.37
4	5	2401	A2M	C4-N9	-2.13	1.33	1.37
4	5	4293	PSU	O4'-C1'	-2.13	1.40	1.43
4	5	4636	PSU	C6-C5	2.13	1.37	1.35
4	5	2050	OMG	C8-N9	-2.12	1.32	1.37
4	5	237	B9B	C5'-C4'	2.12	1.57	1.51
50	9	484	A2M	C6-N1	-2.12	1.29	1.35
4	5	2773	OMG	C6-N1	2.12	1.42	1.38
4	5	3723	A2M	C3'-C4'	2.12	1.58	1.53
4	5	1625	OMG	C4-N9	-2.11	1.32	1.38
4	5	2424	OMG	C6-N1	2.11	1.42	1.38
4	5	398	A2M	C4-N9	-2.10	1.33	1.37
4	5	1522	OMG	C5-C6	2.10	1.52	1.44
4	5	4531	PSU	C4-C5	-2.10	1.38	1.44
4	5	3729	PSU	C4-C5	-2.10	1.38	1.44
4	5	4571	A2M	C6-N1	-2.09	1.29	1.35
50	9	509	OMG	C5-C6	2.09	1.52	1.44
4	5	1883	OMG	C4-N9	-2.09	1.32	1.38
4	5	4636	PSU	O4'-C1'	-2.09	1.41	1.43
50	9	1850	MA6	C5-C6	-2.09	1.36	1.41
4	5	373	OMG	C6-N1	2.09	1.42	1.38
4	5	2401	A2M	C6-N1	-2.08	1.30	1.35
4	5	4306	OMU	C5-C4	2.08	1.48	1.43
4	5	1517	2MG	C5-C6	2.08	1.52	1.44
50	9	683	OMG	C6-N1	2.08	1.42	1.38
4	5	4403	PSU	O4'-C1'	-2.08	1.41	1.43
50	9	1031	A2M	C3'-C4'	2.08	1.58	1.53
4	5	4523	A2M	C6-N1	-2.07	1.30	1.35
4	5	4523	A2M	C3'-C4'	2.07	1.58	1.53
4	5	237	B9B	C5-N7	-2.07	1.35	1.39
4	5	237	B9B	C5-C6	-2.07	1.37	1.41
50	9	484	A2M	C5'-C4'	2.07	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	1456	B8Q	C4-N3	-2.07	1.45	1.48
50	9	159	A2M	C6-N1	-2.07	1.30	1.35
50	9	1678	A2M	C3'-C4'	2.07	1.58	1.53
50	9	823	PSU	O4'-C1'	-2.07	1.41	1.43
50	9	1806	M7A	C5-C6	-2.06	1.35	1.40
4	5	729	2MG	C8-N9	-2.06	1.32	1.37
4	5	2401	A2M	C5'-C4'	2.06	1.57	1.51
50	9	116	OMU	C6-N1	2.06	1.43	1.38
4	5	3825	A2M	C4-N9	-2.05	1.33	1.37
50	9	1031	A2M	C6-N1	-2.05	1.30	1.35
4	5	4442	PSU	O4'-C1'	-2.05	1.41	1.43
4	5	4872	2MG	C6-N1	2.05	1.42	1.38
4	5	4196	OMG	C5-C6	2.05	1.52	1.44
4	5	4296	B8H	C2-N1	-2.04	1.34	1.38
4	5	4370	OMG	C5-C6	2.04	1.52	1.44
50	9	1248	B8N	O4'-C1'	-2.04	1.41	1.43
4	5	4296	B8H	O4'-C1'	-2.04	1.41	1.43
4	5	4450	PSU	C6-C5	2.04	1.37	1.35
4	5	3792	OMG	C5-C6	2.04	1.52	1.44
4	5	1524	A2M	C5'-C4'	2.04	1.57	1.51
4	5	4870	OMG	C5-C6	2.03	1.52	1.44
4	5	1582	PSU	C4-C5	-2.03	1.38	1.44
4	5	1316	OMG	C6-N1	2.03	1.42	1.38
4	5	4355	E6G	C4-N9	-2.03	1.33	1.37
4	5	1322	1MA	CM1-N1	-2.02	1.42	1.46
4	5	2773	OMG	C5-C6	2.02	1.52	1.44
4	5	3867	A2M	C6-N1	-2.02	1.30	1.35
50	9	1678	A2M	C5'-C4'	2.02	1.57	1.51
4	5	4690	B8K	C5-C4	2.01	1.43	1.37
4	5	4628	PSU	C4-C5	-2.01	1.38	1.44
50	9	1337	4AC	O7-C7	-2.01	1.18	1.23
50	9	166	A2M	C5'-C4'	2.01	1.57	1.51
4	5	3825	A2M	C6-N1	-2.01	1.30	1.35

All (1002) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4529	B8W	N2-C2-N3	19.57	146.56	117.22
4	5	2380	B8W	N2-C2-N3	19.30	146.16	117.22
4	5	4185	B8W	N2-C2-N3	18.22	144.54	117.22
4	5	4129	B8W	N2-C2-N3	18.11	144.38	117.22
4	5	4472	B8W	N2-C2-N3	17.85	143.99	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4529	B8W	N2-C2-N1	-16.50	92.48	117.22
4	5	2380	B8W	N2-C2-N1	-15.47	94.02	117.22
4	5	4472	B8W	N2-C2-N1	-14.91	94.86	117.22
4	5	4185	B8W	N2-C2-N1	-14.63	95.29	117.22
4	5	4129	B8W	N2-C2-N1	-14.57	95.37	117.22
4	5	4564	M7A	C5-C6-N6	13.08	145.97	123.75
50	9	1832	6MZ	C4-N9-C8	12.81	119.18	105.74
4	5	4220	6MZ	C4-N9-C8	12.44	118.80	105.74
50	9	1806	M7A	C5-C6-N6	12.28	144.62	123.75
4	5	4529	B8W	C1'-N9-C8	-11.92	100.65	127.09
4	5	2380	B8W	C1'-N9-C8	-11.60	101.35	127.09
4	5	4083	5MU	C5-C4-N3	11.32	125.16	115.32
4	5	4564	M7A	N6-C6-N1	-10.90	94.09	118.38
4	5	4129	B8W	C1'-N9-C8	-10.61	103.54	127.09
4	5	4472	B8W	C1'-N9-C8	-10.60	103.58	127.09
4	5	4529	B8W	C4-N9-C1'	10.60	151.41	126.63
50	9	814	5MU	C5-C4-N3	10.49	124.44	115.32
50	9	1806	M7A	N6-C6-N1	-10.19	95.67	118.38
4	5	4185	B8W	C1'-N9-C8	-10.18	104.50	127.09
4	5	2380	B8W	C4-N9-C1'	9.94	149.89	126.63
50	9	1832	6MZ	N9-C8-N7	-9.92	99.87	113.94
4	5	4129	B8W	O6-C6-C5	9.86	129.06	117.17
4	5	4220	6MZ	N9-C8-N7	-9.47	100.49	113.94
4	5	4472	B8W	C4-N9-C1'	9.41	148.65	126.63
4	5	4129	B8W	C4-N9-C1'	9.35	148.51	126.63
4	5	4220	6MZ	C5-C6-N1	9.17	128.00	118.15
50	9	1850	MA6	N1-C6-N6	-8.71	106.24	116.86
50	9	814	5MU	C5-C6-N1	-8.54	114.04	123.31
50	9	1851	MA6	N1-C6-N6	-8.47	106.54	116.86
4	5	4083	5MU	C5-C6-N1	-8.46	114.12	123.31
4	5	4185	B8W	C4-N9-C1'	8.45	146.40	126.63
4	5	4872	2MG	N1-C2-N2	8.14	124.87	116.56
4	5	4185	B8W	O6-C6-C5	8.14	126.99	117.17
4	5	1517	2MG	C2-N3-C4	7.92	121.91	112.00
4	5	4194	I4U	O4-C4-C5	7.89	121.05	115.45
4	5	237	B9B	C5-C4-N3	-7.86	118.90	127.18
50	9	1832	6MZ	C5-C6-N1	7.70	126.41	118.15
4	5	2786	B9H	C31-N3-C2	7.65	126.69	117.29
4	5	1659	I4U	O4-C4-C5	7.51	120.78	115.45
4	5	4296	B8H	C4-N3-C2	-7.41	117.62	127.34
4	5	4296	B8H	N3-C2-N1	7.40	122.37	115.22
4	5	4129	B8W	C61-O6-C6	7.20	123.93	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4220	6MZ	N3-C4-N9	7.11	139.26	127.17
4	5	4355	E6G	C5-C4-N3	-7.05	119.75	127.18
4	5	3762	B8H	N3-C2-N1	7.02	122.01	115.22
4	5	3762	B8H	C4-N3-C2	-6.96	118.21	127.34
4	5	1517	2MG	C5-C4-N3	-6.94	117.34	128.39
50	9	1219	B8Q	C1'-N1-C2	6.94	128.40	117.04
4	5	1574	B9B	C5-C4-N3	-6.81	120.00	127.18
4	5	4529	B8W	O6-C6-C5	6.78	125.35	117.17
4	5	2754	B9B	C5-C4-N3	-6.74	120.08	127.18
4	5	4872	2MG	C2-N3-C4	6.69	120.37	112.00
50	9	568	E3C	C1'-N1-C2	6.69	127.98	117.04
4	5	4690	B8K	C5-C6-N1	6.64	122.63	110.94
4	5	1860	B8H	C4-N3-C2	-6.63	118.65	127.34
4	5	4690	B8K	C72-C71-N7	6.58	128.52	118.80
4	5	729	2MG	C5-C4-N3	-6.57	117.93	128.39
4	5	1860	B8H	N3-C2-N1	6.55	121.55	115.22
50	9	1806	M7A	N3-C4-N9	6.51	135.02	126.88
4	5	1797	E7G	C4-C5-N7	6.30	110.05	104.94
4	5	1348	P4U	O4-C4-C5	6.26	119.89	115.45
4	5	4371	MHG	C2-N3-C4	6.24	119.81	112.00
4	5	1883	OMG	C5-C4-N3	-6.23	118.47	128.39
4	5	4529	B8W	C5-C4-N3	-6.18	120.67	127.18
50	9	1678	A2M	N3-C2-N1	-6.14	119.29	128.58
50	9	166	A2M	C5-C4-N3	-6.10	118.31	126.72
4	5	3825	A2M	N3-C2-N1	-6.10	119.35	128.58
4	5	2380	B8W	C5-C4-N3	-6.10	120.76	127.18
4	5	4690	B8K	C4-C5-N7	6.09	109.86	104.93
4	5	4523	A2M	N3-C2-N1	-6.06	119.40	128.58
50	9	27	A2M	N3-C2-N1	-6.04	119.43	128.58
4	5	2401	A2M	N3-C2-N1	-6.03	119.45	128.58
4	5	1326	A2M	N3-C2-N1	-6.01	119.48	128.58
50	9	1832	6MZ	N3-C4-N9	6.01	137.38	127.17
4	5	3897	B8K	C4-C5-N7	6.01	109.79	104.93
50	9	1031	A2M	N3-C2-N1	-6.01	119.49	128.58
6	8	14	OMU	C4-N3-C2	-6.00	119.16	126.61
4	5	1534	A2M	C5-C4-N3	-5.99	118.47	126.72
4	5	3899	BGH	C5-C6-N1	5.98	121.47	110.94
4	5	4371	MHG	C4-C5-N7	5.98	109.79	104.94
50	9	1806	M7A	N3-C2-N1	-5.98	119.54	128.58
4	5	3792	OMG	C5-C4-N3	-5.97	118.89	128.39
50	9	1850	MA6	C5-C6-N6	5.95	134.74	125.33
4	5	2297	E7G	C4-C5-N7	5.94	109.76	104.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4564	M7A	N3-C2-N1	-5.93	119.61	128.58
50	9	1850	MA6	N1-C2-N3	-5.91	119.63	128.58
4	5	3723	A2M	N3-C2-N1	-5.91	119.64	128.58
4	5	4220	6MZ	N1-C2-N3	-5.91	119.64	128.58
50	9	166	A2M	N3-C2-N1	-5.90	119.65	128.58
50	9	116	OMU	C4-N3-C2	-5.89	119.30	126.61
4	5	4530	UR3	C4-N3-C2	-5.87	119.86	124.58
4	5	1871	A2M	N3-C2-N1	-5.86	119.71	128.58
4	5	1322	1MA	N1-C2-N3	-5.85	119.05	126.00
4	5	4306	OMU	C4-N3-C2	-5.85	119.35	126.61
4	5	398	A2M	N3-C2-N1	-5.82	119.77	128.58
4	5	4636	PSU	C4-N3-C2	-5.79	118.40	126.37
4	5	3897	B8K	C72-C71-N7	5.78	127.32	118.80
4	5	729	2MG	C2-N3-C4	5.77	119.22	112.00
4	5	3897	B8K	C5-C6-N1	5.75	121.06	110.94
4	5	4500	PSU	C4-N3-C2	-5.75	118.45	126.37
4	5	4442	PSU	N1-C2-N3	5.73	121.21	115.17
4	5	1524	A2M	N3-C2-N1	-5.72	119.92	128.58
4	5	1524	A2M	C5-C4-N3	-5.72	118.85	126.72
50	9	121	OMU	C4-N3-C2	-5.70	119.53	126.61
4	5	3785	A2M	N3-C2-N1	-5.69	119.96	128.58
4	5	4571	A2M	N3-C2-N1	-5.69	119.97	128.58
4	5	1625	OMG	C5-C4-N3	-5.68	119.35	128.39
4	5	3899	BGH	C72-C71-N7	5.67	127.17	118.80
4	5	1534	A2M	N3-C2-N1	-5.66	120.02	128.58
50	9	1851	MA6	N1-C2-N3	-5.65	120.03	128.58
4	5	4564	M7A	N3-C4-N9	5.63	133.92	126.88
50	9	484	A2M	N3-C2-N1	-5.62	120.07	128.58
4	5	3867	A2M	C5-C4-N3	-5.61	118.99	126.72
4	5	4083	5MU	N3-C2-N1	5.57	122.14	114.89
4	5	729	2MG	N9-C4-N3	5.56	137.06	125.95
4	5	4185	B8W	C61-O6-C6	5.55	122.39	117.20
50	9	568	E3C	C4-N3-C2	-5.54	112.01	122.00
50	9	159	A2M	N3-C2-N1	-5.53	120.22	128.58
50	9	668	A2M	N3-C2-N1	-5.53	120.22	128.58
4	5	4472	B8W	C5-C4-N3	-5.52	121.36	127.18
4	5	4355	E6G	C4-C5-C6	5.49	120.61	115.22
4	5	4628	PSU	N1-C2-N3	5.49	120.96	115.17
50	9	822	PSU	N1-C2-N3	5.48	120.95	115.17
50	9	1031	A2M	C5-C4-N3	-5.47	119.18	126.72
50	9	683	OMG	C5-C4-N3	-5.43	119.75	128.39
50	9	1851	MA6	C5-C6-N6	5.41	133.90	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4220	6MZ	C5-C4-N9	-5.41	99.92	105.81
4	5	1909	P7G	C4-C5-N7	5.39	110.34	106.71
4	5	4371	MHG	C5-C6-N1	5.39	120.43	110.94
4	5	4450	PSU	N1-C2-N3	5.38	120.84	115.17
4	5	4415	1MA	C5-C4-N3	-5.37	119.36	127.27
4	5	1605	7MG	C5-C6-N1	5.37	120.39	110.94
4	5	4450	PSU	C4-N3-C2	-5.37	118.98	126.37
50	9	1248	B8N	C5-C4-N3	5.36	125.89	116.15
4	5	4620	OMU	C4-N3-C2	-5.36	119.96	126.61
4	5	2363	A2M	C5-C4-N3	-5.36	119.33	126.72
4	5	4129	B8W	O6-C6-N1	-5.36	111.84	118.96
4	5	4442	PSU	C4-N3-C2	-5.36	118.99	126.37
4	5	2424	OMG	C5-C4-N3	-5.34	119.89	128.39
50	9	1219	B8Q	O2-C2-N3	-5.33	115.48	122.95
4	5	1522	OMG	C5-C4-N3	-5.32	119.92	128.39
50	9	1832	6MZ	N1-C2-N3	-5.31	120.55	128.58
4	5	3867	A2M	N3-C2-N1	-5.30	120.56	128.58
4	5	4637	OMG	C5-C4-N3	-5.30	119.96	128.39
4	5	3729	PSU	N1-C2-N3	5.28	120.74	115.17
4	5	1883	OMG	C2-N3-C4	5.25	121.34	112.30
50	9	1678	A2M	N6-C6-N1	-5.25	106.69	118.38
4	5	2050	OMG	C5-C4-N3	-5.24	120.05	128.39
50	9	509	OMG	C5-C4-N3	-5.24	120.06	128.39
4	5	2401	A2M	C5-C4-N3	-5.24	119.51	126.72
4	5	4870	OMG	C5-C4-N3	-5.22	120.08	128.39
4	5	2363	A2M	N3-C2-N1	-5.22	120.68	128.58
4	5	1517	2MG	C2-N1-C6	-5.22	118.24	124.55
4	5	4185	B8W	N9-C8-N7	-5.21	106.54	113.94
4	5	3825	A2M	C5-C4-N3	-5.21	119.54	126.72
4	5	4500	PSU	N1-C2-N3	5.20	120.66	115.17
4	5	4196	OMG	C5-C4-N3	-5.19	120.13	128.39
50	9	644	OMG	C5-C4-N3	-5.19	120.13	128.39
50	9	568	E3C	O2-C2-N3	-5.18	115.47	122.10
4	5	4636	PSU	N1-C2-N3	5.17	120.62	115.17
4	5	1677	PSU	C4-N3-C2	-5.16	119.27	126.37
4	5	1322	1MA	C5-C4-N3	-5.15	119.69	127.27
4	5	1871	A2M	C5-C4-N3	-5.13	119.65	126.72
4	5	4571	A2M	C5-C4-N3	-5.13	119.66	126.72
4	5	1683	PSU	N1-C2-N3	5.12	120.57	115.17
50	9	27	A2M	C5-C4-N3	-5.12	119.67	126.72
4	5	2522	7MG	C5-C6-N1	5.11	119.94	110.94
4	5	4628	PSU	C4-N3-C2	-5.10	119.34	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4370	OMG	C5-C4-N3	-5.10	120.27	128.39
4	5	4523	A2M	C5-C4-N3	-5.10	119.70	126.72
4	5	1797	E7G	C5-C6-N1	5.09	119.89	110.94
4	5	3718	A2M	C5-C4-N3	-5.08	119.73	126.72
4	5	3867	A2M	N6-C6-N1	-5.07	107.08	118.38
4	5	3792	OMG	C2-N3-C4	5.06	121.02	112.30
4	5	398	A2M	C5-C4-N3	-5.05	119.76	126.72
4	5	4623	OMG	C5-C4-N3	-5.05	120.36	128.39
50	9	822	PSU	C4-N3-C2	-5.05	119.42	126.37
4	5	2363	A2M	N6-C6-N1	-5.04	107.15	118.38
50	9	159	A2M	N6-C6-N1	-5.04	107.16	118.38
50	9	166	A2M	N6-C6-N1	-5.03	107.18	118.38
4	5	1582	PSU	N1-C2-N3	5.01	120.45	115.17
4	5	3785	A2M	C5-C4-N3	-5.01	119.82	126.72
4	5	4403	PSU	N1-C2-N3	4.99	120.44	115.17
4	5	1524	A2M	N6-C6-N1	-4.98	107.28	118.38
50	9	1851	MA6	C5-C4-N3	-4.97	119.87	126.72
4	5	4129	B8W	C5-C4-N3	-4.97	121.95	127.18
4	5	4083	5MU	O4-C4-C5	-4.96	119.24	124.92
4	5	4415	1MA	N1-C2-N3	-4.96	120.10	126.00
4	5	2297	E7G	C5-C6-N1	4.96	119.67	110.94
4	5	3899	BGH	C2-N3-C4	4.96	120.84	112.30
50	9	1219	B8Q	C6-N1-C2	-4.96	117.75	121.80
4	5	1517	2MG	N1-C2-N2	4.95	121.62	116.56
50	9	1248	B8N	C4-N3-C2	-4.95	119.53	125.62
4	5	4872	2MG	C1'-N9-C4	-4.95	111.87	126.49
50	9	814	5MU	N3-C2-N1	4.95	121.33	114.89
4	5	1659	I4U	C5-C4-N3	-4.92	117.63	124.86
50	9	1830	UR3	C1'-N1-C2	4.92	125.10	117.04
50	9	484	A2M	C5-C4-N3	-4.92	119.94	126.72
4	5	1534	A2M	N6-C6-N1	-4.90	107.45	118.38
4	5	4293	PSU	N1-C2-N3	4.89	120.33	115.17
4	5	3880	P7G	C4-C5-N7	4.88	110.00	106.71
4	5	4293	PSU	C4-N3-C2	-4.88	119.65	126.37
4	5	4355	E6G	C61-O6-C6	-4.88	112.73	117.57
50	9	1081	PSU	C4-N3-C2	-4.87	119.66	126.37
4	5	1683	PSU	C4-N3-C2	-4.87	119.66	126.37
4	5	1326	A2M	N6-C6-N1	-4.87	107.53	118.38
50	9	1830	UR3	C4-N3-C2	-4.86	120.67	124.58
4	5	237	B9B	N3-C4-N9	4.86	133.16	126.99
4	5	4523	A2M	N6-C6-N1	-4.85	107.58	118.38
4	5	1456	B8Q	C31-N3-C4	4.84	123.14	114.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	683	OMG	C2-N3-C4	4.82	120.61	112.30
50	9	484	A2M	N6-C6-N1	-4.82	107.64	118.38
4	5	1326	A2M	C5-C4-N3	-4.82	120.08	126.72
4	5	4872	2MG	C2-N1-C6	-4.81	118.73	124.55
4	5	3729	PSU	C4-N3-C2	-4.80	119.75	126.37
4	5	1522	OMG	C2-N3-C4	4.80	120.56	112.30
4	5	3723	A2M	C5-C4-N3	-4.79	120.12	126.72
50	9	119	PSU	C4-N3-C2	-4.78	119.79	126.37
4	5	3785	A2M	N6-C6-N1	-4.76	107.77	118.38
4	5	729	2MG	C2-N1-C6	-4.76	118.80	124.55
4	5	4550	7MG	C5-C6-N1	4.75	119.31	110.94
4	5	1517	2MG	N9-C4-N3	4.75	135.45	125.95
4	5	4472	B8W	C4-C5-C6	4.75	119.88	115.22
4	5	1871	A2M	N6-C6-N1	-4.74	107.81	118.38
4	5	2401	A2M	N6-C6-N1	-4.73	107.83	118.38
4	5	2424	OMG	C2-N3-C4	4.71	120.42	112.30
4	5	4531	PSU	C4-N3-C2	-4.71	119.88	126.37
4	5	3718	A2M	N3-C2-N1	-4.70	121.46	128.58
4	5	4083	5MU	C4-N3-C2	-4.70	121.18	127.34
4	5	1582	PSU	C4-N3-C2	-4.70	119.90	126.37
50	9	1832	6MZ	C1'-N9-C8	-4.70	116.67	127.09
50	9	27	A2M	N6-C6-N1	-4.69	107.93	118.38
4	5	4690	B8K	C2-N3-C4	4.69	120.38	112.30
4	5	4571	A2M	N6-C6-N1	-4.69	107.93	118.38
50	9	1678	A2M	C5-C4-N3	-4.68	120.27	126.72
4	5	4403	PSU	C4-N3-C2	-4.67	119.94	126.37
4	5	1677	PSU	N1-C2-N3	4.67	120.09	115.17
4	5	2364	OMG	C5-C4-N3	-4.67	120.96	128.39
50	9	1081	PSU	N1-C2-N3	4.66	120.09	115.17
50	9	823	PSU	C4-N3-C2	-4.65	119.97	126.37
4	5	373	OMG	C5-C4-N3	-4.64	121.00	128.39
50	9	1850	MA6	N9-C8-N7	-4.64	107.36	113.94
4	5	1605	7MG	C2-N3-C4	4.63	120.28	112.30
4	5	4494	OMG	C2-N3-C4	4.61	120.25	112.30
4	5	2297	E7G	C2-N3-C4	4.60	120.22	112.30
50	9	814	5MU	O4-C4-C5	-4.59	119.66	124.92
4	5	3715	PSU	N1-C2-N3	4.59	120.01	115.17
4	5	398	A2M	N6-C6-N1	-4.58	108.18	118.38
4	5	3825	A2M	N6-C6-N1	-4.57	108.19	118.38
4	5	2773	OMG	C5-C4-N3	-4.57	121.11	128.39
4	5	4872	2MG	C1'-N9-C8	4.57	139.70	126.73
4	5	2508	PSU	C4-N3-C2	-4.56	120.09	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4196	OMG	C2-N3-C4	4.54	120.12	112.30
50	9	1832	6MZ	C5-N7-C8	4.53	110.57	103.45
4	5	4355	E6G	N3-C4-N9	4.53	132.74	126.99
4	5	4597	UR3	C4-N3-C2	-4.52	120.94	124.58
50	9	159	A2M	C5-C4-N3	-4.52	120.49	126.72
4	5	4531	PSU	N1-C2-N3	4.52	119.93	115.17
4	5	4870	OMG	C2-N3-C4	4.51	120.07	112.30
4	5	4637	OMG	C2-N3-C4	4.49	120.04	112.30
4	5	237	B9B	C4-C5-C6	4.49	119.63	115.22
4	5	3715	PSU	C4-N3-C2	-4.49	120.19	126.37
4	5	4494	OMG	C5-C4-N3	-4.47	121.28	128.39
4	5	2508	PSU	N1-C2-N3	4.46	119.88	115.17
4	5	3764	PSU	C4-N3-C2	-4.46	120.22	126.37
4	5	2380	B8W	N9-C8-N7	-4.46	107.61	113.94
4	5	1625	OMG	C2-N3-C4	4.45	119.97	112.30
4	5	4550	7MG	C2-N3-C4	4.45	119.96	112.30
4	5	3718	A2M	N6-C6-N1	-4.44	108.48	118.38
4	5	4185	B8W	C5-C4-N3	-4.44	122.50	127.18
4	5	4129	B8W	N9-C8-N7	-4.44	107.64	113.94
50	9	823	PSU	N1-C2-N3	4.44	119.85	115.17
4	5	3723	A2M	N6-C6-N1	-4.43	108.51	118.38
4	5	2522	7MG	C2-N3-C4	4.43	119.92	112.30
4	5	3785	A2M	N9-C8-N7	-4.42	107.67	113.94
50	9	1248	B8N	C1'-C5-C4	4.41	124.31	117.61
4	5	3899	BGH	C4-C5-N7	4.41	108.50	104.93
50	9	612	PSU	C4-N3-C2	-4.41	120.29	126.37
50	9	668	A2M	C5-C4-N3	-4.40	120.65	126.72
4	5	2364	OMG	C2-N3-C4	4.38	119.84	112.30
4	5	4472	B8W	O6-C6-C5	4.38	122.45	117.17
50	9	1830	UR3	C6-N1-C2	-4.37	118.23	121.80
4	5	1797	E7G	C2-N3-C4	4.36	119.81	112.30
4	5	4370	OMG	C2-N3-C4	4.36	119.80	112.30
4	5	1348	P4U	C5-C4-N3	-4.36	118.47	124.86
4	5	4623	OMG	C2-N3-C4	4.34	119.77	112.30
50	9	668	A2M	N9-C8-N7	-4.33	107.79	113.94
4	5	4220	6MZ	C5-C4-N3	-4.33	120.76	126.72
4	5	4529	B8W	C4-C5-C6	4.32	119.47	115.22
4	5	4129	B8W	O4'-C1'-N9	4.32	116.39	108.09
4	5	1322	1MA	C2-N3-C4	4.32	121.00	112.53
50	9	644	OMG	C2-N3-C4	4.32	119.74	112.30
4	5	3899	BGH	C5-C4-N9	4.31	111.85	106.33
50	9	668	A2M	N6-C6-N1	-4.30	108.80	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4306	OMU	N3-C2-N1	4.30	120.49	114.89
4	5	373	OMG	C2-N3-C4	4.29	119.69	112.30
4	5	1909	P7G	N9-C8-N7	4.29	109.44	103.37
4	5	2754	B9B	C4-C5-C6	4.28	119.43	115.22
4	5	4296	B8H	O2-C2-N1	-4.26	118.47	122.78
4	5	2380	B8W	O6-C6-C5	4.24	122.28	117.17
50	9	1832	6MZ	C5-C4-N9	-4.24	101.19	105.81
4	5	4872	2MG	C5-C4-N3	-4.22	121.67	128.39
4	5	1574	B9B	O6-C6-C5	4.21	122.29	116.73
4	5	2754	B9B	N2-C2-N3	4.20	123.53	117.22
4	5	237	B9B	N2-C2-N3	4.20	123.52	117.22
4	5	1871	A2M	C2'-C1'-N9	-4.20	106.84	113.75
4	5	2754	B9B	N9-C8-N7	-4.19	107.99	113.94
4	5	1574	B9B	N9-C8-N7	-4.18	108.00	113.94
4	5	1316	OMG	C2-N3-C4	4.17	119.48	112.30
50	9	1243	PSU	C6-N1-C2	-4.15	118.84	122.69
4	5	1574	B9B	N2-C2-N3	4.14	123.43	117.22
4	5	1456	B8Q	O2-C2-N3	-4.13	117.16	122.95
50	9	1031	A2M	N6-C6-N1	-4.12	109.20	118.38
50	9	509	OMG	C2-N3-C4	4.11	119.38	112.30
4	5	237	B9B	N9-C8-N7	-4.10	108.12	113.94
4	5	2773	OMG	C2-N3-C4	4.09	119.35	112.30
4	5	2522	7MG	C5-C4-N3	-4.07	120.48	128.13
4	5	1883	OMG	C2-N1-C6	-4.07	117.73	125.11
4	5	3897	B8K	C2-N3-C4	4.07	119.30	112.30
4	5	1883	OMG	N9-C4-N3	4.07	134.08	125.95
4	5	2363	A2M	N9-C8-N7	-4.06	108.17	113.94
6	8	14	OMU	C5-C4-N3	4.06	120.49	114.80
50	9	121	OMU	N3-C2-N1	4.06	120.17	114.89
4	5	4872	2MG	N2-C2-N3	-4.05	115.35	120.51
50	9	1031	A2M	N9-C8-N7	-4.05	108.19	113.94
50	9	1851	MA6	C4-C5-C6	4.04	120.09	115.91
4	5	1574	B9B	N3-C4-N9	4.04	132.12	126.99
4	5	3762	B8H	O2-C2-N1	-4.03	118.70	122.78
4	5	4355	E6G	N9-C8-N7	-4.03	108.22	113.94
4	5	1574	B9B	C4-C5-C6	4.03	119.18	115.22
4	5	4083	5MU	O2-C2-N1	-4.02	117.57	122.80
4	5	4129	B8W	C4-C5-N7	-4.01	105.99	110.58
50	9	612	PSU	N1-C2-N3	4.01	119.40	115.17
50	9	814	5MU	C4-N3-C2	-4.00	122.09	127.34
4	5	1534	A2M	N9-C8-N7	-4.00	108.26	113.94
4	5	4530	UR3	C5-C4-N3	3.99	120.30	115.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1625	OMG	N9-C4-N3	3.99	133.94	125.95
4	5	1524	A2M	N9-C8-N7	-3.98	108.28	113.94
50	9	119	PSU	N1-C2-N3	3.98	119.36	115.17
4	5	4335	5MC	C5-C6-N1	-3.98	118.99	123.31
50	9	159	A2M	N9-C8-N7	-3.97	108.30	113.94
4	5	2754	B9B	N3-C4-N9	3.96	132.02	126.99
4	5	4185	B8W	O6-C6-N1	-3.96	113.70	118.96
4	5	3764	PSU	N1-C2-N3	3.96	119.34	115.17
50	9	1219	B8Q	N3-C2-N1	3.94	122.65	117.16
4	5	1316	OMG	C5-C4-N3	-3.94	122.12	128.39
4	5	4690	B8K	C5-C4-N9	3.94	111.38	106.33
6	8	14	OMU	O4-C4-C5	-3.93	118.38	125.16
4	5	4529	B8W	C61-O6-C6	3.93	120.88	117.20
4	5	2297	E7G	C5-C4-N3	-3.93	120.75	128.13
50	9	166	A2M	C2-N3-C4	3.93	121.42	111.83
4	5	1605	7MG	C5-C4-N3	-3.93	120.76	128.13
4	5	4529	B8W	N9-C8-N7	-3.93	108.37	113.94
50	9	1850	MA6	C2-N1-C6	3.92	121.41	111.83
4	5	2522	7MG	C4-C5-N7	3.92	110.01	105.38
4	5	3897	B8K	N9-C8-N7	3.91	108.47	103.31
50	9	116	OMU	C5-C4-N3	3.91	120.27	114.80
50	9	1678	A2M	N9-C8-N7	-3.89	108.41	113.94
50	9	1832	6MZ	C5-C4-N3	-3.88	121.37	126.72
4	5	4628	PSU	O2-C2-N1	-3.87	118.79	122.79
4	5	2050	OMG	C2-N3-C4	3.87	118.97	112.30
4	5	3792	OMG	N9-C4-N3	3.87	133.69	125.95
50	9	166	A2M	C5'-C4'-C3'	-3.85	101.36	115.21
4	5	4690	B8K	C6-C5-C4	-3.84	115.64	122.40
4	5	4415	1MA	C2-N3-C4	3.84	120.06	112.53
4	5	2522	7MG	C5-C4-N9	3.84	111.25	106.33
50	9	814	5MU	C1'-N1-C2	3.83	124.46	117.59
50	9	116	OMU	N3-C2-N1	3.82	119.86	114.89
4	5	2380	B8W	N3-C4-N9	3.82	131.84	126.99
4	5	1866	UR3	C6-N1-C2	-3.82	118.68	121.80
4	5	4571	A2M	N9-C8-N7	-3.81	108.53	113.94
50	9	1678	A2M	C5-C6-N6	3.81	132.73	123.29
4	5	4523	A2M	N9-C8-N7	-3.81	108.53	113.94
4	5	1860	B8H	O2-C2-N1	-3.81	118.93	122.78
4	5	4472	B8W	N9-C8-N7	-3.81	108.53	113.94
4	5	1326	A2M	C5-C6-N6	3.80	132.71	123.29
4	5	1797	E7G	C5-C4-N3	-3.80	121.00	128.13
4	5	4442	PSU	O2-C2-N1	-3.80	118.87	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	237	B9B	O6-C6-C5	3.79	121.74	116.73
50	9	484	A2M	O4'-C1'-N9	3.79	115.37	108.09
4	5	4550	7MG	C5-C4-N9	3.78	111.17	106.33
4	5	2401	A2M	N9-C8-N7	-3.77	108.58	113.94
50	9	1851	MA6	N9-C8-N7	-3.77	108.58	113.94
4	5	1456	B8Q	N3-C2-N1	3.76	122.40	117.16
4	5	1326	A2M	N9-C8-N7	-3.75	108.61	113.94
4	5	2380	B8W	C61-O6-C6	-3.75	113.69	117.20
50	9	159	A2M	C5-C6-N6	3.73	132.53	123.29
4	5	2363	A2M	C5-C6-N6	3.73	132.52	123.29
4	5	1534	A2M	C2-N3-C4	3.73	120.94	111.83
50	9	822	PSU	O2-C2-N1	-3.71	118.96	122.79
4	5	4529	B8W	N3-C4-N9	3.71	131.70	126.99
4	5	4550	7MG	C4-C5-N7	3.71	109.76	105.38
4	5	2050	OMG	C2-N1-C6	-3.70	118.39	125.11
50	9	568	E3C	C6-N1-C2	-3.70	118.77	121.80
4	5	1316	OMG	N9-C8-N7	-3.70	106.54	113.40
50	9	1248	B8N	N3-C2-N1	3.70	121.24	116.72
4	5	1605	7MG	C4-C5-N7	3.70	109.75	105.38
4	5	2380	B8W	N1-C2-N3	-3.70	119.82	125.48
50	9	1806	M7A	C71-N7-C5	-3.69	108.05	123.44
4	5	2380	B8W	C4-C5-C6	3.68	118.84	115.22
4	5	4494	OMG	N9-C8-N7	-3.68	106.58	113.40
50	9	121	OMU	C5-C4-N3	3.68	119.95	114.80
4	5	1348	P4U	O2-C2-N3	-3.67	116.54	122.33
4	5	4447	5MC	C5-C6-N1	-3.67	119.33	123.31
4	5	3867	A2M	N9-C8-N7	-3.67	108.73	113.94
4	5	3792	OMG	C2-N1-C6	-3.66	118.47	125.11
4	5	4690	B8K	N9-C8-N7	3.66	108.13	103.31
50	9	1243	PSU	N1-C2-N3	3.64	119.01	115.17
4	5	4296	B8H	C5-C4-N3	3.64	124.57	116.55
4	5	3723	A2M	N9-C8-N7	-3.64	108.77	113.94
4	5	4220	6MZ	C2-N3-C4	3.64	120.72	111.83
50	9	1850	MA6	C5-C4-N3	-3.63	121.72	126.72
4	5	1860	B8H	C5-C4-N3	3.63	124.54	116.55
4	5	1534	A2M	N3-C4-N9	3.63	133.33	127.17
4	5	4371	MHG	C5-C4-N3	-3.62	121.33	128.13
4	5	4620	OMU	N3-C2-N1	3.62	119.61	114.89
4	5	1871	A2M	C5-C6-N6	3.62	132.26	123.29
4	5	3867	A2M	C2-N3-C4	3.62	120.68	111.83
50	9	1031	A2M	C2-N3-C4	3.62	120.68	111.83
4	5	1522	OMG	C2-N1-C6	-3.62	118.55	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4550	7MG	C5-C4-N3	-3.62	121.34	128.13
50	9	1031	A2M	N3-C4-N9	3.62	133.32	127.17
50	9	509	OMG	C2-N1-C6	-3.62	118.55	125.11
4	5	1524	A2M	C2-N3-C4	3.62	120.67	111.83
4	5	2401	A2M	C2-N3-C4	3.62	120.66	111.83
4	5	4564	M7A	C2-N3-C4	3.62	120.66	111.83
4	5	4870	OMG	N9-C4-N3	3.61	133.18	125.95
4	5	4129	B8W	C5-N7-C8	3.61	109.12	103.45
4	5	1524	A2M	C4'-O4'-C1'	-3.60	101.51	109.47
4	5	4523	A2M	C2-N3-C4	3.60	120.61	111.83
4	5	4637	OMG	C2-N1-C6	-3.59	118.59	125.11
4	5	4371	MHG	C2-N1-C6	-3.59	120.21	124.55
50	9	484	A2M	C5-C6-N6	3.59	132.17	123.29
4	5	2786	B9H	C4-N3-C2	-3.59	115.54	122.00
4	5	3867	A2M	C5-C6-N6	3.58	132.16	123.29
4	5	3825	A2M	C2-N3-C4	3.58	120.58	111.83
50	9	166	A2M	N3-C4-N9	3.58	133.26	127.17
4	5	4083	5MU	C5M-C5-C4	3.58	122.61	118.78
4	5	3897	B8K	C6-C5-C4	-3.57	116.11	122.40
4	5	4623	OMG	C2-N1-C6	-3.57	118.63	125.11
4	5	4523	A2M	C5-C6-N6	3.57	132.11	123.29
4	5	4129	B8W	C2-N1-C6	3.57	120.92	115.96
4	5	2050	OMG	N9-C4-N3	3.56	133.07	125.95
50	9	568	E3C	C1'-N1-C6	-3.56	113.17	120.78
4	5	3899	BGH	N9-C8-N7	3.54	107.98	103.31
4	5	4529	B8W	C3'-C2'-C1'	3.54	108.15	101.46
4	5	4194	I4U	C5-C4-N3	-3.54	119.67	124.86
4	5	1524	A2M	C5-C6-N6	3.53	132.04	123.29
4	5	3782	5MC	C1'-N1-C6	-3.53	115.34	121.15
4	5	4220	6MZ	C5-N7-C8	3.53	109.00	103.45
50	9	1678	A2M	C2-N3-C4	3.53	120.44	111.83
50	9	166	A2M	C5-C6-N6	3.52	132.01	123.29
4	5	3899	BGH	C5-C4-N3	-3.51	121.54	128.13
50	9	116	OMU	O4-C4-C5	-3.51	119.11	125.16
50	9	644	OMG	N9-C4-N3	3.51	132.97	125.95
4	5	1605	7MG	C5-C4-N9	3.50	110.82	106.33
4	5	4083	5MU	C5M-C5-C6	-3.50	118.11	122.85
4	5	4620	OMU	C5-C4-N3	3.50	119.70	114.80
4	5	398	A2M	N9-C8-N7	-3.50	108.98	113.94
4	5	2380	B8W	C4'-O4'-C1'	-3.49	101.75	109.47
4	5	4185	B8W	C2-N1-C6	3.49	120.81	115.96
4	5	1524	A2M	N3-C4-N9	3.48	133.09	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	27	A2M	C2-N3-C4	3.48	120.33	111.83
4	5	4185	B8W	N1-C2-N3	-3.48	120.15	125.48
4	5	4306	OMU	C5-C4-N3	3.48	119.67	114.80
4	5	4185	B8W	C5-N7-C8	3.48	108.92	103.45
50	9	1832	6MZ	C2-N3-C4	3.47	120.31	111.83
4	5	3825	A2M	N9-C8-N7	-3.47	109.02	113.94
4	5	4872	2MG	N9-C8-N7	-3.47	106.97	113.40
4	5	4185	B8W	C4-C5-N7	-3.46	106.62	110.58
50	9	27	A2M	C5-C6-N6	3.46	131.85	123.29
4	5	2424	OMG	C2-N1-C6	-3.46	118.83	125.11
50	9	1851	MA6	C2-N1-C6	3.44	120.23	111.83
50	9	1851	MA6	C2-N3-C4	3.44	120.22	111.83
4	5	1871	A2M	N9-C8-N7	-3.43	109.07	113.94
4	5	398	A2M	C2-N3-C4	3.43	120.21	111.83
4	5	3718	A2M	C5-C6-N6	3.43	131.78	123.29
4	5	3762	B8H	C5-C4-N3	3.43	124.10	116.55
4	5	4083	5MU	C1'-N1-C6	3.43	126.79	121.15
50	9	1842	4AC	C5-C4-N3	-3.43	117.24	122.60
50	9	683	OMG	N9-C4-N3	3.43	132.80	125.95
50	9	27	A2M	N9-C8-N7	-3.42	109.08	113.94
4	5	2522	7MG	N9-C8-N7	3.42	108.21	103.37
4	5	4129	B8W	C4-C5-C6	3.42	118.58	115.22
4	5	4129	B8W	N1-C2-N3	-3.42	120.25	125.48
4	5	1574	B9B	N3-C2-N1	-3.41	120.26	125.48
50	9	1678	A2M	C2'-C1'-N9	3.41	119.36	113.75
4	5	4571	A2M	C5-C6-N6	3.40	131.71	123.29
50	9	1248	B8N	C31-N3-C4	3.40	121.99	117.18
4	5	3899	BGH	C2'-C1'-N9	-3.40	107.23	114.14
4	5	4571	A2M	C2-N3-C4	3.40	120.13	111.83
50	9	644	OMG	C2-N1-C6	-3.39	118.96	125.11
50	9	1832	6MZ	C9-N6-C6	3.39	125.99	122.85
4	5	4185	B8W	O4'-C1'-N9	3.39	114.59	108.09
4	5	4220	6MZ	C1'-N9-C8	-3.37	119.61	127.09
4	5	4196	OMG	N9-C4-N3	3.37	132.70	125.95
4	5	2773	OMG	N9-C8-N7	-3.37	107.16	113.40
4	5	1871	A2M	C2-N3-C4	3.36	120.04	111.83
4	5	4623	OMG	N9-C4-N3	3.36	132.66	125.95
4	5	3785	A2M	C2-N3-C4	3.35	120.02	111.83
4	5	237	B9B	C61-O6-C6	-3.35	111.83	117.66
4	5	4597	UR3	C5-C4-N3	3.35	119.45	115.04
4	5	4636	PSU	C6-C5-C4	3.34	120.43	118.17
4	5	4185	B8W	C4'-O4'-C1'	-3.34	102.08	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	3723	A2M	C2-N3-C4	3.34	119.98	111.83
4	5	1534	A2M	C5-C6-N6	3.34	131.55	123.29
4	5	1348	P4U	C1'-N1-C2	3.34	125.81	118.44
4	5	4370	OMG	C2-N1-C6	-3.33	119.08	125.11
4	5	1522	OMG	N9-C8-N7	-3.32	107.24	113.40
4	5	3723	A2M	C5-C6-N6	3.32	131.50	123.29
4	5	1322	1MA	N9-C8-N7	-3.32	107.25	113.40
4	5	2297	E7G	C5-C4-N9	3.30	110.57	106.33
4	5	398	A2M	C5-C6-N6	3.30	131.47	123.29
4	5	2363	A2M	C2-N3-C4	3.30	119.90	111.83
4	5	4620	OMU	O4-C4-C5	-3.30	119.47	125.16
4	5	4450	PSU	C6-C5-C4	3.30	120.40	118.17
50	9	166	A2M	N9-C8-N7	-3.30	109.25	113.94
4	5	3729	PSU	C6-N1-C2	-3.30	119.63	122.69
4	5	2050	OMG	N9-C8-N7	-3.30	107.29	113.40
4	5	4129	B8W	C5-C6-N1	-3.29	119.08	123.49
4	5	1625	OMG	C2-N1-C6	-3.29	119.14	125.11
50	9	484	A2M	C2-N3-C4	3.29	119.86	111.83
50	9	644	OMG	N9-C8-N7	-3.28	107.31	113.40
50	9	683	OMG	C2-N1-C6	-3.28	119.17	125.11
4	5	373	OMG	N9-C8-N7	-3.27	107.33	113.40
50	9	668	A2M	C5-C6-N6	3.27	131.39	123.29
4	5	3897	B8K	C5-C4-N9	3.26	110.51	106.33
4	5	1883	OMG	C5-C6-N1	3.26	121.55	113.25
4	5	1326	A2M	C2-N3-C4	3.25	119.78	111.83
4	5	3825	A2M	C5-C6-N6	3.25	131.34	123.29
4	5	2380	B8W	C3'-C2'-C1'	3.25	107.60	101.46
50	9	1850	MA6	C4-C5-C6	3.25	119.27	115.91
4	5	237	B9B	N3-C2-N1	-3.25	120.51	125.48
50	9	1219	B8Q	C1'-N1-C6	-3.24	113.85	120.78
4	5	4196	OMG	C2-N1-C6	-3.23	119.25	125.11
50	9	668	A2M	O4'-C1'-N9	-3.23	101.88	108.09
4	5	4129	B8W	C5-C4-N9	3.23	109.33	105.81
4	5	4494	OMG	C2-N1-C6	-3.23	119.26	125.11
4	5	2754	B9B	N3-C2-N1	-3.22	120.55	125.48
4	5	4371	MHG	N1-C2-N2	3.21	119.84	116.56
50	9	568	E3C	C32-C31-N3	3.21	120.60	112.69
4	5	4083	5MU	C6-N1-C2	-3.21	118.11	121.30
50	9	1219	B8Q	C31-N3-C4	3.20	120.29	114.76
4	5	4185	B8W	C4-N9-C8	3.19	109.09	105.74
50	9	1842	4AC	C6-C5-C4	3.19	120.85	117.00
50	9	668	A2M	C4'-O4'-C1'	-3.19	102.42	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	2786	B9H	O2-C2-N1	-3.19	115.67	122.78
4	5	2401	A2M	C5-C6-N6	3.19	131.18	123.29
4	5	3792	OMG	C5-C6-N1	3.19	121.36	113.25
4	5	2401	A2M	N3-C4-N9	3.19	132.59	127.17
4	5	4637	OMG	N9-C8-N7	-3.19	107.49	113.40
4	5	4442	PSU	C6-N1-C2	-3.18	119.74	122.69
50	9	159	A2M	C2-N3-C4	3.17	119.58	111.83
50	9	814	5MU	C6-N1-C2	-3.17	118.15	121.30
4	5	2364	OMG	C2-N1-C6	-3.17	119.36	125.11
4	5	4185	B8W	C5-C6-N1	-3.16	119.25	123.49
4	5	1866	UR3	C5-C4-N3	3.16	119.20	115.04
4	5	3899	BGH	C6-C5-C4	-3.16	116.85	122.40
4	5	3785	A2M	C5-C6-N6	3.16	131.10	123.29
50	9	119	PSU	O2-C2-N1	-3.15	119.54	122.79
4	5	4870	OMG	N9-C8-N7	-3.15	107.55	113.40
4	5	1522	OMG	N9-C4-N3	3.15	132.25	125.95
4	5	3867	A2M	N3-C4-N9	3.15	132.52	127.17
50	9	159	A2M	C2'-C1'-N9	-3.15	108.58	113.75
50	9	1806	M7A	C2-N3-C4	3.14	119.50	111.83
4	5	3785	A2M	N3-C4-N9	3.14	132.50	127.17
4	5	4293	PSU	C6-N1-C2	-3.13	119.79	122.69
4	5	2424	OMG	N9-C4-N3	3.13	132.21	125.95
4	5	3729	PSU	O2-C2-N1	-3.13	119.56	122.79
4	5	4500	PSU	O2-C2-N1	-3.12	119.57	122.79
4	5	2754	B9B	O6-C6-C5	3.12	120.85	116.73
4	5	4564	M7A	C5-C4-N3	-3.11	119.36	126.56
6	8	14	OMU	N3-C2-N1	3.11	118.94	114.89
4	5	1582	PSU	C6-N1-C2	-3.11	119.81	122.69
50	9	1031	A2M	C2'-C1'-N9	-3.11	108.64	113.75
50	9	121	OMU	O4-C4-C5	-3.11	119.80	125.16
4	5	4494	OMG	O6-C6-C5	-3.11	118.33	126.53
4	5	4623	OMG	N9-C8-N7	-3.10	107.65	113.40
4	5	4185	B8W	C4-C5-C6	3.10	118.27	115.22
4	5	4529	B8W	O6-C6-N1	-3.10	114.84	118.96
50	9	668	A2M	C2-N3-C4	3.09	119.38	111.83
4	5	4335	5MC	CM5-C5-C6	-3.08	118.68	122.85
4	5	4690	B8K	C5-C4-N3	-3.07	122.36	128.13
4	5	4870	OMG	C2-N1-C6	-3.07	119.55	125.11
4	5	4355	E6G	N3-C2-N1	-3.07	120.78	125.48
50	9	1830	UR3	C5-C4-N3	3.06	119.07	115.04
4	5	2363	A2M	C5-N7-C8	3.06	108.26	103.45
4	5	1683	PSU	C6-N1-C2	-3.06	119.85	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4872	2MG	C5-C6-N1	3.06	121.04	113.25
4	5	4494	OMG	C5-C6-N1	3.04	121.00	113.25
4	5	4371	MHG	C5-C4-N9	3.04	110.23	106.33
4	5	4472	B8W	O4'-C1'-N9	3.04	113.92	108.09
4	5	1625	OMG	C1'-N9-C8	-3.03	118.12	126.73
50	9	121	OMU	O2-C2-N1	-3.02	118.86	122.80
4	5	1326	A2M	N3-C4-N9	3.02	132.31	127.17
4	5	1517	2MG	C5-C6-N1	3.02	120.95	113.25
4	5	1797	E7G	C5-C4-N9	3.02	110.20	106.33
4	5	4370	OMG	N9-C4-N3	3.02	131.99	125.95
4	5	1871	A2M	N3-C4-N9	3.02	132.30	127.17
4	5	2363	A2M	N3-C4-N9	3.02	132.29	127.17
50	9	814	5MU	C5M-C5-C6	-3.01	118.77	122.85
4	5	4500	PSU	C6-C5-C4	3.01	120.21	118.17
4	5	398	A2M	N3-C4-N9	3.01	132.28	127.17
4	5	1316	OMG	C2-N1-C6	-3.01	119.66	125.11
4	5	2424	OMG	C5-C6-N1	3.01	120.91	113.25
50	9	568	E3C	C31-N3-C2	3.01	121.26	117.49
4	5	4529	B8W	O4'-C1'-N9	3.00	113.86	108.09
4	5	3785	A2M	C2'-C1'-N9	-3.00	108.81	113.75
4	5	2364	OMG	O6-C6-C5	-3.00	118.61	126.53
4	5	1517	2MG	CM2-N2-C2	-3.00	117.20	123.65
4	5	1883	OMG	N9-C8-N7	-3.00	107.84	113.40
4	5	4529	B8W	C2-N1-C6	3.00	120.13	115.96
4	5	1522	OMG	C5-C6-N1	2.99	120.88	113.25
4	5	1866	UR3	C1'-N1-C2	2.99	121.94	117.04
50	9	1850	MA6	C4-N9-C8	2.99	108.88	105.74
50	9	509	OMG	N9-C4-N3	2.99	131.93	125.95
4	5	4597	UR3	C6-N1-C2	-2.98	119.36	121.80
4	5	4690	B8K	C2-N1-C6	-2.98	119.71	125.11
4	5	1534	A2M	C5-N7-C8	2.98	108.13	103.45
4	5	1625	OMG	O6-C6-C5	-2.98	118.68	126.53
4	5	3715	PSU	O2-C2-N1	-2.97	119.72	122.79
4	5	4523	A2M	O4'-C4'-C3'	-2.97	99.26	105.15
4	5	3825	A2M	N3-C4-N9	2.97	132.22	127.17
4	5	4531	PSU	O2-C2-N1	-2.97	119.73	122.79
4	5	4872	2MG	CM2-N2-C2	-2.96	117.28	123.65
4	5	4370	OMG	N9-C8-N7	-2.96	107.91	113.40
50	9	1850	MA6	C5-N7-C8	2.96	108.10	103.45
4	5	2364	OMG	N9-C8-N7	-2.96	107.92	113.40
4	5	4620	OMU	O2-C2-N1	-2.96	118.95	122.80
4	5	4529	B8W	N1-C2-N3	-2.95	120.95	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1517	2MG	O6-C6-C5	-2.95	118.74	126.53
4	5	4472	B8W	N3-C4-N9	2.94	130.73	126.99
4	5	4472	B8W	C2'-C1'-N9	-2.94	105.99	113.30
50	9	484	A2M	N9-C8-N7	-2.94	109.76	113.94
4	5	1625	OMG	N9-C8-N7	-2.94	107.94	113.40
50	9	1337	4AC	C6-C5-C4	2.94	120.54	117.00
4	5	4523	A2M	C5-C4-N9	2.94	109.02	105.81
50	9	517	OMC	O2-C2-N3	-2.94	117.70	122.33
4	5	3718	A2M	C2-N3-C4	2.93	118.99	111.83
50	9	1710	OMC	O2-C2-N3	-2.93	117.72	122.33
50	9	1850	MA6	C2-N3-C4	2.92	118.96	111.83
50	9	1374	5MC	C5-C6-N1	-2.91	120.15	123.31
50	9	1851	MA6	C5-C4-N9	2.91	108.98	105.81
4	5	2773	OMG	C2-N1-C6	-2.91	119.83	125.11
4	5	4415	1MA	N9-C4-N3	2.91	133.53	126.90
4	5	4623	OMG	O6-C6-C5	-2.91	118.86	126.53
4	5	4403	PSU	C6-N1-C2	-2.90	120.00	122.69
4	5	3792	OMG	N9-C8-N7	-2.89	108.04	113.40
4	5	3899	BGH	C2-N1-C6	-2.89	119.87	125.11
50	9	1830	UR3	O2-C2-N3	-2.89	117.34	121.33
4	5	1797	E7G	C2-N1-C6	-2.89	119.87	125.11
4	5	4623	OMG	C5-C6-N1	2.89	120.60	113.25
4	5	4628	PSU	C6-N1-C2	-2.88	120.02	122.69
4	5	3782	5MC	C5-C4-N4	-2.88	117.33	121.39
4	5	1316	OMG	O6-C6-C5	-2.88	118.92	126.53
50	9	1248	B8N	O4-C4-C5	-2.88	117.59	122.58
4	5	4472	B8W	C5-C6-N1	-2.88	119.63	123.49
50	9	683	OMG	N9-C8-N7	-2.88	108.06	113.40
50	9	1851	MA6	C5-N7-C8	2.88	107.97	103.45
4	5	2380	B8W	C4-N9-C8	2.88	108.76	105.74
4	5	4637	OMG	C5-C6-N1	2.88	120.57	113.25
4	5	4415	1MA	N9-C8-N7	-2.88	108.07	113.40
4	5	4483	B8T	C6-C5-C4	2.87	120.46	117.00
4	5	4870	OMG	C5-C6-N1	2.87	120.55	113.25
4	5	1605	7MG	N9-C8-N7	2.87	107.43	103.37
50	9	814	5MU	O2-C2-N3	-2.87	116.20	121.49
4	5	1316	OMG	C5-C6-N1	2.86	120.54	113.25
4	5	4529	B8W	C5-N7-C8	2.86	107.95	103.45
50	9	1842	4AC	O2-C2-N3	-2.86	117.82	122.33
50	9	1031	A2M	C5-C6-N6	2.86	130.36	123.29
4	5	4571	A2M	N3-C4-N9	2.86	132.02	127.17
4	5	4355	E6G	C6-C5-N7	-2.85	130.48	133.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	822	PSU	C6-N1-C2	-2.85	120.05	122.69
50	9	644	OMG	C5-C6-N1	2.83	120.47	113.25
4	5	3764	PSU	O2-C2-N1	-2.83	119.87	122.79
50	9	612	PSU	O2-C2-N1	-2.83	119.87	122.79
4	5	4472	B8W	N1-C2-N3	-2.83	121.14	125.48
4	5	4196	OMG	O6-C6-C5	-2.83	119.06	126.53
4	5	3715	PSU	C6-N1-C2	-2.82	120.07	122.69
4	5	2424	OMG	N9-C8-N7	-2.82	108.16	113.40
4	5	373	OMG	C2-N1-C6	-2.82	119.99	125.11
4	5	4637	OMG	N9-C4-N3	2.82	131.60	125.95
50	9	683	OMG	C5-C6-N1	2.82	120.43	113.25
4	5	2050	OMG	O6-C6-C5	-2.82	119.10	126.53
4	5	2297	E7G	C2-N1-C6	-2.81	120.01	125.11
4	5	1605	7MG	C2-N1-C6	-2.81	120.02	125.11
4	5	373	OMG	N9-C4-N3	2.81	131.57	125.95
4	5	3785	A2M	O4'-C1'-N9	2.81	113.48	108.09
4	5	237	B9B	C5-N7-C8	2.81	107.86	103.45
4	5	4529	B8W	C5-C6-N1	-2.80	119.74	123.49
4	5	4185	B8W	C2'-C1'-N9	-2.80	106.34	113.30
4	5	2522	7MG	C2-N1-C6	-2.80	120.03	125.11
4	5	2773	OMG	N9-C4-N3	2.80	131.55	125.95
4	5	3723	A2M	N3-C4-N9	2.80	131.93	127.17
50	9	1842	4AC	O7-C7-CM7	-2.80	117.08	122.05
4	5	3782	5MC	C5-C6-N1	-2.79	120.28	123.31
50	9	1832	6MZ	C6-C5-N7	2.79	135.48	132.43
4	5	4450	PSU	O2-C2-N1	-2.79	119.91	122.79
4	5	4355	E6G	C5-C6-N1	-2.79	119.76	123.49
4	5	1574	B9B	O6-C6-N1	-2.78	116.31	120.02
50	9	1851	MA6	C4-C5-N7	-2.76	107.42	110.58
4	5	4185	B8W	C5-C4-N9	2.76	108.82	105.81
4	5	4494	OMG	N9-C4-N3	2.76	131.48	125.95
4	5	2380	B8W	C2-N1-C6	2.76	119.80	115.96
4	5	2861	OMC	O2-C2-N3	-2.76	117.98	122.33
4	5	1582	PSU	O2-C2-N1	-2.75	119.95	122.79
50	9	509	OMG	O6-C6-C5	-2.75	119.27	126.53
4	5	3718	A2M	C5-C4-N9	2.74	108.80	105.81
4	5	2364	OMG	C5-C6-N1	2.74	120.22	113.25
4	5	4196	OMG	N9-C8-N7	-2.73	108.33	113.40
50	9	484	A2M	C5-C4-N9	2.73	108.79	105.81
4	5	237	B9B	C2-N3-C4	2.73	120.82	113.51
4	5	3899	BGH	O6-C6-N1	-2.73	114.99	120.11
4	5	729	2MG	N9-C8-N7	-2.72	108.35	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	729	2MG	O6-C6-C5	-2.72	119.34	126.53
4	5	4472	B8W	C3'-C2'-C1'	2.72	106.60	101.46
4	5	1522	OMG	O6-C6-C5	-2.71	119.38	126.53
4	5	1625	OMG	C5-C6-N1	2.70	120.13	113.25
50	9	668	A2M	C4-N9-C8	2.70	108.58	105.74
4	5	4335	5MC	C1'-N1-C6	-2.70	116.70	121.15
4	5	2773	OMG	O6-C6-C5	-2.70	119.40	126.53
4	5	4370	OMG	O6-C6-C5	-2.70	119.41	126.53
50	9	644	OMG	O6-C6-C5	-2.70	119.41	126.53
4	5	4196	OMG	C5-C6-N1	2.70	120.11	113.25
4	5	4690	B8K	O6-C6-C5	-2.69	121.01	127.62
4	5	1524	A2M	C5-N7-C8	2.68	107.67	103.45
4	5	3867	A2M	C3'-C2'-C1'	2.68	107.94	102.81
4	5	4370	OMG	C5-C6-N1	2.67	120.06	113.25
50	9	683	OMG	O6-C6-C5	-2.67	119.48	126.53
50	9	1337	4AC	C5-C4-N3	-2.67	118.42	122.60
4	5	4293	PSU	O2-C2-N1	-2.67	120.04	122.79
4	5	2364	OMG	N9-C4-N3	2.67	131.29	125.95
4	5	729	2MG	C5-C6-N1	2.67	120.04	113.25
50	9	509	OMG	N9-C8-N7	-2.67	108.46	113.40
4	5	1797	E7G	N9-C8-N7	2.66	107.14	103.37
50	9	27	A2M	N3-C4-N9	2.66	131.70	127.17
50	9	668	A2M	C5'-C4'-C3'	-2.66	105.62	115.21
4	5	2050	OMG	C5-C6-N1	2.66	120.03	113.25
4	5	2861	OMC	C1'-N1-C2	2.66	124.32	118.44
4	5	1574	B9B	C5-N7-C8	2.66	107.63	103.45
4	5	2508	PSU	O2-C2-N1	-2.65	120.05	122.79
4	5	3785	A2M	C5-N7-C8	2.65	107.61	103.45
4	5	237	B9B	O6-C6-N1	-2.64	116.49	120.02
50	9	509	OMG	C5-C6-N1	2.64	119.97	113.25
4	5	4355	E6G	O6-C6-N1	2.63	123.53	120.02
4	5	3897	B8K	C5-C4-N3	-2.62	123.20	128.13
50	9	668	A2M	N3-C4-N9	2.62	131.63	127.17
4	5	373	OMG	O6-C6-C5	-2.62	119.62	126.53
50	9	1219	B8Q	C31-N3-C2	2.62	121.81	117.70
4	5	2424	OMG	O6-C6-C5	-2.61	119.63	126.53
50	9	823	PSU	C6-N1-C2	-2.61	120.27	122.69
50	9	116	OMU	O2-C2-N1	-2.61	119.40	122.80
4	5	4355	E6G	C5-N7-C8	2.61	107.55	103.45
4	5	2380	B8W	C5-N7-C8	2.61	107.55	103.45
4	5	1883	OMG	O6-C6-C5	-2.61	119.66	126.53
50	9	159	A2M	O4'-C4'-C3'	-2.60	99.99	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	3718	A2M	C6-C5-C4	2.60	120.73	117.18
4	5	729	2MG	N2-C2-N3	2.60	123.82	120.51
4	5	4355	E6G	N2-C2-N1	2.60	121.12	117.22
4	5	4637	OMG	O6-C6-C5	-2.60	119.68	126.53
4	5	2363	A2M	C4-C5-N7	-2.59	107.62	110.58
50	9	27	A2M	C5-C4-N9	2.59	108.63	105.81
4	5	3792	OMG	O6-C6-C5	-2.59	119.70	126.53
4	5	4494	OMG	C2'-C1'-N9	-2.59	109.33	114.24
4	5	4447	5MC	CM5-C5-C4	-2.58	116.26	120.51
50	9	1031	A2M	C5-N7-C8	2.58	107.51	103.45
4	5	3880	P7G	N9-C8-N7	2.58	107.03	103.37
4	5	3897	B8K	O3'-C3'-C4'	-2.58	103.66	111.08
4	5	4450	PSU	C6-N1-C2	-2.58	120.30	122.69
4	5	2754	B9B	C5-N7-C8	2.58	107.50	103.45
50	9	166	A2M	C5-N7-C8	2.58	107.50	103.45
50	9	1806	M7A	C4-N9-C1'	-2.57	120.64	126.63
4	5	237	B9B	C3'-C2'-C1'	2.56	106.31	101.46
4	5	4523	A2M	C5-N7-C8	2.56	107.47	103.45
4	5	2363	A2M	C3'-C2'-C1'	2.55	107.68	102.81
4	5	1659	I4U	C6-N1-C2	-2.54	116.16	120.46
4	5	4597	UR3	C1'-N1-C2	2.54	121.20	117.04
50	9	1678	A2M	C5-C4-N9	2.54	108.58	105.81
50	9	1806	M7A	C5-C4-N3	-2.54	120.69	126.56
4	5	3897	B8K	C2-N1-C6	-2.53	120.51	125.11
50	9	822	PSU	O4'-C1'-C2'	2.53	108.65	105.15
4	5	3718	A2M	N3-C4-N9	2.53	131.47	127.17
4	5	4355	E6G	C2-N1-C6	2.53	119.48	115.96
4	5	1534	A2M	C4-C5-N7	-2.52	107.69	110.58
50	9	1337	4AC	O7-C7-CM7	-2.52	117.58	122.05
4	5	4220	6MZ	C9-N6-C6	-2.51	120.52	122.85
4	5	1605	7MG	O6-C6-C5	-2.50	121.47	127.62
4	5	2297	E7G	N9-C8-N7	2.50	106.92	103.37
4	5	4536	OMC	C1'-N1-C2	2.50	123.96	118.44
4	5	373	OMG	C5-C6-N1	2.50	119.61	113.25
50	9	159	A2M	C5-N7-C8	2.49	107.36	103.45
4	5	4306	OMU	O2-C2-N1	-2.49	119.56	122.80
4	5	4671	B8T	C6-C5-C4	2.49	120.00	117.00
4	5	1456	B8Q	C6-N1-C2	-2.48	119.77	121.80
4	5	3792	OMG	C1'-N9-C8	-2.48	119.68	126.73
4	5	729	2MG	C6-C5-C4	2.48	122.56	118.83
4	5	4564	M7A	C71-N7-C5	-2.48	113.12	123.44
50	9	1243	PSU	C4-N3-C2	-2.46	122.98	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	2754	B9B	C4-N9-C1'	-2.46	120.89	126.63
4	5	3867	A2M	C5-C4-N9	2.46	108.49	105.81
50	9	159	A2M	C5-C4-N9	2.46	108.49	105.81
4	5	1574	B9B	C2-N3-C4	2.45	120.08	113.51
4	5	3867	A2M	C5-N7-C8	2.45	107.30	103.45
4	5	2773	OMG	C5-C6-N1	2.45	119.49	113.25
4	5	4870	OMG	O6-C6-C5	-2.45	120.07	126.53
4	5	3909	OMC	O2-C2-N3	-2.44	118.48	122.33
4	5	4371	MHG	N1-C2-N3	-2.44	119.56	123.68
4	5	4296	B8H	O4-C4-N3	-2.44	115.52	120.11
4	5	4571	A2M	C5-N7-C8	2.43	107.27	103.45
50	9	1850	MA6	C4-C5-N7	-2.43	107.80	110.58
4	5	1326	A2M	C5-N7-C8	2.43	107.27	103.45
50	9	1842	4AC	CM7-C7-N4	2.43	119.18	115.27
4	5	1683	PSU	O2-C2-N1	-2.42	120.29	122.79
50	9	668	A2M	C5-N7-C8	2.42	107.26	103.45
4	5	4472	B8W	C2-N1-C6	2.42	119.33	115.96
4	5	1797	E7G	O6-C6-C5	-2.42	121.68	127.62
4	5	4523	A2M	N3-C4-N9	2.42	131.28	127.17
4	5	4636	PSU	C5-C6-N1	-2.42	118.79	122.14
4	5	1517	2MG	N9-C8-N7	-2.41	108.92	113.40
50	9	484	A2M	N3-C4-N9	2.41	131.27	127.17
4	5	3785	A2M	C4-N9-C8	2.41	108.27	105.74
4	5	4185	B8W	C3'-C2'-C1'	2.41	106.02	101.46
4	5	2754	B9B	C4-N9-C8	2.40	108.26	105.74
4	5	1534	A2M	C6-C5-C4	2.40	120.46	117.18
4	5	4550	7MG	N9-C8-N7	2.40	106.77	103.37
4	5	3897	B8K	O6-C6-C5	-2.40	121.72	127.62
4	5	4083	5MU	O4-C4-N3	-2.40	115.60	120.11
50	9	1678	A2M	C5-N7-C8	2.40	107.22	103.45
50	9	166	A2M	C5-C4-N9	2.40	108.42	105.81
4	5	4194	I4U	C2'-C3'-C4'	2.40	107.24	102.61
4	5	2297	E7G	O6-C6-C5	-2.40	121.74	127.62
4	5	4536	OMC	O2-C2-N3	-2.39	118.56	122.33
4	5	1871	A2M	C3'-C2'-C1'	2.39	107.39	102.81
4	5	4872	2MG	O6-C6-C5	-2.39	120.23	126.53
4	5	1456	B8Q	C1'-N1-C2	2.38	120.94	117.04
4	5	4403	PSU	O4'-C1'-C2'	2.38	108.45	105.15
4	5	4531	PSU	C6-N1-C2	-2.38	120.48	122.69
50	9	822	PSU	C6-C5-C4	2.37	119.78	118.17
4	5	2754	B9B	C2-N3-C4	2.37	119.86	113.51
50	9	1081	PSU	O4'-C1'-C2'	2.37	108.43	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	814	5MU	C5M-C5-C4	2.37	121.31	118.78
4	5	3782	5MC	C1'-N1-C2	2.37	123.67	118.44
4	5	4403	PSU	O4-C4-N3	-2.36	115.67	120.11
4	5	4371	MHG	O6-C6-C5	-2.36	121.83	127.62
4	5	4872	2MG	C6-C5-N7	2.36	134.58	130.29
4	5	1574	B9B	C4-N9-C1'	-2.35	121.13	126.63
50	9	823	PSU	O2-C2-N1	-2.35	120.37	122.79
4	5	2363	A2M	C5-C4-N9	2.35	108.37	105.81
4	5	2380	B8W	C2-N3-C4	2.34	119.79	113.51
4	5	4472	B8W	C5-N7-C8	2.34	107.13	103.45
50	9	1678	A2M	N3-C4-N9	2.34	131.14	127.17
50	9	1851	MA6	N3-C4-N9	2.34	131.14	127.17
4	5	1322	1MA	C8-N7-C5	2.34	108.42	104.26
4	5	3764	PSU	C6-N1-C2	-2.33	120.53	122.69
4	5	4636	PSU	O2-C2-N1	-2.33	120.39	122.79
4	5	1316	OMG	N9-C4-N3	2.33	130.60	125.95
50	9	1081	PSU	C6-N1-C2	-2.32	120.54	122.69
50	9	166	A2M	C6-C5-C4	2.32	120.34	117.18
4	5	2363	A2M	C6-C5-C4	2.32	120.34	117.18
4	5	3718	A2M	N9-C8-N7	-2.32	110.65	113.94
4	5	4872	2MG	N1-C2-N3	-2.31	119.78	123.68
4	5	4523	A2M	C2'-C3'-C4'	-2.31	97.02	101.99
4	5	4530	UR3	C3U-N3-C4	2.31	121.08	117.87
4	5	4872	2MG	C4-C5-N7	-2.31	107.01	110.67
4	5	2401	A2M	C5-N7-C8	2.31	107.07	103.45
50	9	814	5MU	C6-C5-C4	2.31	119.92	118.02
4	5	2380	B8W	O4'-C1'-N9	2.30	112.51	108.09
4	5	4571	A2M	C5-C4-N9	2.30	108.32	105.81
50	9	1243	PSU	O2-C2-N1	-2.30	120.42	122.79
4	5	4194	I4U	C4'-O4'-C1'	-2.30	104.40	109.47
4	5	1322	1MA	C1'-N9-C4	-2.29	119.71	126.49
50	9	814	5MU	C1'-N1-C6	-2.29	117.38	121.15
4	5	3867	A2M	O3'-C3'-C2'	-2.29	104.77	111.19
50	9	1337	4AC	N4-C4-N3	2.29	117.59	113.87
50	9	159	A2M	C4-C5-N7	-2.29	107.97	110.58
50	9	166	A2M	C2'-C3'-C4'	2.28	106.90	101.99
4	5	1797	E7G	N9-C4-N3	2.28	128.80	125.46
4	5	1524	A2M	C6-C5-C4	2.28	120.29	117.18
4	5	4355	E6G	C2-N3-C4	2.27	119.60	113.51
4	5	3897	B8K	O4'-C1'-C2'	-2.27	101.76	106.62
50	9	159	A2M	N3-C4-N9	2.27	131.02	127.17
4	5	3825	A2M	C5-N7-C8	2.27	107.01	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1625	OMG	C1'-N9-C4	2.26	133.16	126.49
4	5	3899	BGH	C4'-O4'-C1'	-2.26	104.48	109.47
4	5	3723	A2M	C5-N7-C8	2.26	107.00	103.45
4	5	2508	PSU	C6-N1-C2	-2.25	120.60	122.69
50	9	814	5MU	O4-C4-N3	-2.25	115.88	120.11
4	5	4306	OMU	O4-C4-C5	-2.25	121.28	125.16
50	9	1031	A2M	C6-C5-C4	2.25	120.25	117.18
4	5	1574	B9B	C4-N9-C8	2.25	108.10	105.74
4	5	398	A2M	C2'-C1'-N9	-2.24	110.06	113.75
4	5	1574	B9B	C2-N1-C6	2.24	119.08	115.96
4	5	3785	A2M	C4'-O4'-C1'	-2.24	104.51	109.47
4	5	4690	B8K	C4'-O4'-C1'	-2.24	104.52	109.47
4	5	373	OMG	CM2-O2'-C2'	-2.24	108.72	114.47
4	5	1860	B8H	O4-C4-N3	-2.24	115.91	120.11
4	5	3825	A2M	C5-C4-N9	2.23	108.25	105.81
4	5	1871	A2M	C6-C5-C4	2.23	120.23	117.18
4	5	398	A2M	C5-N7-C8	2.23	106.96	103.45
4	5	3867	A2M	C4-C5-N7	-2.23	108.03	110.58
4	5	4550	7MG	N1-C2-N3	-2.22	119.26	123.32
4	5	4523	A2M	C4-C5-N7	-2.21	108.05	110.58
50	9	1678	A2M	C4-C5-N7	-2.21	108.05	110.58
4	5	4690	B8K	N1-C2-N3	-2.21	119.28	123.32
4	5	2522	7MG	O6-C6-C5	-2.21	122.21	127.62
4	5	4220	6MZ	C4-N9-C1'	-2.20	121.48	126.63
4	5	1316	OMG	C8-N9-C4	2.20	110.15	106.03
4	5	2297	E7G	N9-C4-N3	2.19	128.67	125.46
4	5	4872	2MG	C8-N7-C5	2.19	108.16	104.26
4	5	1871	A2M	C5-N7-C8	2.19	106.89	103.45
4	5	1534	A2M	C5-C4-N9	2.19	108.19	105.81
50	9	644	OMG	C1'-N9-C8	-2.18	120.53	126.73
4	5	4494	OMG	N1-C2-N3	-2.18	119.33	123.32
50	9	27	A2M	C5-N7-C8	2.18	106.88	103.45
4	5	237	B9B	C5'-C4'-C3'	-2.17	107.39	115.21
50	9	484	A2M	C5'-C4'-C3'	-2.17	107.39	115.21
50	9	1842	4AC	C1'-N1-C2	2.16	123.22	118.44
4	5	4870	OMG	C1'-N9-C8	-2.16	120.59	126.73
4	5	4529	B8W	C4-C5-N7	-2.16	108.11	110.58
6	8	14	OMU	O2-C2-N1	-2.16	119.99	122.80
50	9	1248	B8N	O4'-C1'-C2'	2.15	108.13	105.15
4	5	1677	PSU	O4'-C1'-C2'	2.15	108.13	105.15
4	5	4637	OMG	C8-N7-C5	2.15	108.09	104.26
4	5	4530	UR3	O2-C2-N3	-2.15	118.36	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	2773	OMG	C8-N7-C5	2.15	108.09	104.26
50	9	1842	4AC	N4-C4-N3	2.14	117.35	113.87
50	9	1248	B8N	O4-C4-N3	-2.14	116.51	119.99
4	5	3782	5MC	N4-C4-N3	2.13	122.37	118.51
4	5	4129	B8W	C2-N3-C4	2.13	119.22	113.51
50	9	612	PSU	C6-N1-C2	-2.13	120.72	122.69
4	5	3899	BGH	N1-C2-N3	-2.13	119.43	123.32
4	5	4371	MHG	C6-C5-C4	-2.13	118.66	122.40
4	5	3899	BGH	O4'-C4'-C3'	-2.12	100.94	105.15
4	5	4872	2MG	C5-C4-N9	2.12	109.45	105.66
4	5	3867	A2M	O3'-C3'-C4'	-2.12	104.99	111.08
4	5	4550	7MG	O6-C6-C5	-2.12	122.42	127.62
4	5	1322	1MA	N9-C4-N3	2.11	131.71	126.90
4	5	4185	B8W	O4'-C4'-C3'	-2.11	100.96	105.15
4	5	4442	PSU	C6-C5-C4	2.10	119.59	118.17
4	5	3867	A2M	C6-C5-C4	2.10	120.05	117.18
50	9	1374	5MC	C5-C4-N3	-2.10	119.60	121.75
4	5	4529	B8W	C4-N9-C8	2.10	107.94	105.74
4	5	4550	7MG	C6-C5-C4	-2.09	118.72	122.40
4	5	3762	B8H	O4-C4-N3	-2.09	116.17	120.11
4	5	4597	UR3	C3U-N3-C2	2.09	120.97	117.33
4	5	4129	B8W	O4'-C4'-C3'	-2.08	101.02	105.15
4	5	4403	PSU	O2-C2-N1	-2.08	120.64	122.79
4	5	4571	A2M	C6-C5-C4	2.08	120.02	117.18
4	5	1517	2MG	N1-C2-N3	-2.08	120.18	123.68
4	5	1677	PSU	C6-C5-C4	2.08	119.58	118.17
50	9	1031	A2M	C4-N9-C8	2.08	107.92	105.74
4	5	2422	OMC	O2-C2-N3	-2.07	119.06	122.33
4	5	4371	MHG	C71-C72-C73	-2.07	108.59	114.13
4	5	1605	7MG	C6-C5-C4	-2.07	118.76	122.40
4	5	237	B9B	C4-C5-N7	-2.07	108.22	110.58
4	5	1524	A2M	C5-C4-N9	2.07	108.07	105.81
4	5	1866	UR3	C4-N3-C2	-2.07	122.92	124.58
4	5	4129	B8W	C4-N9-C8	2.06	107.91	105.74
50	9	1081	PSU	O2-C2-N1	-2.06	120.66	122.79
4	5	4194	I4U	O4'-C1'-C2'	-2.06	102.21	106.62
4	5	3785	A2M	O3'-C3'-C4'	2.06	117.00	111.08
4	5	1677	PSU	O2-C2-N1	-2.06	120.66	122.79
4	5	4523	A2M	O4'-C1'-N9	2.06	112.04	108.09
4	5	1326	A2M	C6-C5-C4	2.06	119.99	117.18
4	5	1316	OMG	N1-C2-N3	-2.06	119.56	123.32
4	5	4529	B8W	C2-N3-C4	2.05	119.01	113.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4185	B8W	C2-N3-C4	2.05	118.99	113.51
4	5	1871	A2M	C5-C4-N9	2.04	108.04	105.81
50	9	159	A2M	C4-N9-C8	2.04	107.88	105.74
4	5	4550	7MG	C2-N1-C6	-2.04	121.41	125.11
4	5	1797	E7G	C6-C5-C4	-2.04	118.81	122.40
4	5	4371	MHG	N9-C4-N3	2.04	128.44	125.46
50	9	119	PSU	C6-N1-C2	-2.04	120.80	122.69
4	5	1522	OMG	C8-N7-C5	2.03	107.89	104.26
4	5	4483	B8T	O2-C2-N3	-2.03	119.13	122.33
4	5	1677	PSU	C6-N1-C2	-2.03	120.81	122.69
4	5	1322	1MA	C4-C5-N7	-2.03	107.45	110.67
50	9	668	A2M	C3'-C2'-C1'	2.03	106.69	102.81
4	5	3887	OMC	O2-C2-N3	-2.02	119.14	122.33
50	9	1678	A2M	O3'-C3'-C2'	-2.02	105.52	111.19
50	9	484	A2M	C5-N7-C8	2.02	106.63	103.45
4	5	1605	7MG	N9-C4-N3	2.02	128.42	125.46
4	5	1883	OMG	C8-N7-C5	2.02	107.86	104.26
4	5	4472	B8W	C6-C5-N7	-2.02	131.45	133.82
4	5	237	B9B	C4-N9-C8	2.01	107.85	105.74
4	5	4442	PSU	O4'-C1'-C2'	2.01	107.94	105.15
4	5	3880	P7G	O4'-C1'-N9	-2.01	106.55	109.30
4	5	2786	B9H	C32-C31-N3	2.01	116.67	112.53
4	5	4636	PSU	O4'-C1'-C2'	2.01	107.93	105.15
4	5	1348	P4U	C1'-N1-C6	-2.01	116.48	120.78
50	9	484	A2M	C6-C5-C4	2.01	119.92	117.18
4	5	2754	B9B	C2-N1-C6	2.00	118.75	115.96
4	5	4571	A2M	C4-C5-N7	-2.00	108.29	110.58
4	5	4296	B8H	O4'-C1'-C2'	2.00	107.92	105.15
4	5	4494	OMG	C8-N9-C4	2.00	109.78	106.03
4	5	4500	PSU	C5-C6-N1	-2.00	119.36	122.14
4	5	4571	A2M	O3'-C3'-C4'	-2.00	105.34	111.08

There are no chirality outliers.

All (192) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	333	MLZ	N-CA-CB-CG
9	C	333	MLZ	C-CA-CB-CG
9	C	333	MLZ	CD-CE-NZ-CM
4	5	237	B9B	C5-C6-O6-C61
4	5	237	B9B	N1-C6-O6-C61
4	5	237	B9B	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	5	237	B9B	O4'-C4'-C5'-O5'
4	5	1348	P4U	N3-C4-O4-C41
4	5	1348	P4U	O4'-C4'-C5'-O5'
4	5	1574	B9B	C5-C6-O6-C61
4	5	1574	B9B	N1-C6-O6-C61
4	5	1797	E7G	O4'-C4'-C5'-O5'
4	5	1866	UR3	O4'-C4'-C5'-O5'
4	5	2364	OMG	O4'-C4'-C5'-O5'
4	5	2380	B8W	C5-C6-O6-C61
4	5	2380	B8W	N1-C6-O6-C61
4	5	2786	B9H	C32-C31-N3-C2
4	5	3762	B8H	O4'-C4'-C5'-O5'
4	5	3792	OMG	O4'-C4'-C5'-O5'
4	5	3897	B8K	O4'-C4'-C5'-O5'
4	5	3899	BGH	O4'-C4'-C5'-O5'
4	5	4129	B8W	C5-C6-O6-C61
4	5	4129	B8W	N1-C6-O6-C61
4	5	4185	B8W	C5-C6-O6-C61
4	5	4185	B8W	N1-C6-O6-C61
4	5	4194	I4U	O4'-C4'-C5'-O5'
4	5	4220	6MZ	C5-C6-N6-C9
4	5	4220	6MZ	N1-C6-N6-C9
4	5	4306	OMU	C1'-C2'-O2'-CM2
4	5	4355	E6G	C5-C6-O6-C61
4	5	4355	E6G	N1-C6-O6-C61
4	5	4371	MHG	C2'-C1'-N9-C8
4	5	4371	MHG	C71-C72-C73-C75
4	5	4403	PSU	C2'-C1'-C5-C4
4	5	4403	PSU	O4'-C1'-C5-C4
4	5	4403	PSU	O4'-C1'-C5-C6
4	5	4447	5MC	C2'-C1'-N1-C2
4	5	4447	5MC	C2'-C1'-N1-C6
4	5	4450	PSU	O4'-C4'-C5'-O5'
4	5	4472	B8W	C5-C6-O6-C61
4	5	4472	B8W	N1-C6-O6-C61
4	5	4500	PSU	O4'-C4'-C5'-O5'
4	5	4529	B8W	C5-C6-O6-C61
4	5	4529	B8W	N1-C6-O6-C61
4	5	4637	OMG	O4'-C4'-C5'-O5'
4	5	4870	OMG	O4'-C4'-C5'-O5'
4	5	4872	2MG	O4'-C4'-C5'-O5'
6	8	14	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
44	m	72	MLZ	CD-CE-NZ-CM
50	9	116	OMU	C1'-C2'-O2'-CM2
50	9	116	OMU	C3'-C4'-C5'-O5'
50	9	116	OMU	O4'-C4'-C5'-O5'
50	9	121	OMU	O4'-C4'-C5'-O5'
50	9	166	A2M	O4'-C4'-C5'-O5'
50	9	166	A2M	C3'-C4'-C5'-O5'
50	9	568	E3C	O4'-C1'-N1-C2
50	9	568	E3C	O4'-C1'-N1-C6
50	9	668	A2M	O4'-C4'-C5'-O5'
50	9	668	A2M	C3'-C4'-C5'-O5'
50	9	683	OMG	O4'-C4'-C5'-O5'
50	9	683	OMG	C3'-C4'-C5'-O5'
50	9	1248	B8N	O4'-C4'-C5'-O5'
50	9	1703	OMC	O4'-C4'-C5'-O5'
50	9	1830	UR3	O4'-C1'-N1-C6
50	9	1830	UR3	O4'-C1'-N1-C2
50	9	1832	6MZ	C5-C6-N6-C9
50	9	1832	6MZ	N1-C6-N6-C9
50	9	1851	MA6	O4'-C4'-C5'-O5'
50	9	1851	MA6	C3'-C4'-C5'-O5'
4	5	398	A2M	O4'-C4'-C5'-O5'
4	5	1348	P4U	C3'-C4'-C5'-O5'
4	5	1582	PSU	C3'-C4'-C5'-O5'
4	5	2380	B8W	C3'-C4'-C5'-O5'
4	5	2380	B8W	O4'-C4'-C5'-O5'
4	5	2424	OMG	O4'-C4'-C5'-O5'
4	5	2424	OMG	C3'-C4'-C5'-O5'
4	5	3729	PSU	O4'-C4'-C5'-O5'
4	5	3792	OMG	C3'-C4'-C5'-O5'
4	5	3867	A2M	O4'-C4'-C5'-O5'
4	5	3867	A2M	C3'-C4'-C5'-O5'
4	5	3880	P7G	O4'-C4'-C5'-O5'
4	5	3899	BGH	C3'-C4'-C5'-O5'
4	5	4129	B8W	O4'-C4'-C5'-O5'
4	5	4355	E6G	O4'-C4'-C5'-O5'
4	5	4415	1MA	C3'-C4'-C5'-O5'
4	5	4450	PSU	C3'-C4'-C5'-O5'
4	5	4500	PSU	C3'-C4'-C5'-O5'
4	5	4523	A2M	O4'-C4'-C5'-O5'
4	5	4529	B8W	O4'-C4'-C5'-O5'
4	5	4636	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	5	4636	PSU	O4'-C4'-C5'-O5'
50	9	121	OMU	C3'-C4'-C5'-O5'
50	9	159	A2M	O4'-C4'-C5'-O5'
50	9	159	A2M	C3'-C4'-C5'-O5'
50	9	1243	PSU	C3'-C4'-C5'-O5'
50	9	1243	PSU	O4'-C4'-C5'-O5'
4	5	1582	PSU	O4'-C4'-C5'-O5'
4	5	2364	OMG	C3'-C4'-C5'-O5'
4	5	4185	B8W	O4'-C4'-C5'-O5'
4	5	4415	1MA	O4'-C4'-C5'-O5'
4	5	4637	OMG	C3'-C4'-C5'-O5'
4	5	4870	OMG	C3'-C4'-C5'-O5'
50	9	568	E3C	C3'-C4'-C5'-O5'
50	9	568	E3C	O4'-C4'-C5'-O5'
4	5	1348	P4U	O4-C41-C42-C43
4	5	4870	OMG	C3'-C2'-O2'-CM2
4	5	1797	E7G	C3'-C4'-C5'-O5'
4	5	1866	UR3	C3'-C4'-C5'-O5'
4	5	3762	B8H	C3'-C4'-C5'-O5'
4	5	3785	A2M	C3'-C4'-C5'-O5'
4	5	3897	B8K	C3'-C4'-C5'-O5'
4	5	4472	B8W	O4'-C4'-C5'-O5'
4	5	4872	2MG	C3'-C4'-C5'-O5'
4	5	3701	OMC	C2'-C1'-N1-C6
4	5	729	2MG	O4'-C4'-C5'-O5'
4	5	3729	PSU	C3'-C4'-C5'-O5'
4	5	3785	A2M	O4'-C4'-C5'-O5'
4	5	3880	P7G	C3'-C4'-C5'-O5'
4	5	4194	I4U	C3'-C4'-C5'-O5'
4	5	4371	MHG	O4'-C4'-C5'-O5'
50	9	1248	B8N	C3'-C4'-C5'-O5'
50	9	1703	OMC	C3'-C4'-C5'-O5'
4	5	2754	B9B	O6-C61-C62-C63
50	9	1337	4AC	O4'-C4'-C5'-O5'
50	9	1851	MA6	C5-C6-N6-C9
4	5	398	A2M	C3'-C4'-C5'-O5'
4	5	2754	B9B	C5-C6-O6-C61
4	5	1534	A2M	C4'-C5'-O5'-P
4	5	1625	OMG	C4'-C5'-O5'-P
4	5	1909	P7G	C72-C71-N7-C8
4	5	2401	A2M	C3'-C4'-C5'-O5'
4	5	4371	MHG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	5	2786	B9H	C32-C31-N3-C4
4	5	2297	E7G	C72-C71-N7-C8
4	5	3701	OMC	C2'-C1'-N1-C2
4	5	3701	OMC	O4'-C1'-N1-C6
4	5	4371	MHG	C71-C72-C73-C74
4	5	4355	E6G	C62-C61-O6-C6
4	5	4293	PSU	O4'-C4'-C5'-O5'
50	9	1850	MA6	O4'-C4'-C5'-O5'
4	5	3701	OMC	O4'-C1'-N1-C2
4	5	3701	OMC	C3'-C2'-O2'-CM2
4	5	3785	A2M	C3'-C2'-O2'-CM'
50	9	159	A2M	C4'-C5'-O5'-P
50	9	644	OMG	C4'-C5'-O5'-P
50	9	1851	MA6	C4'-C5'-O5'-P
4	5	1677	PSU	O4'-C1'-C5-C4
4	5	4450	PSU	O4'-C1'-C5-C4
4	5	729	2MG	C3'-C4'-C5'-O5'
4	5	1883	OMG	C3'-C4'-C5'-O5'
4	5	4293	PSU	C3'-C4'-C5'-O5'
4	5	4523	A2M	C3'-C4'-C5'-O5'
4	5	4194	I4U	C42-C41-O4-C4
4	5	2754	B9B	C4'-C5'-O5'-P
4	5	4500	PSU	C4'-C5'-O5'-P
4	5	4447	5MC	O4'-C1'-N1-C6
50	9	668	A2M	C3'-C2'-O2'-CM'
4	5	1574	B9B	C2'-C1'-N9-C8
4	5	1909	P7G	O4'-C4'-C5'-O5'
4	5	2861	OMC	O4'-C4'-C5'-O5'
4	5	1326	A2M	C4'-C5'-O5'-P
4	5	3897	B8K	C4'-C5'-O5'-P
4	5	4530	UR3	C4'-C5'-O5'-P
4	5	2363	A2M	O4'-C4'-C5'-O5'
4	5	4355	E6G	C3'-C4'-C5'-O5'
4	5	4447	5MC	O4'-C1'-N1-C2
4	5	2754	B9B	C2'-C1'-N9-C8
4	5	1316	OMG	C1'-C2'-O2'-CM2
4	5	1909	P7G	C72-C71-N7-C5
50	9	644	OMG	C1'-C2'-O2'-CM2
50	9	1710	OMC	C1'-C2'-O2'-CM2
4	5	3887	OMC	C4'-C5'-O5'-P
4	5	4620	OMU	C3'-C4'-C5'-O5'
4	5	4450	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
4	5	4636	PSU	O4'-C1'-C5-C6
4	5	1659	I4U	C42-C41-O4-C4
4	5	4194	I4U	C43-C41-O4-C4
4	5	4371	MHG	C2'-C1'-N9-C4
4	5	4870	OMG	C4'-C5'-O5'-P
4	5	1348	P4U	C2'-C1'-N1-C2
4	5	4523	A2M	C3'-C2'-O2'-CM'
50	9	668	A2M	C2'-C1'-N9-C8
4	5	1534	A2M	O4'-C4'-C5'-O5'
4	5	4529	B8W	C3'-C4'-C5'-O5'
4	5	1883	OMG	C4'-C5'-O5'-P
50	9	814	5MU	C2'-C1'-N1-C2
50	9	1219	B8Q	C2'-C1'-N1-C2
4	5	3785	A2M	C2'-C1'-N9-C8
50	9	1337	4AC	C3'-C4'-C5'-O5'
4	5	3701	OMC	C4'-C5'-O5'-P
4	5	3899	BGH	C4'-C5'-O5'-P
50	9	1081	PSU	C4'-C5'-O5'-P

There are no ring outliers.

48 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	9	1678	A2M	1	0
4	5	1871	A2M	1	0
4	5	398	A2M	1	0
4	5	3897	B8K	1	0
4	5	4500	PSU	1	0
4	5	1574	B9B	2	0
4	5	3718	A2M	3	0
4	5	1326	A2M	1	0
4	5	4571	A2M	1	0
50	9	166	A2M	1	0
4	5	4523	A2M	1	0
4	5	2422	OMC	1	0
4	5	4403	PSU	1	0
4	5	4220	6MZ	1	0
50	9	1850	MA6	2	0
4	5	1625	OMG	1	0
50	9	159	A2M	2	0
4	5	2297	E7G	1	0
4	5	4296	B8H	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	5	1316	OMG	2	0
50	9	1842	4AC	1	0
4	5	3762	B8H	6	0
4	5	3723	A2M	3	0
4	5	237	B9B	1	0
9	C	333	MLZ	1	0
4	5	1605	7MG	2	0
4	5	2522	7MG	1	0
4	5	3825	A2M	1	0
50	9	1031	A2M	2	0
50	9	27	A2M	1	0
4	5	4870	OMG	1	0
4	5	4620	OMU	2	0
50	9	509	OMG	1	0
4	5	1524	A2M	1	0
4	5	2773	OMG	1	0
4	5	4415	1MA	1	0
4	5	1866	UR3	2	0
4	5	4472	B8W	1	0
4	5	2364	OMG	1	0
4	5	3909	OMC	1	0
50	9	116	OMU	1	0
4	5	1456	B8Q	1	0
6	8	14	OMU	1	0
4	5	3899	BGH	1	0
4	5	729	2MG	1	0
4	5	1860	B8H	5	0
50	9	814	5MU	1	0
4	5	2754	B9B	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	5	43
50	9	18
6	8	1
2	2	1
28	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	40.26
1	5	1252:C	O3'	1271:G	P	35.28
1	5	1405:C	O3'	1406:G	P	20.05
1	5	1219:G	O3'	1233:G	P	19.96
1	5	1406(C):G	O3'	1411:C	P	18.99
1	5	1411:C	O3'	1411(A):G	P	18.31
1	9	834:C	O3'	841:G	P	17.82
1	9	323:C	O3'	329:G	P	17.67
1	9	697:G	O3'	729:C	P	17.28
1	5	523:C	O3'	638:G	P	17.26
1	9	1761:U	O3'	1771:G	P	17.22
1	9	756:C	O3'	788:G	P	17.19
1	9	1417:C	O3'	1423:C	P	16.88
1	5	4101:C	O3'	4107:G	P	16.87
1	5	4138:C	O3'	4146:G	P	16.05
1	5	990:U	O3'	1064:G	P	15.99
1	5	1696:C	O3'	1720:C	P	15.87
1	9	130:G	O3'	140:U	P	15.86
1	5	4777:C	O3'	4859:C	P	15.85
1	5	1406:G	O3'	1406(A):G	P	15.56

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	760:G	O3'	904:C	P	15.37
1	5	3976:C	O3'	4039:G	P	14.31
1	5	5022:U	O3'	5028:G	P	13.97
1	5	922:C	O3'	922(A):G	P	13.56
1	5	1364:U	O3'	1368:A	P	13.45
1	8	79:G	O3'	85:U	P	13.18
1	5	738:C	O3'	738(A):C	P	12.82
1	5	2901:G	O3'	3597:G	P	12.78
1	5	182:G	O3'	189:G	P	12.60
1	5	921:C	O3'	922:C	P	11.48
1	5	4729:A	O3'	4735:G	P	10.05
1	5	922(B):C	O3'	923:C	P	9.10
1	5	1180:C	O3'	1183:C	P	8.92
1	5	738(A):C	O3'	739:G	P	8.73
1	9	225:G	O3'	287:U	P	8.33
1	5	935:A	O3'	935(A):G	P	7.20
1	5	481:G	O3'	481(A):C	P	6.85
1	5	512:U	O3'	515:C	P	6.78
1	9	745:C	O3'	749:U	P	6.74
1	5	737:C	O3'	738:C	P	6.37
1	5	500:G	O3'	504:G	P	6.21
1	5	480:C	O3'	481:G	P	5.99
1	5	1239:C	O3'	1244:G	P	5.62
1	9	736:C	O3'	743:U	P	5.29
1	5	935(A):G	O3'	936:C	P	4.93
1	9	322:C	O3'	323:C	P	4.92
1	9	1432:U	O3'	1438:A	P	4.81
1	5	934:C	O3'	935:A	P	4.66
1	5	4740:G	O3'	4743:G	P	4.61
1	5	170:C	O3'	171:U	P	4.59
1	5	1100:U	O3'	1168:G	P	4.20
1	9	309:G	O3'	310:C	P	4.18
1	9	304:C	O3'	305:U	P	4.17
1	9	798:G	O3'	799:U	P	4.13
1	2	16:C	O3'	18:G	P	3.88
1	5	4899:G	O3'	4902:C	P	3.28
1	5	1438:U	O3'	1440:U	P	3.27
1	5	751:G	O3'	752:G	P	3.24
1	5	5020:G	O3'	5021:C	P	3.21
1	9	902:G	O3'	903:A	P	3.20
1	9	903:A	O3'	904:A	P	3.20
1	5	267:G	O3'	268:G	P	3.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	1295:A	O3'	1296:U	P	3.17
1	W	13:ILE	C	14:TYR	N	1.18

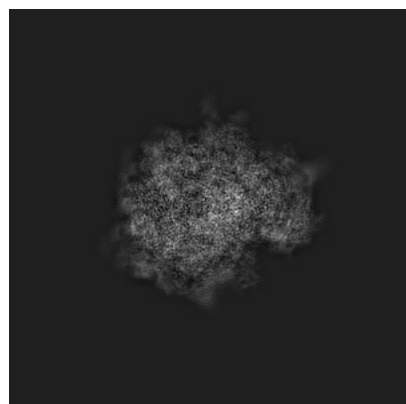
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9237. These allow visual inspection of the internal detail of the map and identification of artifacts.

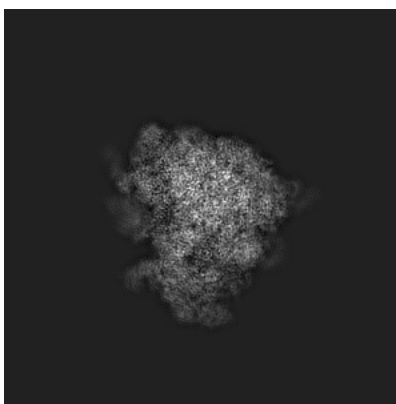
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

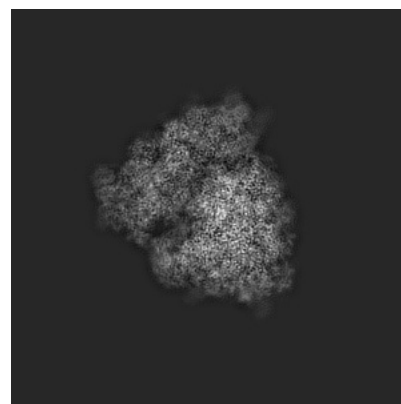
6.1.1 Primary map



X

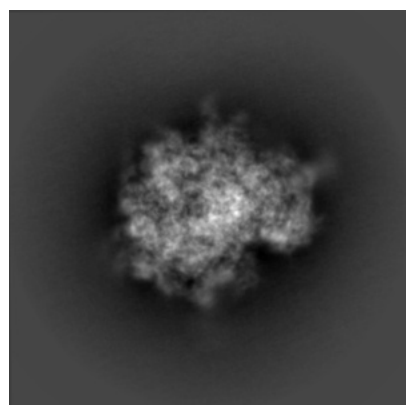


Y

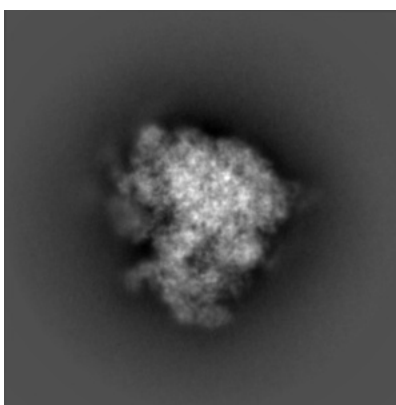


Z

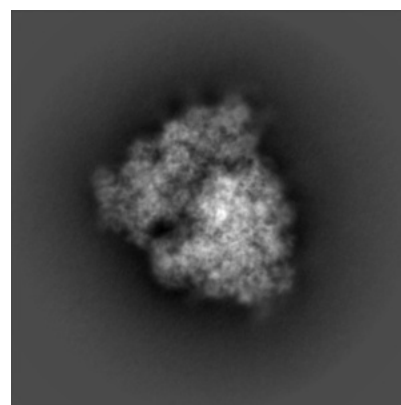
6.1.2 Raw map



X



Y



Z

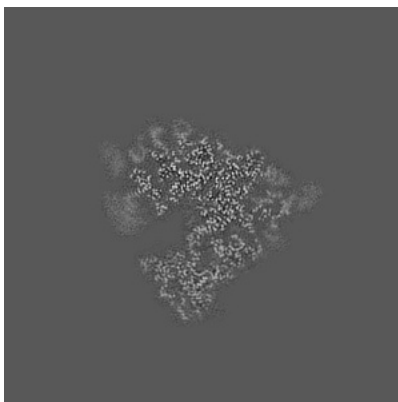
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

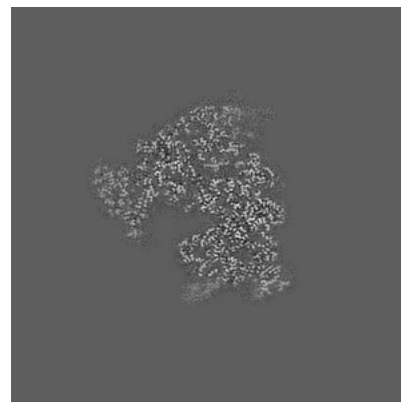
6.2.1 Primary map



X Index: 200

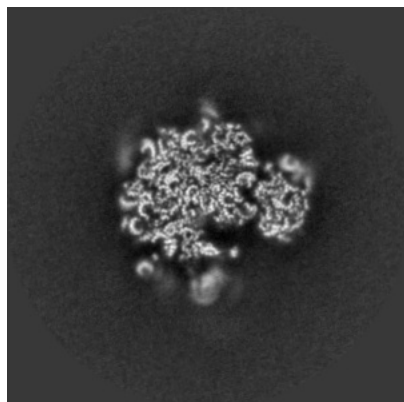


Y Index: 200

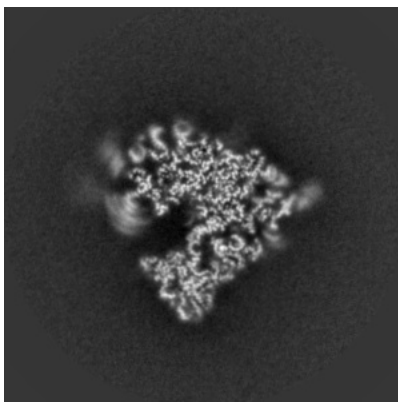


Z Index: 200

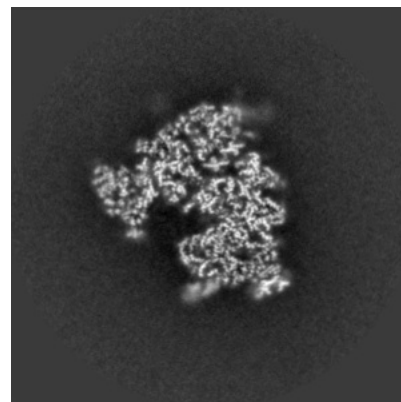
6.2.2 Raw map



X Index: 200



Y Index: 200

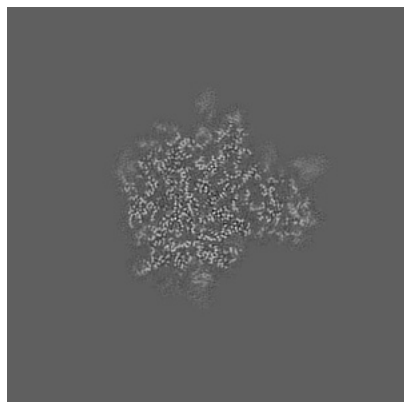


Z Index: 200

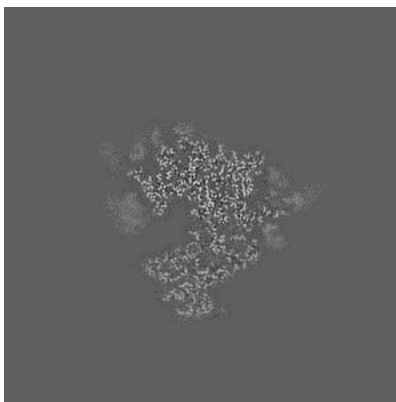
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

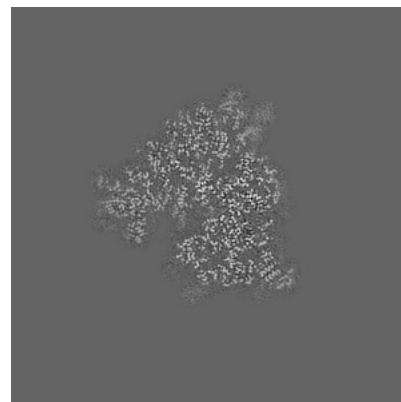
6.3.1 Primary map



X Index: 213

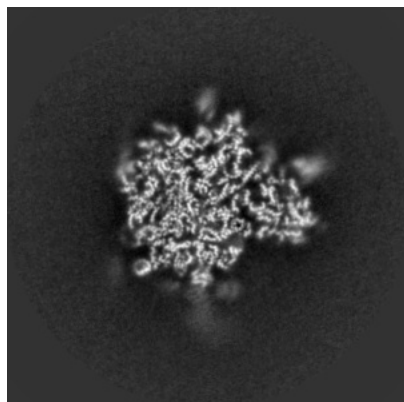


Y Index: 204

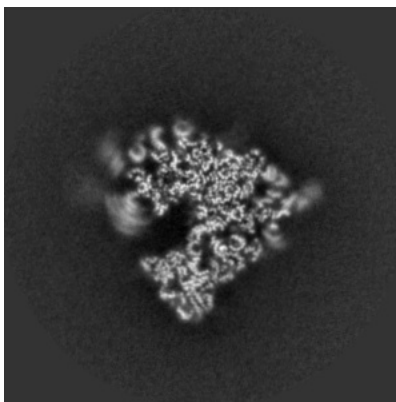


Z Index: 193

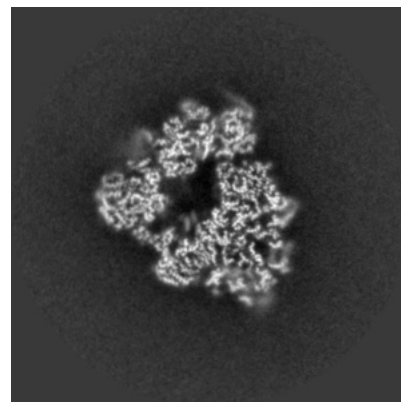
6.3.2 Raw map



X Index: 213



Y Index: 201

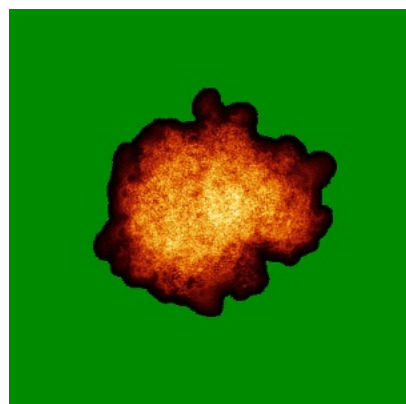


Z Index: 176

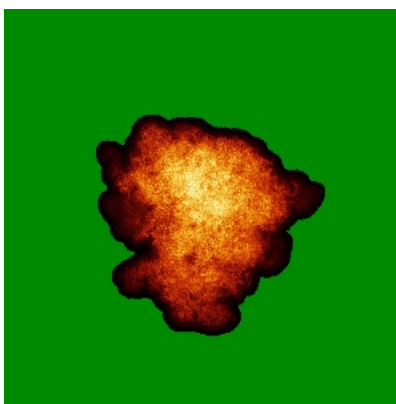
The images above show the largest variance slices of the map in three orthogonal directions.

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

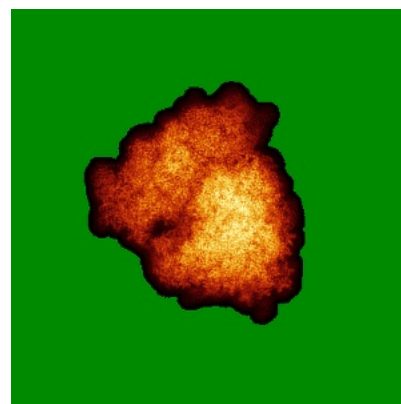
6.4.1 Primary map



X

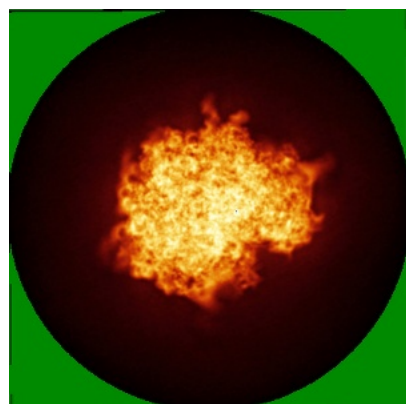


Y

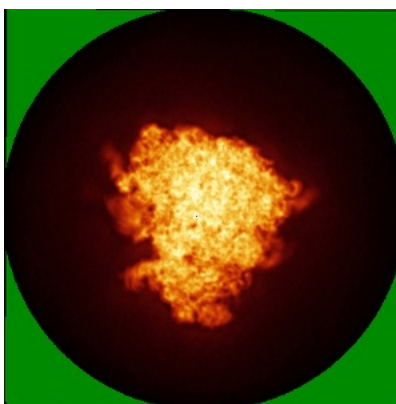


Z

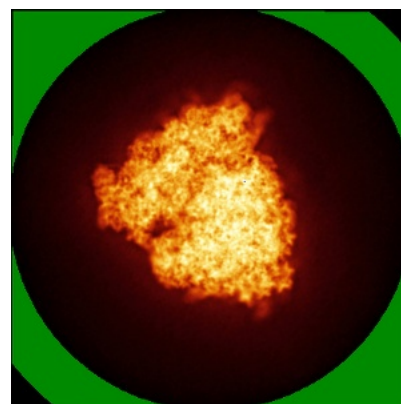
6.4.2 Raw map



X



Y

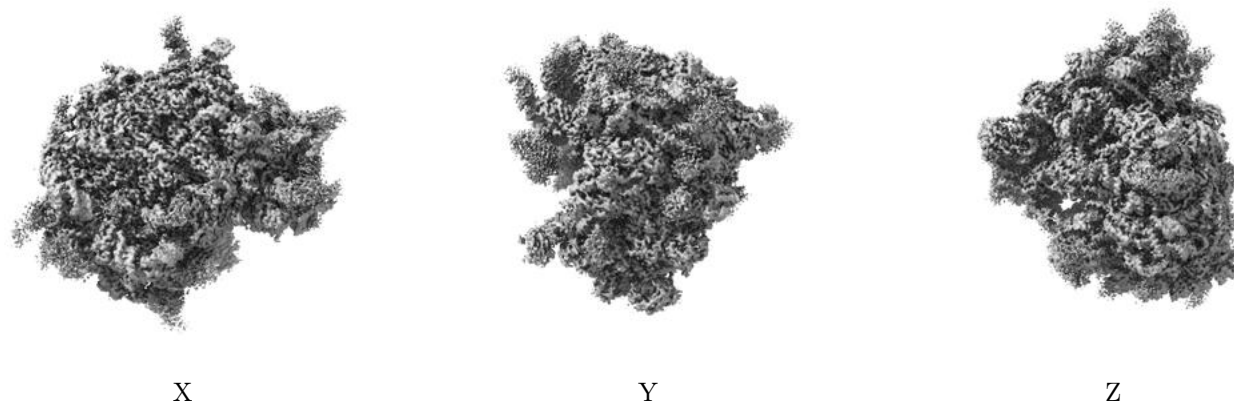


Z

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.

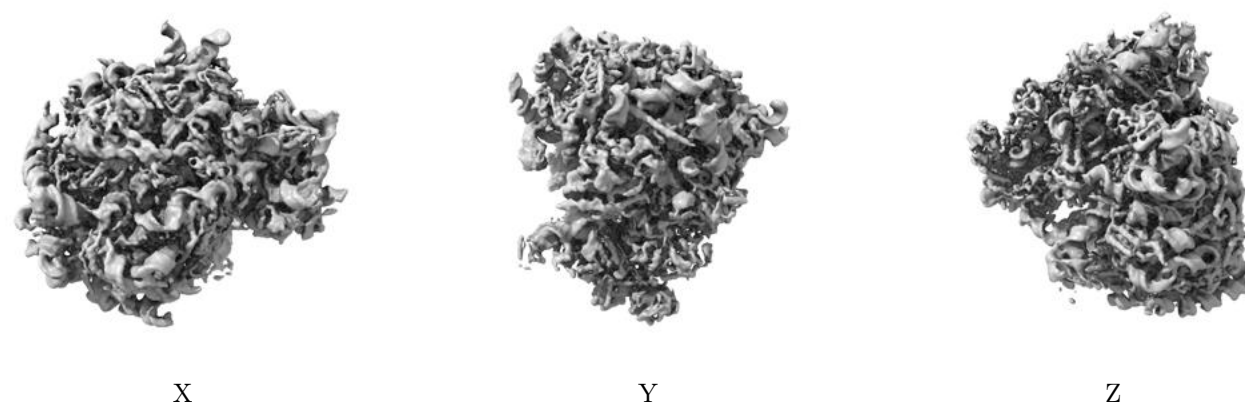
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

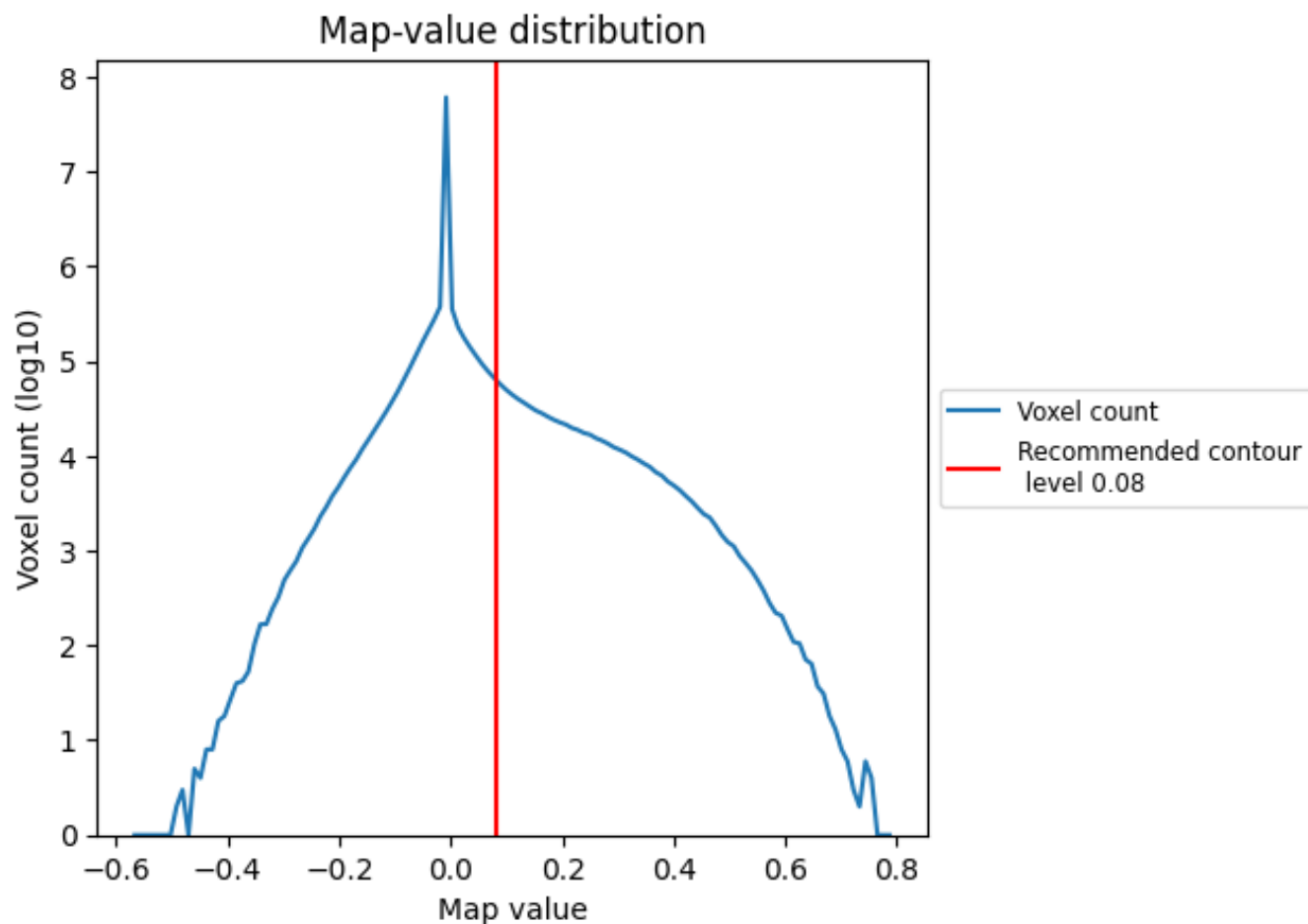
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

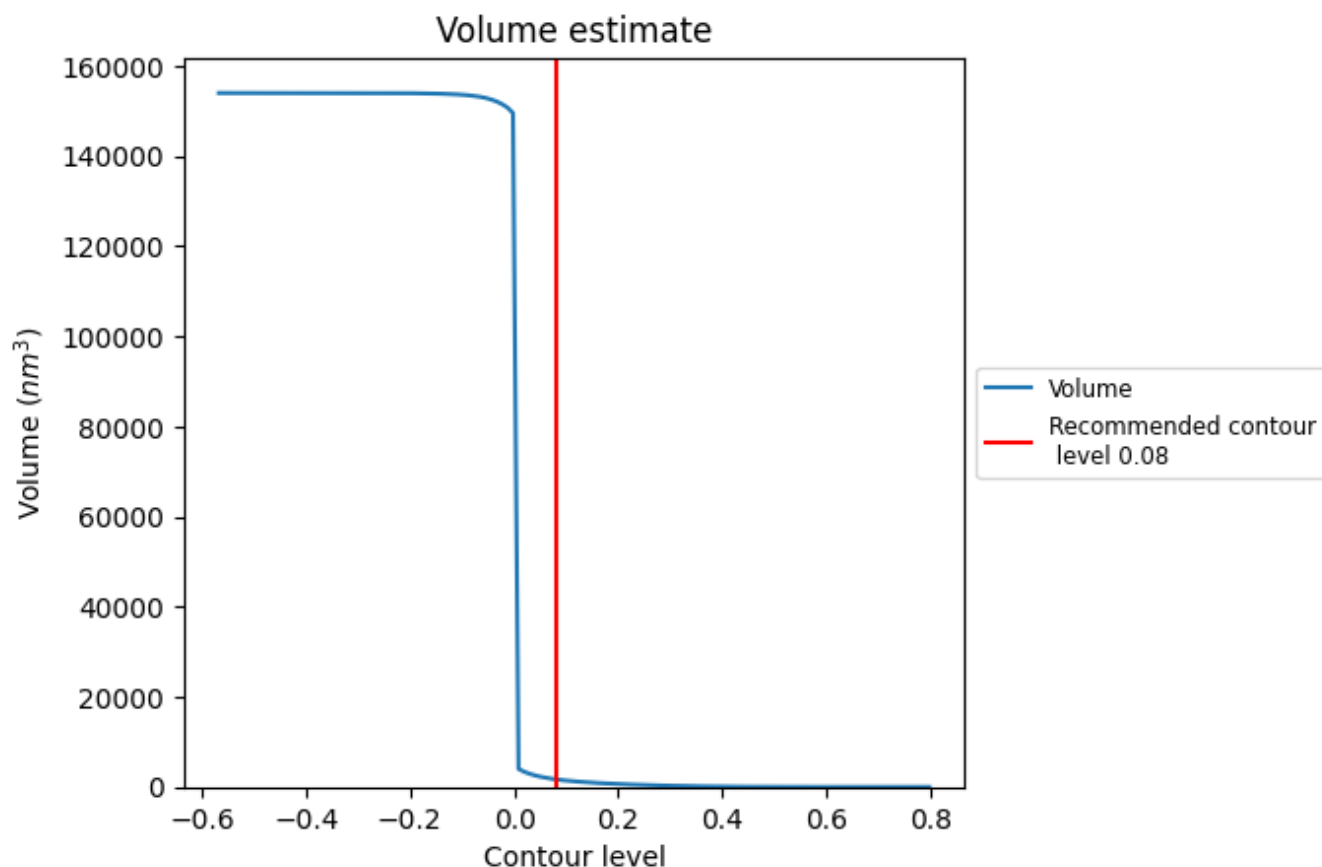
This section contains the results of statistical analysis of the map.

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.

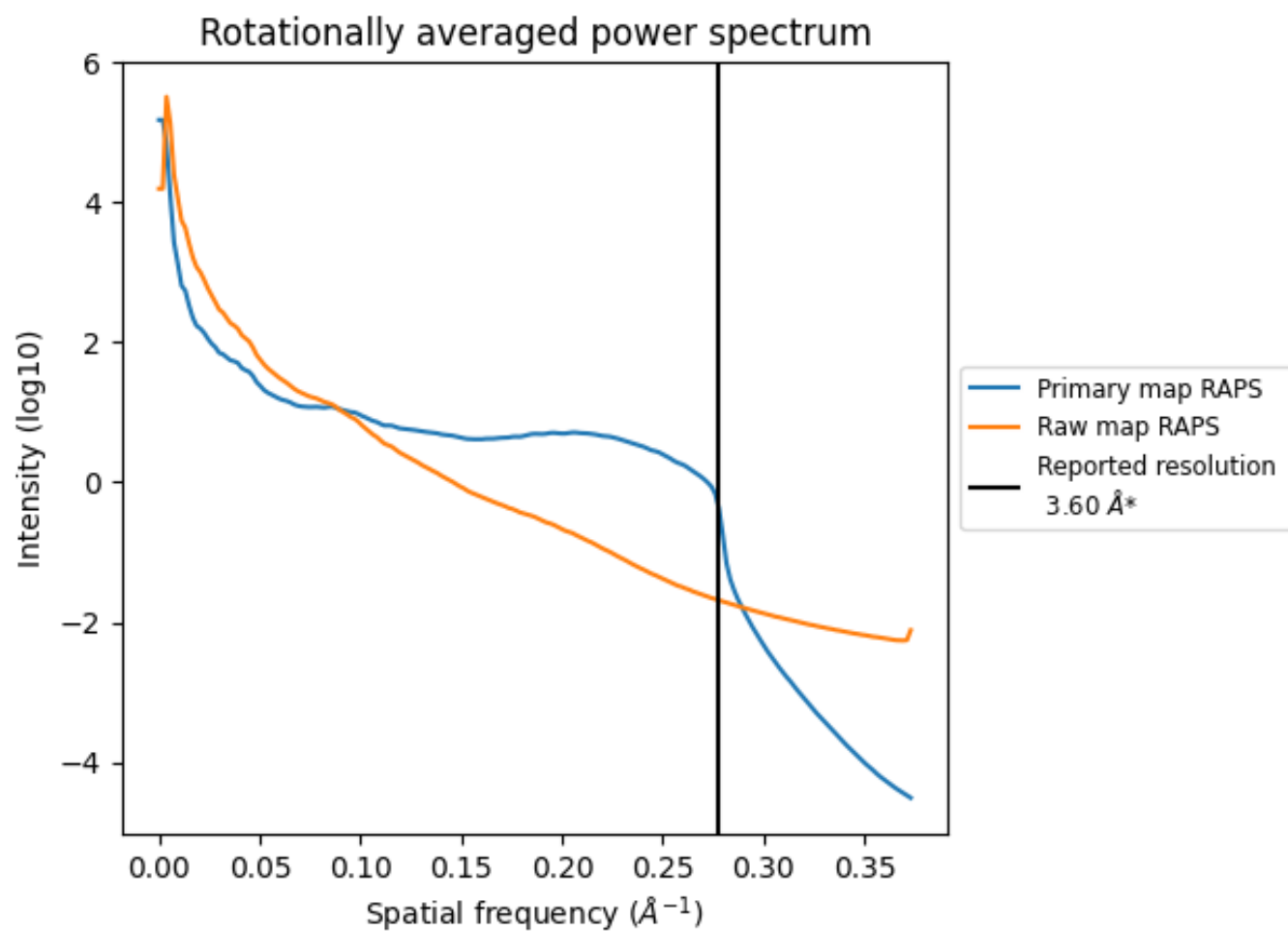
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1689 nm³; this corresponds to an approximate mass of 1525 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 ⓘ

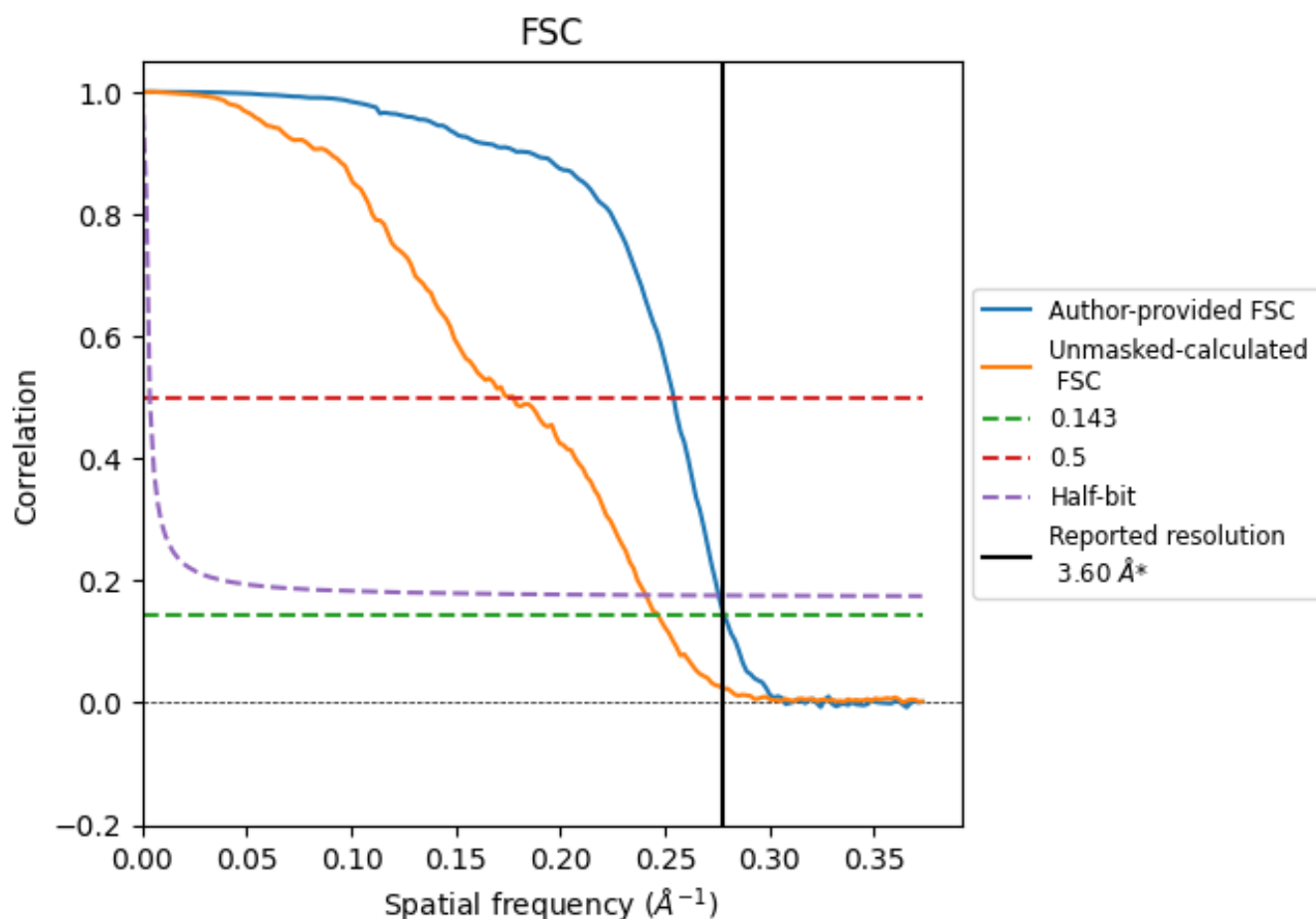


*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

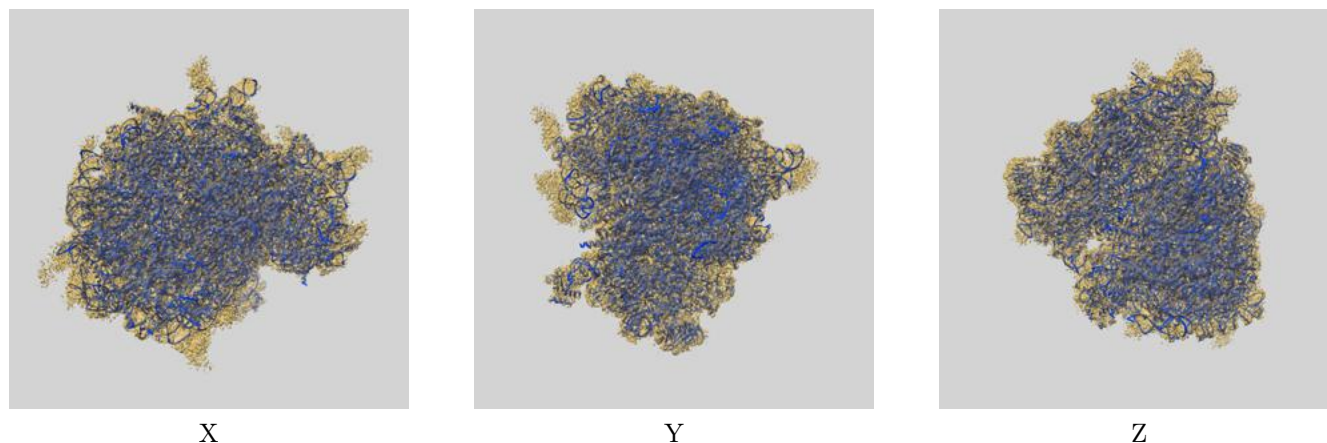
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	3.93	3.63
Unmasked-calculated*	4.05	5.64	4.15

*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 4.05 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

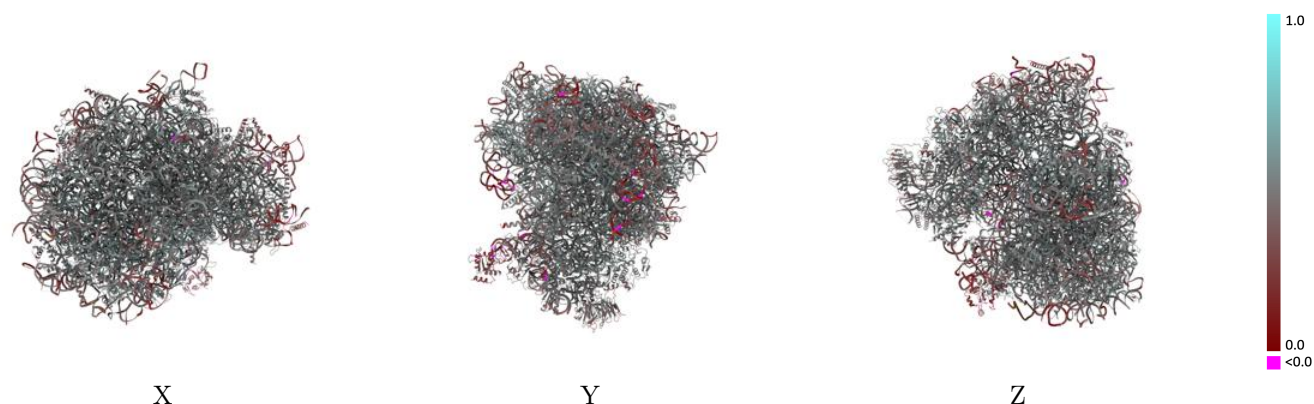
This section contains information regarding the fit between EMDB map EMD-9237 and PDB model 6MTB. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



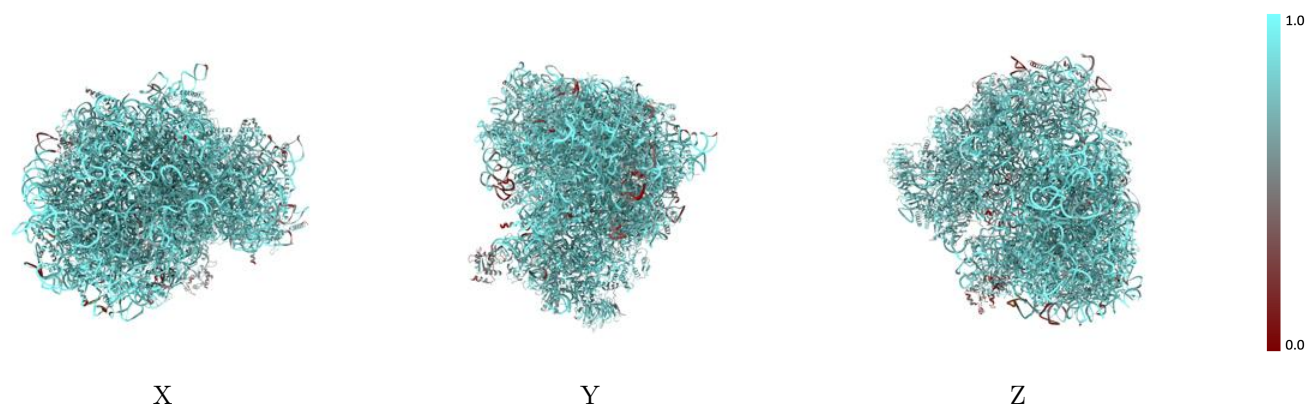
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



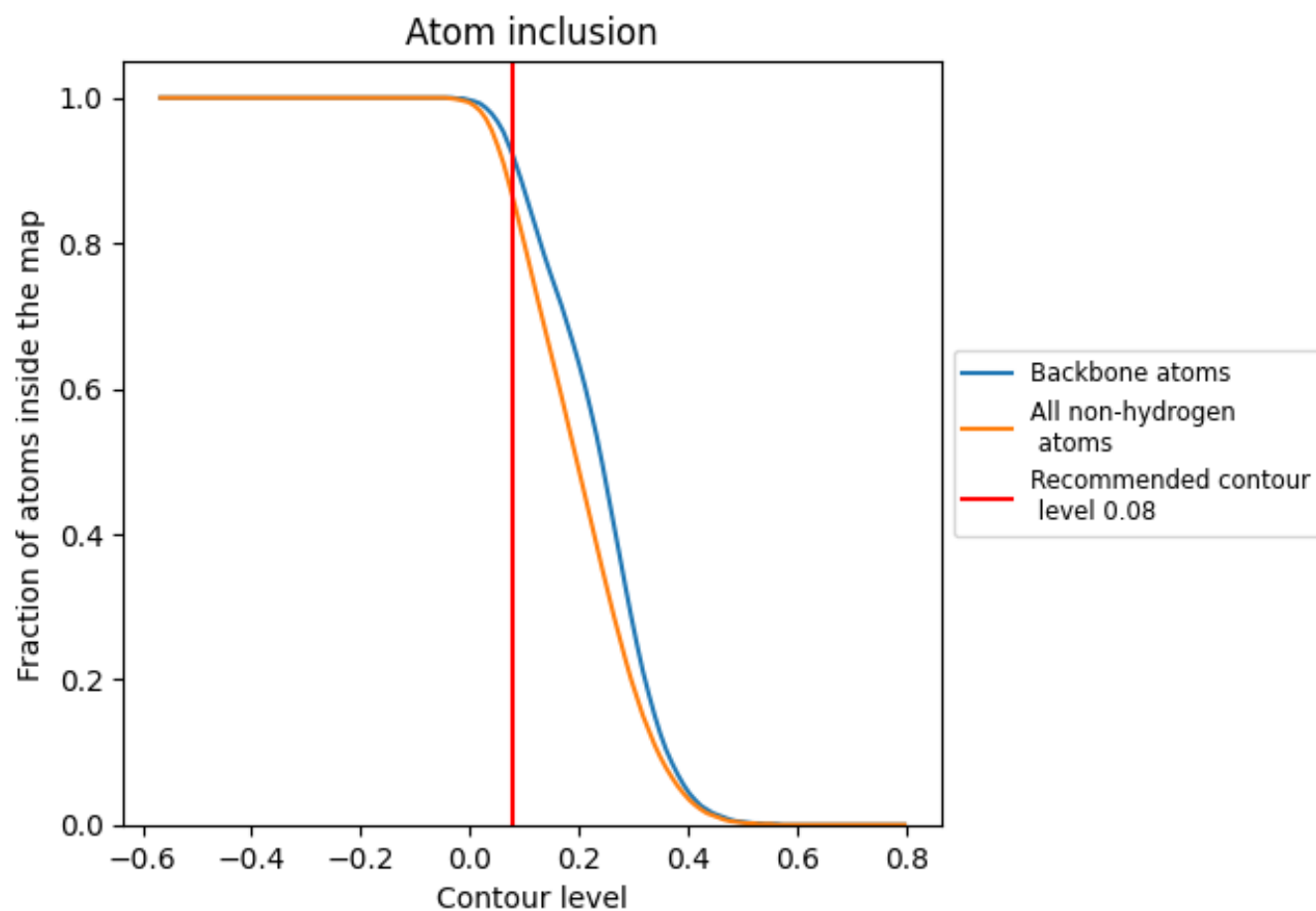
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.4680
1	 0.7920	 0.4930
2	 0.6470	 0.3510
4	 0.7520	 0.2920
5	 0.8980	 0.4560
7	 0.9420	 0.4880
8	 0.9170	 0.4670
9	 0.8910	 0.4460
A	 0.8670	 0.5320
AA	 0.8420	 0.4980
B	 0.8880	 0.5300
BB	 0.8040	 0.4950
C	 0.8590	 0.5210
CC	 0.8470	 0.5130
D	 0.8680	 0.5000
DD	 0.7610	 0.4620
E	 0.8730	 0.5080
EE	 0.8370	 0.5010
F	 0.8480	 0.5150
FF	 0.8150	 0.4790
G	 0.8030	 0.4790
GG	 0.7830	 0.4510
H	 0.8440	 0.5170
HH	 0.7420	 0.4480
I	 0.8500	 0.5210
II	 0.8030	 0.4860
J	 0.8370	 0.4920
JJ	 0.8210	 0.4880
KK	 0.7570	 0.4400
L	 0.8180	 0.4970
LL	 0.8150	 0.5110
M	 0.8640	 0.5060
MM	 0.4520	 0.2670
N	 0.8640	 0.5280
NN	 0.8200	 0.4970



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Chain	Atom inclusion	Q-score
O	 0.8730	 0.5230
OO	 0.8000	 0.4920
P	 0.8810	 0.5300
PP	 0.7720	 0.4510
Q	 0.8660	 0.5280
QQ	 0.8090	 0.4810
R	 0.8220	 0.4840
RR	 0.7930	 0.4730
S	 0.8670	 0.5230
SS	 0.7920	 0.4650
T	 0.8500	 0.5180
TT	 0.8280	 0.4690
U	 0.7740	 0.4490
UU	 0.7390	 0.4520
V	 0.8610	 0.5280
VV	 0.8410	 0.5060
W	 0.7590	 0.4570
WW	 0.8530	 0.5180
X	 0.8370	 0.5100
XX	 0.8420	 0.5170
Y	 0.8350	 0.5040
YY	 0.8080	 0.4700
Z	 0.8670	 0.5110
ZZ	 0.7940	 0.4610
a	 0.8730	 0.5260
aa	 0.8350	 0.5190
b	 0.7670	 0.4620
bb	 0.7950	 0.4950
c	 0.8350	 0.5000
cc	 0.7640	 0.5000
d	 0.8440	 0.5110
dd	 0.8480	 0.4810
e	 0.8860	 0.5370
ee	 0.7490	 0.4780
f	 0.9050	 0.5410
ff	 0.4580	 0.1230
g	 0.8450	 0.5140
gg	 0.7360	 0.4260
h	 0.8220	 0.5000
i	 0.8350	 0.4940
j	 0.8780	 0.5240
k	 0.7610	 0.4700

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Chain	Atom inclusion	Q-score
l	 0.8760	 0.5230
m	 0.8800	 0.5120
n	 0.8120	 0.5060
o	 0.8410	 0.5270
p	 0.8230	 0.5200
r	 0.8740	 0.5220
u	 0.4500	 0.2750