



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 05:18 AM EDT

PDB ID : 6MTC / pdb_00006mtc
EMDB ID : EMD-9239
Title : Rabbit 80S ribosome with Z-site tRNA and IFRD2 (unrotated state)
Authors : Brown, A.; Baird, M.R.; Yip, M.C.J.; Murray, J.; Shao, S.
Deposited on : 2018-10-19
Resolution : 3.40 Å (reported)
Based on initial model : 5LZV

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

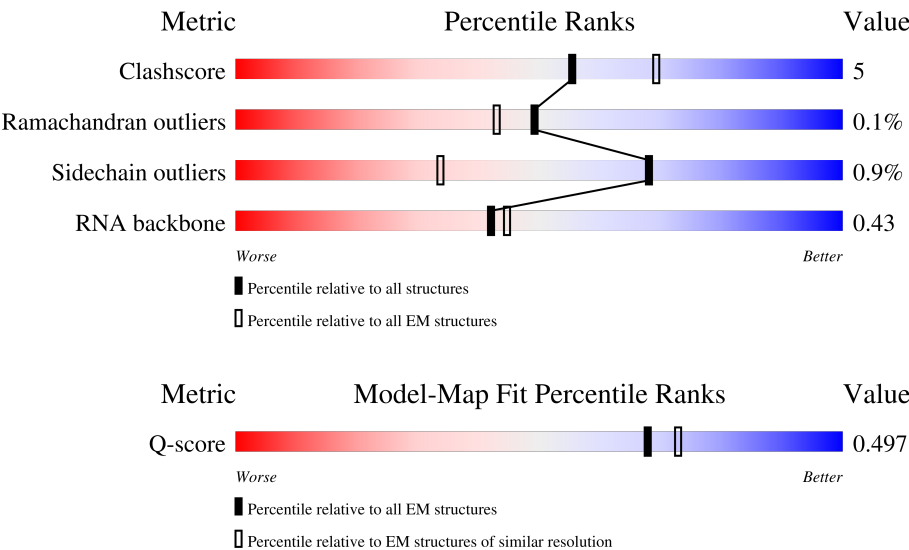
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	4	75	5% 40% 48% 12%
2	5	3597	60% 32% 7%
3	7	120	72% 27%

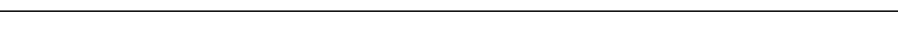
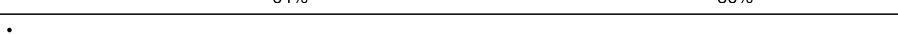
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Mol	Chain	Length	Quality of chain
4	8	151	
5	A	248	
6	B	394	
7	C	362	
8	D	293	
9	E	291	
10	F	225	
11	G	319	
12	H	190	
13	I	214	
14	J	170	
15	L	210	
16	M	138	
17	N	203	
18	O	199	
19	P	153	
20	Q	187	
21	R	180	
22	S	176	
23	T	159	
24	U	99	
25	V	131	
26	W	157	
27	X	118	
28	Y	134	

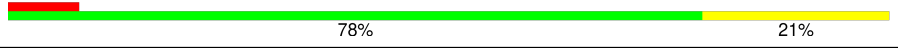
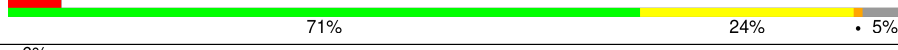
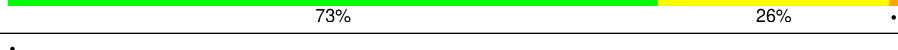
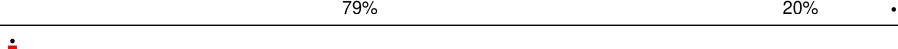
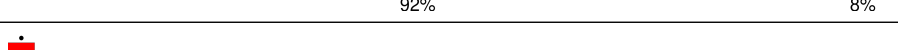
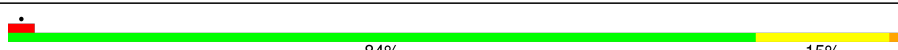
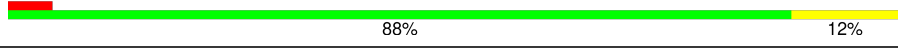
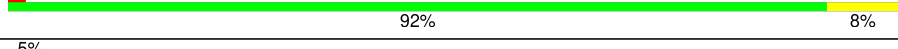
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Mol	Chain	Length	Quality of chain
29	Z	135	
30	a	147	
31	b	245	
32	c	98	
33	d	107	
34	e	128	
35	f	109	
36	g	114	
37	h	122	
38	i	102	
39	j	86	
40	k	69	
41	l	50	
42	m	52	
43	n	25	
44	o	103	
45	p	91	
46	r	124	
47	u	206	
48	v	441	
49	9	1698	
50	AA	217	
51	BB	213	
52	CC	221	
53	DD	228	

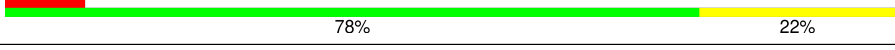
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Mol	Chain	Length	Quality of chain
54	EE	262	
55	FF	204	
56	GG	237	
57	HH	194	
58	II	206	
59	JJ	185	
60	KK	96	
61	LL	158	
62	MM	117	
63	NN	149	
64	OO	136	
65	PP	120	
66	QQ	142	
67	RR	132	
68	SS	144	
69	TT	141	
70	UU	100	
71	VV	83	
72	WW	129	
73	XX	141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

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Mol	Chain	Length	Quality of chain
79	dd	55	
80	ee	55	
81	ff	68	
82	gg	313	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	B8W	5	4185	-	X	-	-

2 Entry composition [i](#)

There are 84 unique types of molecules in this entry. The entry contains 216975 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 Z-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	3597	Total	C	N	O	P	0	0
			77254	34469	14127	25061	3597		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	151	Total	C	N	O	P	0	0
			3209	1433	564	1062	150		

- Molecule 5 is a protein called 60S ribosomal protein L8.

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

- Molecule 6 is a protein called 60S ribosomal protein L3.

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

- Molecule 7 is a protein called 60S ribosomal protein L4.

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

- Molecule 8 is a protein called 60S ribosomal protein L5.

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

- Molecule 9 is a protein called 60S ribosomal protein L6.

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

- Molecule 10 is a protein called 60S ribosomal protein L7.

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

- Molecule 11 is a protein called 60S ribosomal protein L7a.

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

- Molecule 12 is a protein called 60S ribosomal protein L9.

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

- Molecule 13 is a protein called 60S ribosomal protein L10.

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

- Molecule 14 is a protein called 60S ribosomal protein L11.

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

- Molecule 15 is a protein called 60S ribosomal protein L13.

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

- Molecule 16 is a protein called 60S ribosomal protein L14.

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

- Molecule 17 is a protein called 60S Ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

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

- Molecule 19 is a protein called 60S ribosomal protein L17.

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

- Molecule 20 is a protein called 60S ribosomal protein L18.

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

- Molecule 21 is a protein called 60S ribosomal protein L19.

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

- Molecule 22 is a protein called 60S ribosomal protein L18a.

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

- Molecule 23 is a protein called 60S ribosomal protein L21.

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

- Molecule 24 is a protein called 60S ribosomal protein L22.

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

- Molecule 25 is a protein called 60S ribosomal protein L23.

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

- Molecule 26 is a protein called 60S ribosomal protein L24.

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

- Molecule 27 is a protein called 60S ribosomal protein L23a.

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

- Molecule 28 is a protein called 60S ribosomal protein L26.

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

- Molecule 29 is a protein called 60S ribosomal protein L27.

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

- Molecule 30 is a protein called 60S ribosomal protein L27a.

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

- Molecule 31 is a protein called 60S ribosomal protein L29.

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

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

- Molecule 33 is a protein called 60S ribosomal protein L31.

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

- Molecule 34 is a protein called 60S ribosomal protein L32.

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

- Molecule 35 is a protein called 60S ribosomal protein L35a.

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

- Molecule 36 is a protein called 60S ribosomal protein L34.

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

- Molecule 37 is a protein called 60S ribosomal protein L35.

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

- Molecule 38 is a protein called 60S ribosomal protein L36.

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

- Molecule 39 is a protein called 60S ribosomal protein L37.

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

- Molecule 40 is a protein called 60S ribosomal protein L38.

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

- Molecule 41 is a protein called 60S ribosomal protein L39.

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

- Molecule 42 is a protein called 60S ribosomal protein L40.

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

- Molecule 43 is a protein called 60S ribosomal protein L41.

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

- Molecule 44 is a protein called 60S ribosomal protein L36a.

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

- Molecule 45 is a protein called 60S ribosomal protein L37a.

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

- Molecule 46 is a protein called 60S ribosomal protein L28.

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

- Molecule 47 is a protein called 60S ribosomal protein L10a.

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

- Molecule 48 is a protein called Interferon-related developmental regulator 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	354	Total	C	N	O	S	0	0
			2737	1725	493	506	13		

- Molecule 49 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	9	1698	Total	C	N	O	P	0	0
			36291	16217	6509	11868	1697		

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

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

- Molecule 51 is a protein called 40S ribosomal protein S3a.

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

- Molecule 52 is a protein called 40S ribosomal protein S2.

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

- Molecule 53 is a protein called 40S ribosomal protein S3.

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

- Molecule 54 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 55 is a protein called 40S ribosomal protein S5.

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

- Molecule 56 is a protein called 40S ribosomal protein S6.

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

- Molecule 57 is a protein called 40S ribosomal protein S7.

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

- Molecule 58 is a protein called 40S ribosomal protein S8.

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

- Molecule 59 is a protein called 40S ribosomal protein S9.

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

- Molecule 60 is a protein called 40S ribosomal protein S10.

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

- Molecule 61 is a protein called 40S ribosomal protein S11.

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

- Molecule 62 is a protein called 40S ribosomal protein S12.

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

- Molecule 63 is a protein called 40S ribosomal protein S13.

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

- Molecule 64 is a protein called 40S ribosomal protein S14.

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

- Molecule 65 is a protein called 40S ribosomal protein S15.

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

- Molecule 66 is a protein called 40S ribosomal protein S16.

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

- Molecule 67 is a protein called 40S ribosomal protein S17.

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

- Molecule 68 is a protein called 40S ribosomal protein S18.

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

- Molecule 69 is a protein called 40S ribosomal protein S19.

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

- Molecule 70 is a protein called 40S ribosomal protein S20.

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

- Molecule 71 is a protein called 40S ribosomal protein S21.

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

- Molecule 72 is a protein called 40S ribosomal protein S15a.

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

- Molecule 73 is a protein called 40S ribosomal protein S23.

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

- Molecule 74 is a protein called 40S ribosomal protein S24.

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

- Molecule 75 is a protein called 40S ribosomal protein S25.

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

- Molecule 76 is a protein called 40S ribosomal protein S26.

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

- Molecule 77 is a protein called 40S ribosomal protein S27.

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

- Molecule 78 is a protein called 40S ribosomal protein S28.

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

- Molecule 79 is a protein called 40S ribosomal protein S29.

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

- Molecule 80 is a protein called 40S ribosomal protein S30.

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

- Molecule 81 is a protein called 40S ribosomal protein S27a.

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

- Molecule 82 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
83	5	199	Total	Mg	0
			199	199	
83	7	7	Total	Mg	0
			7	7	
83	8	6	Total	Mg	0
			6	6	

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Mol	Chain	Residues	Atoms		AltConf
83	A	1	Total 1	Mg 1	0
83	B	1	Total 1	Mg 1	0
83	P	2	Total 2	Mg 2	0
83	V	1	Total 1	Mg 1	0
83	j	1	Total 1	Mg 1	0
83	9	77	Total 77	Mg 77	0
83	LL	1	Total 1	Mg 1	0
83	TT	1	Total 1	Mg 1	0

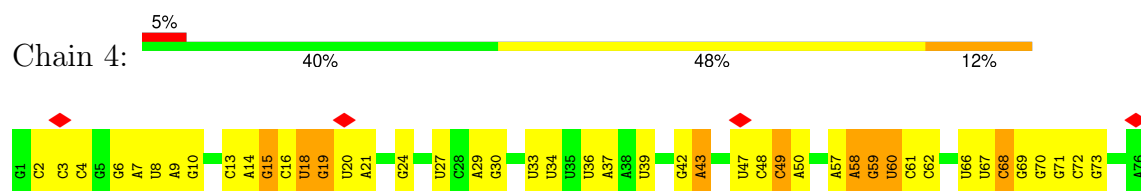
- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

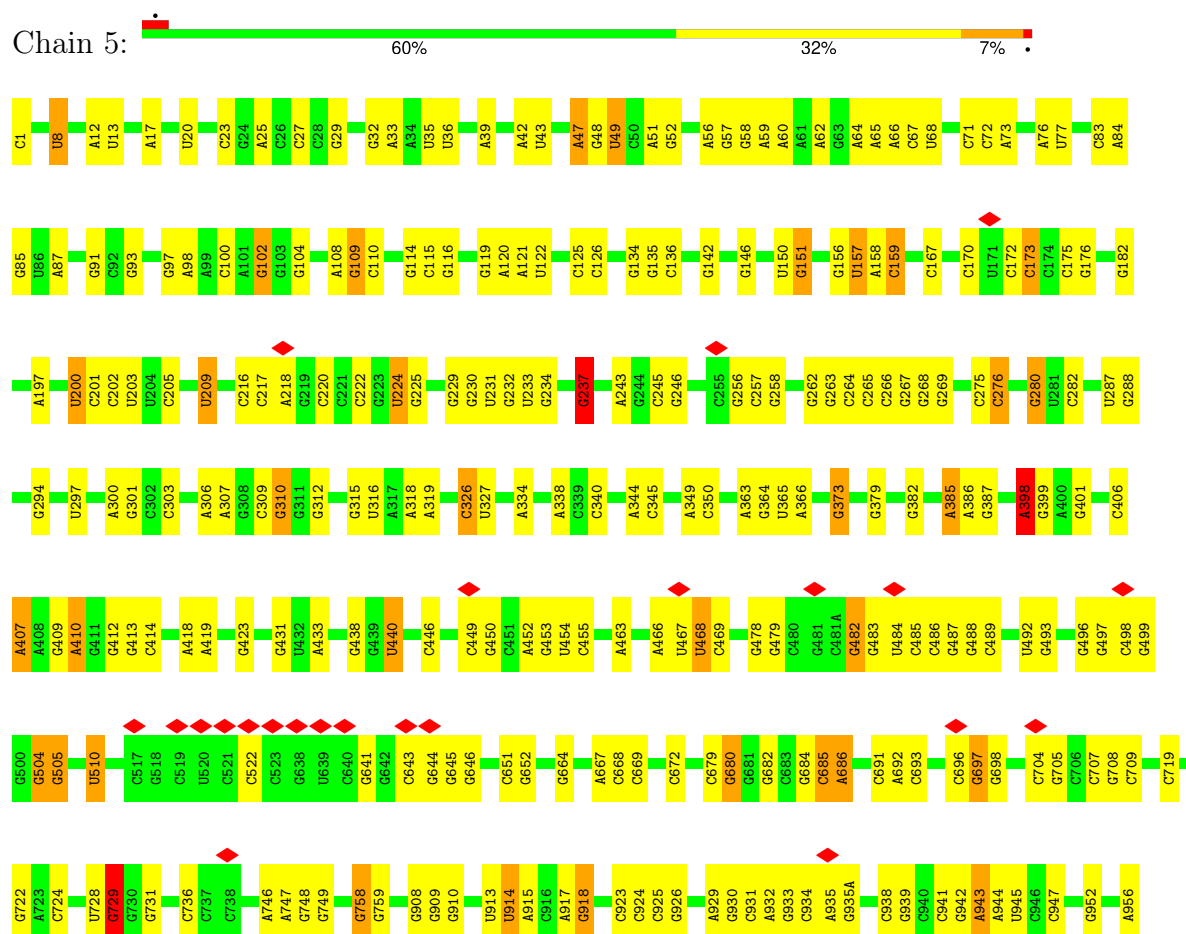
3 Residue-property plots

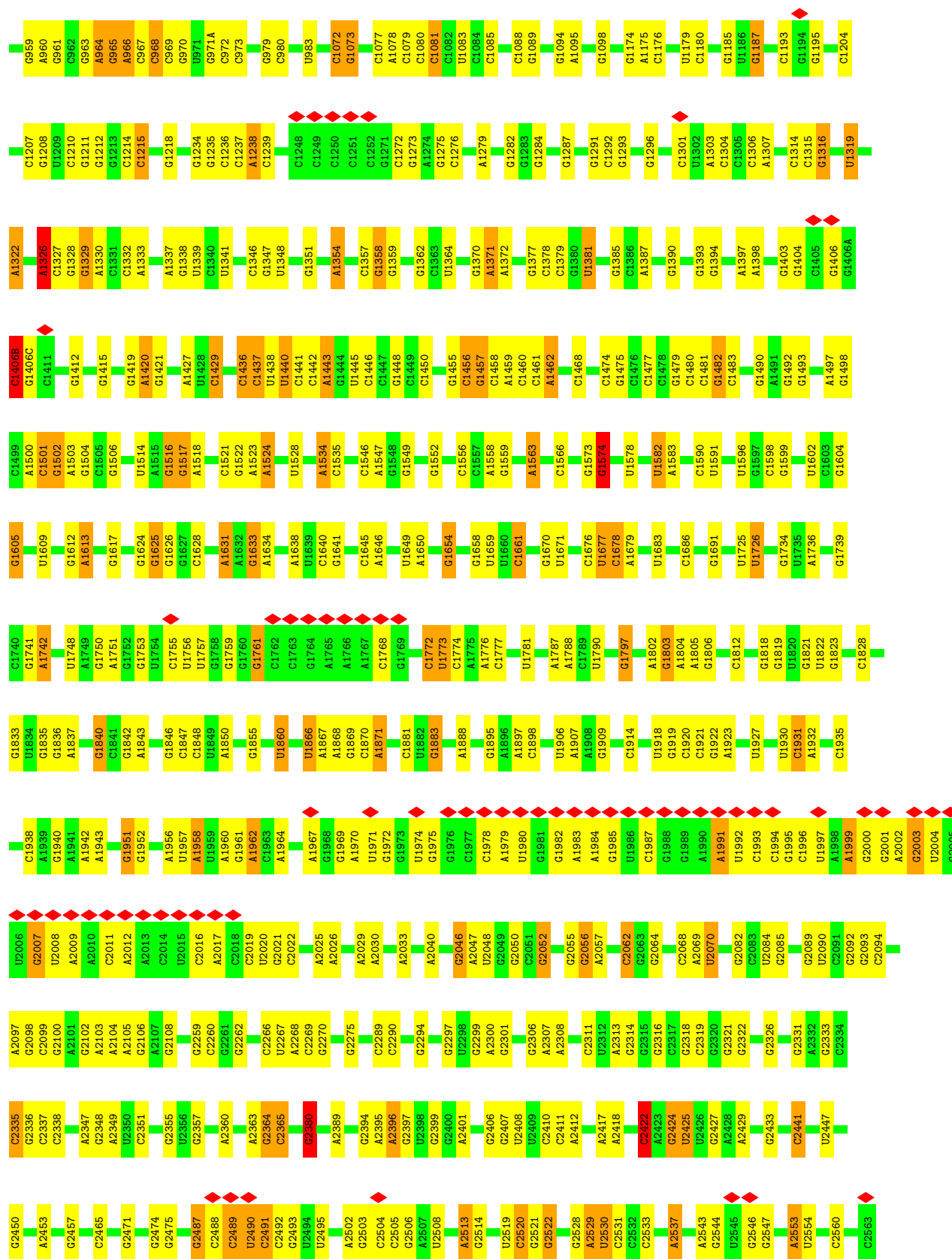
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Z-site tRNA

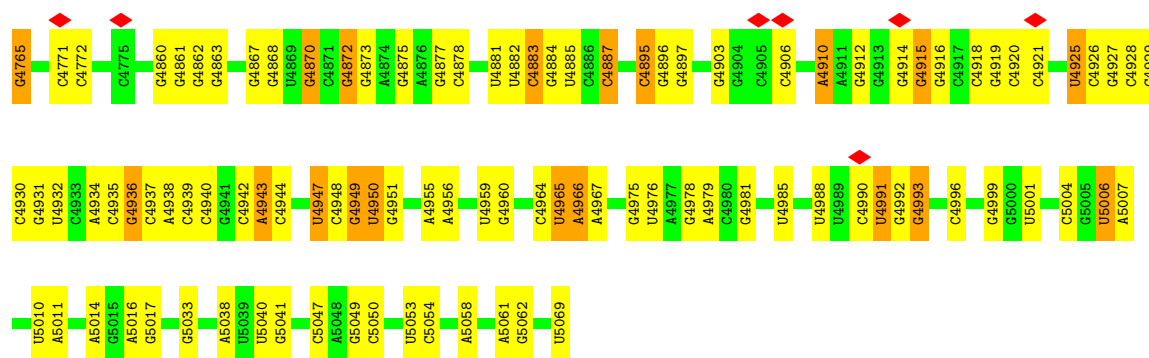


• Molecule 2: 28S rRNA

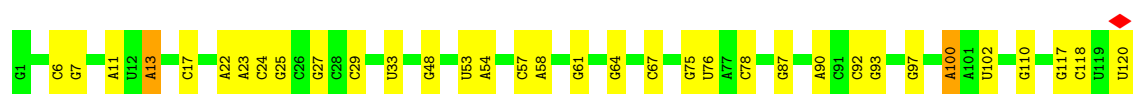




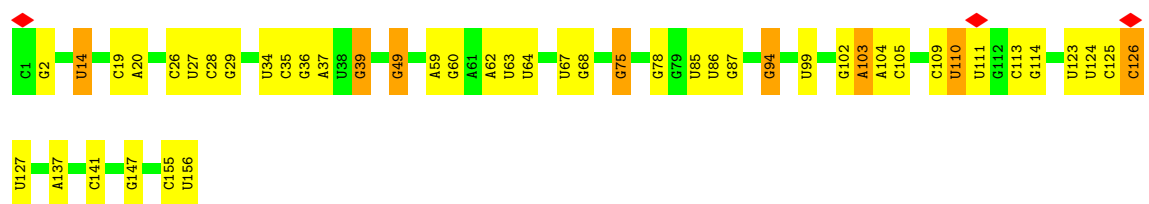
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G4578	U4579	C4582	C4583	A4584	U4585	U4587	U4588	A4589	A4590	U4594	A4595	U4596	U4597	U4598	A4599	A4600	A4601	C4602	U4608	A4611	G4617	G4618	U4619	U4620	A4621	A4622	A4623	G4624	U4626	U4627	U4628	U4629	G4633	U4634	A4635	U4636	U4637	U4638	G4639	U4646	C4653	U4656	G4657	A4658	A4659	A4660	U4664	C4665	G4666	A4667	A4668	A4669	A4670		
C4476	A4477	G4478	U4482	C4483	A4488	A4489	U4494	U4495	U4496	U4497	U4498	U4499	U4500	U4501	C4502	A4507	A4510	A4511	U4512	A4513	U4514	U4515	U4516	A4517	A4518	C4519	U4520	U4521	U4522	A4523	A4524	A4525	U4526	U4527	U4528	U4529	U4530	U4531	C4536	A4548	U4549	U4550	U4558	A4559	A4560	A4564	C4565	U4566	G4567	U4570	A4571	U4572	G4573	U4574	G4575
A4376	A4377	A4378	A4379	A4380	C4387	A4388	C4391	A4394	U4395	C4398	U4399	C4400	C4401	C4402	U4403	U4404	C4405	A4415	U4419	C4420	C4421	A4422	C4426	C4429	C4430	U4431	U4439	C4440	A4441	U4442	U4445	U4446	C4447	U4448	A4449	U4450	G4454	U4457	A4464	A4467	A4472	G4473	A4474	C4475	A4476	A4477	A4478	A4479	A4480	A4481	A4482	A4483			
A4271	G4272	A4273	A4274	G4275	A4281	A4282	U4289	U4290	U4291	A4292	U4293	U4294	U4295	A4296	A4304	C4305	U4306	C4307	C4308	A4313	C4314	A4317	C4318	C4319	C4320	G4326	C4327	G4330	G4331	C4332	C4335	G4338	C4339	A4348	C4349	U4354	G4355	U4359	U4360	G4364	A4368	A4369	C4370	U4371	U4372	G4373	A4374	A4375							
G4168	G4169	A4170	C4171	A4172	U4173	U4174	U4175	U4183	U4184	U4185	U4188	U4189	U4190	C4191	U4192	U4193	U4194	U4195	U4196	U4197	U4209	A4212	C4215	U4219	A4220	U4225	G4228	U4229	U4232	A4233	U4238	A4239	C4240	C4241	U4242	A4251	G4254	A4255	U4258	U4259	U4260	C4261	U4265	U4266	A4267	A4268	A4269	A4270	A4271						
A4073	C4074	A4075	A4076	A4077	C4078	G4081	G4082	U4083	C4084	A4085	C4086	G4087	C4088	U4089	G4095	C4096	C4097	A4098	G4099	C4100	U4101	G4107	G4108	C4109	C4110	U4113	C4116	C4119	U4120	C4121	G4124	C4125	C4126	A4127	U4128	G4129	G4135	G4136	G4151	U4152	C4153	U4154	C4155	U4156	A4157	C4158	C4162	U4163	C4164						
G3933	G3938	G3939	U3940	G3946	C3947	C3948	U3949	U3950	C3951	A3952	G3953	A3954	A3955	U3956	U3957	C3958	U3959	A3960	C3961	A3962	A3963	U3964	A3965	A3966	G3969	G3975	C3976	G4039	G4042	G4043	U4044	G4045	A4046	A4047	A4050	C4051	A4052	U4053	C4054	U4055	A4056	U4060	G4061	A4062	U4065	U4066	U4067	U4068	U4069						
G3823	A3824	A3825	U3838	G3839	U3840	C3843	U3848	A3849	U3853	A3860	C3865	A3866	U3867	A3868	A3869	C3870	A3871	A3876	C3877	C3878	C3879	C3880	C3887	C3888	C3889	U3892	C3897	C3898	C3899	G3900	A3901	A3902	G3903	C3904	A3905	A3906	G3907	C3909	C3910	C3911	U3915	G3916	U3927	A3928	U3932	U3933	U3934	U3935	U3936						
A3717	A3718	A3719	G3720	U3721	G3722	A3723	A3724	A3726	U3729	A3733	U3734	G3735	G3740	G3753	A3756	A3759	U3762	A3763	U3764	G3765	A3766	U3773	A3774	A3775	G3776	G3777	C3782	A3783	A3784	A3785	U3786	G3787	U3790	C3791	G3792	U3802	C3810	G3811	C3812	A3813	U3814	A3817	U3818	G3819	U3820	U3821	U3822	U3823							
U3606	U3607	A3609	C3617	G3618	G3619	C3620	A3621	C3622	C3623	A3624	G3625	C3626	A3635	U3641	C3646	C3650	A3651	U3657	A3662	A3663	C3664	G3672	C3673	U3679	C3680	A3681	C3682	C3683	C3684	C3685	U3688	G3689	U3690	G3691	A3692	U3697	A3698	C3701	U3709	G3710	A3711	A3712	U3713	U3714	A3604	C3605	C3606	C3607	C3608						
G2680	G2686	U2687	A2695	A2696	A2697	U2706	U2707	U2708	U2709	C2710	G2711	G2714	G2715	G2716	G2724	A2725	G2726	G2739	U2740	U2741	G2742	A2743	G2744	A2745	A2746	C2756	G2759	U2763	A2764	U2769	G2773	G2778	U2782	A2783	C2786	A2787	U2788	A2789	U2790	G2793	C2794	C2795	C2796	C2797	C2798	C2799	C2800	C2801							
A2798	U2803	C2804	U2810	C2811	A2812	C2813	C2814	U2819	G2822	U2826	U2827	U2828	U2829	A2835	U2836	U2837	C2838	G2842	A2845	C2846	G2847	C2848	G2855	C2856	A2857	C2861	C2867	C2868	U2869	C2875	C2876	G2877	C2878	A2879	U2880	A2881	C2884	C2892	G2897	A2898	C2899	A2900	A2901	A2902	A2903	A2904	A2905	A2906	A2907	A2908					
U2580	A2581	C2582	U2583	U2584	U2585	U2586	U2587	U2588	U2589	A2590	A2591	A2592	C2593	U2594	U2595	U2596	U2597	U2598	U2599	A2600	A2601	C2607	A2611	G2612	C2613	C2616	C2617	C2618	C2619	C2620	U2626	C2627	G2638	U2639	G2649	C2653	U2661	C2662	C2663	C2668	A2676	C2677	C2678	C2679	C2680	C2681	C2682	C2683	C2684						



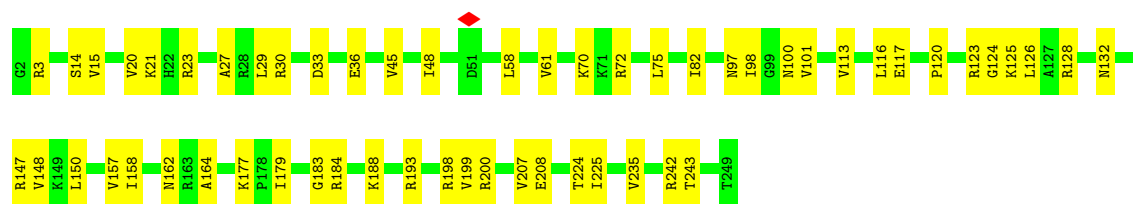
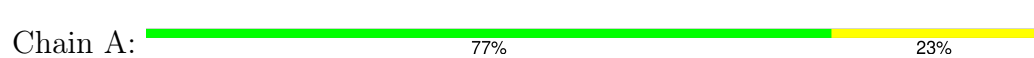
• Molecule 3: 5S rRNA



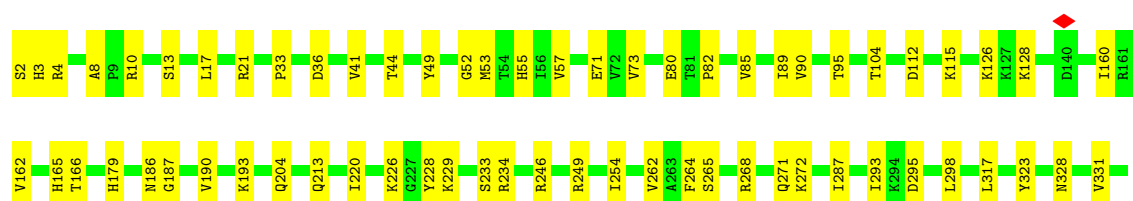
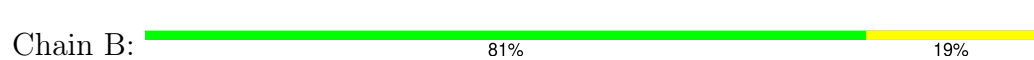
• Molecule 4: 5.8S rRNA



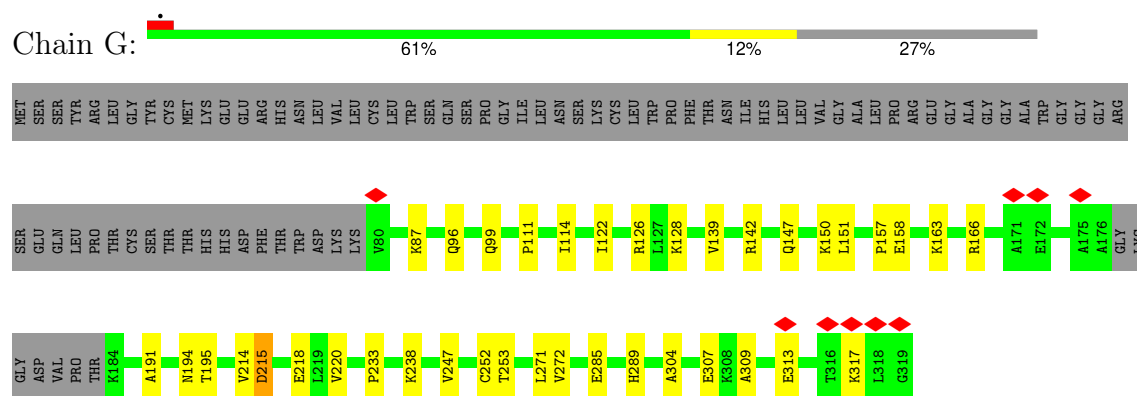
• Molecule 5: 60S ribosomal protein L8



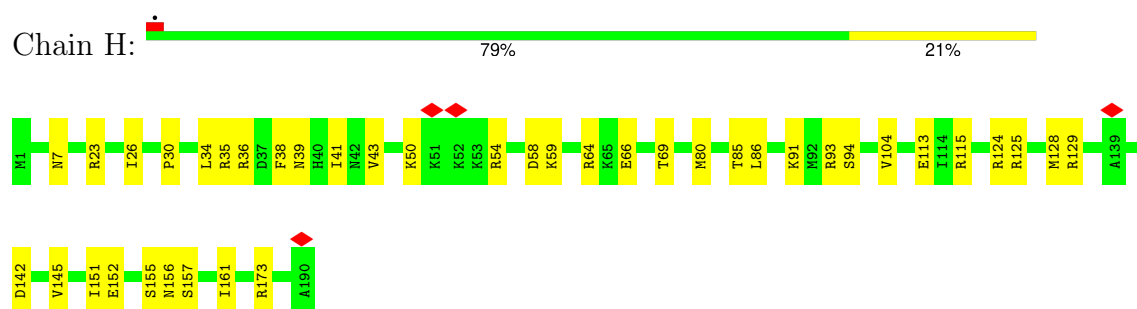
• Molecule 6: 60S ribosomal protein L3



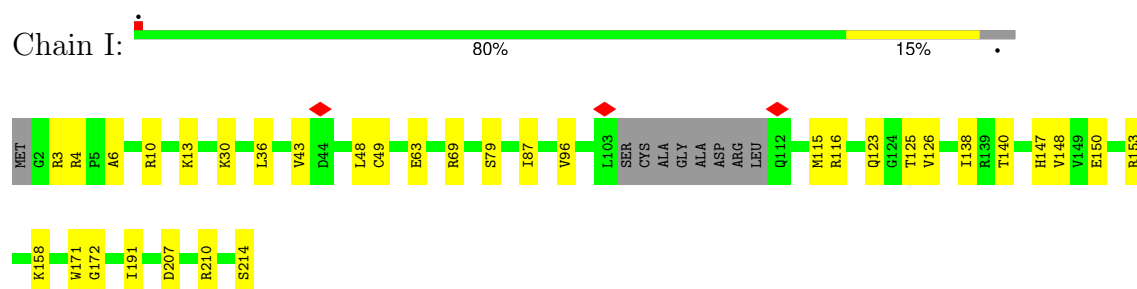
- Molecule 11: 60S ribosomal protein L7a



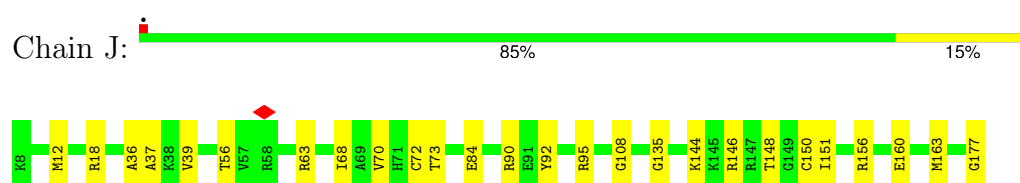
- Molecule 12: 60S ribosomal protein L9



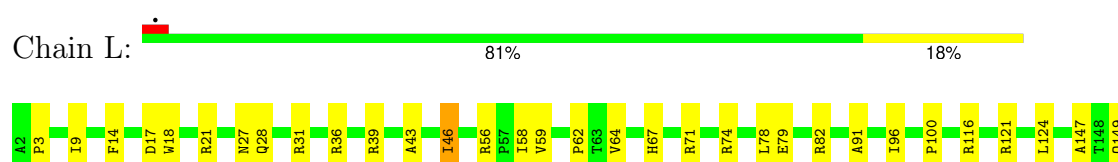
- Molecule 13: 60S ribosomal protein L10

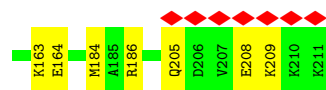


- Molecule 14: 60S ribosomal protein L11

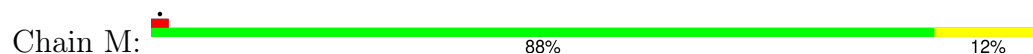


- Molecule 15: 60S ribosomal protein L13

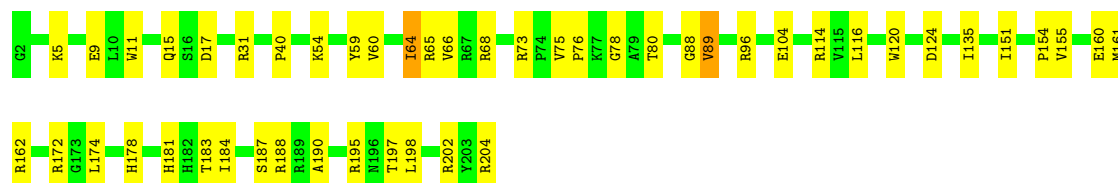




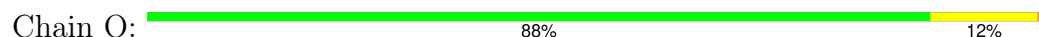
- Molecule 16: 60S ribosomal protein L14



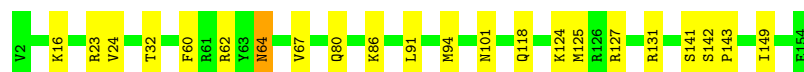
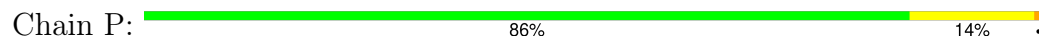
- Molecule 17: 60S Ribosomal protein L15



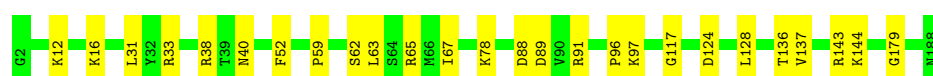
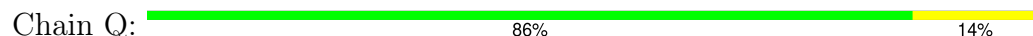
- Molecule 18: 60S ribosomal protein L13a



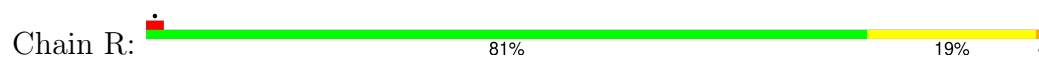
- Molecule 19: 60S ribosomal protein L17



- Molecule 20: 60S ribosomal protein L18

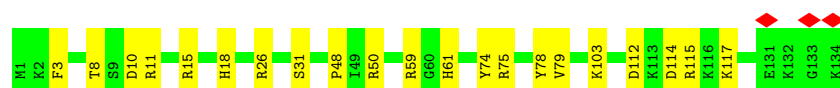


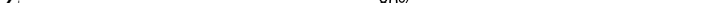
- Molecule 21: 60S ribosomal protein L19

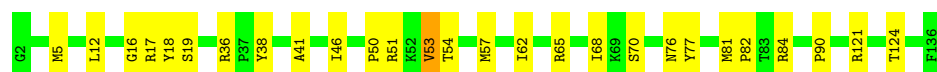




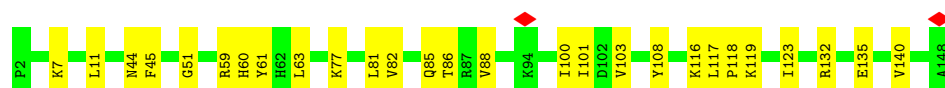
- Chain Y: 84% 16%

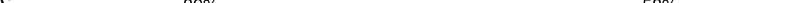


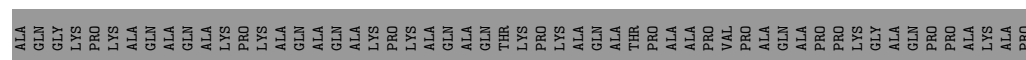
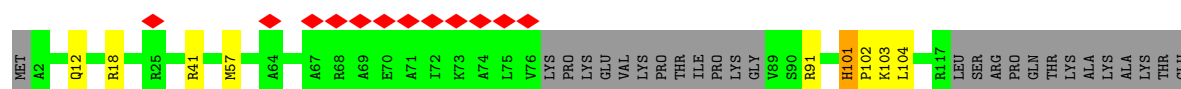
- Chain Z:  80% 19%

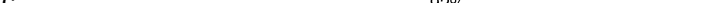


- Chain a: 82% 18%



- Chain b:  5% 39% 58%



- Chain c:  92% 8%



- WORLDWIDE
PDB
PROTEIN DATA BANK

Chain d:  83% 17%



- Molecule 34: 60S ribosomal protein L32

Chain e:  88% 12%



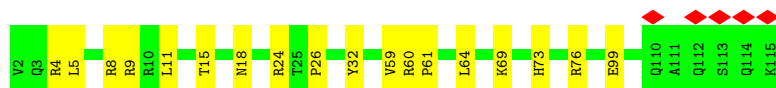
- Molecule 35: 60S ribosomal protein L35a

Chain f:  84% 16%



- Molecule 36: 60S ribosomal protein L34

Chain g:  84% 16%



- Molecule 37: 60S ribosomal protein L35

Chain h:  92% 8%



- Molecule 38: 60S ribosomal protein L36

Chain i:  93% 7%



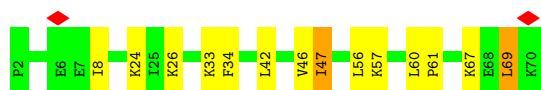
- Molecule 39: 60S ribosomal protein L37

Chain j:  88% 12%



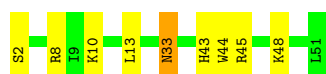
- Molecule 40: 60S ribosomal protein L38

Chain k:  80% 17%



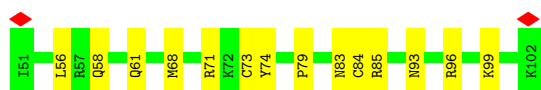
- Molecule 41: 60S ribosomal protein L39

Chain l:  82% 16%



- Molecule 42: 60S ribosomal protein L40

Chain m:  73% 27%



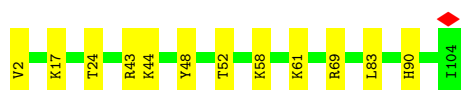
- Molecule 43: 60S ribosomal protein L41

Chain n:  64% 36%



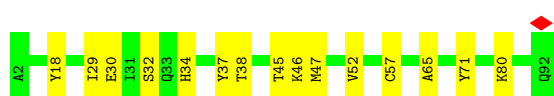
- Molecule 44: 60S ribosomal protein L36a

Chain o:  88% 12%



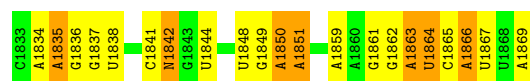
- Molecule 45: 60S ribosomal protein L37a

Chain p:  84% 16%

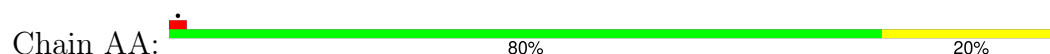


- Molecule 46: 60S ribosomal protein L28

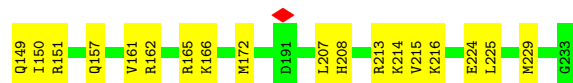
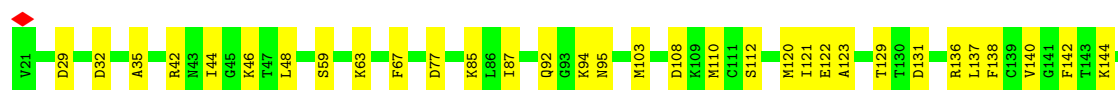
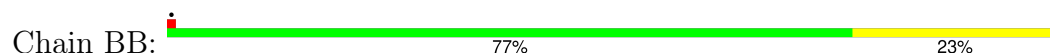
Chain r:  85% 15%



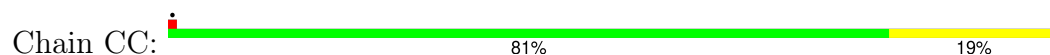
- Molecule 50: 40S ribosomal protein SA



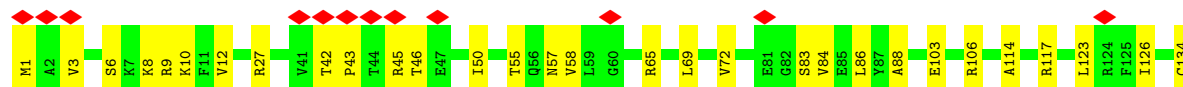
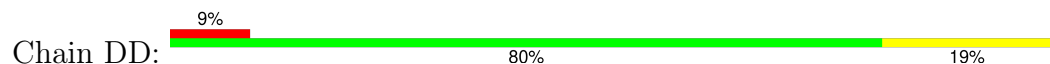
- Molecule 51: 40S ribosomal protein S3a



- Molecule 52: 40S ribosomal protein S2

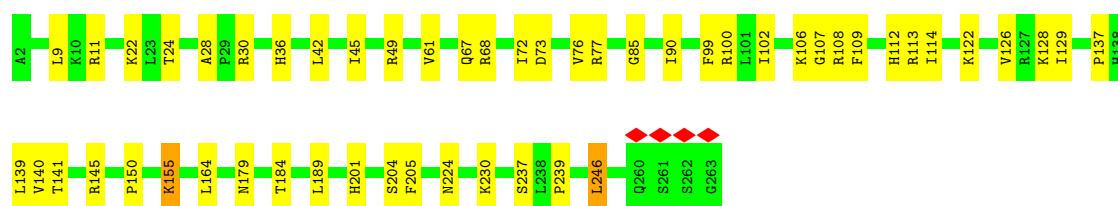


- Molecule 53: 40S ribosomal protein S3



- Molecule 54: 40S ribosomal protein S4, X isoform

Chain EE: 



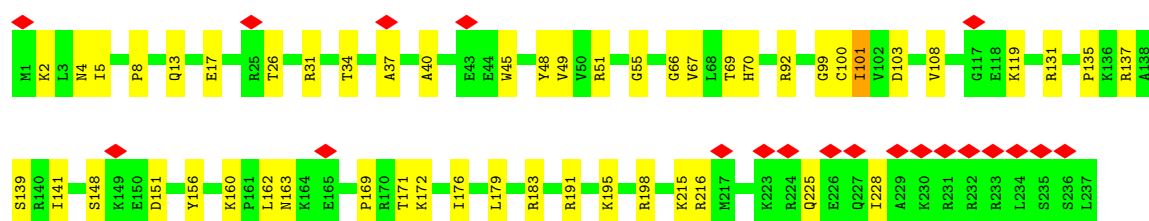
- Molecule 55: 40S ribosomal protein S5

Chain FF: 



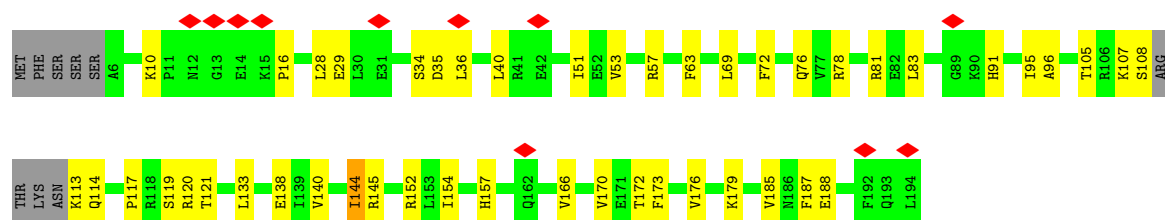
- Molecule 56: 40S ribosomal protein S6

Chain GG: 



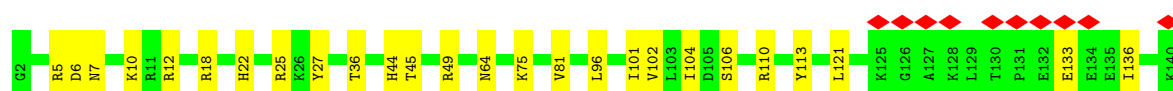
- Molecule 57: 40S ribosomal protein S7

Chain HH: 



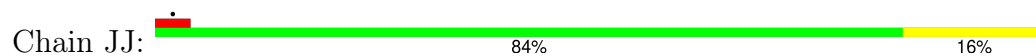
- Molecule 58: 40S ribosomal protein S8

Chain II: 

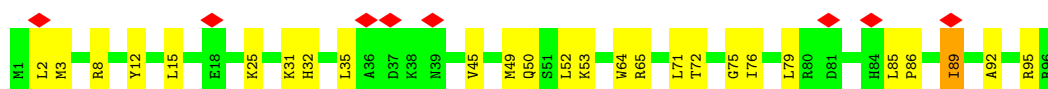
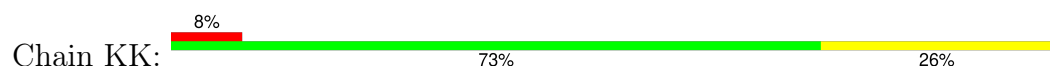




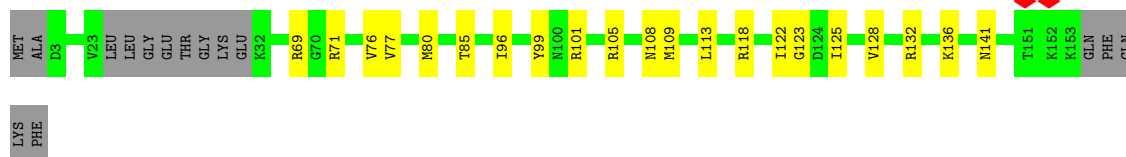
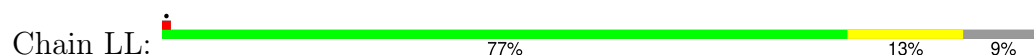
- Molecule 59: 40S ribosomal protein S9



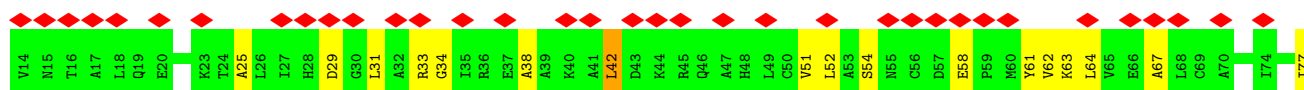
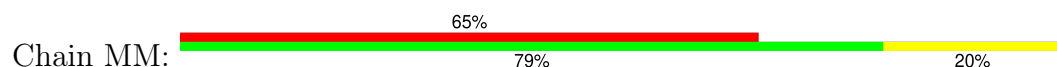
- Molecule 60: 40S ribosomal protein S10



- Molecule 61: 40S ribosomal protein S11



- Molecule 62: 40S ribosomal protein S12

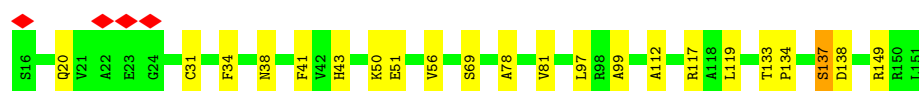


- Molecule 63: 40S ribosomal protein S13



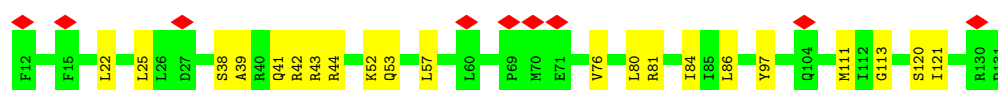
- Molecule 64: 40S ribosomal protein S14

Chain OO:  84% 15%



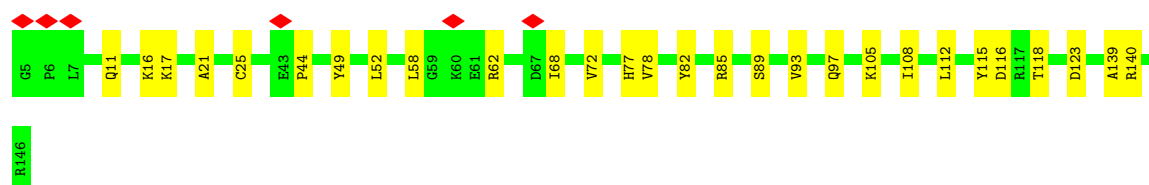
- Molecule 65: 40S ribosomal protein S15

Chain PP:  8% 82% 18%



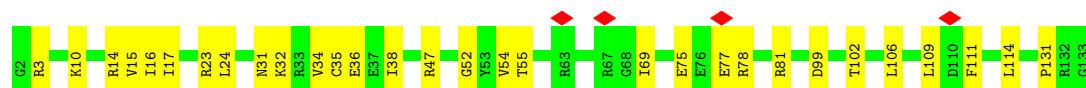
- Molecule 66: 40S ribosomal protein S16

Chain QQ:  80% 20%



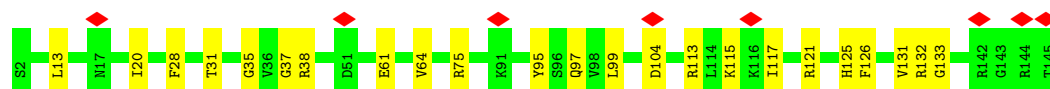
- Molecule 67: 40S ribosomal protein S17

Chain RR:  77% 23%



- Molecule 68: 40S ribosomal protein S18

Chain SS:  6% 84% 16%



- Molecule 69: 40S ribosomal protein S19

Chain TT:  84% 15%

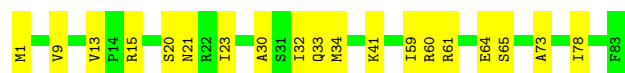
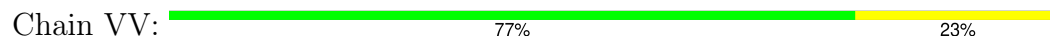


- Molecule 70: 40S ribosomal protein S20

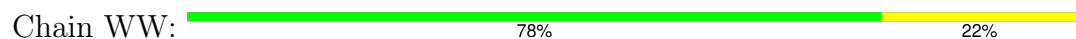
Chain UU:  9% 77% 22%



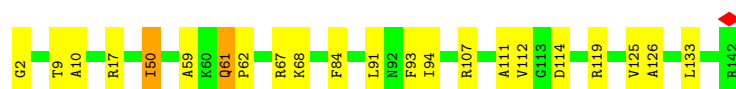
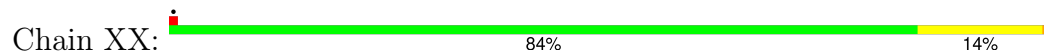
- Molecule 71: 40S ribosomal protein S21



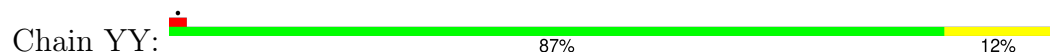
- Molecule 72: 40S ribosomal protein S15a



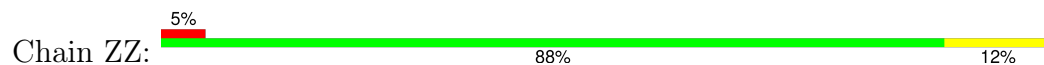
- Molecule 73: 40S ribosomal protein S23



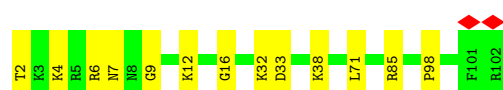
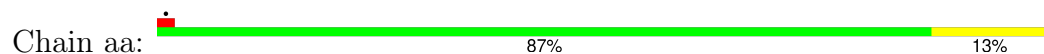
- Molecule 74: 40S ribosomal protein S24



- Molecule 75: 40S ribosomal protein S25



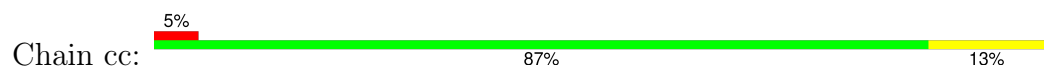
- Molecule 76: 40S ribosomal protein S26



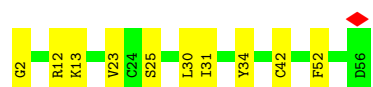
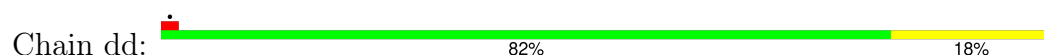
- Molecule 77: 40S ribosomal protein S27



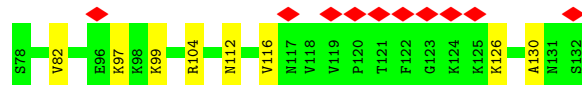
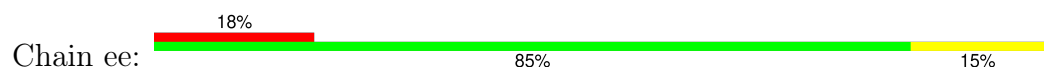
- Molecule 78: 40S ribosomal protein S28



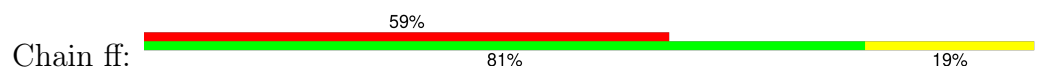
- Molecule 79: 40S ribosomal protein S29



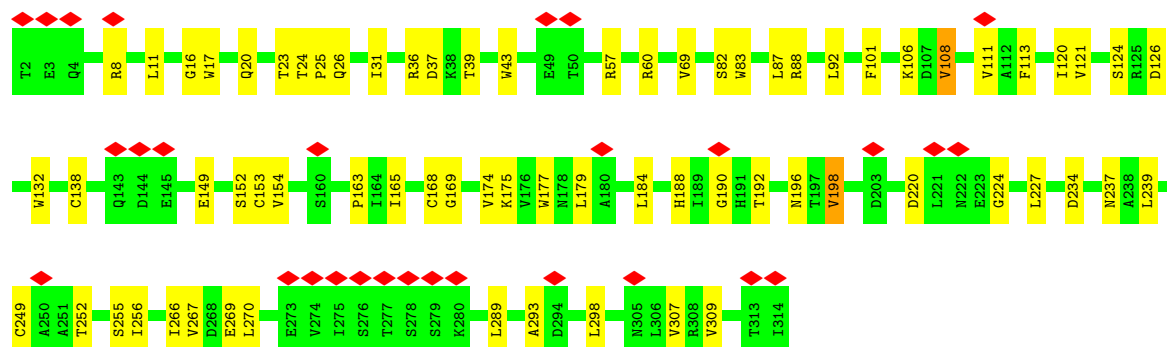
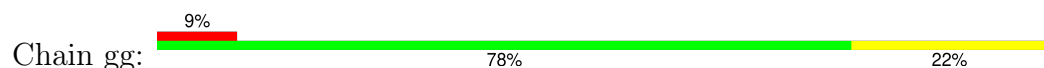
- Molecule 80: 40S ribosomal protein S30



- Molecule 81: 40S ribosomal protein S27a



- Molecule 82: Receptor of activated protein C kinase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74031	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	1.018	Depositor
Minimum map value	-0.622	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.1	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: B8H, 6MZ, PSU, I4U, 4AC, E3C, MG, OMC, MLZ, B8W, OMU, B9H, UR3, E7G, B8K, B8N, 5MC, A2M, P4U, B9B, 7MG, P7G, MA6, ZN, M7A, BGH, 2MG, OMG, B8T, E6G, 1MA, MHG, 5MU, B8Q

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	4	0.22	0/1779	0.45	0/2771
2	5	0.45	3/83825 (0.0%)	0.50	11/130614 (0.0%)
3	7	0.42	0/2858	0.42	0/4455
4	8	0.45	0/3559	0.46	0/5543
5	A	0.54	0/1936	0.76	1/2596 (0.0%)
6	B	0.48	0/3240	0.68	0/4339
7	C	0.49	0/2927	0.65	0/3932
8	D	0.39	0/2437	0.59	2/3264 (0.1%)
9	E	0.39	0/1762	0.64	1/2362 (0.0%)
10	F	0.49	0/1911	0.72	0/2549
11	G	0.43	0/1910	0.66	0/2569
12	H	0.43	0/1535	0.69	0/2063
13	I	0.43	0/1702	0.58	0/2272
14	J	0.39	0/1385	0.71	0/1852
15	L	0.42	0/1733	0.67	0/2316
16	M	0.44	0/1158	0.67	0/1547
17	N	0.52	0/1746	0.70	2/2338 (0.1%)
18	O	0.48	0/1662	0.67	0/2222
19	P	0.49	0/1268	0.67	0/1700
20	Q	0.49	0/1539	0.72	0/2054
21	R	0.47	0/1524	0.74	1/2013 (0.0%)
22	S	0.50	0/1501	0.68	0/2012
23	T	0.47	0/1326	0.66	0/1770
24	U	0.36	0/823	0.69	0/1104
25	V	0.46	0/993	0.63	0/1332
26	W	0.41	0/873	0.74	0/1158
27	X	0.43	0/984	0.61	0/1323
28	Y	0.42	0/1132	0.68	0/1504
29	Z	0.43	0/1130	0.63	0/1507
30	a	0.51	0/1191	0.63	0/1590

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	b	0.37	0/861	0.67	0/1138
32	c	0.46	0/771	0.66	0/1034
33	d	0.43	0/903	0.71	0/1216
34	e	0.48	0/1071	0.63	0/1429
35	f	0.50	0/895	0.70	0/1198
36	g	0.45	0/916	0.71	0/1220
37	h	0.41	0/1021	0.65	0/1348
38	i	0.40	0/841	0.64	0/1112
39	j	0.49	0/720	0.72	0/952
40	k	0.45	1/575 (0.2%)	0.65	1/761 (0.1%)
41	l	0.51	0/459	0.74	0/608
42	m	0.44	0/425	0.74	0/561
43	n	0.43	0/240	0.77	0/305
44	o	0.43	0/855	0.57	0/1128
45	p	0.48	0/718	0.66	0/953
46	r	0.50	0/1010	0.70	0/1354
47	u	0.29	0/1680	0.75	3/2255 (0.1%)
48	v	0.32	0/2779	0.72	0/3751
49	9	0.38	0/39723	0.47	0/61870
50	AA	0.42	0/1747	0.67	0/2374
51	BB	0.42	0/1756	0.72	0/2350
52	CC	0.43	0/1753	0.69	0/2369
53	DD	0.32	0/1796	0.67	2/2417 (0.1%)
54	EE	0.39	0/2118	0.66	0/2849
55	FF	0.39	0/1492	0.69	1/2005 (0.0%)
56	GG	0.33	0/1946	0.65	0/2590
57	HH	0.35	0/1510	0.70	0/2022
58	II	0.42	0/1715	0.68	0/2287
59	JJ	0.37	0/1550	0.62	0/2069
60	KK	0.32	0/834	0.73	2/1125 (0.2%)
61	LL	0.43	0/1195	0.64	0/1597
62	MM	0.30	0/918	0.72	2/1233 (0.2%)
63	NN	0.42	0/1226	0.70	0/1649
64	OO	0.45	0/1029	0.67	1/1380 (0.1%)
65	PP	0.36	0/1017	0.67	0/1358
66	QQ	0.34	0/1146	0.65	0/1534
67	RR	0.36	0/1082	0.70	0/1452
68	SS	0.31	0/1208	0.69	2/1618 (0.1%)
69	TT	0.32	0/1115	0.60	0/1493
70	UU	0.33	0/805	0.65	0/1081
71	VV	0.42	0/643	0.63	0/860
72	WW	0.46	0/1051	0.73	0/1406
73	XX	0.40	0/1116	0.68	2/1490 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	YY	0.34	0/1028	0.57	0/1366
75	ZZ	0.29	0/604	0.56	0/810
76	aa	0.47	1/828 (0.1%)	0.70	0/1109
77	bb	0.37	0/665	0.63	0/891
78	cc	0.34	0/490	0.61	0/656
79	dd	0.36	0/470	0.59	0/623
80	ee	0.32	0/447	0.66	0/587
81	ff	0.25	0/567	0.58	0/753
82	gg	0.29	0/2493	0.63	0/3394
All	All	0.42	5/229172 (0.0%)	0.57	34/335661 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	B	0	1
7	C	0	1
11	G	0	1
12	H	0	1
15	L	0	2
17	N	0	3
18	O	0	1
23	T	0	1
31	b	0	1
33	d	0	1
40	k	0	1
47	u	0	2
52	CC	0	1
54	EE	0	1
71	VV	0	1
72	WW	0	1
73	XX	0	1
81	ff	0	1
All	All	0	22

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	k	61	PRO	CA-C	5.65	1.55	1.52
2	5	4523	A2M	O3'-P	5.64	1.61	1.56

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3785	A2M	O3'-P	5.22	1.61	1.56
76	aa	98	PRO	CA-C	-5.20	1.48	1.52
2	5	1534	A2M	O3'-P	5.04	1.61	1.56

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4056	A	OP1-P-O3'	-9.67	78.98	108.00
64	OO	137	SER	N-CA-C	-6.58	103.72	111.03
2	5	4056	A	OP2-P-O3'	-6.48	88.57	108.00
5	A	15	VAL	N-CA-C	-6.26	106.61	113.43
40	k	61	PRO	O-C-N	6.13	124.03	121.15
55	FF	88	MET	CG-SD-CE	-6.07	87.56	100.90
17	N	120	TRP	CA-C-N	-5.97	116.50	122.77
17	N	120	TRP	C-N-CA	-5.97	116.50	122.77
53	DD	43	PRO	CA-C-N	5.59	132.22	121.54
53	DD	43	PRO	C-N-CA	5.59	132.22	121.54
2	5	2046	G	P-O3'-C3'	5.51	128.47	120.20
21	R	99	MET	CA-CB-CG	-5.48	103.13	114.10
2	5	2695	A	P-O3'-C3'	5.41	128.32	120.20
2	5	1406(B)	C	P-O3'-C3'	5.32	126.08	119.70
2	5	4925	U	P-O3'-C3'	5.28	128.12	120.20
9	E	180	GLY	N-CA-C	-5.26	101.61	112.34
62	MM	54	SER	CA-C-N	5.25	131.58	121.54
62	MM	54	SER	C-N-CA	5.25	131.58	121.54
47	u	145	VAL	CA-C-N	5.22	131.51	121.54
47	u	145	VAL	C-N-CA	5.22	131.51	121.54
2	5	1072	C	P-O3'-C3'	5.20	127.99	120.20
2	5	3888	G	C2'-C3'-O3'	5.19	121.48	113.70
2	5	2695	A	C2'-C3'-O3'	5.17	117.25	109.50
68	SS	99	LEU	CA-C-N	5.16	129.40	121.19
68	SS	99	LEU	C-N-CA	5.16	129.40	121.19
2	5	3876	A	P-O3'-C3'	5.11	127.86	120.20
73	XX	126	ALA	CA-C-N	5.07	131.22	121.54
73	XX	126	ALA	C-N-CA	5.07	131.22	121.54
47	u	25	ARG	CA-CB-CG	5.05	124.20	114.10
2	5	4947	U	C2'-C3'-O3'	5.03	121.25	113.70
60	KK	2	LEU	CA-C-N	5.02	138.35	121.27
60	KK	2	LEU	C-N-CA	5.02	138.35	121.27
8	D	229	ASN	CA-C-N	5.01	131.11	121.54
8	D	229	ASN	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B	55	HIS	Peptide
7	C	73	VAL	Peptide
52	CC	187	ARG	Peptide
54	EE	155	LYS	Peptide
11	G	215	ASP	Peptide
12	H	50	LYS	Peptide
15	L	209	LYS	Peptide
15	L	46	ILE	Peptide
17	N	184	ILE	Peptide
17	N	76	PRO	Peptide
17	N	78	GLY	Peptide
18	O	110	PRO	Peptide
23	T	80	VAL	Peptide
71	VV	32	ILE	Peptide
72	WW	54	ASP	Peptide
73	XX	61	GLN	Peptide
31	b	101	HIS	Peptide
33	d	95	ASP	Peptide
81	ff	137	ASP	Peptide
40	k	69	LEU	Peptide
47	u	117	ILE	Peptide
47	u	60	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4	1593	0	809	11	0
2	5	77254	0	38800	555	0
3	7	2558	0	1296	17	0
4	8	3209	0	1631	25	0
5	A	1898	0	1993	41	0
6	B	3172	0	3310	54	0
7	C	2884	0	3054	36	0
8	D	2391	0	2424	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	1729	0	1887	20	0
10	F	1875	0	1995	25	0
11	G	1879	0	2027	29	0
12	H	1516	0	1595	28	0
13	I	1664	0	1712	19	0
14	J	1362	0	1399	16	0
15	L	1702	0	1820	29	0
16	M	1137	0	1209	12	0
17	N	1701	0	1749	33	0
18	O	1630	0	1778	17	0
19	P	1242	0	1274	17	0
20	Q	1515	0	1634	21	0
21	R	1508	0	1664	27	0
22	S	1462	0	1508	25	0
23	T	1298	0	1366	16	0
24	U	809	0	833	7	0
25	V	979	0	1039	21	0
26	W	860	0	903	17	0
27	X	967	0	1040	9	0
28	Y	1115	0	1205	16	0
29	Z	1107	0	1182	15	0
30	a	1162	0	1209	20	0
31	b	848	0	920	8	0
32	c	761	0	794	4	0
33	d	888	0	930	11	0
34	e	1053	0	1147	12	0
35	f	876	0	912	12	0
36	g	906	0	998	11	0
37	h	1013	0	1147	10	0
38	i	830	0	916	6	0
39	j	705	0	737	8	0
40	k	569	0	637	8	0
41	l	447	0	480	8	0
42	m	430	0	466	10	0
43	n	239	0	289	10	0
44	o	842	0	913	9	0
45	p	708	0	756	12	0
46	r	994	0	1051	12	0
47	u	1654	0	1760	33	0
48	v	2737	0	2782	24	0
49	9	36291	0	18321	273	0
50	AA	1710	0	1708	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	BB	1729	0	1803	35	0
52	CC	1716	0	1806	25	0
53	DD	1768	0	1866	31	0
54	EE	2076	0	2177	32	0
55	FF	1471	0	1522	24	0
56	GG	1923	0	2089	40	0
57	HH	1488	0	1582	29	0
58	II	1686	0	1772	21	0
59	JJ	1525	0	1640	21	0
60	KK	810	0	836	18	0
61	LL	1175	0	1249	16	0
62	MM	908	0	939	16	0
63	NN	1202	0	1289	11	0
64	OO	1016	0	1039	16	0
65	PP	997	0	1045	13	0
66	QQ	1128	0	1195	19	0
67	RR	1068	0	1121	21	0
68	SS	1190	0	1249	15	0
69	TT	1097	0	1132	20	0
70	UU	795	0	862	14	0
71	VV	636	0	637	12	0
72	WW	1034	0	1080	24	0
73	XX	1098	0	1167	16	0
74	YY	1011	0	1083	10	0
75	ZZ	598	0	656	8	0
76	aa	814	0	865	9	0
77	bb	651	0	672	5	0
78	cc	488	0	514	6	0
79	dd	459	0	449	10	0
80	ee	443	0	492	6	0
81	ff	555	0	566	11	0
82	gg	2436	0	2393	44	0
83	5	199	0	0	0	0
83	7	7	0	0	0	0
83	8	6	0	0	0	0
83	9	77	0	0	0	0
83	A	1	0	0	0	0
83	B	1	0	0	0	0
83	LL	1	0	0	0	0
83	P	2	0	0	0	0
83	TT	1	0	0	0	0
83	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	j	1	0	0	0	0
84	aa	1	0	0	0	0
84	dd	1	0	0	0	0
84	ff	1	0	0	0	0
84	g	1	0	0	0	0
84	j	1	0	0	0	0
84	m	1	0	0	0	0
84	o	1	0	0	0	0
84	p	1	0	0	0	0
All	All	216975	0	161796	1824	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 5.

All (1824) 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)
2:5:1860:B8H:C4	2:5:1860:B8H:C5	1.82	1.57
2:5:4296:B8H:C5	2:5:4296:B8H:C4	1.83	1.56
2:5:1860:B8H:C6	2:5:1860:B8H:N1	1.68	1.54
2:5:3762:B8H:C6	2:5:3762:B8H:N1	1.68	1.54
2:5:3762:B8H:C4	2:5:3762:B8H:C5	1.82	1.54
2:5:4296:B8H:N1	2:5:4296:B8H:C6	1.67	1.54
49:9:166:A2M:C1'	49:9:166:A2M:O4'	1.64	1.28
49:9:159:A2M:C1'	49:9:159:A2M:O4'	1.64	1.26
2:5:4523:A2M:C1'	2:5:4523:A2M:O4'	1.63	1.25
2:5:3718:A2M:C1'	2:5:3718:A2M:O4'	1.63	1.24
49:9:1031:A2M:C1'	49:9:1031:A2M:O4'	1.63	1.23
2:5:4571:A2M:C1'	2:5:4571:A2M:O4'	1.63	1.17
2:5:3723:A2M:C1'	2:5:3723:A2M:O4'	1.63	1.16
2:5:398:A2M:C1'	2:5:398:A2M:O4'	1.63	1.15
2:5:3899:BGH:C4'	2:5:3899:BGH:O4'	1.65	1.13
2:5:2754:B9B:C1'	2:5:2754:B9B:O4'	1.64	1.12
2:5:3951:G:N1	2:5:4062:A:H2	1.47	1.12
2:5:1574:B9B:C1'	2:5:1574:B9B:O4'	1.64	1.10
2:5:237:B9B:C1'	2:5:237:B9B:O4'	1.65	1.07
2:5:4887:C:N4	2:5:4932:U:H3	1.61	0.96
2:5:3951:G:N1	2:5:4062:A:C2	2.25	0.94
7:C:218:VAL:O	7:C:222:ARG:HB2	1.67	0.93
2:5:3952:A:H2	2:5:4061:G:H1	0.98	0.91
1:4:6:G:H1	1:4:67:U:H3	1.20	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:2845:A:H61	2:5:3843:C:H42	1.21	0.88
2:5:3762:B8H:N1	2:5:3762:B8H:C5	2.36	0.87
2:5:4887:C:H42	2:5:4932:U:H3	0.86	0.82
2:5:3952:A:C2	2:5:4061:G:N1	2.47	0.82
2:5:3952:A:H2	2:5:4061:G:N1	1.79	0.80
51:BB:67:PHE:O	51:BB:85:LYS:HA	1.82	0.79
62:MM:25:ALA:O	62:MM:29:ASP:HA	1.84	0.76
62:MM:34:GLY:O	62:MM:38:ALA:HB2	1.86	0.76
2:5:4296:B8H:C5	2:5:4296:B8H:N1	2.35	0.74
50:AA:126:ASP:O	50:AA:130:ASP:HB2	1.88	0.74
81:ff:141:CYS:O	81:ff:145:CYS:HA	1.87	0.74
2:5:1860:B8H:C6	2:5:1860:B8H:C2	2.65	0.73
2:5:2845:A:H61	2:5:3843:C:N4	1.85	0.73
2:5:2845:A:N6	2:5:3843:C:H42	1.85	0.73
47:u:53:VAL:O	47:u:154:THR:HA	1.88	0.72
2:5:4296:B8H:C6	2:5:4296:B8H:C2	2.65	0.72
2:5:3762:B8H:C6	2:5:3762:B8H:C2	2.66	0.71
2:5:4162:C:H5	11:G:126:ARG:HH12	1.37	0.71
49:9:1416:C:HO2'	69:TT:3:GLY:N	1.87	0.71
53:DD:45:ARG:HA	53:DD:83:SER:O	1.91	0.71
49:9:1623:A:H62	68:SS:132:ARG:HH21	1.37	0.70
81:ff:132:MET:HG2	81:ff:141:CYS:HB2	1.73	0.70
49:9:1590:C:H5'	69:TT:82:ARG:HH12	1.56	0.70
57:HH:144:ILE:HD11	57:HH:152:ARG:HD3	1.74	0.70
49:9:1396:A:O2'	49:9:1398:G:N7	2.24	0.69
76:aa:12:LYS:HD3	76:aa:16:GLY:H	1.57	0.69
9:E:115:MET:O	46:r:87:ARG:NH1	2.26	0.69
12:H:94:SER:HB3	12:H:142:ASP:HB3	1.73	0.69
2:5:4523:A2M:H5''	2:5:4524:G:H5'	1.74	0.69
13:I:36:LEU:HD11	13:I:69:ARG:HH21	1.58	0.68
28:Y:59:ARG:HB2	28:Y:103:LYS:HG2	1.76	0.68
50:AA:10:MET:HE2	50:AA:15:VAL:HG22	1.75	0.68
54:EE:137:PRO:HB2	54:EE:150:PRO:HD2	1.76	0.68
49:9:351:G:OP1	58:II:7:ASN:ND2	2.27	0.68
55:FF:71:ARG:NH1	55:FF:148:ASN:OD1	2.26	0.68
51:BB:48:LEU:HB2	64:OO:51:GLU:HG2	1.76	0.68
53:DD:123:LEU:HD11	53:DD:152:PHE:HB3	1.75	0.67
70:UU:80:PHE:HB3	79:dd:52:PHE:HB3	1.74	0.67
49:9:1834:A:H2	49:9:1837:G:H1	1.43	0.67
53:DD:46:THR:HB	53:DD:84:VAL:HG12	1.77	0.67
2:5:2521:G:H2'	2:5:2522:7MG:H82	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:117:GLU:HB3	5:A:162:ASN:HB2	1.75	0.67
13:I:210:ARG:O	13:I:214:SER:HB2	1.94	0.67
2:5:1351:G:OP1	7:C:33:ARG:NH1	2.28	0.66
56:GG:31:ARG:HG2	56:GG:101:ILE:HG22	1.76	0.66
49:9:1091:C:HO2'	72:WW:2:VAL:N	1.92	0.66
48:v:284:ALA:HB2	48:v:335:VAL:HG23	1.77	0.66
2:5:4895:C:O2	16:M:132:ARG:NH2	2.29	0.66
50:AA:80:ARG:NH1	50:AA:165:ASN:O	2.29	0.66
57:HH:72:PHE:O	57:HH:76:GLN:HB2	1.95	0.66
2:5:3952:A:N1	2:5:4061:G:O6	2.29	0.65
34:e:7:LEU:HB2	34:e:93:LYS:HB3	1.78	0.65
2:5:3688:U:OP2	5:A:198:ARG:NH2	2.30	0.65
42:m:71:ARG:HE	42:m:96:ARG:HB3	1.62	0.65
2:5:1459:A:OP1	20:Q:65:ARG:NH2	2.29	0.65
8:D:50:ARG:O	8:D:64:ILE:HA	1.97	0.65
54:EE:106:LYS:HE3	54:EE:108:ARG:HH22	1.60	0.65
61:LL:101:ARG:HB2	73:XX:10:ALA:HB2	1.78	0.65
2:5:469:C:N3	9:E:108:ARG:NH1	2.44	0.65
2:5:4296:B8H:C6	2:5:4296:B8H:CN1	2.73	0.64
50:AA:52:LYS:HB2	67:RR:109:LEU:HD21	1.79	0.64
59:JJ:136:ARG:NH1	59:JJ:159:PHE:O	2.30	0.64
49:9:1096:G:OP1	72:WW:20:ARG:NH1	2.30	0.64
2:5:4525:C:OP1	6:B:246:ARG:NH1	2.31	0.64
59:JJ:136:ARG:HA	59:JJ:141:VAL:HA	1.80	0.64
13:I:150:GLU:OE2	13:I:153:ARG:NH1	2.30	0.64
2:5:2406:G:N7	41:l:2:SER:N	2.46	0.63
21:R:42:ARG:HA	21:R:45:ILE:HD12	1.79	0.63
2:5:979:G:OP1	9:E:49:ASN:ND2	2.31	0.63
57:HH:117:PRO:HG2	57:HH:120:ARG:HD3	1.81	0.63
2:5:1860:B8H:C5	2:5:1860:B8H:N1	2.38	0.63
47:u:52:THR:HA	47:u:155:ILE:O	1.98	0.63
4:8:75:G:OP2	28:Y:74:TYR:OH	2.16	0.63
2:5:3956:G:C6	2:5:3966:A:C5	2.87	0.63
51:BB:137:LEU:HB3	51:BB:172:MET:HE2	1.80	0.63
48:v:131:LYS:O	48:v:135:GLN:HB2	1.99	0.62
4:8:49:G:H5'	37:h:47:ILE:HD11	1.79	0.62
21:R:15:LEU:HD23	21:R:52:ARG:HB3	1.82	0.62
13:I:30:LYS:HD3	13:I:63:GLU:HG3	1.80	0.62
20:Q:67:ILE:HD12	20:Q:96:PRO:HD2	1.80	0.62
82:gg:266:ILE:HD11	82:gg:269:GLU:HB2	1.82	0.62
32:c:31:TYR:OH	32:c:59:GLU:OE2	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DD:134:CYS:SG	53:DD:135:GLU:N	2.72	0.62
2:5:1:C:H42	4:8:156:U:H3	1.48	0.62
21:R:35:ALA:O	21:R:40:GLN:NE2	2.31	0.62
6:B:254:ILE:HD13	6:B:268:ARG:HH22	1.64	0.62
22:S:8:ARG:NH1	22:S:35:PRO:O	2.32	0.62
26:W:6:CYS:HB3	26:W:10:GLY:H	1.63	0.62
53:DD:172:VAL:HG22	53:DD:185:LYS:HG2	1.82	0.62
19:P:23:ARG:NH1	19:P:125:MET:SD	2.73	0.62
49:9:1148:A:OP1	76:aa:6:ARG:NH2	2.33	0.62
2:5:2429:A:H5''	41:l:43:HIS:HE2	1.63	0.62
49:9:312:G:O2'	56:GG:191:ARG:NH1	2.33	0.62
49:9:940:U:H3	49:9:1002:U:H3	1.46	0.62
26:W:80:ARG:NH1	56:GG:8:PRO:O	2.33	0.61
62:MM:96:ARG:HH22	62:MM:100:PRO:HG3	1.65	0.61
49:9:616:A:OP1	73:XX:68:LYS:NZ	2.33	0.61
49:9:1610:G:OP2	68:SS:132:ARG:NH1	2.33	0.61
2:5:200:U:O4	28:Y:103:LYS:NZ	2.32	0.61
2:5:2847:G:OP1	25:V:101:ASN:ND2	2.34	0.61
48:v:272:SER:O	48:v:276:ARG:NH1	2.34	0.61
53:DD:226:GLN:NE2	82:gg:224:GLY:O	2.33	0.61
82:gg:24:THR:HG22	82:gg:26:GLN:H	1.66	0.61
49:9:316:G:H3'	56:GG:183:ARG:HH22	1.66	0.61
32:c:56:ARG:HA	32:c:59:GLU:HG2	1.83	0.61
2:5:4939:C:OP1	9:E:190:ARG:NH1	2.34	0.61
55:FF:50:PRO:HG2	55:FF:90:VAL:HG22	1.83	0.60
2:5:294:G:OP2	44:o:43:ARG:NH2	2.32	0.60
21:R:102:LEU:HD22	21:R:138:LEU:HD13	1.83	0.60
49:9:960:U:H5''	64:OO:149:ARG:HH22	1.66	0.60
62:MM:52:LEU:HD21	62:MM:62:VAL:HG23	1.83	0.60
82:gg:8:ARG:HB3	82:gg:309:VAL:HG23	1.82	0.60
5:A:116:LEU:HB3	5:A:126:LEU:HB2	1.83	0.60
55:FF:55:ARG:NH2	66:QQ:123:ASP:OD1	2.34	0.60
2:5:2262:G:OP2	46:r:98:ARG:NH2	2.35	0.60
8:D:65:ALA:HB2	8:D:74:ILE:HG13	1.83	0.60
54:EE:179:ASN:HD22	54:EE:230:LYS:HA	1.67	0.60
49:9:989:C:O2	76:aa:32:LYS:NZ	2.35	0.60
48:v:209:GLU:OE2	48:v:259:ARG:NH2	2.35	0.60
49:9:1103:C:OP1	51:BB:157:GLN:NE2	2.34	0.60
2:5:3641:U:OP2	2:5:3646:A:N6	2.34	0.60
2:5:2007:G:H21	2:5:2012:A:H62	1.49	0.60
2:5:2299:G:OP2	7:C:204:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:10:ARG:NH1	6:B:265:SER:O	2.35	0.60
25:V:82:ILE:HG22	25:V:83:ARG:HG3	1.84	0.60
49:9:587:A:H5'	49:9:592:C:H41	1.67	0.60
56:GG:55:GLY:HA3	56:GG:108:VAL:O	2.01	0.60
60:KK:31:LYS:NZ	60:KK:35:LEU:O	2.33	0.60
60:KK:92:ALA:HA	60:KK:95:ARG:HE	1.65	0.60
70:UU:53:PRO:HA	70:UU:88:LEU:O	2.01	0.60
2:5:67:C:OP2	2:5:312:G:N2	2.34	0.60
11:G:158:GLU:OE1	11:G:166:ARG:NH2	2.35	0.60
49:9:1192:U:OP2	73:XX:119:ARG:NH2	2.35	0.60
50:AA:36:GLN:O	50:AA:53:ARG:NH1	2.34	0.60
2:5:1503:A:H4'	2:5:1504:G:H5'	1.84	0.59
2:5:2489:C:O2'	2:5:2491:C:N4	2.34	0.59
2:5:2626:U:O4	24:U:97:ARG:NH1	2.35	0.59
10:F:93:ARG:NH2	10:F:95:ARG:O	2.35	0.59
16:M:104:MET:HE2	18:O:199:HIS:HB3	1.84	0.59
22:S:92:ASN:ND2	23:T:156:TYR:O	2.35	0.59
2:5:2793:G:H5'	2:5:2794:C:H5''	1.83	0.59
2:5:4930:C:H5'	9:E:269:GLN:HG2	1.84	0.59
49:9:694:G:H1	49:9:732:U:H3	1.50	0.59
49:9:1617:G:N1	49:9:1620:A:OP2	2.35	0.59
56:GG:66:GLY:N	56:GG:100:CYS:SG	2.75	0.59
63:NN:49:GLN:HA	63:NN:52:VAL:HG22	1.83	0.59
82:gg:16:GLY:H	82:gg:37:ASP:HB2	1.65	0.59
2:5:1362:G:OP1	15:L:39:ARG:NH2	2.34	0.59
2:5:2103:A:O2'	31:b:103:LYS:NZ	2.35	0.59
2:5:2811:G:N1	2:5:2814:C:OP2	2.32	0.59
49:9:1658:G:OP2	49:9:1660:C:N4	2.35	0.59
2:5:3951:G:O6	2:5:4062:A:N1	2.35	0.59
3:7:6:C:H4'	8:D:52:ILE:HD13	1.83	0.59
2:5:1860:B8H:C6	2:5:1860:B8H:CN1	2.76	0.59
2:5:3762:B8H:C6	2:5:3762:B8H:CN1	2.74	0.59
16:M:35:ARG:NH2	22:S:99:ASP:OD1	2.35	0.59
28:Y:50:ARG:HB2	28:Y:115:ARG:HH22	1.67	0.59
45:p:38:THR:HA	45:p:45:THR:HA	1.83	0.59
50:AA:147:LEU:O	50:AA:165:ASN:ND2	2.35	0.59
2:5:1870:C:H2'	2:5:1871:A2M:H8	1.84	0.59
2:5:2528:G:H4'	2:5:2783:A:H4'	1.84	0.59
2:5:4380:A:OP1	44:o:58:LYS:NZ	2.34	0.59
5:A:97:ASN:OD1	5:A:100:ASN:ND2	2.36	0.59
29:Z:84:ARG:NH1	36:g:99:GLU:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:21:ARG:HB3	17:N:197:THR:HG22	1.83	0.59
66:QQ:97:GLN:OE1	66:QQ:105:LYS:NZ	2.33	0.59
2:5:1319:U:N3	2:5:1322:1MA:OP2	2.35	0.59
49:9:637:U:OP2	80:ee:97:LYS:NZ	2.36	0.59
2:5:338:A:OP1	15:L:31:ARG:NH1	2.35	0.59
2:5:728:U:OP1	10:F:75:ARG:NH2	2.36	0.59
49:9:1293:A:H61	49:9:1306:U:H3	1.48	0.59
64:OO:99:ALA:H	64:OO:133:THR:HG22	1.67	0.59
2:5:1645:C:OP1	7:C:80:ARG:NH2	2.36	0.58
2:5:4558:U:OP2	6:B:246:ARG:NH2	2.36	0.58
2:5:4765:G:OP1	12:H:23:ARG:NE	2.36	0.58
23:T:119:ALA:HA	23:T:122:LYS:HB2	1.84	0.58
65:PP:111:MET:HA	68:SS:117:ILE:HD11	1.85	0.58
2:5:3877:A:O2'	2:5:4400:G:N2	2.35	0.58
47:u:48:ARG:NH2	47:u:159:MET:O	2.36	0.58
49:9:1143:A:OP2	52:CC:187:ARG:NH2	2.36	0.58
2:5:1358:G:N2	2:5:1381:U:O4	2.35	0.58
2:5:1931:C:N4	2:5:2040:A:O2'	2.36	0.58
4:8:94:G:OP2	39:j:72:ARG:NH2	2.36	0.58
12:H:59:LYS:HE2	12:H:66:GLU:HB3	1.84	0.58
49:9:525:A:OP2	80:ee:99:LYS:NZ	2.37	0.58
50:AA:122:LEU:HG	50:AA:142:LEU:HD23	1.84	0.58
50:AA:214:GLU:OE2	67:RR:81:ARG:NH2	2.36	0.58
55:FF:40:ALA:HB3	55:FF:67:PRO:HA	1.85	0.58
49:9:496:C:OP1	54:EE:49:ARG:NH1	2.36	0.58
67:RR:16:ILE:HG22	67:RR:24:LEU:HD11	1.86	0.58
2:5:1840:G:OP2	10:F:201:LYS:NZ	2.36	0.58
2:5:1895:G:O2'	2:5:1907:A:N3	2.35	0.58
2:5:2583:C:OP2	36:g:76:ARG:NH1	2.32	0.58
2:5:2836:A:H4'	6:B:229:LYS:HA	1.83	0.58
22:S:34:ALA:HB1	22:S:39:VAL:HG13	1.85	0.58
47:u:26:ARG:HH12	47:u:209:THR:HB	1.66	0.58
49:9:1398:G:O2'	82:gg:88:ARG:NH2	2.36	0.58
2:5:4087:G:H1	11:G:99:GLN:HE22	1.51	0.58
3:7:27:G:OP1	14:J:146:ARG:NH1	2.37	0.58
16:M:89:THR:HG22	16:M:91:TRP:H	1.66	0.58
28:Y:112:ASP:H	28:Y:115:ARG:HB3	1.68	0.58
51:BB:32:ASP:OD1	51:BB:46:LYS:NZ	2.36	0.58
52:CC:134:ASN:OD1	52:CC:167:ARG:NH1	2.36	0.58
55:FF:145:ARG:HB2	78:cc:49:PRO:HD2	1.86	0.58
2:5:230:G:OP1	28:Y:15:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:1215:C:OP2	10:F:58:LYS:NZ	2.37	0.58
2:5:1739:G:N3	2:5:1742:A:N6	2.51	0.58
4:8:85:U:O4	28:Y:50:ARG:NH2	2.36	0.58
8:D:53:VAL:HG11	8:D:159:VAL:HA	1.85	0.58
49:9:1205:C:O2'	49:9:1834:A:N6	2.37	0.58
2:5:4212:A:N1	23:T:3:ASN:ND2	2.46	0.58
50:AA:63:ARG:HD3	50:AA:185:MET:HE1	1.85	0.58
2:5:262:G:H2'	2:5:263:G:H8	1.69	0.58
2:5:1081:C:H42	2:5:1218:G:H1	1.51	0.58
2:5:1364:U:OP2	15:L:36:ARG:NH2	2.36	0.58
2:5:1919:G:N2	22:S:163:HIS:O	2.36	0.58
2:5:2020:U:H2'	2:5:2021:G:H8	1.69	0.58
20:Q:89:ASP:OD1	20:Q:91:ARG:NH2	2.37	0.58
48:v:332:PHE:HA	48:v:335:VAL:HG12	1.84	0.58
59:JJ:63:LEU:HD22	59:JJ:70:ARG:HB2	1.85	0.58
82:gg:25:PRO:HA	82:gg:293:ALA:HB1	1.86	0.58
2:5:4517:A:OP2	6:B:2:SER:N	2.37	0.58
49:9:925:G:H1	49:9:1017:U:H3	1.49	0.58
57:HH:63:PHE:HA	57:HH:95:ILE:O	2.04	0.58
2:5:303:C:OP2	17:N:68:ARG:NH2	2.37	0.57
2:5:1670:G:OP1	31:b:12:GLN:NE2	2.37	0.57
8:D:55:VAL:HG12	8:D:60:ILE:HG12	1.85	0.57
12:H:85:THR:HG23	12:H:86:LEU:HG	1.86	0.57
2:5:2422:OMC:OP1	19:P:127:ARG:NH2	2.37	0.57
2:5:3651:A:OP2	5:A:200:ARG:NH1	2.37	0.57
17:N:96:ARG:NH1	17:N:104:GLU:OE1	2.37	0.57
25:V:13:LYS:HB2	25:V:128:LEU:HD11	1.86	0.57
2:5:85:G:O2'	2:5:97:G:O6	2.22	0.57
2:5:729:2MG:N2	22:S:66:GLN:O	2.37	0.57
49:9:433:A:H5''	58:II:22:HIS:HB3	1.86	0.57
49:9:1507:G:N2	81:ff:87:THR:O	2.37	0.57
64:OO:97:LEU:HD11	64:OO:112:ALA:HB1	1.85	0.57
49:9:874:G:N3	57:HH:114:GLN:NE2	2.51	0.57
49:9:1623:A:H5''	68:SS:133:GLY:HA3	1.85	0.57
54:EE:126:VAL:HA	54:EE:141:THR:HA	1.87	0.57
58:II:101:ILE:HD12	58:II:190:LEU:HD11	1.85	0.57
70:UU:54:VAL:HG22	70:UU:88:LEU:HB2	1.87	0.57
72:WW:42:MET:HE2	72:WW:49:GLU:HA	1.87	0.57
2:5:1316:OMG:OP1	34:e:43:ASN:ND2	2.37	0.57
2:5:4896:G:H2'	2:5:4897:G:H8	1.69	0.57
10:F:41:LEU:HD11	31:b:102:PRO:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:227:VAL:HG13	22:S:39:VAL:HG23	1.86	0.57
17:N:181:HIS:O	17:N:195:ARG:NH2	2.34	0.57
46:r:65:LYS:O	46:r:102:TYR:OH	2.20	0.57
49:9:165:G:N2	49:9:165:G:OP2	2.37	0.57
53:DD:190:LEU:HD23	53:DD:199:GLY:HA2	1.87	0.57
67:RR:31:ASN:HA	67:RR:34:VAL:HG12	1.85	0.57
21:R:173:ARG:HA	21:R:176:ARG:HG2	1.87	0.57
24:U:111:GLU:OE2	24:U:113:ARG:NH1	2.37	0.57
35:f:50:VAL:HG22	35:f:69:VAL:HG12	1.87	0.57
49:9:951:C:O2'	64:OO:50:LYS:NZ	2.35	0.57
55:FF:19:LEU:HD12	55:FF:109:LEU:HD11	1.87	0.57
65:PP:52:LYS:HG2	65:PP:80:LEU:HD21	1.85	0.57
11:G:139:VAL:HG11	11:G:238:LYS:HE2	1.87	0.57
22:S:80:ILE:HG12	22:S:129:VAL:HG22	1.87	0.57
49:9:1550:G:H3'	49:9:1579:A:H61	1.69	0.57
58:II:27:TYR:HB3	58:II:49:ARG:HH12	1.70	0.57
2:5:2837:U:OP1	6:B:249:ARG:NH1	2.37	0.57
29:Z:54:THR:H	29:Z:57:MET:HE2	1.69	0.57
49:9:111:A:O2'	61:LL:69:ARG:NH1	2.38	0.57
49:9:527:C:H4'	59:JJ:121:LYS:HD3	1.87	0.57
56:GG:151:ASP:OD1	56:GG:151:ASP:N	2.38	0.57
65:PP:81:ARG:NH1	65:PP:120:SER:OG	2.38	0.57
82:gg:23:THR:HG22	82:gg:31:ILE:HD11	1.86	0.57
2:5:2616:C:OP1	21:R:60:ARG:NH1	2.37	0.57
5:A:70:LYS:HD2	5:A:72:ARG:HH12	1.70	0.57
22:S:13:VAL:HG23	22:S:62:VAL:HB	1.87	0.57
49:9:94:G:HO2'	49:9:508:A:HO2'	1.51	0.57
49:9:1650:A:H5''	66:QQ:139:ALA:HB2	1.86	0.57
82:gg:20:GLN:NE2	82:gg:69:VAL:O	2.36	0.57
82:gg:87:LEU:HB2	82:gg:101:PHE:HB2	1.85	0.57
2:5:942:G:OP1	10:F:244:ARG:NH1	2.38	0.57
2:5:4327:C:OP1	23:T:70:HIS:NE2	2.37	0.57
5:A:179:ILE:HG23	5:A:184:ARG:HB2	1.87	0.57
36:g:60:ARG:HD3	36:g:61:PRO:HD2	1.87	0.57
44:o:44:LYS:HE3	44:o:52:THR:HB	1.86	0.57
54:EE:112:HIS:NE2	54:EE:237:SER:OG	2.36	0.57
2:5:4583:C:O2'	2:5:4718:G:N2	2.38	0.56
11:G:111:PRO:HD2	11:G:114:ILE:HD12	1.86	0.56
21:R:151:ARG:HE	61:LL:118:ARG:HE	1.52	0.56
26:W:105:ARG:NH2	56:GG:148:SER:OG	2.38	0.56
39:j:19:CYS:SG	39:j:20:ARG:N	2.77	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BB:35:ALA:O	51:BB:42:ARG:NH1	2.38	0.56
2:5:1604:G:H2'	2:5:1605:7MG:H82	1.86	0.56
16:M:12:VAL:HG22	16:M:60:PHE:HB2	1.88	0.56
49:9:1206:G:N2	49:9:1835:A:OP1	2.38	0.56
49:9:1863:A:OP2	76:aa:4:LYS:NZ	2.37	0.56
57:HH:144:ILE:HB	57:HH:154:ILE:HG22	1.87	0.56
2:5:2380:B8W:N2	2:5:2425:U:OP1	2.37	0.56
2:5:4910:A:H4'	6:B:95:THR:HG22	1.86	0.56
5:A:225:ILE:HD11	5:A:235:VAL:H	1.70	0.56
49:9:126:G:OP2	56:GG:195:LYS:NZ	2.38	0.56
58:II:142:SER:O	58:II:146:GLN:HB2	2.04	0.56
1:4:58:A:O2'	1:4:61:C:N4	2.38	0.56
2:5:364:G:O6	39:j:52:LYS:NZ	2.38	0.56
2:5:2566:G:H2'	2:5:2567:G:H8	1.69	0.56
3:7:87:G:N2	3:7:90:A:OP2	2.39	0.56
47:u:20:GLY:HA2	47:u:22:GLN:HG2	1.87	0.56
49:9:153:G:N3	56:GG:13:GLN:NE2	2.51	0.56
55:FF:99:ILE:HD13	55:FF:171:GLU:HB3	1.87	0.56
62:MM:85:LEU:HA	62:MM:88:TRP:HD1	1.70	0.56
64:OO:56:VAL:HG12	64:OO:81:VAL:HG23	1.88	0.56
2:5:382:G:N1	2:5:385:A:OP2	2.36	0.56
2:5:2337:C:H4'	46:r:19:LYS:HB2	1.87	0.56
26:W:105:ARG:HE	56:GG:151:ASP:HB3	1.70	0.56
57:HH:36:LEU:HG	57:HH:40:LEU:HD23	1.87	0.56
30:a:85:GLN:HA	30:a:88:VAL:HG22	1.88	0.56
49:9:1036:A:N3	49:9:1844:U:O2'	2.36	0.56
49:9:1451:G:OP1	67:RR:32:LYS:NZ	2.37	0.56
49:9:1562:C:H2'	49:9:1563:G:H8	1.71	0.56
59:JJ:108:ARG:NH2	59:JJ:154:GLN:OE1	2.39	0.56
2:5:1502:G:OP2	20:Q:62:SER:OG	2.23	0.56
2:5:1573:G:OP1	21:R:92:LYS:NZ	2.39	0.56
2:5:3722:G:H2'	2:5:3723:A2M:H8	1.88	0.56
2:5:4981:G:O6	6:B:21:ARG:NH2	2.39	0.56
6:B:234:ARG:NH2	6:B:268:ARG:O	2.35	0.56
49:9:1014:G:N2	77:bb:51:GLN:OE1	2.39	0.56
2:5:2697:A:O3'	2:5:2711:G:N2	2.39	0.56
2:5:2810:U:H5''	21:R:70:ARG:HH22	1.71	0.56
2:5:3853:U:O2'	2:5:4979:A:N3	2.39	0.56
2:5:4943:A:OP1	9:E:157:THR:OG1	2.21	0.56
51:BB:121:ILE:HG12	51:BB:161:VAL:HG13	1.88	0.56
2:5:1077:C:OP1	2:5:1215:C:O2'	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:1516:G:O2'	15:L:18:TRP:NE1	2.38	0.55
2:5:2322:G:OP1	34:e:36:ARG:NH1	2.39	0.55
2:5:4429:C:N3	13:I:158:LYS:NZ	2.46	0.55
5:A:126:LEU:HD13	5:A:150:LEU:HD21	1.87	0.55
49:9:1587:G:H5''	69:TT:77:LYS:HD3	1.87	0.55
75:ZZ:68:ILE:HB	75:ZZ:109:TYR:HB2	1.88	0.55
2:5:32:G:N1	2:5:49:U:OP2	2.34	0.55
2:5:1420:A:N7	30:a:116:LYS:NZ	2.55	0.55
2:5:1654:G:N2	2:5:1678:C:OP1	2.39	0.55
36:g:11:LEU:O	36:g:18:ASN:ND2	2.39	0.55
69:TT:42:HIS:HB3	69:TT:93:SER:HB3	1.87	0.55
82:gg:163:PRO:HB2	82:gg:179:LEU:HB3	1.87	0.55
2:5:1991:A:N6	2:5:2003:G:OP1	2.40	0.55
6:B:71:GLU:OE1	26:W:1:MET:N	2.40	0.55
7:C:152:LEU:HD23	7:C:251:ILE:HG12	1.88	0.55
8:D:37:VAL:HG12	8:D:50:ARG:HD3	1.89	0.55
9:E:181:PRO:HD2	9:E:184:LEU:HD12	1.87	0.55
10:F:121:PHE:O	10:F:204:ASN:ND2	2.35	0.55
2:5:2465:C:H1'	2:5:3672:G:H1	1.71	0.55
2:5:2627:C:OP1	24:U:92:LYS:NZ	2.39	0.55
2:5:2725:A:N6	21:R:88:ARG:O	2.40	0.55
2:5:4761:G:H2'	2:5:4762:A:H8	1.71	0.55
2:5:1927:U:H3	2:5:2056:G:H1	1.53	0.55
2:5:3762:B8H:C5	2:5:3762:B8H:C2	2.84	0.55
2:5:4296:B8H:C5	2:5:4296:B8H:C2	2.83	0.55
22:S:69:GLU:HG3	22:S:72:PRO:HB3	1.88	0.55
48:v:325:ARG:HA	48:v:328:GLN:HG2	1.89	0.55
49:9:581:U:OP1	59:JJ:133:ARG:NH2	2.39	0.55
49:9:1060:A:O2'	49:9:1062:A:N7	2.38	0.55
2:5:966:A:O4'	2:5:968:C:N4	2.39	0.55
2:5:4522:G:O2'	2:5:4525:C:OP2	2.25	0.55
2:5:4764:A:O2'	12:H:43:VAL:O	2.22	0.55
47:u:64:SER:HB3	47:u:107:TYR:HD1	1.71	0.55
49:9:1597:C:OP2	75:ZZ:85:ARG:NH1	2.39	0.55
55:FF:32:ASP:HB3	55:FF:35:LEU:H	1.72	0.55
2:5:4862:G:H2'	2:5:4863:G:H8	1.71	0.55
49:9:659:G:HO2'	49:9:662:G:HO2'	1.52	0.55
49:9:1644:C:H4'	66:QQ:140:ARG:HB2	1.88	0.55
2:5:8:U:H5''	17:N:40:PRO:HG3	1.88	0.55
2:5:3604:A:H5''	21:R:71:ARG:HH12	1.72	0.55
2:5:4078:C:OP1	17:N:31:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:147:GLN:HA	11:G:150:LYS:HG2	1.89	0.55
27:X:110:LYS:NZ	27:X:121:VAL:O	2.40	0.55
72:WW:111:MET:HE3	72:WW:116:ALA:HA	1.89	0.55
2:5:83:C:O2'	2:5:100:C:N4	2.39	0.55
2:5:2846:G:O2'	25:V:19:GLY:O	2.25	0.55
2:5:4054:C:O2	47:u:35:GLN:NE2	2.32	0.55
3:7:24:C:O2	3:7:117:G:N2	2.34	0.55
44:o:2:VAL:N	44:o:90:HIS:O	2.40	0.55
49:9:72:C:O2'	49:9:74:G:OP2	2.24	0.55
2:5:407:A:O2'	2:5:410:A:OP1	2.24	0.55
2:5:2016:C:H2'	2:5:2017:A:H8	1.72	0.55
2:5:3692:A:H62	2:5:3823:G:H21	1.54	0.55
2:5:4045:G:OP2	47:u:98:LYS:NZ	2.35	0.55
2:5:4622:A:H4'	6:B:13:SER:HB2	1.89	0.55
2:5:4735:G:N1	2:5:4965:U:N3	2.55	0.55
4:8:27:U:H4'	7:C:53:ALA:HB3	1.89	0.55
17:N:174:LEU:HA	17:N:183:THR:HG21	1.89	0.55
49:9:1092:G:OP1	63:NN:2:GLY:N	2.40	0.55
49:9:1566:G:N7	69:TT:101:ARG:NH1	2.50	0.55
51:BB:122:GLU:O	51:BB:165:ARG:NH2	2.39	0.55
2:5:935:A:H5'	2:5:935(A):G:H4'	1.88	0.54
2:5:5038:A:OP1	26:W:61:LYS:NZ	2.35	0.54
9:E:144:ARG:NE	35:f:110:ILE:OXT	2.38	0.54
14:J:18:ARG:HG3	14:J:135:GLY:HA3	1.89	0.54
57:HH:145:ARG:HD2	72:WW:51:GLU:HB3	1.89	0.54
33:d:36:VAL:HG11	33:d:44:ARG:HD3	1.88	0.54
50:AA:77:ILE:HG12	50:AA:99:ILE:HB	1.88	0.54
74:YY:34:THR:HG23	74:YY:69:THR:HG21	1.90	0.54
2:5:300:A:H2'	2:5:301:G:H8	1.71	0.54
2:5:4251:A:H5''	14:J:108:GLY:HA3	1.88	0.54
49:9:1139:C:N4	49:9:1149:A:N7	2.55	0.54
51:BB:225:LEU:HD11	51:BB:229:MET:HE2	1.89	0.54
65:PP:44:ARG:HG2	65:PP:84:ILE:HD11	1.89	0.54
68:SS:61:GLU:HA	68:SS:64:VAL:HG22	1.89	0.54
72:WW:23:ARG:HD3	77:bb:4:ALA:HB2	1.89	0.54
2:5:1552:G:O2'	2:5:1574:B9B:N2	2.40	0.54
2:5:4618:G:H5''	25:V:15:ARG:HB2	1.89	0.54
24:U:37:ALA:HA	24:U:65:ARG:HH22	1.72	0.54
30:a:82:VAL:HG21	30:a:101:ILE:HG12	1.90	0.54
49:9:885:U:O2	49:9:901:G:O6	2.25	0.54
49:9:1745:A:O3'	56:GG:31:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:AA:33:GLN:NE2	71:VV:64:GLU:OE2	2.36	0.54
2:5:1628:C:OP1	5:A:14:SER:OG	2.25	0.54
49:9:1488:C:O2'	49:9:1490:G:OP2	2.24	0.54
65:PP:41:GLN:NE2	65:PP:113:GLY:O	2.41	0.54
72:WW:44:HIS:NE2	72:WW:112:ASP:OD2	2.41	0.54
2:5:2739:C:O2	5:A:188:LYS:NZ	2.40	0.54
4:8:26:C:O2'	7:C:53:ALA:O	2.26	0.54
40:k:24:LYS:HD3	40:k:69:LEU:HD11	1.89	0.54
60:KK:85:LEU:HB3	60:KK:89:ILE:HD11	1.89	0.54
2:5:2778:G:N1	4:8:113:C:OP1	2.41	0.54
2:5:1970:A:N6	2:5:2016:C:OP2	2.40	0.54
49:9:57:U:O2'	49:9:499:G:N3	2.39	0.54
53:DD:69:LEU:HA	53:DD:72:VAL:HB	1.90	0.54
62:MM:87:GLU:O	62:MM:93:LYS:NZ	2.41	0.54
10:F:93:ARG:HB2	10:F:113:LEU:HB3	1.90	0.54
15:L:56:ARG:O	15:L:116:ARG:NH2	2.41	0.54
28:Y:18:HIS:O	28:Y:78:TYR:OH	2.25	0.54
49:9:943:U:OP1	51:BB:214:LYS:NZ	2.41	0.54
55:FF:58:ALA:HB3	55:FF:62:ARG:HH11	1.71	0.54
73:XX:107:ARG:HD3	73:XX:112:VAL:HG22	1.90	0.54
2:5:1279:A:O2'	7:C:323:ARG:NH2	2.41	0.54
2:5:2706:G:O2'	2:5:2709:C:N4	2.41	0.54
2:5:3685:C:OP1	5:A:193:ARG:NH1	2.40	0.54
2:5:3969:G:H1'	47:u:166:ALA:HB3	1.90	0.54
17:N:160:GLU:HG2	17:N:161:MET:HG3	1.89	0.54
59:JJ:137:VAL:HG22	59:JJ:157:ILE:HG12	1.90	0.54
19:P:16:LYS:HG2	19:P:149:ILE:HG12	1.89	0.53
52:CC:183:LYS:HD3	52:CC:194:ARG:HH21	1.72	0.53
73:XX:91:LEU:HB3	80:ee:82:VAL:HG21	1.89	0.53
2:5:4677:U:O2'	2:5:4713:G:N2	2.38	0.53
49:9:10:G:H21	52:CC:114:LYS:HA	1.72	0.53
49:9:1005:G:OP2	51:BB:162:ARG:NH1	2.40	0.53
49:9:1301:A:OP2	79:dd:2:GLY:N	2.42	0.53
63:NN:45:LEU:HG	63:NN:49:GLN:HG3	1.89	0.53
2:5:2411:C:H2'	2:5:2412:A:H8	1.74	0.53
2:5:4293:PSU:H5'	44:o:83:LEU:HD21	1.90	0.53
6:B:160:ILE:HD11	6:B:190:VAL:HG13	1.89	0.53
14:J:56:THR:HG23	14:J:63:ARG:HA	1.91	0.53
56:GG:2:LYS:NZ	56:GG:17:GLU:OE2	2.41	0.53
2:5:1315:C:OP1	34:e:44:ARG:NH2	2.39	0.53
10:F:91:VAL:O	10:F:119:GLY:HA2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:9:1013:U:OP1	49:9:1129:G:O2'	2.27	0.53
49:9:1373:C:O2'	67:RR:10:LYS:NZ	2.32	0.53
1:4:29:A:H2'	1:4:30:G:H8	1.74	0.53
2:5:1390:G:N2	2:5:1393:G:OP2	2.38	0.53
7:C:315:LYS:HD2	10:F:167:ALA:HB1	1.91	0.53
2:5:114:G:N2	2:5:276:C:O2'	2.41	0.53
2:5:158:A:H5''	2:5:159:C:H2'	1.91	0.53
49:9:851:C:O2'	49:9:852:G:N2	2.41	0.53
49:9:925:G:OP1	63:NN:121:ARG:NH2	2.41	0.53
55:FF:49:LEU:HB3	55:FF:51:HIS:H	1.73	0.53
48:v:216:CYS:HB2	48:v:267:LEU:HD23	1.90	0.53
49:9:1497:G:N7	60:KK:25:LYS:NZ	2.48	0.53
53:DD:55:THR:HA	53:DD:58:VAL:HG22	1.91	0.53
54:EE:73:ASP:OD2	54:EE:145:ARG:NH2	2.41	0.53
68:SS:13:LEU:HB2	68:SS:20:ILE:HB	1.89	0.53
2:5:2848:G:O2'	2:5:3838:U:O4	2.24	0.53
2:5:3620:G:OP1	2:5:3622:C:N4	2.42	0.53
2:5:3663:A:N6	2:5:4168:G:O2'	2.42	0.53
26:W:80:ARG:HD2	56:GG:131:ARG:HG3	1.90	0.53
27:X:129:ARG:HD3	27:X:135:LYS:HE3	1.91	0.53
49:9:1864:U:O2'	49:9:1866:A:N7	2.41	0.53
67:RR:31:ASN:HD21	67:RR:55:THR:HG22	1.73	0.53
2:5:664:G:O2'	2:5:668:C:N4	2.41	0.53
2:5:3782:5MC:OP2	43:n:23:ARG:NH1	2.42	0.53
9:E:163:LYS:HG2	9:E:277:VAL:HG12	1.91	0.53
49:9:1446:A:H5''	70:UU:58:THR:HG23	1.90	0.53
71:VV:15:ARG:HH11	71:VV:33:GLN:HG3	1.74	0.53
82:gg:132:TRP:CD1	82:gg:138:CYS:HA	2.43	0.53
2:5:4586:G:OP1	18:O:72:HIS:N	2.41	0.53
49:9:64:A:H2	49:9:83:A:H62	1.56	0.53
49:9:1590:C:OP1	69:TT:82:ARG:NH1	2.42	0.53
49:9:1598:G:O6	75:ZZ:85:ARG:NE	2.42	0.53
2:5:4594:U:H2'	2:5:4595:G:H8	1.74	0.52
15:L:14:PHE:HE1	17:N:198:LEU:HD11	1.73	0.52
17:N:68:ARG:NH1	17:N:124:ASP:O	2.40	0.52
30:a:81:LEU:HD21	30:a:103:VAL:HG23	1.91	0.52
49:9:1673:U:H5''	66:QQ:78:VAL:HG22	1.91	0.52
59:JJ:19:PRO:O	59:JJ:24:ARG:NH2	2.42	0.52
59:JJ:109:ARG:HH21	59:JJ:146:SER:HB3	1.74	0.52
69:TT:75:MET:HE3	69:TT:78:ILE:HD13	1.91	0.52
72:WW:52:ILE:HG22	72:WW:61:ILE:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:YY:91:LEU:HD22	74:YY:96:LEU:HD11	1.91	0.52
2:5:2062:C:O2'	22:S:111:ARG:NH1	2.42	0.52
2:5:4289:U:HO2'	2:5:4320:G:HO2'	1.54	0.52
9:E:189:LEU:HD21	9:E:256:VAL:HG11	1.90	0.52
15:L:186:ARG:HE	38:i:9:VAL:HG11	1.72	0.52
51:BB:29:ASP:OD2	51:BB:94:LYS:NZ	2.39	0.52
52:CC:149:THR:HA	52:CC:152:ARG:HG2	1.90	0.52
2:5:1558:A:H2'	2:5:1559:G:H8	1.75	0.52
16:M:125:ASN:HA	16:M:128:LYS:HG2	1.92	0.52
22:S:132:ILE:HG23	22:S:136:LYS:HB3	1.91	0.52
49:9:1584:G:OP1	69:TT:77:LYS:NZ	2.38	0.52
49:9:1654:G:OP1	69:TT:90:SER:OG	2.27	0.52
51:BB:108:ASP:O	51:BB:112:SER:HB2	2.09	0.52
2:5:1357:C:O2'	7:C:114:ARG:NH2	2.42	0.52
2:5:3961:G:H1'	2:5:4045:G:H21	1.75	0.52
7:C:292:ILE:HG21	20:Q:31:LEU:HD11	1.92	0.52
49:9:383:G:H4'	61:LL:132:ARG:HD2	1.90	0.52
49:9:944:A:H5''	64:OO:134:PRO:HB2	1.91	0.52
2:5:419:A:N3	2:5:1332:C:O2'	2.40	0.52
2:5:2290:C:HO2'	2:5:2322:G:HO2'	1.52	0.52
6:B:41:VAL:HA	6:B:187:GLY:HA3	1.91	0.52
6:B:57:VAL:HG22	6:B:73:VAL:HG12	1.92	0.52
49:9:1579:A:H4'	49:9:1581:C:H5	1.74	0.52
2:5:1860:B8H:C5	2:5:1860:B8H:C2	2.85	0.52
5:A:116:LEU:HD21	5:A:148:VAL:HG11	1.92	0.52
9:E:291:PHE:HZ	35:f:110:ILE:HD13	1.75	0.52
49:9:520:A:O2'	49:9:825:A:N3	2.39	0.52
82:gg:152:SER:H	82:gg:169:GLY:HA2	1.73	0.52
6:B:33:PRO:O	6:B:186:ASN:ND2	2.42	0.52
49:9:508:A:H3'	49:9:509:OMG:H8	1.75	0.52
49:9:1220:A:N3	49:9:1677:U:O2'	2.38	0.52
49:9:1677:U:H2'	49:9:1678:A2M:H8	1.92	0.52
82:gg:153:CYS:SG	82:gg:154:VAL:N	2.83	0.52
2:5:1492:G:O2'	31:b:41:ARG:NH1	2.43	0.52
49:9:1549:U:OP1	79:dd:34:TYR:OH	2.27	0.52
2:5:175:C:H2'	2:5:176:G:H8	1.75	0.52
2:5:1563:A:N6	49:9:1028:A:N1	2.58	0.52
2:5:3717:A:OP2	2:5:3735:G:N2	2.37	0.52
2:5:3951:G:H1	2:5:4062:A:H2	0.66	0.52
2:5:4238:G:H2'	2:5:4239:A:H8	1.75	0.52
5:A:29:LEU:O	5:A:123:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:229:LYS:HD3	6:B:272:LYS:HD3	1.92	0.52
43:n:2:ARG:NH1	49:9:1841:C:OP2	2.36	0.52
2:5:173:C:H1'	37:h:112:ARG:HG2	1.92	0.52
2:5:1517:2MG:HN2	7:C:103:ALA:HA	1.75	0.52
2:5:2782:U:OP2	41:l:10:LYS:NZ	2.41	0.52
4:8:29:G:H5''	15:L:27:ASN:HB3	1.92	0.52
53:DD:69:LEU:HD12	53:DD:86:LEU:HD13	1.91	0.52
57:HH:157:HIS:HA	57:HH:188:GLU:O	2.10	0.52
66:QQ:89:SER:HB2	66:QQ:112:LEU:HD21	1.91	0.52
2:5:4220:6MZ:OP1	23:T:2:THR:N	2.43	0.51
3:7:17:C:OP1	14:J:156:ARG:NH2	2.41	0.51
71:VV:20:SER:HB3	71:VV:59:ILE:HD11	1.92	0.51
2:5:66:A:N6	2:5:282:C:O2'	2.43	0.51
2:5:197:A:N3	2:5:222:C:O2'	2.40	0.51
2:5:736:C:OP1	16:M:74:ARG:NH1	2.42	0.51
2:5:1736:A:N3	3:7:78:C:O2'	2.42	0.51
2:5:4056:A:H1'	47:u:164:CYS:HB3	1.93	0.51
2:5:4688:C:O2'	12:H:155:SER:OG	2.26	0.51
10:F:133:ARG:HA	10:F:136:GLU:HB2	1.90	0.51
13:I:96:VAL:HG12	13:I:125:THR:HG22	1.91	0.51
49:9:1617:G:O6	65:PP:43:ARG:NH1	2.43	0.51
49:9:1841:C:H2'	49:9:1842:4AC:H6	1.92	0.51
50:AA:42:LYS:HD2	50:AA:46:ILE:HG23	1.92	0.51
51:BB:129:THR:OG1	51:BB:131:ASP:O	2.25	0.51
54:EE:68:ARG:HG3	54:EE:76:VAL:HG11	1.91	0.51
72:WW:30:CYS:N	72:WW:59:GLY:O	2.38	0.51
1:4:15:G:H2'	1:4:59:G:H1	1.76	0.51
2:5:1646:A:O2'	39:j:49:TRP:O	2.27	0.51
2:5:2869:U:O2'	2:5:2881:A:N7	2.38	0.51
25:V:16:ILE:HB	25:V:88:TYR:HB2	1.92	0.51
58:II:110:ARG:HA	58:II:121:LEU:HD21	1.91	0.51
70:UU:62:ARG:HE	70:UU:81:GLN:HE21	1.59	0.51
2:5:1598:C:H2'	2:5:1599:G:H8	1.76	0.51
2:5:2396:A:N6	2:5:2814:C:O2	2.44	0.51
17:N:187:SER:OG	17:N:188:ARG:N	2.42	0.51
49:9:1245:G:O2'	49:9:1492:U:OP1	2.28	0.51
57:HH:170:VAL:HG13	57:HH:187:PHE:HB2	1.92	0.51
72:WW:103:VAL:HA	72:WW:112:ASP:HA	1.92	0.51
82:gg:165:ILE:HG23	82:gg:177:TRP:HB2	1.92	0.51
2:5:307:A:N3	2:5:310:G:O2'	2.44	0.51
2:5:3897:B8K:O2'	2:5:3898:G:OP2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:3951:G:C2	2:5:4062:A:H2	2.26	0.51
5:A:116:LEU:O	5:A:125:LYS:N	2.44	0.51
6:B:10:ARG:HH22	6:B:265:SER:HB2	1.75	0.51
7:C:333:MLZ:HCM3	9:E:57:GLY:H	1.74	0.51
16:M:97:ALA:HB2	18:O:203:VAL:HB	1.91	0.51
73:XX:67:ARG:HB3	73:XX:84:PHE:HE1	1.75	0.51
2:5:1326:A2M:OP2	2:5:4445:U:O2'	2.27	0.51
2:5:2607:C:H5''	21:R:96:MET:HE1	1.93	0.51
2:5:3683:C:OP1	5:A:132:ASN:ND2	2.42	0.51
14:J:84:GLU:OE2	14:J:92:TYR:OH	2.29	0.51
49:9:540:U:H1'	49:9:543:C:H41	1.76	0.51
49:9:1017:U:H5'	63:NN:55:ARG:HG2	1.92	0.51
52:CC:179:THR:HG21	52:CC:198:ALA:H	1.75	0.51
53:DD:8:LYS:HE3	70:UU:59:LYS:HD2	1.92	0.51
2:5:102:G:OP1	15:L:71:ARG:NH2	2.38	0.51
2:5:2520:C:H2'	2:5:2521:G:H8	1.74	0.51
2:5:2877:G:N2	2:5:3824:A:O2'	2.36	0.51
6:B:85:VAL:HG22	6:B:204:GLN:HG2	1.92	0.51
11:G:214:VAL:HG21	11:G:220:VAL:HG21	1.92	0.51
21:R:99:MET:HE1	21:R:128:LYS:HA	1.91	0.51
35:f:7:CYS:HB2	35:f:103:VAL:HG13	1.91	0.51
48:v:114:GLU:OE2	48:v:115:ARG:NH1	2.44	0.51
48:v:288:GLU:OE1	48:v:360:SER:OG	2.29	0.51
49:9:65:C:H4'	56:GG:172:LYS:HE2	1.93	0.51
54:EE:45:ILE:HA	54:EE:61:VAL:HG21	1.93	0.51
2:5:1661:C:OP1	34:e:36:ARG:NH2	2.43	0.51
2:5:1994:C:H2'	2:5:1995:G:H8	1.76	0.51
2:5:4693:C:OP1	12:H:64:ARG:NH2	2.43	0.51
16:M:12:VAL:HA	16:M:25:VAL:O	2.10	0.51
49:9:1228:A:H2'	49:9:1229:G:C8	2.46	0.51
49:9:1593:C:O2	69:TT:12:GLN:NE2	2.33	0.51
53:DD:1:MET:HE2	53:DD:3:VAL:HB	1.93	0.51
54:EE:45:ILE:HG13	54:EE:61:VAL:HG11	1.92	0.51
55:FF:24:SER:OG	55:FF:26:ASP:OD1	2.28	0.51
57:HH:108:SER:OG	57:HH:113:LYS:NZ	2.39	0.51
62:MM:67:ALA:HB1	81:f:114:ILE:HD11	1.93	0.51
66:QQ:85:ARG:NH2	66:QQ:116:ASP:OD2	2.43	0.51
69:TT:126:GLN:OE1	69:TT:129:ARG:NH2	2.44	0.51
2:5:1631:A:C8	5:A:199:VAL:HG21	2.46	0.51
2:5:1759:G:H1	2:5:1773:U:H3	1.58	0.51
2:5:4053:A:O2'	2:5:4054:C:O5'	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:70:MET:HA	10:F:73:MET:HG2	1.92	0.51
12:H:91:LYS:HG2	12:H:145:VAL:HG22	1.92	0.51
20:Q:97:LYS:NZ	20:Q:117:GLY:O	2.44	0.51
33:d:36:VAL:HG23	33:d:41:ARG:HG2	1.92	0.51
49:9:1616:U:H3	49:9:1620:A:H2	1.59	0.51
50:AA:85:ARG:HH21	50:AA:201:LEU:HD12	1.75	0.51
51:BB:35:ALA:HB2	51:BB:44:ILE:HD11	1.92	0.51
2:5:1906:U:H2'	2:5:1907:A:H8	1.75	0.51
47:u:35:GLN:HB2	47:u:205:TYR:HB2	1.92	0.51
49:9:687:C:O3'	57:HH:121:THR:OG1	2.29	0.51
49:9:862:A:N3	72:WW:105:THR:OG1	2.43	0.51
49:9:1568:C:OP1	69:TT:96:SER:OG	2.22	0.51
50:AA:19:LEU:HD21	67:RR:106:LEU:HD11	1.93	0.51
74:YY:41:ARG:NH2	74:YY:52:PRO:O	2.42	0.51
2:5:224:U:HO2'	2:5:243:A:HO2'	1.59	0.50
4:8:110:U:OP2	41:l:8:ARG:NH1	2.44	0.50
6:B:89:ILE:HG22	6:B:162:VAL:HG23	1.93	0.50
43:n:21:ARG:NH2	49:9:1175:G:OP1	2.45	0.50
49:9:639:C:H2'	49:9:640:A:H8	1.75	0.50
62:MM:63:LYS:HB3	81:ff:108:VAL:HG21	1.93	0.50
74:YY:7:ILE:HD11	74:YY:40:ILE:HG22	1.93	0.50
2:5:2427:G:OP1	21:R:5:ARG:NH2	2.44	0.50
25:V:42:VAL:HA	25:V:61:VAL:HG23	1.94	0.50
46:r:85:ASN:N	46:r:85:ASN:OD1	2.42	0.50
47:u:59:PRO:HB2	47:u:170:GLY:H	1.76	0.50
52:CC:106:VAL:HG22	52:CC:128:VAL:HG22	1.93	0.50
66:QQ:16:LYS:HG3	66:QQ:17:LYS:H	1.76	0.50
26:W:81:ALA:HB2	26:W:87:LEU:HB2	1.93	0.50
48:v:239:GLN:HG2	48:v:365:ARG:HH22	1.75	0.50
57:HH:78:ARG:HA	57:HH:81:ARG:HG2	1.93	0.50
70:UU:31:SER:HB2	70:UU:107:GLU:HG2	1.92	0.50
2:5:66:A:O2'	2:5:326:C:O2	2.30	0.50
2:5:668:C:H4'	7:C:6:PRO:HB3	1.94	0.50
2:5:3908:A:N7	2:5:4449:A:N6	2.59	0.50
2:5:3963:A:O2'	2:5:3965:A:OP2	2.29	0.50
5:A:177:LYS:HB2	45:p:29:ILE:HG21	1.93	0.50
16:M:27:ILE:HA	16:M:38:VAL:HG23	1.94	0.50
20:Q:179:GLY:H	30:a:51:GLY:HA2	1.77	0.50
37:h:31:LEU:HB3	37:h:47:ILE:HG22	1.93	0.50
47:u:36:ILE:HB	47:u:165:LEU:HB2	1.93	0.50
47:u:74:CYS:SG	47:u:75:ASP:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:MM:34:GLY:O	62:MM:38:ALA:CB	2.56	0.50
82:gg:57:ARG:NH2	82:gg:92:LEU:O	2.44	0.50
2:5:440:U:O2'	35:f:91:ASN:O	2.28	0.50
2:5:973:C:O2	2:5:1282:G:N2	2.36	0.50
2:5:3811:G:O2'	2:5:3814:U:OP2	2.30	0.50
2:5:4124:G:N2	11:G:96:GLN:O	2.44	0.50
2:5:4318:C:H4'	44:o:17:LYS:HA	1.93	0.50
6:B:49:TYR:OH	6:B:179:HIS:ND1	2.39	0.50
9:E:153:LEU:HD13	9:E:197:VAL:HG11	1.94	0.50
49:9:663:C:OP2	73:XX:2:GLY:N	2.44	0.50
57:HH:138:GLU:OE2	63:NN:19:ARG:NH2	2.41	0.50
2:5:399:G:N2	19:P:101:ASN:OD1	2.43	0.50
2:5:2580:U:O2	29:Z:76:ASN:ND2	2.44	0.50
2:5:2877:G:H21	2:5:3824:A:HO2'	1.57	0.50
7:C:11:TYR:HE2	7:C:149:GLU:HG2	1.76	0.50
8:D:146:LEU:HG	8:D:163:LEU:HD13	1.92	0.50
17:N:5:LYS:HG3	38:i:40:VAL:HG11	1.93	0.50
49:9:600:G:H2'	49:9:601:G:H8	1.77	0.50
49:9:824:C:H1'	59:JJ:144:ILE:HD11	1.94	0.50
51:BB:103:MET:HB3	51:BB:215:VAL:HB	1.94	0.50
80:ee:112:ASN:HA	80:ee:116:VAL:HG12	1.94	0.50
2:5:4476:C:O2'	2:5:4478:G:OP2	2.26	0.50
4:8:102:G:OP2	4:8:104:A:O2'	2.28	0.50
21:R:139:MET:O	21:R:143:HIS:ND1	2.45	0.50
23:T:64:VAL:HG22	23:T:74:ILE:HG22	1.94	0.50
52:CC:251:LEU:HD23	71:VV:23:ILE:HG13	1.94	0.50
2:5:2457:G:OP1	17:N:65:ARG:NH1	2.44	0.50
4:8:155:C:OP2	11:G:142:ARG:NH2	2.45	0.50
7:C:94:ASN:N	7:C:94:ASN:OD1	2.42	0.50
29:Z:36:ARG:NH1	29:Z:38:TYR:OH	2.42	0.50
45:p:47:MET:HE2	45:p:71:TYR:HE1	1.76	0.50
46:r:63:VAL:HG22	46:r:79:ARG:HD3	1.93	0.50
62:MM:25:ALA:O	62:MM:29:ASP:CA	2.57	0.50
82:gg:11:LEU:HB2	82:gg:307:VAL:HB	1.94	0.50
21:R:99:MET:HE2	21:R:127:VAL:HG12	1.94	0.50
49:9:1495:G:N2	79:dd:42:CYS:SG	2.78	0.50
49:9:1740:C:OP1	58:II:44:HIS:ND1	2.37	0.50
51:BB:144:LYS:HD3	51:BB:208:HIS:HB3	1.94	0.50
82:gg:113:PHE:HA	82:gg:120:ILE:HG22	1.92	0.50
2:5:1985:G:O2'	2:5:2003:G:OP2	2.28	0.49
2:5:4617:G:O2'	25:V:13:LYS:O	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:120:PRO:HA	5:A:162:ASN:HB3	1.94	0.49
58:II:6:ASP:OD1	58:II:6:ASP:N	2.42	0.49
2:5:1185:G:O2'	8:D:278:ASP:OD2	2.29	0.49
2:5:1686:C:O2'	31:b:18:ARG:NH2	2.45	0.49
7:C:189:MET:HG2	7:C:195:LYS:HE2	1.93	0.49
49:9:126:G:OP1	56:GG:198:ARG:NH2	2.38	0.49
55:FF:102:LEU:HD13	75:ZZ:110:THR:HG22	1.94	0.49
74:YY:20:ARG:HD2	74:YY:74:MET:HG3	1.95	0.49
82:gg:20:GLN:HE21	82:gg:69:VAL:H	1.61	0.49
82:gg:220:ASP:HB2	82:gg:227:LEU:HD11	1.94	0.49
2:5:243:A:H5''	28:Y:3:PHE:HD2	1.77	0.49
2:5:1942:A:H2'	2:5:1943:A:C8	2.47	0.49
2:5:2308:A:N3	4:8:19:C:O2'	2.39	0.49
2:5:3635:A:H61	45:p:18:TYR:H	1.59	0.49
2:5:4949:G:H4'	2:5:4950:U:H5'	1.93	0.49
24:U:84:LYS:HB2	24:U:110:TYR:CZ	2.47	0.49
42:m:84:CYS:SG	42:m:85:ARG:N	2.85	0.49
55:FF:201:LYS:HA	55:FF:204:ARG:HE	1.77	0.49
68:SS:115:LYS:HD3	68:SS:126:PHE:HB2	1.94	0.49
82:gg:174:VAL:HB	82:gg:188:HIS:HB2	1.94	0.49
2:5:510:U:H5''	30:a:86:THR:HG22	1.94	0.49
2:5:2335:C:H2'	2:5:2336:G:H8	1.78	0.49
49:9:537:C:N3	49:9:547:G:N2	2.60	0.49
49:9:1305:C:OP2	81:ff:93:HIS:ND1	2.38	0.49
49:9:1679:A:OP1	55:FF:60:ARG:NH2	2.46	0.49
54:EE:11:ARG:HA	54:EE:28:ALA:HB2	1.94	0.49
54:EE:42:LEU:HD13	54:EE:109:PHE:HB2	1.94	0.49
1:4:49:C:H2'	1:4:50:A:H8	1.77	0.49
2:5:87:A:H4'	30:a:63:LEU:HD13	1.94	0.49
2:5:3952:A:N1	2:5:4061:G:C6	2.81	0.49
2:5:4238:G:H2'	2:5:4239:A:C8	2.48	0.49
2:5:4338:G:N1	2:5:4373:G:OP1	2.34	0.49
9:E:156:LEU:HD11	9:E:198:ILE:HG13	1.95	0.49
11:G:147:GLN:HG3	11:G:271:LEU:HD21	1.93	0.49
35:f:59:THR:OG1	35:f:65:ASN:OD1	2.30	0.49
49:9:385:G:O2'	58:II:10:LYS:NZ	2.45	0.49
49:9:1570:G:HO2'	49:9:1614:A:HO2'	1.60	0.49
56:GG:67:VAL:HG12	56:GG:69:THR:HG22	1.95	0.49
13:I:87:ILE:HG22	13:I:138:ILE:HG12	1.94	0.49
25:V:31:ASN:ND2	25:V:115:SER:OG	2.38	0.49
45:p:46:LYS:O	45:p:57:CYS:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:u:39:LYS:HA	47:u:202:ARG:HG3	1.93	0.49
49:9:1718:G:O2'	49:9:1815:A:N6	2.45	0.49
66:QQ:21:ALA:HB2	66:QQ:72:VAL:HG13	1.94	0.49
67:RR:36:GLU:HG3	67:RR:47:ARG:HH11	1.78	0.49
2:5:1823:G:O2'	8:D:44:TYR:O	2.30	0.49
14:J:150:CYS:SG	14:J:151:ILE:N	2.85	0.49
48:v:434:ARG:HH21	49:9:961:G:H8	1.60	0.49
49:9:5:U:H2'	49:9:6:G:H8	1.78	0.49
49:9:1415:C:O2'	69:TT:132:ASP:OD2	2.28	0.49
53:DD:114:ALA:HB3	53:DD:117:ARG:HG2	1.95	0.49
54:EE:99:PHE:HE1	54:EE:113:ARG:HG2	1.77	0.49
54:EE:129:ILE:HD11	54:EE:155:LYS:HA	1.95	0.49
56:GG:160:LYS:O	56:GG:171:THR:HA	2.13	0.49
57:HH:145:ARG:HH21	72:WW:49:GLU:HG3	1.78	0.49
82:gg:106:LYS:HD3	82:gg:126:ASP:HB3	1.94	0.49
82:gg:289:LEU:HD11	82:gg:298:LEU:HD12	1.93	0.49
2:5:1883:OMG:HM22	2:5:2070:U:H3	1.77	0.49
2:5:2756:G:O6	29:Z:51:ARG:NH2	2.36	0.49
2:5:4873:G:C8	18:O:179:LYS:HE3	2.47	0.49
2:5:4992:G:H2'	2:5:4993:G:C8	2.48	0.49
10:F:178:LEU:HD21	10:F:203:ALA:HA	1.94	0.49
22:S:112:ASP:OD1	22:S:116:ARG:NH1	2.44	0.49
49:9:658:U:O2	73:XX:17:ARG:NH2	2.46	0.49
54:EE:100:ARG:HH12	54:EE:122:LYS:HA	1.77	0.49
60:KK:12:TYR:HB3	60:KK:79:LEU:HD11	1.95	0.49
72:WW:111:MET:HE1	72:WW:119:LYS:HD2	1.94	0.49
2:5:438:G:N2	35:f:23:GLU:OE2	2.32	0.49
12:H:26:ILE:HG12	12:H:35:ARG:HG2	1.93	0.49
12:H:36:ARG:HH11	12:H:38:PHE:HE1	1.61	0.49
18:O:54:TYR:HD2	18:O:145:VAL:HG21	1.78	0.49
43:n:11:ARG:HH11	49:9:1183:A:H5'	1.78	0.49
55:FF:50:PRO:HB3	55:FF:69:VAL:HG12	1.94	0.49
2:5:965:G:N2	2:5:966:A:N7	2.59	0.49
11:G:233:PRO:HG2	11:G:272:VAL:HG13	1.94	0.49
47:u:112:ALA:HB1	47:u:117:ILE:HD11	1.95	0.49
53:DD:218:LEU:HB3	82:gg:192:THR:HG22	1.95	0.49
56:GG:37:ALA:HA	56:GG:49:VAL:HG12	1.95	0.49
57:HH:34:SER:OG	57:HH:35:ASP:N	2.45	0.49
78:cc:10:LYS:O	78:cc:58:LEU:HB2	2.13	0.49
2:5:121:A:OP1	11:G:163:LYS:NZ	2.38	0.48
2:5:1176:C:O3'	8:D:268:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:4394:A:H3'	2:5:4395:U:H2'	1.95	0.48
2:5:4474:A:H5'	42:m:99:LYS:HB2	1.95	0.48
2:5:4753:U:OP1	35:f:100:ARG:NH1	2.46	0.48
32:c:45:LEU:HD23	32:c:96:ILE:HD12	1.95	0.48
40:k:24:LYS:HA	40:k:67:LYS:O	2.14	0.48
44:o:24:THR:HG23	44:o:69:ARG:HB3	1.95	0.48
49:9:1536:G:H2'	49:9:1537:A:C8	2.48	0.48
53:DD:58:VAL:HA	53:DD:65:ARG:HH21	1.78	0.48
2:5:2529:A:O2'	2:5:2531:C:OP2	2.31	0.48
28:Y:8:THR:HB	28:Y:10:ASP:H	1.79	0.48
49:9:146:G:N1	49:9:174:OMC:O2	2.46	0.48
49:9:1299:A:O2'	49:9:1301:A:OP1	2.29	0.48
2:5:1942:A:OP2	2:5:2040:A:N6	2.42	0.48
3:7:61:G:O2'	8:D:279:ARG:NH1	2.42	0.48
6:B:165:HIS:ND1	6:B:166:THR:O	2.42	0.48
15:L:147:ALA:HB1	37:h:120:ALA:HB3	1.95	0.48
46:r:52:GLU:HB2	46:r:61:VAL:HG23	1.95	0.48
49:9:1304:U:H5''	81:ff:93:HIS:HB2	1.94	0.48
49:9:1518:C:H5''	49:9:1519:U:H5''	1.96	0.48
50:AA:155:ARG:NH1	71:VV:61:ARG:O	2.47	0.48
60:KK:15:LEU:HD21	60:KK:71:LEU:HD13	1.95	0.48
54:EE:67:GLN:NE2	74:YY:17:LEU:O	2.47	0.48
57:HH:69:LEU:HG	57:HH:96:ALA:HB2	1.94	0.48
60:KK:49:MET:HA	60:KK:52:LEU:HB2	1.95	0.48
65:PP:53:GLN:HG2	65:PP:80:LEU:HD23	1.95	0.48
2:5:115:C:O2'	2:5:276:C:OP1	2.30	0.48
2:5:914:U:N3	2:5:918:G:N7	2.62	0.48
2:5:1073:G:H1	2:5:1238:A:H2	1.62	0.48
2:5:2492:C:H2'	2:5:2493:G:C8	2.48	0.48
3:7:67:C:H4'	23:T:20:ARG:HH12	1.77	0.48
5:A:147:ARG:HG2	5:A:157:VAL:HG22	1.95	0.48
23:T:42:ILE:HD11	23:T:74:ILE:HD11	1.95	0.48
24:U:60:VAL:HG11	24:U:76:VAL:HG13	1.94	0.48
25:V:106:VAL:HA	25:V:112:MET:HA	1.96	0.48
49:9:185:G:O6	49:9:214:U:O2	2.31	0.48
59:JJ:107:GLU:HA	59:JJ:112:THR:HG21	1.95	0.48
2:5:1460:C:H5''	20:Q:144:LYS:HG2	1.94	0.48
2:5:4431:U:OP2	13:I:3:ARG:NH2	2.36	0.48
2:5:4689:U:H4'	12:H:151:ILE:HD12	1.94	0.48
3:7:11:A:O2'	3:7:13:A:OP2	2.31	0.48
29:Z:50:PRO:HD3	29:Z:68:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:n:15:ARG:NH1	49:9:1183:A:OP1	2.46	0.48
47:u:171:HIS:CE1	47:u:174:MET:HE2	2.48	0.48
2:5:1556:C:O2'	2:5:2669:C:OP1	2.25	0.48
2:5:2566:G:H2'	2:5:2567:G:C8	2.49	0.48
2:5:2759:G:H1'	2:5:2764:A:H2	1.78	0.48
2:5:3940:U:H5''	11:G:128:LYS:HD2	1.95	0.48
2:5:4661:G:N2	2:5:5004:C:O3'	2.47	0.48
6:B:80:GLU:OE1	6:B:323:TYR:OH	2.25	0.48
7:C:78:ARG:HB3	7:C:88:GLY:HA2	1.96	0.48
15:L:79:GLU:OE1	15:L:82:ARG:NH2	2.46	0.48
49:9:640:A:H2'	49:9:641:A:C8	2.49	0.48
62:MM:51:VAL:HG22	62:MM:77:ILE:HB	1.95	0.48
82:gg:111:VAL:HA	82:gg:121:VAL:O	2.13	0.48
2:5:724:C:H1'	7:C:343:GLN:HE21	1.78	0.48
20:Q:16:LYS:O	20:Q:33:ARG:NH2	2.47	0.48
36:g:61:PRO:HA	36:g:64:LEU:HD13	1.94	0.48
48:v:147:VAL:HA	48:v:193:VAL:HG21	1.96	0.48
49:9:522:A:H5''	59:JJ:145:PRO:HD2	1.95	0.48
55:FF:47:LYS:NZ	66:QQ:115:TYR:O	2.46	0.48
60:KK:50:GLN:HA	60:KK:53:LYS:HG2	1.95	0.48
1:4:7:A:O2'	1:4:49:C:O5'	2.31	0.48
2:5:3697:U:H5''	2:5:3698:G:H5'	1.95	0.48
2:5:4594:U:H2'	2:5:4595:G:C8	2.49	0.48
9:E:253:GLN:NE2	9:E:257:ASP:OD2	2.34	0.48
49:9:1033:G:N1	49:9:1080:A:O2'	2.37	0.48
82:gg:39:THR:HG22	82:gg:60:ARG:HG2	1.96	0.48
82:gg:121:VAL:HG11	82:gg:165:ILE:HD11	1.96	0.48
2:5:1952:G:OP1	22:S:139:ARG:NE	2.38	0.48
2:5:4454:G:O2'	2:5:4500:PSU:O2'	2.31	0.48
5:A:33:ASP:N	5:A:33:ASP:OD1	2.43	0.48
21:R:8:LYS:HB2	21:R:24:LEU:HD11	1.96	0.48
30:a:103:VAL:HG22	30:a:108:TYR:HB2	1.95	0.48
33:d:20:VAL:HG12	33:d:91:LYS:HA	1.94	0.48
33:d:64:ILE:HG23	33:d:68:LEU:HD23	1.95	0.48
48:v:97:GLU:HA	48:v:100:ARG:HG2	1.95	0.48
49:9:116:OMU:HM23	49:9:116:OMU:H1'	1.71	0.48
49:9:355:G:OP1	61:LL:105:ARG:NH1	2.46	0.48
49:9:921:G:C5	72:WW:28:ARG:HD2	2.49	0.48
58:II:81:VAL:HG22	58:II:102:VAL:HG12	1.95	0.48
2:5:3953:G:N2	2:5:4060:U:O2	2.40	0.47
7:C:305:PRO:HD3	20:Q:38:ARG:HH22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:u:31:THR:HA	47:u:171:HIS:HA	1.96	0.47
50:AA:157:VAL:O	71:VV:65:SER:OG	2.31	0.47
82:gg:177:TRP:HA	82:gg:184:LEU:HA	1.96	0.47
2:5:1341:U:O3'	17:N:204:ARG:NH1	2.47	0.47
2:5:2411:C:H2'	2:5:2412:A:C8	2.49	0.47
2:5:2878:G:H4'	2:5:3825:A2M:H5''	1.95	0.47
2:5:4212:A:N6	2:5:4219:A:OP2	2.42	0.47
9:E:96:THR:HG22	9:E:109:VAL:HG22	1.95	0.47
49:9:1101:U:H2'	49:9:1102:G:C8	2.49	0.47
52:CC:171:GLY:O	72:WW:98:GLN:NE2	2.41	0.47
2:5:709:C:H1'	2:5:4942:C:H5	1.80	0.47
2:5:1440:U:OP1	10:F:33:ARG:NH2	2.47	0.47
2:5:4478:G:O2'	2:5:4602:A:N1	2.47	0.47
6:B:36:ASP:OD1	6:B:36:ASP:N	2.46	0.47
7:C:137:VAL:HG21	7:C:150:LEU:HD21	1.96	0.47
12:H:23:ARG:HH21	12:H:39:ASN:HA	1.79	0.47
25:V:82:ILE:HG23	25:V:121:VAL:HA	1.96	0.47
42:m:58:GLN:HA	42:m:61:GLN:HG2	1.94	0.47
49:9:1442:U:N3	66:QQ:11:GLN:OE1	2.47	0.47
49:9:1557:C:OP1	79:dd:13:LYS:NZ	2.41	0.47
49:9:1636:G:H8	55:FF:164:ARG:HH22	1.61	0.47
52:CC:65:LYS:HG3	52:CC:273:LEU:HD22	1.95	0.47
61:LL:128:VAL:HA	61:LL:141:ASN:O	2.14	0.47
64:OO:38:ASN:HA	64:OO:69:SER:HB3	1.97	0.47
66:QQ:85:ARG:HH12	66:QQ:118:THR:HG23	1.78	0.47
82:gg:152:SER:OG	82:gg:168:CYS:SG	2.65	0.47
2:5:2835:A:O2'	6:B:228:TYR:O	2.30	0.47
2:5:4883:C:N4	9:E:184:LEU:O	2.31	0.47
4:8:36:G:O2'	4:8:103:A:N1	2.43	0.47
11:G:215:ASP:OD1	11:G:215:ASP:N	2.37	0.47
30:a:59:ARG:NH1	30:a:61:TYR:OH	2.48	0.47
30:a:119:LYS:HA	30:a:140:VAL:HG13	1.96	0.47
49:9:26:U:H2'	49:9:27:A2M:H8	1.97	0.47
49:9:814:5MU:OP1	54:EE:22:LYS:NZ	2.47	0.47
50:AA:5:LEU:HD11	71:VV:41:LYS:HA	1.95	0.47
51:BB:149:GLN:HE21	51:BB:151:ARG:HB3	1.79	0.47
67:RR:23:ARG:NH1	82:gg:149:GLU:OE1	2.47	0.47
76:aa:7:ASN:O	76:aa:9:GLY:N	2.48	0.47
2:5:57:G:H5''	17:N:154:PRO:HB2	1.96	0.47
2:5:1468:C:OP1	30:a:132:ARG:NH2	2.47	0.47
2:5:1914:C:H4'	18:O:89:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:2318:G:N2	2:5:2321:G:OP2	2.42	0.47
2:5:4129:B8W:O6	2:5:4156:G:N2	2.47	0.47
6:B:317:LEU:HB2	6:B:372:SER:HB2	1.95	0.47
9:E:155:ILE:O	9:E:162:GLY:N	2.42	0.47
12:H:7:ASN:HB3	12:H:58:ASP:HB3	1.96	0.47
17:N:114:ARG:NH1	17:N:151:ILE:O	2.39	0.47
25:V:43:LYS:NZ	25:V:62:MET:SD	2.88	0.47
49:9:397:G:OP2	61:LL:108:ASN:ND2	2.48	0.47
49:9:1262:C:O2'	79:dd:12:ARG:NH1	2.48	0.47
49:9:1513:C:H2'	49:9:1514:G:H8	1.78	0.47
49:9:1550:G:O2'	49:9:1558:C:O2	2.31	0.47
49:9:1589:A:N3	49:9:1653:U:O2'	2.43	0.47
66:QQ:49:TYR:HA	66:QQ:52:LEU:HB2	1.95	0.47
67:RR:75:GLU:HA	67:RR:78:ARG:HG2	1.95	0.47
67:RR:111:PHE:HB3	67:RR:114:LEU:HD21	1.97	0.47
73:XX:94:ILE:HG22	73:XX:125:VAL:HG11	1.97	0.47
2:5:1500:A:H5''	2:5:1501:C:H5'	1.95	0.47
2:5:1982:G:N2	2:5:2009:A:O2'	2.39	0.47
2:5:4626:A:H4'	6:B:53:MET:HG3	1.96	0.47
4:8:67:U:H2'	4:8:68:G:H8	1.80	0.47
6:B:90:VAL:HG22	6:B:104:THR:HG23	1.97	0.47
13:I:43:VAL:O	13:I:171:TRP:NE1	2.42	0.47
72:WW:3:ARG:HH22	72:WW:28:ARG:NH2	2.12	0.47
2:5:62:A:N3	2:5:77:U:O2'	2.40	0.47
2:5:1502:G:H22	30:a:77:LYS:HD3	1.80	0.47
2:5:1558:A:H2'	2:5:1559:G:C8	2.50	0.47
2:5:2696:A:H5'	40:k:26:LYS:HE2	1.96	0.47
2:5:4405:G:O6	2:5:4439:U:O2	2.33	0.47
2:5:4419:U:OP1	2:5:4421:C:N4	2.47	0.47
7:C:284:MET:HE3	20:Q:124:ASP:HB3	1.97	0.47
11:G:304:ALA:HA	11:G:307:GLU:HG2	1.96	0.47
13:I:6:ALA:O	13:I:10:ARG:HB2	2.14	0.47
25:V:87:SER:HA	25:V:97:TYR:HB3	1.97	0.47
43:n:2:ARG:HB3	43:n:5:TRP:CD1	2.50	0.47
49:9:352:U:O2	61:LL:71:ARG:NE	2.41	0.47
49:9:532:C:H2'	49:9:533:A:C8	2.50	0.47
49:9:603:C:N4	49:9:620:G:O6	2.47	0.47
49:9:996:A:H2'	49:9:997:A:C8	2.49	0.47
49:9:1265:A:O2'	49:9:1327:G:OP2	2.25	0.47
50:AA:123:VAL:HG13	50:AA:145:ILE:HB	1.97	0.47
53:DD:57:ASN:O	53:DD:65:ARG:NH2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:66:A:H61	2:5:282:C:HO2'	1.62	0.47
2:5:1761:G:O6	2:5:1772:C:N4	2.47	0.47
4:8:14:OMU:HM23	4:8:14:OMU:H1'	1.55	0.47
5:A:45:VAL:HG22	5:A:61:VAL:HG22	1.97	0.47
8:D:41:LYS:HD2	23:T:93:ILE:HG12	1.96	0.47
14:J:90:ARG:NH2	14:J:108:GLY:O	2.44	0.47
32:c:48:LEU:HD11	32:c:60:ILE:HG21	1.97	0.47
33:d:23:ARG:NH1	33:d:25:TYR:OH	2.42	0.47
47:u:171:HIS:HD2	47:u:173:LYS:HG2	1.78	0.47
49:9:692:G:H2'	49:9:693:A:H8	1.79	0.47
51:BB:120:MET:HG3	51:BB:142:PHE:HE1	1.80	0.47
62:MM:58:GLU:HG3	62:MM:61:TYR:CZ	2.50	0.47
68:SS:31:THR:HG23	68:SS:37:GLY:HA2	1.96	0.47
8:D:289:ARG:HA	8:D:292:GLU:HG2	1.96	0.47
17:N:155:VAL:O	17:N:162:ARG:NH2	2.48	0.47
22:S:76:LYS:HD2	22:S:131:GLU:HG3	1.96	0.47
29:Z:51:ARG:HB3	29:Z:65:ARG:HH11	1.80	0.47
49:9:154:U:O2	56:GG:4:ASN:ND2	2.42	0.47
49:9:1866:A:H61	76:aa:85:ARG:H	1.62	0.47
52:CC:254:ASP:HB3	71:VV:1:MET:H1	1.80	0.47
54:EE:90:ILE:HB	54:EE:99:PHE:HB2	1.96	0.47
67:RR:17:ILE:HD11	67:RR:54:VAL:HA	1.97	0.47
2:5:3725:G:N7	38:i:67:LYS:NZ	2.49	0.47
2:5:4735:G:O6	2:5:4965:U:O4	2.32	0.47
6:B:317:LEU:HD21	6:B:381:THR:HA	1.98	0.47
47:u:67:VAL:HG21	47:u:144:MET:HE1	1.96	0.47
49:9:448:A:H5''	58:II:25:ARG:HA	1.97	0.47
49:9:959:G:OP2	64:OO:38:ASN:ND2	2.45	0.47
51:BB:92:GLN:HB3	51:BB:95:ASN:HB2	1.97	0.47
53:DD:103:GLU:OE2	53:DD:173:ARG:NH1	2.44	0.47
56:GG:26:THR:HG21	56:GG:40:ALA:HB3	1.96	0.47
66:QQ:58:LEU:HD13	66:QQ:108:ILE:HD11	1.97	0.47
71:VV:73:ALA:HB1	71:VV:78:ILE:HB	1.95	0.47
82:gg:82:SER:OG	82:gg:83:TRP:N	2.48	0.47
2:5:27:C:O2'	2:5:60:A:N3	2.40	0.46
2:5:151:G:N7	11:G:194:ASN:ND2	2.54	0.46
5:A:20:VAL:HG12	5:A:23:ARG:HD2	1.97	0.46
5:A:116:LEU:N	5:A:126:LEU:O	2.48	0.46
11:G:191:ALA:O	11:G:195:THR:OG1	2.33	0.46
21:R:163:ARG:HH21	49:9:873:G:H22	1.61	0.46
22:S:127:MET:HE1	23:T:155:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:f:54:LYS:O	35:f:66:LYS:NZ	2.42	0.46
49:9:1579:A:O2'	49:9:1581:C:OP2	2.27	0.46
49:9:1808:U:H2'	49:9:1809:A:C8	2.50	0.46
73:XX:59:ALA:HB1	73:XX:114:ASP:HB3	1.96	0.46
2:5:1346:C:H2'	2:5:1347:G:H8	1.80	0.46
19:P:60:PHE:HD2	19:P:67:VAL:HG21	1.81	0.46
49:9:1232:U:H3	49:9:1526:G:H1	1.63	0.46
65:PP:57:LEU:HD21	65:PP:86:LEU:HD12	1.97	0.46
74:YY:83:LYS:HE3	74:YY:96:LEU:HD13	1.98	0.46
75:ZZ:88:LEU:HD23	75:ZZ:91:LEU:HD12	1.97	0.46
82:gg:31:ILE:HG22	82:gg:43:TRP:HB2	1.98	0.46
2:5:1332:C:H2'	2:5:1333:A:C8	2.50	0.46
2:5:2848:G:N2	2:5:3839:G:OP2	2.38	0.46
8:D:54:ARG:NH2	8:D:147:ASP:OD2	2.42	0.46
17:N:116:LEU:HD22	17:N:135:ILE:HD11	1.97	0.46
30:a:132:ARG:HA	30:a:135:GLU:HG2	1.96	0.46
49:9:1792:G:H2'	49:9:1793:A:H8	1.81	0.46
56:GG:67:VAL:HB	56:GG:99:GLY:HA2	1.97	0.46
56:GG:135:PRO:HB2	56:GG:141:ILE:HD13	1.97	0.46
70:UU:63:ILE:HD12	79:dd:31:ILE:HD11	1.96	0.46
18:O:15:LEU:HB2	18:O:18:ARG:HB3	1.97	0.46
49:9:532:C:H2'	49:9:533:A:H8	1.80	0.46
49:9:641:A:O2'	49:9:645:C:OP1	2.33	0.46
49:9:1204:A:O2'	49:9:1700:C:OP2	2.30	0.46
49:9:1259:A:N6	49:9:1519:U:O5'	2.48	0.46
51:BB:137:LEU:HG	51:BB:215:VAL:HG22	1.96	0.46
57:HH:154:ILE:HG13	57:HH:185:VAL:HG13	1.98	0.46
76:aa:38:LYS:HB2	76:aa:71:LEU:HB2	1.97	0.46
2:5:1429:C:O2'	20:Q:136:THR:O	2.33	0.46
2:5:2489:C:H4'	2:5:2490:U:H5	1.81	0.46
2:5:2877:G:N2	2:5:3824:A:HO2'	2.13	0.46
2:5:4700:A:H2	12:H:69:THR:HG22	1.79	0.46
2:5:4996:C:H4'	33:d:26:THR:HG23	1.96	0.46
3:7:48:G:O2'	8:D:222:GLN:O	2.33	0.46
8:D:19:LYS:HB2	8:D:24:ARG:HG3	1.96	0.46
22:S:47:PHE:HE1	22:S:125:GLN:HG3	1.81	0.46
49:9:1656:G:H1	49:9:1668:U:H3	1.64	0.46
2:5:643:C:H2'	2:5:644:G:H8	1.81	0.46
2:5:1450:C:OP1	20:Q:40:ASN:ND2	2.48	0.46
2:5:2588:C:OP2	2:5:2769:U:O2'	2.31	0.46
2:5:2743:A:H1'	5:A:21:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:4473:A:O2'	42:m:96:ARG:NH2	2.41	0.46
16:M:119:ARG:NH2	16:M:123:ILE:HD11	2.29	0.46
20:Q:33:ARG:HE	20:Q:52:PHE:HZ	1.63	0.46
46:r:64:MET:HB2	46:r:78:VAL:HG23	1.97	0.46
47:u:114:GLU:HB2	47:u:138:LEU:HD11	1.97	0.46
49:9:639:C:H2'	49:9:640:A:C8	2.50	0.46
49:9:649:U:H2'	49:9:650:A:H8	1.80	0.46
49:9:894:G:H2'	49:9:895:G:H8	1.79	0.46
49:9:1345:G:OP1	49:9:1688:C:O2'	2.32	0.46
56:GG:215:LYS:HE2	56:GG:216:ARG:HH11	1.81	0.46
70:UU:26:SER:HB3	70:UU:32:LEU:HD12	1.98	0.46
71:VV:30:ALA:O	71:VV:60:ARG:NH1	2.46	0.46
2:5:68:U:OP1	17:N:178:HIS:ND1	2.37	0.46
2:5:3720:G:H22	2:5:3733:A:H2	1.64	0.46
2:5:3870:C:H2'	2:5:3871:A:H8	1.81	0.46
7:C:170:LEU:HD23	7:C:221:PHE:HZ	1.80	0.46
11:G:151:LEU:HD13	11:G:271:LEU:HD12	1.98	0.46
11:G:285:GLU:O	11:G:289:HIS:HB2	2.16	0.46
27:X:65:ALA:HB2	37:h:69:LEU:HD11	1.98	0.46
40:k:34:PHE:HE2	40:k:47:ILE:HD11	1.81	0.46
49:9:1354:G:N2	49:9:1357:A:OP2	2.39	0.46
52:CC:88:ILE:HD13	52:CC:94:ILE:HD11	1.97	0.46
64:OO:137:SER:OG	64:OO:138:ASP:N	2.48	0.46
2:5:1326:A2M:HM'3	2:5:1326:A2M:HI'	1.87	0.46
2:5:1327:C:H2'	2:5:1328:G:H8	1.81	0.46
2:5:1590:C:H4'	2:5:2857:A:H5'	1.98	0.46
2:5:2812:A:OP1	21:R:83:GLY:N	2.46	0.46
47:u:50:SER:OG	47:u:158:GLN:OE1	2.33	0.46
49:9:677:G:H21	49:9:1028:A:H62	1.64	0.46
52:CC:167:ARG:HA	52:CC:181:PRO:HD3	1.98	0.46
68:SS:121:ARG:HG3	68:SS:131:VAL:HB	1.98	0.46
75:ZZ:50:PHE:HB3	75:ZZ:55:TYR:HB2	1.96	0.46
2:5:685:C:O2'	2:5:686:A:O4'	2.33	0.46
2:5:1094:G:H2'	2:5:1095:A:H8	1.81	0.46
2:5:1406:G:OP2	2:5:1406(B):C:O2'	2.34	0.46
2:5:1951:G:O2'	22:S:95:ARG:NH1	2.40	0.46
5:A:158:ILE:HG23	5:A:162:ASN:HD21	1.80	0.46
12:H:129:ARG:HD2	12:H:156:ASN:HB3	1.98	0.46
14:J:160:GLU:HA	14:J:163:MET:HG2	1.97	0.46
23:T:51:GLY:HA3	23:T:92:ARG:HB2	1.98	0.46
49:9:925:G:H2'	49:9:926:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:CC:166:ARG:HG2	52:CC:181:PRO:HG3	1.97	0.46
68:SS:113:ARG:O	68:SS:117:ILE:HB	2.15	0.46
2:5:418:A:H4'	2:5:2311:C:H5'	1.96	0.46
2:5:3726:A:N6	2:5:4359:U:O2'	2.48	0.46
2:5:4260:U:H2'	2:5:4261:C:C6	2.51	0.46
2:5:4467:A:O2'	2:5:4510:A:N3	2.38	0.46
2:5:4646:U:OP1	21:R:59:SER:N	2.40	0.46
2:5:4735:G:C6	2:5:4965:U:N3	2.82	0.46
6:B:112:ASP:HA	6:B:115:LYS:HB2	1.98	0.46
15:L:121:ARG:HA	15:L:124:LEU:HD22	1.98	0.46
27:X:82:THR:HG21	37:h:37:THR:HG22	1.98	0.46
48:v:365:ARG:HA	48:v:365:ARG:HD2	1.54	0.46
49:9:1564:C:OP1	69:TT:121:ARG:NH1	2.49	0.46
50:AA:23:THR:HG22	50:AA:170:SER:HB2	1.98	0.46
59:JJ:113:GLN:OE1	59:JJ:154:GLN:NE2	2.46	0.46
61:LL:99:TYR:O	61:LL:101:ARG:N	2.49	0.46
2:5:33:A:H5''	2:5:47:A:H61	1.81	0.45
2:5:109:G:OP2	15:L:74:ARG:NH2	2.49	0.45
2:5:1633:G:C6	5:A:207:VAL:HG21	2.50	0.45
2:5:4507:A:O2'	25:V:41:SER:OG	2.23	0.45
5:A:27:ALA:O	5:A:128:ARG:NH2	2.48	0.45
6:B:293:ILE:HA	6:B:298:LEU:HA	1.98	0.45
13:I:79:SER:OG	13:I:147:HIS:ND1	2.47	0.45
45:p:32:SER:O	45:p:37:TYR:OH	2.30	0.45
49:9:1270:G:O2'	49:9:1301:A:N7	2.46	0.45
49:9:1309:C:H5''	81:ff:105:TYR:HE1	1.81	0.45
69:TT:96:SER:HB3	69:TT:99:VAL:HG22	1.98	0.45
72:WW:6:VAL:HG22	72:WW:34:ILE:HD11	1.98	0.45
2:5:209:U:H4'	28:Y:59:ARG:HD2	1.98	0.45
2:5:1214:C:O2	31:b:91:ARG:NH1	2.50	0.45
2:5:1364:U:H5	15:L:36:ARG:HH12	1.64	0.45
2:5:3951:G:C6	2:5:4062:A:N1	2.84	0.45
27:X:145:ASP:N	27:X:145:ASP:OD1	2.49	0.45
49:9:38:A:H5''	59:JJ:5:ARG:HD3	1.98	0.45
49:9:1142:G:N2	49:9:1145:A:OP2	2.38	0.45
49:9:1664:A:O2'	49:9:1666:C:N4	2.48	0.45
51:BB:46:LYS:HE3	64:OO:20:GLN:HB2	1.98	0.45
51:BB:59:SER:O	51:BB:63:LYS:HB2	2.16	0.45
51:BB:150:ILE:HG13	67:RR:131:PRO:HA	1.97	0.45
52:CC:69:LEU:HD11	52:CC:273:LEU:HD11	1.97	0.45
53:DD:218:LEU:HD22	82:gg:192:THR:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:HH:53:VAL:HG21	57:HH:172:THR:HA	1.98	0.45
2:5:327:U:O2'	38:i:30:ARG:NH1	2.42	0.45
2:5:423:G:N3	19:P:118:GLN:NE2	2.65	0.45
11:G:309:ALA:O	11:G:313:GLU:HB2	2.15	0.45
12:H:41:ILE:HD11	12:H:69:THR:HB	1.99	0.45
17:N:64:ILE:HD11	17:N:66:VAL:HG13	1.98	0.45
28:Y:26:ARG:NH1	28:Y:75:ARG:O	2.48	0.45
29:Z:53:VAL:HG23	29:Z:62:ILE:HG12	1.98	0.45
56:GG:48:TYR:OH	56:GG:119:LYS:O	2.29	0.45
57:HH:140:VAL:HG12	63:NN:19:ARG:HD2	1.97	0.45
67:RR:52:GLY:O	67:RR:55:THR:OG1	2.31	0.45
70:UU:98:VAL:HA	70:UU:101:ILE:HG22	1.98	0.45
2:5:268:G:H2'	2:5:269:G:H8	1.80	0.45
2:5:4518:A:OP1	2:5:4520:G:O2'	2.29	0.45
5:A:48:ILE:HD13	45:p:65:ALA:HB2	1.99	0.45
15:L:163:LYS:NZ	15:L:164:GLU:O	2.48	0.45
18:O:54:TYR:OH	18:O:73:PHE:O	2.34	0.45
22:S:161:ARG:HD2	22:S:164:LYS:HB2	1.99	0.45
49:9:110:U:H5'	54:EE:205:PHE:HE2	1.82	0.45
49:9:1228:A:H2'	49:9:1229:G:H8	1.81	0.45
54:EE:72:ILE:HD12	54:EE:77:ARG:HB2	1.99	0.45
60:KK:65:ARG:NH2	79:dd:25:SER:OG	2.49	0.45
65:PP:22:LEU:HA	65:PP:25:LEU:HD12	1.97	0.45
2:5:20:U:OP2	4:8:36:G:N1	2.48	0.45
2:5:4095:G:H1	2:5:4113:U:H3	1.63	0.45
2:5:4239:A:H2'	2:5:4240:G:C8	2.52	0.45
15:L:78:LEU:HD13	15:L:100:PRO:HA	1.98	0.45
18:O:47:PHE:HZ	18:O:144:GLU:HG3	1.79	0.45
51:BB:122:GLU:HB3	51:BB:140:VAL:HG23	1.98	0.45
61:LL:80:MET:HE2	61:LL:122:ILE:HG23	1.97	0.45
78:cc:10:LYS:HD3	78:cc:61:SER:HB2	1.98	0.45
81:ff:135:HIS:CD2	81:ff:140:TYR:HB3	2.52	0.45
2:5:4565:C:O2	6:B:268:ARG:NE	2.50	0.45
2:5:5001:U:H4'	6:B:317:LEU:HB3	1.99	0.45
4:8:39:G:H1'	4:8:103:A:H61	1.82	0.45
6:B:52:GLY:HA2	6:B:341:LYS:HE3	1.99	0.45
6:B:220:ILE:HB	6:B:346:THR:HB	1.99	0.45
29:Z:5:MET:HE2	29:Z:82:PRO:HG3	1.99	0.45
49:9:90:G:OP1	49:9:445:A:N6	2.49	0.45
49:9:681:U:H4'	73:XX:9:THR:HG22	1.97	0.45
49:9:1593:C:OP1	75:ZZ:103:HIS:NE2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:GG:162:LEU:O	56:GG:169:PRO:HA	2.15	0.45
68:SS:35:GLY:O	68:SS:97:GLN:NE2	2.47	0.45
70:UU:18:HIS:O	70:UU:92:HIS:HA	2.16	0.45
2:5:29:G:H5''	17:N:172:ARG:HG2	1.99	0.45
2:5:1481:C:O2'	2:5:1482:G:O5'	2.35	0.45
2:5:2399:G:HO2'	2:5:2822:G:HO2'	1.51	0.45
2:5:2533:C:OP1	27:X:139:ARG:NH2	2.49	0.45
26:W:8:PHE:HZ	26:W:49:ILE:HD12	1.82	0.45
49:9:31:U:O2'	49:9:643:A:N1	2.44	0.45
57:HH:51:ILE:HG21	57:HH:179:LYS:HG2	1.98	0.45
66:QQ:25:CYS:HB3	66:QQ:68:ILE:HG12	1.98	0.45
2:5:758:G:H5''	12:H:54:ARG:HH22	1.81	0.45
12:H:34:LEU:HD11	12:H:80:MET:HG3	1.98	0.45
18:O:157:GLU:HA	18:O:160:ARG:HG2	1.99	0.45
22:S:35:PRO:HD2	22:S:39:VAL:HG11	1.99	0.45
34:e:85:LEU:HD11	34:e:111:ILE:HG23	1.99	0.45
59:JJ:38:ARG:HG2	80:ee:104:ARG:HB2	1.99	0.45
64:OO:34:PHE:HB3	64:OO:41:PHE:HB2	1.97	0.45
2:5:52:G:OP2	39:j:48:ASN:ND2	2.49	0.45
2:5:1371:A:N1	4:8:28:C:O2'	2.44	0.45
2:5:1613:A:H5''	5:A:183:GLY:HA2	1.98	0.45
2:5:2543:A:H2	2:5:2773:OMG:HN21	1.65	0.45
19:P:64:ASN:HD22	19:P:64:ASN:N	2.14	0.45
49:9:599:A:H2'	49:9:606:G:H21	1.81	0.45
50:AA:188:THR:HG22	50:AA:189:ILE:HG13	1.98	0.45
2:5:1207:C:H2'	2:5:1208:G:H8	1.82	0.45
2:5:1524:A2M:H61	2:5:3915:U:HO2'	1.60	0.45
2:5:2739:C:H4'	45:p:52:VAL:HG21	1.98	0.45
2:5:4599:A:N6	2:5:4611:A:OP2	2.48	0.45
10:F:79:ASN:HA	23:T:143:THR:HG22	1.99	0.45
12:H:58:ASP:OD1	12:H:58:ASP:N	2.49	0.45
14:J:37:ALA:HA	14:J:70:VAL:HG11	2.00	0.45
21:R:151:ARG:NE	61:LL:118:ARG:HE	2.15	0.45
25:V:69:LYS:NZ	25:V:71:GLU:OE2	2.45	0.45
49:9:146:G:O2'	49:9:147:A:O5'	2.35	0.45
53:DD:219:PRO:HG2	82:gg:190:GLY:HA2	1.99	0.45
2:5:643:C:H2'	2:5:644:G:C8	2.52	0.44
2:5:4081:G:H2'	2:5:4082:G:H8	1.83	0.44
8:D:33:ARG:HH21	8:D:37:VAL:HG11	1.82	0.44
24:U:60:VAL:HG13	24:U:75:GLU:HB3	1.98	0.44
49:9:659:G:O2'	49:9:662:G:O2'	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:9:794:A:H2'	49:9:795:A:H8	1.81	0.44
2:5:1480:C:O2'	2:5:1482:G:OP2	2.34	0.44
2:5:1969:G:O6	2:5:2019:C:N4	2.49	0.44
6:B:3:HIS:ND1	6:B:4:ARG:O	2.45	0.44
6:B:331:VAL:HG21	6:B:347:LEU:HD21	1.99	0.44
46:r:17:LEU:HD21	46:r:19:LYS:HE3	1.99	0.44
49:9:942:G:N2	64:OO:137:SER:OG	2.42	0.44
58:II:113:TYR:OH	58:II:156:ALA:O	2.35	0.44
2:5:1354:A:N1	2:5:1385:G:O2'	2.49	0.44
2:5:3619:G:H22	2:5:3624:A:H1'	1.82	0.44
2:5:3974:G:OP2	2:5:3975:C:N4	2.49	0.44
2:5:4076:G:P	11:G:126:ARG:HE	2.40	0.44
2:5:4194:I4U:O2'	13:I:116:ARG:NH1	2.49	0.44
2:5:4860:G:H5'	18:O:169:ARG:HH11	1.81	0.44
2:5:4896:G:H2'	2:5:4897:G:C8	2.52	0.44
3:7:57:C:H2'	3:7:58:A:H8	1.83	0.44
6:B:8:ALA:HB1	25:V:48:ARG:HH22	1.82	0.44
7:C:12:SER:HA	7:C:155:GLU:HG2	1.98	0.44
20:Q:124:ASP:OD1	20:Q:124:ASP:N	2.50	0.44
26:W:104:GLN:OE1	56:GG:156:TYR:OH	2.36	0.44
47:u:60:ARG:HG2	47:u:63:PHE:HD1	1.82	0.44
49:9:384:U:O4	58:II:5:ARG:NH2	2.44	0.44
49:9:1831:A:H2'	49:9:1832:6MZ:H8	1.99	0.44
51:BB:131:ASP:OD1	51:BB:131:ASP:N	2.48	0.44
52:CC:168:GLY:N	52:CC:179:THR:O	2.45	0.44
52:CC:214:LEU:HD12	52:CC:244:ILE:HD11	1.99	0.44
53:DD:42:THR:OG1	53:DD:45:ARG:O	2.31	0.44
53:DD:142:LEU:HD11	53:DD:182:LEU:HD21	1.99	0.44
54:EE:139:LEU:HG	54:EE:150:PRO:HG3	1.99	0.44
58:II:12:ARG:HE	58:II:18:ARG:HG2	1.82	0.44
60:KK:15:LEU:HG	60:KK:71:LEU:HD22	1.99	0.44
77:bb:36:LYS:HB3	77:bb:43:ILE:HG22	1.99	0.44
82:gg:17:TRP:O	82:gg:36:ARG:N	2.40	0.44
17:N:88:GLY:HA3	44:o:48:TYR:CE2	2.53	0.44
22:S:15:ARG:HH12	22:S:18:PRO:HG3	1.82	0.44
48:v:276:ARG:NE	48:v:328:GLN:OE1	2.42	0.44
49:9:1287:A:OP1	81:f:97:LYS:NZ	2.33	0.44
58:II:106:SER:HB3	58:II:171:LEU:HG	2.00	0.44
65:PP:38:SER:OG	65:PP:39:ALA:N	2.46	0.44
2:5:952:G:H5''	35:f:73:LYS:HE2	2.00	0.44
2:5:3802:U:O4	2:5:4502:C:N4	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:3848:U:H2'	2:5:3849:A:H8	1.83	0.44
18:O:43:ILE:HD11	18:O:138:LEU:HD13	1.99	0.44
19:P:141:SER:OG	19:P:142:SER:N	2.49	0.44
25:V:82:ILE:HD13	25:V:121:VAL:HG22	1.99	0.44
49:9:1693:G:N2	49:9:1834:A:H8	2.15	0.44
62:MM:31:LEU:HA	62:MM:112:LYS:H	1.83	0.44
82:gg:108:VAL:HA	82:gg:124:SER:HA	1.99	0.44
2:5:2553:A:OP2	2:5:2574:G:O2'	2.30	0.44
2:5:4419:U:H5''	2:5:4421:C:H41	1.83	0.44
11:G:317:LYS:HE3	51:BB:224:GLU:HB2	2.00	0.44
12:H:152:GLU:O	12:H:156:ASN:HB2	2.18	0.44
14:J:72:CYS:SG	14:J:73:THR:N	2.91	0.44
57:HH:57:ARG:HH12	57:HH:91:HIS:CD2	2.35	0.44
80:ee:126:LYS:HE3	80:ee:130:ALA:HB1	1.99	0.44
2:5:51:A:N3	2:5:1528:U:O2'	2.51	0.44
2:5:935(A):G:O2'	16:M:19:PRO:O	2.26	0.44
2:5:3717:A:H2'	2:5:3718:A2M:C8	2.47	0.44
2:5:4338:G:N7	44:o:61:LYS:NZ	2.56	0.44
8:D:286:SER:HA	8:D:289:ARG:HG2	1.99	0.44
12:H:113:GLU:HA	12:H:124:ARG:O	2.18	0.44
12:H:113:GLU:HG2	12:H:125:ARG:HG2	1.99	0.44
15:L:17:ASP:O	15:L:21:ARG:NH2	2.51	0.44
15:L:91:ALA:HB1	15:L:96:ILE:HB	1.99	0.44
49:9:84:A:H5''	74:YY:122:LYS:NZ	2.33	0.44
49:9:913:A:N6	57:HH:119:SER:O	2.44	0.44
49:9:1705:C:H2'	49:9:1706:G:C8	2.53	0.44
52:CC:178:HIS:ND1	52:CC:179:THR:HG23	2.33	0.44
54:EE:36:HIS:CG	54:EE:85:GLY:HA3	2.52	0.44
71:VV:34:MET:HB3	71:VV:34:MET:HE3	1.78	0.44
2:5:923:C:H5'	2:5:924:C:H5''	1.99	0.44
2:5:1088:C:H2'	2:5:1089:G:H8	1.82	0.44
2:5:2487:G:O2'	4:8:126:C:OP2	2.30	0.44
2:5:4457:U:OP1	25:V:50:ASN:ND2	2.51	0.44
2:5:4472:B8W:O2'	42:m:74:TYR:O	2.36	0.44
3:7:48:G:OP1	8:D:226:TYR:OH	2.36	0.44
17:N:17:ASP:OD1	17:N:17:ASP:N	2.50	0.44
21:R:13:SER:OG	21:R:38:ARG:NH1	2.45	0.44
36:g:8:ARG:NH2	36:g:32:TYR:O	2.50	0.44
49:9:441:C:H2'	49:9:442:C:C6	2.53	0.44
50:AA:10:MET:HE1	50:AA:51:LEU:HB3	1.99	0.44
51:BB:110:MET:HE1	51:BB:140:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:LL:76:VAL:HG12	61:LL:125:ILE:HG12	1.98	0.44
2:5:1506:G:N3	7:C:116:ASN:ND2	2.61	0.44
2:5:3682:A:H5''	5:A:132:ASN:HD22	1.82	0.44
2:5:4135:G:H2'	2:5:4136:G:H8	1.83	0.44
2:5:4174:U:H2'	2:5:4175:G:H8	1.82	0.44
6:B:44:THR:HG21	6:B:186:ASN:HD22	1.83	0.44
26:W:9:SER:O	26:W:52:THR:OG1	2.34	0.44
49:9:1568:C:H2'	49:9:1569:A:C8	2.52	0.44
49:9:1588:A:H2'	49:9:1589:A:C8	2.53	0.44
55:FF:34:SER:HA	78:cc:55:VAL:HG23	2.00	0.44
60:KK:72:THR:HG23	60:KK:75:GLY:H	1.83	0.44
82:gg:256:ILE:HB	82:gg:270:LEU:HG	2.00	0.44
2:5:1645:C:H2'	2:5:1646:A:C8	2.53	0.43
2:5:4398:C:H41	2:5:4446:U:H3	1.66	0.43
4:8:60:G:OP1	27:X:70:LYS:NZ	2.44	0.43
17:N:9:GLU:HB2	38:i:44:ILE:HG13	2.00	0.43
17:N:54:LYS:H	17:N:59:TYR:HE2	1.64	0.43
18:O:15:LEU:HD12	18:O:18:ARG:HD2	1.99	0.43
18:O:186:GLU:O	18:O:190:SER:HB2	2.18	0.43
19:P:124:LYS:HA	19:P:143:PRO:HD2	2.00	0.43
21:R:106:LEU:HB3	21:R:120:TYR:CE1	2.53	0.43
22:S:76:LYS:NZ	22:S:100:LEU:O	2.41	0.43
29:Z:46:ILE:HA	29:Z:70:SER:HA	1.99	0.43
49:9:28:U:H2'	49:9:29:G:H8	1.83	0.43
49:9:159:A2M:H8	49:9:159:A2M:OP2	2.18	0.43
49:9:1653:U:H3	49:9:1671:G:H1	1.65	0.43
53:DD:106:ARG:HG3	53:DD:175:VAL:HG22	2.00	0.43
54:EE:128:LYS:HB2	54:EE:140:VAL:HB	2.00	0.43
56:GG:5:ILE:HG21	56:GG:45:TRP:HH2	1.83	0.43
72:WW:80:ASP:N	72:WW:80:ASP:OD1	2.45	0.43
73:XX:93:PHE:HB3	73:XX:133:LEU:HD23	2.00	0.43
2:5:1479:G:H21	15:L:184:MET:HE2	1.82	0.43
2:5:1552:G:N2	2:5:1574:B9B:O2'	2.50	0.43
2:5:3932:U:H2'	2:5:3933:G:H8	1.83	0.43
2:5:4078:C:O2'	2:5:4172:A:N6	2.51	0.43
5:A:117:GLU:HG3	5:A:124:GLY:H	1.82	0.43
8:D:64:ILE:HG13	8:D:105:LEU:HD21	1.99	0.43
8:D:108:ARG:CZ	8:D:253:TYR:HB2	2.48	0.43
15:L:64:VAL:HA	15:L:67:HIS:CD2	2.53	0.43
55:FF:51:HIS:ND1	66:QQ:82:TYR:OH	2.43	0.43
56:GG:2:LYS:HG2	56:GG:17:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:KK:64:TRP:CD2	79:dd:23:VAL:HG12	2.53	0.43
5:A:224:THR:HG21	5:A:243:THR:HG21	1.99	0.43
41:l:44:TRP:O	41:l:48:LYS:NZ	2.39	0.43
49:9:1850:MA6:H8	49:9:1850:MA6:O5'	2.18	0.43
50:AA:173:LEU:HD13	50:AA:177:MET:HE2	2.00	0.43
53:DD:9:ARG:HA	53:DD:12:VAL:HG22	2.00	0.43
58:II:36:THR:OG1	58:II:96:LEU:O	2.36	0.43
77:bb:33:MET:HE1	77:bb:73:LEU:HD11	2.00	0.43
2:5:1907:A:H4'	10:F:222:LYS:HE3	2.00	0.43
3:7:92:C:H2'	3:7:93:G:H8	1.82	0.43
6:B:160:ILE:HD12	6:B:193:LYS:HD2	2.00	0.43
27:X:129:ARG:NH2	27:X:131:ASP:OD2	2.51	0.43
34:e:69:MET:HA	34:e:75:ARG:HD3	2.00	0.43
35:f:76:ARG:HH21	35:f:85:ARG:CZ	2.31	0.43
40:k:33:LYS:HG2	40:k:46:VAL:HG22	2.00	0.43
46:r:2:SER:OG	46:r:3:ALA:N	2.51	0.43
49:9:5:U:H2'	49:9:6:G:C8	2.54	0.43
49:9:1256:G:N2	79:dd:30:LEU:O	2.49	0.43
49:9:1536:G:H2'	49:9:1537:A:H8	1.83	0.43
54:EE:246:LEU:H	54:EE:246:LEU:HG	1.64	0.43
55:FF:38:TYR:OH	78:cc:51:ARG:NH1	2.51	0.43
57:HH:166:VAL:HG13	57:HH:173:PHE:HE2	1.82	0.43
75:ZZ:88:LEU:HB3	75:ZZ:109:TYR:HE2	1.83	0.43
82:gg:168:CYS:HB3	82:gg:198:VAL:HG23	1.99	0.43
2:5:232:G:O6	28:Y:61:HIS:N	2.51	0.43
2:5:2397:G:O6	36:g:4:ARG:NH2	2.48	0.43
2:5:2441:C:H4'	36:g:9:ARG:HE	1.84	0.43
2:5:2639:U:H1'	36:g:26:PRO:HA	2.00	0.43
2:5:3892:U:O2'	19:P:80:GLN:OE1	2.30	0.43
2:5:4081:G:H2'	2:5:4082:G:C8	2.53	0.43
2:5:4653:C:OP1	33:d:79:ASN:ND2	2.51	0.43
2:5:4991:U:H2'	2:5:4992:G:H8	1.83	0.43
28:Y:114:ASP:HA	28:Y:117:LYS:HG2	2.01	0.43
31:b:101:HIS:NE2	31:b:104:LEU:HB2	2.33	0.43
48:v:308:THR:HA	48:v:311:THR:HG22	2.01	0.43
49:9:1578:U:H1'	53:DD:6:SER:HB3	2.01	0.43
49:9:1745:A:H1'	56:GG:66:GLY:HA2	2.01	0.43
53:DD:158:ILE:H	53:DD:158:ILE:HG13	1.67	0.43
67:RR:77:GLU:OE2	67:RR:81:ARG:NH1	2.51	0.43
2:5:478:G:H2'	2:5:479:G:H8	1.84	0.43
2:5:1332:C:H2'	2:5:1333:A:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:1790:U:OP2	23:T:13:TYR:OH	2.24	0.43
2:5:1868:A:H61	13:I:115:MET:HE3	1.84	0.43
2:5:2389:A:H4'	33:d:70:LYS:HG3	2.00	0.43
2:5:2491:C:H2'	2:5:2492:C:C6	2.54	0.43
2:5:2581:A:H2'	2:5:2582:A:C8	2.54	0.43
2:5:4627:U:H4'	6:B:373:LYS:HD2	2.01	0.43
11:G:317:LYS:HD2	51:BB:225:LEU:HB3	2.00	0.43
19:P:64:ASN:H	19:P:64:ASN:ND2	2.16	0.43
49:9:562:U:H2'	49:9:563:G:C8	2.54	0.43
50:AA:69:GLU:HB2	52:CC:270:THR:HG21	2.00	0.43
60:KK:85:LEU:HA	60:KK:86:PRO:HD3	1.89	0.43
72:WW:3:ARG:HH22	72:WW:28:ARG:HH21	1.65	0.43
2:5:229:G:H5''	28:Y:11:ARG:HG3	2.00	0.43
2:5:707:C:O2'	2:5:4943:A:N1	2.46	0.43
2:5:1999:A:O2'	2:5:2000:G:O4'	2.32	0.43
2:5:2793:G:H4'	39:j:8:PHE:HD2	1.84	0.43
2:5:3723:A2M:HM'3	2:5:3723:A2M:H1'	1.91	0.43
4:8:37:A:OP2	37:h:89:ARG:NH1	2.40	0.43
5:A:82:ILE:HG22	45:p:65:ALA:HB3	2.00	0.43
7:C:95:MET:HB2	7:C:95:MET:HE3	1.79	0.43
8:D:131:ASN:OD1	8:D:131:ASN:N	2.50	0.43
11:G:157:PRO:HG3	11:G:247:VAL:HG12	1.99	0.43
17:N:187:SER:H	17:N:190:ALA:HB3	1.84	0.43
37:h:4:ILE:O	37:h:56:ARG:NH1	2.52	0.43
47:u:60:ARG:O	47:u:62:LYS:N	2.51	0.43
49:9:168:C:OP1	56:GG:131:ARG:NE	2.52	0.43
49:9:1199:A:H5''	76:aa:2:THR:HB	2.00	0.43
52:CC:146:GLU:HG2	52:CC:149:THR:HG22	2.01	0.43
52:CC:221:ASP:N	52:CC:221:ASP:OD1	2.52	0.43
54:EE:102:ILE:HD13	54:EE:239:PRO:HD3	2.01	0.43
60:KK:15:LEU:HD22	60:KK:49:MET:HE2	2.01	0.43
61:LL:109:MET:HB2	61:LL:109:MET:HE3	1.81	0.43
64:OO:31:CYS:HA	64:OO:43:HIS:O	2.19	0.43
66:QQ:44:PRO:HD3	66:QQ:77:HIS:HB3	2.01	0.43
2:5:651:C:H2'	2:5:652:G:H8	1.83	0.43
2:5:1329:G:H2'	2:5:3865:A:H5'	2.00	0.43
2:5:1461:C:H2'	2:5:1462:A:C8	2.53	0.43
2:5:3959:U:H2'	2:5:3960:A:H8	1.84	0.43
2:5:4354:U:H3	30:a:60:HIS:CE1	2.36	0.43
8:D:152:ARG:HG3	8:D:154:THR:HG23	2.00	0.43
15:L:28:GLN:HB3	17:N:202:ARG:HE	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:78:LYS:HG2	20:Q:137:VAL:HG23	2.00	0.43
49:9:307:G:N2	58:II:45:THR:O	2.51	0.43
49:9:1447:G:OP1	70:UU:85:HIS:ND1	2.52	0.43
52:CC:70:VAL:HG21	52:CC:93:ILE:HG23	2.01	0.43
64:OO:78:ALA:HB1	64:OO:119:LEU:HD12	1.99	0.43
2:5:2394:G:O2'	2:5:2819:U:O4	2.26	0.43
2:5:2520:C:H2'	2:5:2521:G:C8	2.52	0.43
2:5:4966:A:OP1	6:B:128:LYS:NZ	2.52	0.43
5:A:3:ARG:HD2	5:A:208:GLU:HB3	2.01	0.43
5:A:117:GLU:O	5:A:162:ASN:ND2	2.52	0.43
6:B:264:PHE:N	18:O:64:THR:O	2.49	0.43
8:D:236:MET:HE2	8:D:236:MET:HB2	1.95	0.43
17:N:75:VAL:HG11	17:N:80:THR:HG22	2.01	0.43
30:a:117:LEU:HD12	30:a:118:PRO:HD2	2.00	0.43
69:TT:22:LEU:HD23	69:TT:28:LEU:HD22	2.01	0.43
3:7:23:A:N3	3:7:118:C:O2'	2.39	0.43
10:F:181:TYR:CZ	10:F:202:GLU:HG2	2.54	0.43
28:Y:31:SER:HA	28:Y:48:PRO:HA	2.01	0.43
47:u:27:LYS:HE2	47:u:28:PHE:CZ	2.54	0.43
49:9:382:C:H2'	49:9:383:G:H8	1.84	0.43
2:5:4220:6MZ:O5'	2:5:4220:6MZ:H8	2.18	0.42
7:C:4:ALA:O	7:C:29:LYS:NZ	2.48	0.42
15:L:64:VAL:HA	15:L:67:HIS:HD2	1.84	0.42
23:T:74:ILE:HG21	23:T:74:ILE:HD13	1.84	0.42
36:g:69:LYS:HG3	36:g:73:HIS:CD2	2.54	0.42
40:k:8:ILE:HD11	40:k:56:LEU:HD13	2.01	0.42
41:l:33:ASN:HD22	41:l:33:ASN:HA	1.61	0.42
41:l:43:HIS:CE1	41:l:45:ARG:HG2	2.54	0.42
49:9:183:G:O2'	49:9:184:G:O4'	2.36	0.42
57:HH:105:THR:HG23	57:HH:107:LYS:H	1.84	0.42
67:RR:35:CYS:HA	67:RR:38:ILE:HG22	2.01	0.42
68:SS:121:ARG:O	68:SS:125:HIS:ND1	2.48	0.42
82:gg:239:LEU:HA	82:gg:249:CYS:O	2.18	0.42
2:5:1788:A:O2'	2:5:4209:G:O2'	2.31	0.42
2:5:3910:C:H2'	2:5:3911:C:C6	2.54	0.42
4:8:141:C:H5''	17:N:60:VAL:HG21	2.01	0.42
11:G:252:CYS:SG	11:G:253:THR:N	2.92	0.42
47:u:52:THR:HB	47:u:156:LYS:HD3	2.00	0.42
56:GG:176:ILE:HG13	56:GG:179:LEU:HD23	2.00	0.42
56:GG:225:GLN:HA	56:GG:228:ILE:HG22	2.00	0.42
67:RR:99:ASP:OD1	67:RR:102:THR:OG1	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:478:G:H2'	2:5:479:G:C8	2.54	0.42
2:5:1802:A:H5''	2:5:1803:G:H5'	2.01	0.42
2:5:4153:C:H2'	2:5:4154:G:H8	1.85	0.42
3:7:29:C:H4'	14:J:12:MET:HE1	2.01	0.42
11:G:139:VAL:HG21	11:G:238:LYS:HG3	2.01	0.42
15:L:9:ILE:HG21	30:a:45:PHE:HE1	1.84	0.42
47:u:41:TYR:OH	47:u:47:LYS:O	2.37	0.42
49:9:1228:A:O2'	49:9:1634:A:N3	2.43	0.42
52:CC:207:ALA:O	52:CC:211:LYS:CB	2.67	0.42
54:EE:112:HIS:CD2	54:EE:114:ILE:HD11	2.54	0.42
58:II:64:ASN:HA	58:II:75:LYS:HA	2.00	0.42
62:MM:64:LEU:HD11	81:ff:106:TYR:HB2	1.99	0.42
65:PP:121:ILE:H	65:PP:121:ILE:HG13	1.71	0.42
72:WW:7:LEU:HD23	72:WW:34:ILE:HG12	2.02	0.42
2:5:909:G:H2'	2:5:910:G:H8	1.84	0.42
2:5:964:A:H2'	2:5:965:G:C8	2.54	0.42
2:5:2082:G:H5''	20:Q:12:LYS:HG2	2.01	0.42
2:5:3709:U:H6	2:5:3711:A:H61	1.66	0.42
2:5:4723:A:H2'	2:5:4724:A:C8	2.54	0.42
2:5:4915:G:H2'	2:5:4916:G:C8	2.54	0.42
21:R:163:ARG:HH21	49:9:873:G:N2	2.18	0.42
43:n:7:LYS:HE2	43:n:11:ARG:NH2	2.34	0.42
49:9:385:G:H3'	61:LL:136:LYS:HB2	2.02	0.42
49:9:872:A:O2'	49:9:874:G:OP2	2.37	0.42
49:9:1189:A:H2'	49:9:1190:A:H8	1.84	0.42
49:9:1205:C:HO2'	49:9:1834:A:N6	2.17	0.42
67:RR:14:ARG:HG2	67:RR:69:ILE:HD11	2.00	0.42
74:YY:76:TYR:OH	74:YY:86:GLU:OE1	2.33	0.42
82:gg:196:ASN:HD21	82:gg:237:ASN:HA	1.85	0.42
82:gg:234:ASP:OD1	82:gg:234:ASP:N	2.52	0.42
2:5:943:A:N7	10:F:150:ASN:ND2	2.60	0.42
2:5:1442:C:H2'	2:5:1443:A:C8	2.54	0.42
2:5:4088:C:H2'	2:5:4089:G:C8	2.54	0.42
20:Q:88:ASP:OD1	20:Q:89:ASP:N	2.52	0.42
25:V:21:PRO:HA	25:V:54:ALA:HA	2.02	0.42
49:9:1247:C:H1'	49:9:1251:A:C4	2.54	0.42
51:BB:108:ASP:O	51:BB:112:SER:CB	2.67	0.42
52:CC:128:VAL:HG11	52:CC:155:ILE:HG12	2.01	0.42
57:HH:133:LEU:HD21	57:HH:176:VAL:HG11	2.01	0.42
77:bb:8:LEU:HA	77:bb:8:LEU:HD23	1.79	0.42
2:5:1306:C:H2'	2:5:1307:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:1867:A:OP1	13:I:13:LYS:NZ	2.51	0.42
2:5:3848:U:H2'	2:5:3849:A:C8	2.55	0.42
43:n:11:ARG:NH2	49:9:1844:U:OP1	2.52	0.42
48:v:349:VAL:HG13	48:v:356:LEU:HB3	2.01	0.42
49:9:1553:C:O2'	49:9:1554:C:O4'	2.38	0.42
53:DD:50:ILE:HG23	53:DD:88:ALA:HA	2.02	0.42
59:JJ:70:ARG:NH1	59:JJ:94:LEU:HD21	2.35	0.42
68:SS:104:ASP:OD1	68:SS:104:ASP:N	2.50	0.42
2:5:150:U:OP2	11:G:253:THR:OG1	2.31	0.42
2:5:197:A:N1	2:5:225:G:O2'	2.48	0.42
2:5:280:G:O6	17:N:15:GLN:NE2	2.53	0.42
2:5:963:G:O2'	2:5:964:A:H8	2.03	0.42
2:5:1866:UR3:H3U2	2:5:4405:G:H8	1.85	0.42
2:5:2407:G:H2'	41:l:13:LEU:HD22	2.01	0.42
2:5:4240:G:H5'	8:D:152:ARG:HD3	2.01	0.42
5:A:98:ILE:HD13	45:p:80:LYS:HG3	2.01	0.42
6:B:229:LYS:HE3	6:B:233:SER:HB3	2.02	0.42
8:D:166:ALA:HB1	8:D:171:LEU:HD22	2.00	0.42
12:H:93:ARG:HE	42:m:56:LEU:HD21	1.84	0.42
47:u:121:PRO:HA	47:u:125:GLY:HA3	2.02	0.42
49:9:126:G:H5''	56:GG:195:LYS:HD3	2.02	0.42
49:9:190:G:O2'	49:9:209:A:N6	2.52	0.42
49:9:1587:G:N7	69:TT:67:ARG:HD3	2.35	0.42
55:FF:35:LEU:HD22	55:FF:147:VAL:HG23	2.02	0.42
64:OO:117:ARG:HH12	78:cc:40:ARG:HH11	1.67	0.42
82:gg:252:THR:OG1	82:gg:255:SER:O	2.29	0.42
1:4:18:U:H4'	1:4:19:G:H5'	2.00	0.42
2:5:1187:G:H1'	8:D:275:GLN:HE21	1.84	0.42
13:I:207:ASP:HA	13:I:210:ARG:HG2	2.02	0.42
15:L:3:PRO:HG2	30:a:44:ASN:HD22	1.84	0.42
49:9:486:A:H1'	49:9:513:G:H22	1.84	0.42
49:9:1613:G:P	65:PP:42:ARG:HH12	2.43	0.42
63:NN:20:ARG:HH11	72:WW:56:HIS:HB3	1.84	0.42
66:QQ:58:LEU:HB3	66:QQ:62:ARG:HD2	2.02	0.42
70:UU:56:MET:HB3	70:UU:56:MET:HE2	1.70	0.42
2:5:1328:G:O2'	2:5:2349:A:OP1	2.33	0.42
2:5:5010:U:H2'	2:5:5011:A:H8	1.85	0.42
6:B:82:PRO:HB3	6:B:328:ASN:ND2	2.34	0.42
7:C:32:ILE:HD12	7:C:130:ALA:HB2	2.01	0.42
15:L:184:MET:HE3	15:L:184:MET:HB2	1.89	0.42
29:Z:16:GLY:O	29:Z:19:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:9:696:G:H2'	49:9:697:G:H8	1.85	0.42
49:9:928:G:H2'	49:9:929:G:C8	2.55	0.42
49:9:1232:U:H2'	49:9:1233:G:C8	2.55	0.42
49:9:1454:A:C8	67:RR:3:ARG:HD2	2.55	0.42
50:AA:164:ASN:O	50:AA:170:SER:OG	2.27	0.42
62:MM:42:LEU:HD13	62:MM:42:LEU:HA	1.78	0.42
73:XX:107:ARG:NH2	73:XX:111:ALA:O	2.52	0.42
1:4:6:G:H2'	1:4:7:A:C8	2.55	0.42
1:4:27:U:H3	1:4:43:A:H61	1.68	0.42
2:5:287:U:H2'	2:5:288:G:C8	2.55	0.42
2:5:373:OMG:HM21	2:5:1645:C:H4'	2.02	0.42
2:5:398:A2M:O5'	2:5:398:A2M:H8	2.20	0.42
2:5:1521:C:OP1	7:C:100:ARG:NH2	2.48	0.42
2:5:2306:G:O2'	2:5:2331:G:N1	2.49	0.42
2:5:4153:C:H2'	2:5:4154:G:C8	2.55	0.42
2:5:4274:A:H2'	2:5:4275:G:C8	2.54	0.42
2:5:4978:G:OP1	6:B:271:GLN:NE2	2.48	0.42
12:H:113:GLU:OE1	12:H:115:ARG:NH2	2.53	0.42
34:e:26:ASP:N	34:e:26:ASP:OD1	2.50	0.42
48:v:107:LEU:HA	48:v:148:GLN:HE21	1.84	0.42
49:9:1587:G:C5	69:TT:78:ILE:HD11	2.54	0.42
51:BB:138:PHE:O	51:BB:213:ARG:N	2.51	0.42
69:TT:113:VAL:HA	69:TT:123:LEU:HA	2.02	0.42
71:VV:21:ASN:HB3	72:WW:67:GLY:HA3	2.01	0.42
2:5:645:G:H2'	2:5:646:G:H8	1.85	0.41
2:5:1958:A:H5''	2:5:1962:A:H1'	2.02	0.41
2:5:2537:A:OP1	40:k:42:LEU:N	2.52	0.41
2:5:3607:U:H2'	2:5:3608:A:C8	2.55	0.41
2:5:3974:G:O6	2:5:4039:G:N1	2.53	0.41
18:O:22:ILE:HG23	22:S:166:ARG:HH11	1.85	0.41
21:R:96:MET:HE2	21:R:100:ARG:HH12	1.85	0.41
29:Z:41:ALA:HB2	29:Z:77:TYR:HE1	1.84	0.41
47:u:159:MET:HE1	47:u:163:LEU:HD13	2.02	0.41
47:u:183:ILE:HG12	47:u:206:ILE:HD11	2.02	0.41
49:9:170:A:OP1	56:GG:137:ARG:N	2.47	0.41
49:9:434:G:H2'	49:9:435:A:C8	2.55	0.41
49:9:652:U:H2'	49:9:653:A:H8	1.85	0.41
2:5:1812:C:H1'	31:b:57:MET:HE2	2.03	0.41
2:5:3870:C:H2'	2:5:3871:A:C8	2.55	0.41
2:5:4699:U:H1'	2:5:4700:A:H5''	2.02	0.41
2:5:5016:A:N6	2:5:5033:G:O2'	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:287:ILE:HG12	6:B:331:VAL:HG12	2.03	0.41
10:F:89:ALA:HB2	10:F:124:LEU:HD21	2.01	0.41
17:N:73:ARG:HG2	17:N:75:VAL:HG13	2.02	0.41
21:R:81:ARG:HG2	21:R:88:ARG:CZ	2.49	0.41
48:v:315:ASP:OD2	48:v:328:GLN:NE2	2.29	0.41
49:9:604:A:N3	49:9:639:C:O2'	2.53	0.41
49:9:1163:C:H2'	49:9:1164:G:H8	1.85	0.41
51:BB:123:ALA:HB2	51:BB:165:ARG:HB2	2.03	0.41
52:CC:196:ILE:HB	52:CC:223:TYR:HB2	2.01	0.41
54:EE:9:LEU:HB2	54:EE:30:ARG:HD3	2.03	0.41
60:KK:3:MET:HG2	60:KK:8:ARG:HB2	2.02	0.41
69:TT:13:GLU:HA	69:TT:16:ARG:HG2	2.02	0.41
82:gg:175:LYS:HD2	82:gg:184:LEU:HD13	2.02	0.41
2:5:679:C:H2'	2:5:680:G:C8	2.56	0.41
2:5:1427:A:OP2	2:5:1457:G:N2	2.40	0.41
2:5:2338:C:O2	7:C:245:HIS:NE2	2.41	0.41
2:5:4188:U:H2'	2:5:4189:U:C6	2.55	0.41
2:5:4935:C:H2'	2:5:4936:G:H8	1.85	0.41
6:B:33:PRO:HD2	6:B:44:THR:HB	2.02	0.41
9:E:152:ILE:HG21	9:E:273:TYR:HE2	1.86	0.41
10:F:158:TYR:HD2	10:F:165:ARG:HG2	1.85	0.41
10:F:178:LEU:HB3	10:F:183:ILE:HB	2.01	0.41
13:I:36:LEU:HD12	13:I:87:ILE:HD11	2.01	0.41
15:L:46:ILE:O	15:L:149:GLN:NE2	2.53	0.41
19:P:64:ASN:HB2	19:P:80:GLN:NE2	2.35	0.41
20:Q:59:PRO:HG3	20:Q:143:ARG:HA	2.02	0.41
22:S:7:LEU:HD23	22:S:107:THR:HA	2.02	0.41
34:e:90:MET:HG2	46:r:33:LYS:HA	2.02	0.41
49:9:67:C:H41	56:GG:163:ASN:HA	1.85	0.41
49:9:527:C:H2'	49:9:528:A:H8	1.85	0.41
49:9:1350:U:O2	50:AA:110:ASN:ND2	2.51	0.41
49:9:1801:A:H2'	49:9:1802:C:C6	2.54	0.41
59:JJ:136:ARG:HD3	59:JJ:160:SER:HA	2.02	0.41
60:KK:76:ILE:HD12	60:KK:76:ILE:HA	1.89	0.41
2:5:697:G:H2'	2:5:698:G:H8	1.85	0.41
2:5:947:C:OP1	7:C:336:ARG:NH2	2.43	0.41
2:5:1088:C:H2'	2:5:1089:G:C8	2.55	0.41
2:5:2326:G:H5''	34:e:127:ALA:HB1	2.02	0.41
2:5:2514:G:O2'	2:5:2743:A:N6	2.54	0.41
2:5:3928:A:H5'	17:N:89:VAL:HG13	2.01	0.41
6:B:226:LYS:HD2	6:B:272:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:358:LEU:HD23	7:C:361:LYS:HD2	2.01	0.41
12:H:128:MET:HG3	12:H:157:SER:HB2	2.02	0.41
15:L:205:GLN:HA	15:L:208:GLU:HG3	2.02	0.41
19:P:32:THR:HG23	19:P:91:LEU:HD21	2.01	0.41
30:a:100:ILE:HG12	30:a:123:ILE:HB	2.01	0.41
33:d:87:ARG:HH12	33:d:122:VAL:HG11	1.86	0.41
47:u:177:ASP:HA	47:u:180:VAL:HG22	2.02	0.41
49:9:145:G:OP1	56:GG:139:SER:OG	2.34	0.41
50:AA:184:ARG:HG2	50:AA:191:ARG:HG2	2.02	0.41
53:DD:210:ILE:HD13	67:RR:15:VAL:HG12	2.03	0.41
63:NN:37:ILE:HD11	63:NN:63:VAL:HG11	2.01	0.41
2:5:466:A:O2'	2:5:468:U:OP1	2.32	0.41
2:5:2052:G:O2'	2:5:2057:A:N1	2.52	0.41
2:5:2418:A:N1	2:5:2429:A:O2'	2.44	0.41
2:5:4494:OMG:HM21	25:V:22:VAL:HG21	2.03	0.41
18:O:84:VAL:HG11	18:O:102:LEU:HD22	2.03	0.41
35:f:77:ALA:HA	35:f:84:VAL:HG23	2.03	0.41
43:n:1:MET:HB2	49:9:1706:G:H5'	2.02	0.41
48:v:212:PHE:HA	48:v:215:SER:HB3	2.02	0.41
49:9:1643:U:H2'	49:9:1644:C:C6	2.55	0.41
59:JJ:88:ASP:OD1	59:JJ:88:ASP:N	2.52	0.41
65:PP:81:ARG:NH1	65:PP:97:TYR:O	2.45	0.41
2:5:23:C:H4'	39:j:59:THR:HG23	2.01	0.41
2:5:2804:OMC:HM23	2:5:2804:OMC:H1'	1.85	0.41
2:5:4128:A:H2	11:G:87:LYS:HE3	1.85	0.41
2:5:4991:U:H2'	2:5:4992:G:C8	2.55	0.41
7:C:339:THR:O	7:C:343:GLN:OE1	2.38	0.41
20:Q:128:LEU:HD23	20:Q:128:LEU:HA	1.91	0.41
26:W:3:VAL:HG12	26:W:12:LYS:HG2	2.02	0.41
29:Z:12:LEU:HB2	29:Z:81:MET:HB3	2.03	0.41
29:Z:17:ARG:NH2	29:Z:18:TYR:OH	2.54	0.41
34:e:44:ARG:HG3	34:e:49:PHE:CD2	2.55	0.41
51:BB:136:ARG:HB2	51:BB:216:LYS:HB3	2.02	0.41
53:DD:126:ILE:HD11	53:DD:134:CYS:SG	2.61	0.41
1:4:68:C:H2'	1:4:69:G:H8	1.86	0.41
2:5:510:U:OP2	30:a:85:GLN:NE2	2.47	0.41
2:5:2599:G:O2'	2:5:2746:A:N6	2.50	0.41
2:5:3867:A2M:HM'3	2:5:3867:A2M:H1'	1.90	0.41
2:5:4258:C:H5'	14:J:68:ILE:HD11	2.01	0.41
2:5:5006:U:H4'	2:5:5007:A:H5'	2.02	0.41
12:H:104:VAL:HG12	12:H:113:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:173:ARG:NH1	42:m:99:LYS:O	2.54	0.41
19:P:24:VAL:HG23	19:P:86:LYS:HG3	2.03	0.41
21:R:64:ARG:HH11	21:R:64:ARG:HD2	1.74	0.41
26:W:6:CYS:SG	26:W:7:SER:N	2.94	0.41
42:m:83:ASN:ND2	42:m:93:ASN:HA	2.36	0.41
48:v:411:SER:O	48:v:415:LYS:HD2	2.20	0.41
49:9:474:G:O2'	49:9:508:A:OP1	2.29	0.41
49:9:658:U:H1'	73:XX:17:ARG:HH21	1.85	0.41
49:9:1498:A:OP2	53:DD:27:ARG:NH1	2.53	0.41
50:AA:142:LEU:HA	50:AA:143:PRO:HD2	1.98	0.41
55:FF:42:LYS:HD3	55:FF:42:LYS:HA	1.94	0.41
1:4:60:U:H5''	1:4:61:C:H5	1.86	0.41
2:5:257:C:H2'	2:5:258:G:H8	1.86	0.41
2:5:318:A:H2'	2:5:319:A:H8	1.86	0.41
2:5:482:G:H1	2:5:672:C:H42	1.69	0.41
2:5:1338:G:H4'	2:5:1339:U:C6	2.56	0.41
2:5:4239:A:H2'	2:5:4240:G:H8	1.84	0.41
2:5:4274:A:H2'	2:5:4275:G:H8	1.84	0.41
5:A:113:VAL:HB	5:A:164:ALA:HB1	2.03	0.41
7:C:62:THR:HG21	7:C:91:ALA:HB1	2.03	0.41
7:C:209:VAL:HB	7:C:229:LEU:HD13	2.01	0.41
10:F:29:ILE:HD12	10:F:33:ARG:HH12	1.86	0.41
30:a:7:LYS:HE2	30:a:11:LEU:HD11	2.03	0.41
37:h:12:LYS:HE3	37:h:12:LYS:HB2	1.94	0.41
59:JJ:67:ASP:HB3	59:JJ:70:ARG:HB3	2.03	0.41
59:JJ:111:GLN:HE21	59:JJ:123:ILE:HG22	1.84	0.41
74:YY:82:ALA:O	74:YY:86:GLU:HB2	2.21	0.41
2:5:230:G:H2'	2:5:231:U:O4'	2.20	0.41
2:5:344:A:H5'	39:j:75:ARG:HH22	1.86	0.41
2:5:423:G:OP1	19:P:62:ARG:NH2	2.48	0.41
2:5:964:A:H2'	2:5:965:G:H8	1.86	0.41
2:5:1403:G:H2'	2:5:1404:G:C8	2.56	0.41
2:5:1403:G:H2'	2:5:1404:G:H8	1.86	0.41
2:5:1726:U:H5'	10:F:134:ILE:HD11	2.02	0.41
2:5:2519:U:O2'	2:5:2530:U:O2	2.30	0.41
2:5:3860:A:H2	19:P:131:ARG:HH22	1.69	0.41
2:5:3956:G:O6	2:5:3966:A:C6	2.72	0.41
3:7:75:G:N2	3:7:100:A:OP2	2.41	0.41
4:8:19:C:H2'	4:8:20:A:C8	2.56	0.41
6:B:44:THR:HG21	6:B:186:ASN:ND2	2.36	0.41
6:B:213:GLN:HE22	6:B:363:ILE:HB	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:40:ASP:HB2	8:D:43:LYS:HG2	2.02	0.41
9:E:164:ARG:O	9:E:185:ASN:ND2	2.54	0.41
11:G:218:GLU:OE1	17:N:11:TRP:NE1	2.54	0.41
12:H:30:PRO:HD2	12:H:85:THR:HA	2.03	0.41
13:I:49:CYS:HB2	13:I:172:GLY:HA2	2.03	0.41
14:J:36:ALA:HA	14:J:39:VAL:HG12	2.02	0.41
15:L:43:ALA:O	15:L:149:GLN:NE2	2.44	0.41
23:T:33:ILE:H	23:T:33:ILE:HG13	1.80	0.41
26:W:8:PHE:HB3	26:W:36:CYS:HB3	2.03	0.41
27:X:80:PRO:HG2	27:X:155:ILE:HG21	2.03	0.41
33:d:27:ILE:HB	33:d:84:ILE:HG22	2.03	0.41
40:k:57:LYS:HA	40:k:60:LEU:HD23	2.03	0.41
45:p:30:GLU:O	45:p:34:HIS:ND1	2.41	0.41
45:p:37:TYR:HB2	45:p:47:MET:HB2	2.03	0.41
47:u:149:ASP:HA	47:u:152:LYS:HG2	2.02	0.41
48:v:128:LYS:HD3	48:v:129:LYS:HG2	2.02	0.41
48:v:239:GLN:CD	48:v:365:ARG:HH12	2.28	0.41
49:9:919:A:H8	63:NN:64:ARG:HH12	1.68	0.41
49:9:1189:A:H2'	49:9:1190:A:C8	2.56	0.41
49:9:1551:U:OP1	53:DD:9:ARG:NH2	2.52	0.41
54:EE:107:GLY:HA2	54:EE:189:LEU:HD22	2.03	0.41
54:EE:122:LYS:HG2	54:EE:164:LEU:HD21	2.03	0.41
54:EE:184:THR:N	54:EE:224:ASN:O	2.50	0.41
54:EE:201:HIS:HB3	54:EE:204:SER:HB2	2.03	0.41
57:HH:144:ILE:HG23	72:WW:52:ILE:HG13	2.02	0.41
59:JJ:64:ASP:OD2	72:WW:117:ARG:NH1	2.54	0.41
73:XX:50:ILE:H	73:XX:50:ILE:HG13	1.69	0.41
76:aa:33:ASP:OD1	76:aa:33:ASP:N	2.54	0.41
82:gg:163:PRO:O	82:gg:179:LEU:N	2.45	0.41
2:5:1094:G:H2'	2:5:1095:A:C8	2.56	0.41
2:5:1436:C:H5''	2:5:1437:C:H5'	2.03	0.41
2:5:2389:A:H5'	33:d:70:LYS:HE2	2.02	0.41
2:5:4764:A:OP1	22:S:156:HIS:ND1	2.42	0.41
5:A:58:LEU:HD13	5:A:75:LEU:HD23	2.03	0.41
13:I:4:ARG:H	13:I:123:GLN:HE22	1.68	0.41
29:Z:121:ARG:HA	29:Z:124:THR:HG22	2.03	0.41
49:9:533:A:H2'	49:9:534:G:H8	1.86	0.41
49:9:1535:U:O3'	55:FF:88:MET:HE1	2.21	0.41
49:9:1597:C:H4'	49:9:1603:G:C6	2.56	0.41
50:AA:177:MET:HE3	50:AA:177:MET:HB2	1.55	0.41
54:EE:11:ARG:NH2	54:EE:24:THR:OG1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:KK:89:ILE:H	60:KK:89:ILE:HG13	1.58	0.41
2:5:4860:G:H2'	2:5:4861:G:H8	1.86	0.40
3:7:92:C:H2'	3:7:93:G:C8	2.56	0.40
4:8:39:G:H1'	4:8:103:A:N6	2.36	0.40
34:e:38:PRO:HB2	34:e:43:ASN:ND2	2.36	0.40
51:BB:77:ASP:OD1	51:BB:77:ASP:N	2.54	0.40
61:LL:85:THR:HA	61:LL:113:LEU:H	1.86	0.40
66:QQ:58:LEU:HD11	66:QQ:112:LEU:HD11	2.03	0.40
2:5:504:G:H2'	2:5:505:G:H8	1.86	0.40
2:5:651:C:H2'	2:5:652:G:C8	2.56	0.40
2:5:1617:G:H1'	2:5:2513:A:N6	2.36	0.40
2:5:1725:U:H2'	2:5:1726:U:C6	2.56	0.40
2:5:3709:U:H2'	2:5:3710:G:C8	2.57	0.40
2:5:4084:G:O6	5:A:70:LYS:NZ	2.47	0.40
2:5:4088:C:H2'	2:5:4089:G:H8	1.86	0.40
2:5:4578:G:H2'	2:5:4579:U:C6	2.56	0.40
2:5:4620:OMU:HM23	2:5:4620:OMU:H1'	1.75	0.40
2:5:4685:U:H2'	2:5:4686:G:C8	2.56	0.40
5:A:30:ARG:NH1	5:A:36:GLU:OE1	2.54	0.40
13:I:140:THR:HG21	13:I:148:VAL:HG21	2.03	0.40
14:J:95:ARG:NH2	14:J:177:GLY:O	2.44	0.40
49:9:453:C:O2'	56:GG:92:ARG:O	2.35	0.40
49:9:926:A:OP1	63:NN:94:LYS:NZ	2.51	0.40
49:9:932:G:O2'	49:9:934:G:OP2	2.34	0.40
49:9:934:G:H1	49:9:1008:A:H2	1.67	0.40
56:GG:34:THR:O	56:GG:51:ARG:HA	2.21	0.40
57:HH:10:LYS:HE2	57:HH:16:PRO:HA	2.03	0.40
57:HH:133:LEU:HD23	57:HH:133:LEU:HA	1.93	0.40
58:II:133:GLU:HA	58:II:136:ILE:HG22	2.03	0.40
61:LL:77:VAL:O	61:LL:123:GLY:N	2.48	0.40
2:5:156:G:N2	2:5:157:U:O4	2.54	0.40
2:5:487:G:H2'	2:5:488:G:H8	1.87	0.40
2:5:3598:C:H2'	2:5:3599:A:C8	2.57	0.40
2:5:3950:U:H2'	2:5:3951:G:C8	2.56	0.40
6:B:378:ARG:HH11	26:W:11:TYR:HE2	1.69	0.40
19:P:94:MET:HE3	19:P:94:MET:HB2	1.92	0.40
42:m:68:MET:HG2	42:m:79:PRO:HA	2.03	0.40
48:v:108:LEU:HB3	48:v:111:PHE:HB3	2.02	0.40
49:9:380:G:H1'	58:II:5:ARG:NH1	2.36	0.40
49:9:696:G:H2'	49:9:697:G:C8	2.57	0.40
49:9:1599:U:C2	55:FF:166:ILE:HG13	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:GG:70:HIS:CE1	56:GG:103:ASP:HB2	2.56	0.40
68:SS:28:PHE:HE1	68:SS:38:ARG:HH11	1.69	0.40
68:SS:75:ARG:HH11	68:SS:95:TYR:HB2	1.87	0.40
2:5:365:U:H2'	2:5:366:A:H8	1.85	0.40
2:5:1846:G:H2'	2:5:1847:C:C6	2.57	0.40
2:5:3900:G:OP1	2:5:3901:A:O2'	2.31	0.40
2:5:3932:U:H2'	2:5:3933:G:C8	2.56	0.40
2:5:4966:A:H5''	6:B:126:LYS:HE3	2.03	0.40
10:F:156:ARG:HA	10:F:156:ARG:HD3	1.97	0.40
14:J:144:LYS:O	14:J:148:THR:OG1	2.38	0.40
20:Q:63:LEU:O	20:Q:67:ILE:HG12	2.22	0.40
37:h:47:ILE:HD13	37:h:47:ILE:HG21	1.92	0.40
38:i:64:SER:HB2	47:u:39:LYS:HD2	2.03	0.40
46:r:18:ILE:HG23	46:r:25:TYR:HB2	2.02	0.40
49:9:476:A:N3	49:9:488:U:O2'	2.43	0.40
49:9:872:A:N1	49:9:914:U:O4	2.55	0.40
49:9:872:A:N1	49:9:914:U:C4	2.89	0.40
49:9:1051:G:H2'	49:9:1052:A:H8	1.87	0.40
51:BB:166:LYS:HB3	51:BB:166:LYS:HE2	1.87	0.40
62:MM:31:LEU:HD13	62:MM:33:ARG:HB2	2.02	0.40
70:UU:55:ARG:HE	70:UU:87:ARG:CZ	2.35	0.40
2:5:692:A:H2'	2:5:693:C:H6	1.85	0.40
2:5:1338:G:H4'	2:5:1339:U:H6	1.87	0.40
2:5:2613:C:OP1	36:g:24:ARG:NH2	2.54	0.40
2:5:3617:G:O2'	2:5:3620:G:N7	2.50	0.40
6:B:384:GLU:OE2	26:W:14:TYR:OH	2.36	0.40
7:C:336:ARG:HA	7:C:339:THR:HG22	2.03	0.40
8:D:41:LYS:NZ	23:T:32:ARG:O	2.43	0.40
25:V:99:GLU:HB3	26:W:24:THR:HG23	2.03	0.40
43:n:12:ARG:NH2	49:9:1848:U:O4	2.54	0.40
49:9:218:U:O2	58:II:184:ARG:NH2	2.54	0.40
49:9:220:U:H2'	49:9:221:A:C8	2.57	0.40
49:9:656:G:N2	49:9:663:C:H5''	2.36	0.40
50:AA:128:ARG:NH1	50:AA:151:ASP:O	2.50	0.40
53:DD:6:SER:O	53:DD:10:LYS:HB2	2.22	0.40
60:KK:32:HIS:CE1	60:KK:45:VAL:HG11	2.57	0.40
73:XX:107:ARG:HD3	73:XX:107:ARG:HH21	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	246/248 (99%)	218 (89%)	28 (11%)	0	100	100
6	B	392/394 (100%)	364 (93%)	27 (7%)	1 (0%)	36	65
7	C	359/362 (99%)	343 (96%)	16 (4%)	0	100	100
8	D	291/293 (99%)	277 (95%)	14 (5%)	0	100	100
9	E	208/291 (72%)	193 (93%)	15 (7%)	0	100	100
10	F	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
11	G	229/319 (72%)	221 (96%)	8 (4%)	0	100	100
12	H	188/190 (99%)	179 (95%)	9 (5%)	0	100	100
13	I	201/214 (94%)	194 (96%)	7 (4%)	0	100	100
14	J	168/170 (99%)	166 (99%)	2 (1%)	0	100	100
15	L	208/210 (99%)	200 (96%)	7 (3%)	1 (0%)	24	54
16	M	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
17	N	201/203 (99%)	186 (92%)	15 (8%)	0	100	100
18	O	197/199 (99%)	193 (98%)	4 (2%)	0	100	100
19	P	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
20	Q	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
21	R	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
22	S	174/176 (99%)	164 (94%)	9 (5%)	1 (1%)	21	50
23	T	157/159 (99%)	148 (94%)	9 (6%)	0	100	100
24	U	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
25	V	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
26	W	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
27	X	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
28	Y	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
29	Z	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	a	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
31	b	100/245 (41%)	93 (93%)	7 (7%)	0	100	100
32	c	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
33	d	105/107 (98%)	95 (90%)	9 (9%)	1 (1%)	12	40
34	e	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
35	f	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
36	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
37	h	120/122 (98%)	120 (100%)	0	0	100	100
38	i	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
39	j	84/86 (98%)	75 (89%)	9 (11%)	0	100	100
40	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
41	l	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
42	m	49/52 (94%)	43 (88%)	5 (10%)	1 (2%)	6	25
43	n	23/25 (92%)	23 (100%)	0	0	100	100
44	o	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
45	p	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
46	r	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
47	u	204/206 (99%)	173 (85%)	29 (14%)	2 (1%)	12	40
48	v	348/441 (79%)	320 (92%)	28 (8%)	0	100	100
50	AA	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
51	BB	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
52	CC	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
53	DD	226/228 (99%)	217 (96%)	9 (4%)	0	100	100
54	EE	260/262 (99%)	243 (94%)	17 (6%)	0	100	100
55	FF	181/204 (89%)	172 (95%)	9 (5%)	0	100	100
56	GG	235/237 (99%)	226 (96%)	9 (4%)	0	100	100
57	HH	181/194 (93%)	172 (95%)	9 (5%)	0	100	100
58	II	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
59	JJ	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
60	KK	94/96 (98%)	86 (92%)	8 (8%)	0	100	100
61	LL	139/158 (88%)	132 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	MM	115/117 (98%)	102 (89%)	13 (11%)	0	100	100
63	NN	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
64	OO	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
65	PP	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
66	QQ	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
67	RR	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
68	SS	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
69	TT	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
70	UU	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
71	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
72	WW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
73	XX	139/141 (99%)	130 (94%)	7 (5%)	2 (1%)	9	31
74	YY	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
75	ZZ	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
76	aa	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
77	bb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
78	cc	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
79	dd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
80	ee	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
81	ff	66/68 (97%)	58 (88%)	8 (12%)	0	100	100
82	gg	311/313 (99%)	279 (90%)	32 (10%)	0	100	100
All	All	11723/12395 (95%)	11060 (94%)	653 (6%)	10 (0%)	49	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	m	73	CYS
6	B	295	ASP
33	d	96	GLU
47	u	61	PRO
47	u	198	TRP
73	XX	62	PRO
22	S	166	ARG
73	XX	61	GLN
29	Z	90	PRO

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Mol	Chain	Res	Type
15	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	
5	A	190/190 (100%)	188 (99%)	2 (1%)	65	74
6	B	342/342 (100%)	340 (99%)	2 (1%)	78	80
7	C	301/301 (100%)	299 (99%)	2 (1%)	76	78
8	D	247/247 (100%)	246 (100%)	1 (0%)	84	83
9	E	190/251 (76%)	186 (98%)	4 (2%)	47	64
10	F	196/196 (100%)	194 (99%)	2 (1%)	68	75
11	G	200/272 (74%)	199 (100%)	1 (0%)	81	81
12	H	169/169 (100%)	168 (99%)	1 (1%)	78	80
13	I	175/181 (97%)	172 (98%)	3 (2%)	53	67
14	J	143/143 (100%)	143 (100%)	0	100	100
15	L	175/175 (100%)	173 (99%)	2 (1%)	65	74
16	M	117/117 (100%)	117 (100%)	0	100	100
17	N	171/171 (100%)	169 (99%)	2 (1%)	63	72
18	O	171/171 (100%)	170 (99%)	1 (1%)	78	80
19	P	134/134 (100%)	133 (99%)	1 (1%)	76	78
20	Q	164/164 (100%)	164 (100%)	0	100	100
21	R	159/159 (100%)	159 (100%)	0	100	100
22	S	157/157 (100%)	155 (99%)	2 (1%)	61	71
23	T	139/139 (100%)	138 (99%)	1 (1%)	76	78
24	U	89/89 (100%)	89 (100%)	0	100	100
25	V	101/101 (100%)	101 (100%)	0	100	100
26	W	86/126 (68%)	86 (100%)	0	100	100
27	X	106/106 (100%)	105 (99%)	1 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	Y	124/124 (100%)	123 (99%)	1 (1%)	73	77
29	Z	117/117 (100%)	116 (99%)	1 (1%)	70	76
30	a	119/119 (100%)	119 (100%)	0	100	100
31	b	84/184 (46%)	84 (100%)	0	100	100
32	c	84/84 (100%)	83 (99%)	1 (1%)	63	72
33	d	98/98 (100%)	98 (100%)	0	100	100
34	e	114/114 (100%)	113 (99%)	1 (1%)	70	76
35	f	88/88 (100%)	88 (100%)	0	100	100
36	g	98/98 (100%)	95 (97%)	3 (3%)	35	59
37	h	109/109 (100%)	109 (100%)	0	100	100
38	i	86/86 (100%)	85 (99%)	1 (1%)	63	72
39	j	73/73 (100%)	72 (99%)	1 (1%)	59	70
40	k	64/64 (100%)	63 (98%)	1 (2%)	55	68
41	l	47/47 (100%)	46 (98%)	1 (2%)	47	64
42	m	47/47 (100%)	47 (100%)	0	100	100
43	n	24/24 (100%)	24 (100%)	0	100	100
44	o	91/91 (100%)	91 (100%)	0	100	100
45	p	74/74 (100%)	74 (100%)	0	100	100
46	r	108/108 (100%)	107 (99%)	1 (1%)	70	76
47	u	186/186 (100%)	183 (98%)	3 (2%)	55	68
48	v	289/355 (81%)	284 (98%)	5 (2%)	53	67
50	AA	180/181 (99%)	179 (99%)	1 (1%)	78	80
51	BB	194/194 (100%)	192 (99%)	2 (1%)	68	75
52	CC	187/187 (100%)	181 (97%)	6 (3%)	34	58
53	DD	190/190 (100%)	189 (100%)	1 (0%)	81	81
54	EE	224/224 (100%)	223 (100%)	1 (0%)	84	83
55	FF	158/170 (93%)	156 (99%)	2 (1%)	61	71
56	GG	207/207 (100%)	206 (100%)	1 (0%)	81	81
57	HH	165/174 (95%)	161 (98%)	4 (2%)	43	62
58	II	178/178 (100%)	177 (99%)	1 (1%)	78	80
59	JJ	161/161 (100%)	161 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	KK	87/87 (100%)	86 (99%)	1 (1%)	65	74
61	LL	130/142 (92%)	129 (99%)	1 (1%)	73	77
62	MM	99/99 (100%)	98 (99%)	1 (1%)	68	75
63	NN	130/130 (100%)	130 (100%)	0	100	100
64	OO	106/106 (100%)	106 (100%)	0	100	100
65	PP	109/109 (100%)	108 (99%)	1 (1%)	70	76
66	QQ	117/117 (100%)	116 (99%)	1 (1%)	70	76
67	RR	119/119 (100%)	119 (100%)	0	100	100
68	SS	125/125 (100%)	125 (100%)	0	100	100
69	TT	111/111 (100%)	109 (98%)	2 (2%)	51	67
70	UU	92/92 (100%)	89 (97%)	3 (3%)	33	57
71	VV	67/67 (100%)	65 (97%)	2 (3%)	36	59
72	WW	112/112 (100%)	110 (98%)	2 (2%)	51	67
73	XX	113/113 (100%)	112 (99%)	1 (1%)	70	76
74	YY	107/107 (100%)	106 (99%)	1 (1%)	70	76
75	ZZ	66/66 (100%)	66 (100%)	0	100	100
76	aa	88/88 (100%)	88 (100%)	0	100	100
77	bb	75/75 (100%)	75 (100%)	0	100	100
78	cc	55/55 (100%)	54 (98%)	1 (2%)	51	67
79	dd	48/48 (100%)	48 (100%)	0	100	100
80	ee	46/46 (100%)	46 (100%)	0	100	100
81	ff	61/61 (100%)	61 (100%)	0	100	100
82	gg	272/272 (100%)	269 (99%)	3 (1%)	65	74
All	All	10225/10604 (96%)	10138 (99%)	87 (1%)	68	76

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	101	VAL
5	A	242	ARG
6	B	17	LEU
6	B	262	VAL
7	C	57	LEU
7	C	150	LEU

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Mol	Chain	Res	Type
8	D	74	ILE
9	E	51	VAL
9	E	165	VAL
9	E	178	VAL
9	E	215	LEU
10	F	88	LEU
10	F	124	LEU
11	G	122	ILE
12	H	161	ILE
13	I	48	LEU
13	I	126	VAL
13	I	191	ILE
15	L	58	ILE
15	L	59	VAL
17	N	64	ILE
17	N	89	VAL
18	O	22	ILE
19	P	64	ASN
22	S	75	VAL
22	S	168	THR
23	T	96	ILE
27	X	40	ILE
28	Y	79	VAL
29	Z	53	VAL
32	c	65	MET
34	e	13	VAL
36	g	5	LEU
36	g	15	THR
36	g	59	VAL
38	i	29	ARG
39	j	36	LYS
40	k	47	ILE
41	l	33	ASN
46	r	106	LEU
47	u	12	GLU
47	u	80	VAL
47	u	183	ILE
48	v	77	LEU
48	v	113	LEU
48	v	165	LEU
48	v	244	LEU
48	v	387	LEU

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Mol	Chain	Res	Type
50	AA	186	ARG
51	BB	87	ILE
51	BB	207	LEU
52	CC	66	LEU
52	CC	137	VAL
52	CC	205	VAL
52	CC	209	VAL
52	CC	212	LYS
52	CC	248	TYR
53	DD	158	ILE
54	EE	246	LEU
55	FF	102	LEU
55	FF	178	ILE
56	GG	101	ILE
57	HH	28	LEU
57	HH	29	GLU
57	HH	83	LEU
57	HH	144	ILE
58	II	104	ILE
60	KK	89	ILE
61	LL	96	ILE
62	MM	42	LEU
65	PP	76	VAL
66	QQ	93	VAL
69	TT	78	ILE
69	TT	113	VAL
70	UU	48	LEU
70	UU	54	VAL
70	UU	106	ILE
71	VV	9	VAL
71	VV	13	VAL
72	WW	7	LEU
72	WW	104	LEU
73	XX	50	ILE
74	YY	17	LEU
78	cc	17	VAL
82	gg	108	VAL
82	gg	198	VAL
82	gg	267	VAL

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

Mol	Chain	Res	Type
5	A	22	HIS
5	A	162	ASN
7	C	38	ASN
7	C	50	GLN
8	D	122	GLN
8	D	138	GLN
8	D	202	GLN
11	G	134	ASN
11	G	259	GLN
13	I	166	HIS
13	I	177	ASN
14	J	46	GLN
14	J	97	ASN
15	L	19	GLN
17	N	32	GLN
17	N	149	GLN
18	O	50	ASN
18	O	180	GLN
19	P	64	ASN
19	P	97	ASN
20	Q	7	HIS
21	R	39	GLN
21	R	141	HIS
22	S	37	HIS
23	T	139	HIS
25	V	27	ASN
26	W	30	GLN
28	Y	65	GLN
29	Z	78	ASN
30	a	44	ASN
30	a	120	GLN
31	b	12	GLN
31	b	19	ASN
32	c	19	GLN
33	d	30	HIS
33	d	34	HIS
34	e	52	GLN
34	e	107	ASN
35	f	56	ASN
38	i	80	HIS
39	j	76	HIS
41	l	25	GLN
43	n	22	GLN

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Mol	Chain	Res	Type
44	o	3	ASN
44	o	90	HIS
47	u	73	HIS
48	v	148	GLN
48	v	252	HIS
48	v	381	HIS
48	v	384	ASN
50	AA	9	GLN
51	BB	43	ASN
51	BB	202	GLN
53	DD	74	GLN
53	DD	159	HIS
54	EE	36	HIS
54	EE	138	HIS
55	FF	74	ASN
55	FF	79	HIS
55	FF	82	ASN
56	GG	177	GLN
57	HH	91	HIS
57	HH	126	HIS
57	HH	157	HIS
57	HH	186	ASN
58	II	168	GLN
60	KK	32	HIS
60	KK	77	GLN
64	OO	113	GLN
66	QQ	48	GLN
66	QQ	77	HIS
66	QQ	80	GLN
67	RR	31	ASN
72	WW	24	GLN
73	XX	31	HIS
73	XX	61	GLN
75	ZZ	112	ASN
79	dd	3	HIS
81	ff	135	HIS
82	gg	4	GLN
82	gg	215	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	4	74/75 (98%)	35 (47%)	1 (1%)
2	5	3558/3597 (98%)	899 (25%)	68 (1%)
3	7	119/120 (99%)	14 (11%)	0
4	8	149/151 (98%)	27 (18%)	1 (0%)
49	9	1682/1698 (99%)	391 (23%)	20 (1%)
All	All	5582/5641 (98%)	1366 (24%)	90 (1%)

All (1366) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	4	2	C
1	4	3	C
1	4	4	C
1	4	8	U
1	4	9	A
1	4	10	G
1	4	13	C
1	4	14	A
1	4	15	G
1	4	16	C
1	4	18	U
1	4	19	G
1	4	20	U
1	4	21	A
1	4	24	G
1	4	33	U
1	4	34	U
1	4	36	U
1	4	37	A
1	4	39	U
1	4	42	G
1	4	43	A
1	4	47	U
1	4	48	C
1	4	49	C
1	4	57	A
1	4	58	A
1	4	59	G
1	4	60	U
1	4	62	C
1	4	66	U
1	4	68	C
1	4	70	G

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Mol	Chain	Res	Type
1	4	71	G
1	4	73	G
2	5	8	U
2	5	12	A
2	5	13	U
2	5	17	A
2	5	25	A
2	5	35	U
2	5	36	U
2	5	39	A
2	5	42	A
2	5	43	U
2	5	48	G
2	5	49	U
2	5	56	A
2	5	58	G
2	5	59	A
2	5	64	A
2	5	65	A
2	5	71	C
2	5	72	C
2	5	73	A
2	5	76	A
2	5	84	A
2	5	91	G
2	5	93	G
2	5	98	A
2	5	102	G
2	5	104	G
2	5	108	A
2	5	109	G
2	5	110	C
2	5	116	G
2	5	119	G
2	5	120	A
2	5	122	U
2	5	126	C
2	5	134	G
2	5	135	G
2	5	136	C
2	5	142	G
2	5	146	G

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Mol	Chain	Res	Type
2	5	151	G
2	5	157	U
2	5	159	C
2	5	167	C
2	5	170	C
2	5	172	C
2	5	173	C
2	5	182	G
2	5	200	U
2	5	201	C
2	5	202	C
2	5	203	U
2	5	205	C
2	5	209	U
2	5	216	C
2	5	218	A
2	5	220	C
2	5	224	U
2	5	233	U
2	5	234	G
2	5	237	B9B
2	5	245	C
2	5	246	G
2	5	256	G
2	5	264	C
2	5	265	C
2	5	266	C
2	5	267	G
2	5	275	C
2	5	276	C
2	5	280	G
2	5	297	U
2	5	306	A
2	5	309	C
2	5	310	G
2	5	315	G
2	5	316	U
2	5	326	C
2	5	334	A
2	5	340	C
2	5	345	C
2	5	349	A

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Mol	Chain	Res	Type
2	5	350	C
2	5	363	A
2	5	379	G
2	5	386	A
2	5	387	G
2	5	398	A2M
2	5	401	G
2	5	406	C
2	5	407	A
2	5	409	G
2	5	410	A
2	5	412	G
2	5	413	G
2	5	414	C
2	5	431	G
2	5	433	A
2	5	440	U
2	5	446	C
2	5	449	C
2	5	450	G
2	5	452	A
2	5	453	G
2	5	454	U
2	5	455	C
2	5	463	A
2	5	467	U
2	5	468	U
2	5	482	G
2	5	483	G
2	5	484	U
2	5	486	C
2	5	489	C
2	5	492	U
2	5	493	G
2	5	496	G
2	5	497	G
2	5	498	C
2	5	499	G
2	5	505	G
2	5	510	U
2	5	522	C
2	5	641	G

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Mol	Chain	Res	Type
2	5	667	A
2	5	669	C
2	5	680	G
2	5	682	G
2	5	684	G
2	5	685	C
2	5	686	A
2	5	691	C
2	5	696	C
2	5	697	G
2	5	704	C
2	5	705	G
2	5	708	G
2	5	719	C
2	5	722	G
2	5	729	2MG
2	5	731	G
2	5	746	A
2	5	747	A
2	5	748	G
2	5	749	G
2	5	758	G
2	5	759	G
2	5	908	G
2	5	913	U
2	5	914	U
2	5	915	A
2	5	917	A
2	5	918	G
2	5	925	C
2	5	926	G
2	5	929	A
2	5	931	C
2	5	932	A
2	5	933	G
2	5	934	C
2	5	938	C
2	5	939	G
2	5	941	C
2	5	943	A
2	5	944	A
2	5	945	U

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Mol	Chain	Res	Type
2	5	956	A
2	5	959	G
2	5	960	A
2	5	961	G
2	5	964	A
2	5	965	G
2	5	966	A
2	5	967	C
2	5	968	C
2	5	969	C
2	5	970	G
2	5	971(A)	G
2	5	972	C
2	5	980	C
2	5	983	U
2	5	1072	C
2	5	1073	G
2	5	1078	A
2	5	1079	C
2	5	1080	C
2	5	1081	C
2	5	1083	U
2	5	1085	C
2	5	1098	G
2	5	1174	G
2	5	1175	A
2	5	1179	U
2	5	1180	C
2	5	1187	G
2	5	1193	C
2	5	1195	G
2	5	1204	C
2	5	1210	C
2	5	1211	G
2	5	1212	G
2	5	1215	C
2	5	1234	G
2	5	1235	G
2	5	1236	C
2	5	1237	C
2	5	1238	A
2	5	1239	C

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Mol	Chain	Res	Type
2	5	1272	C
2	5	1273	G
2	5	1275	G
2	5	1276	C
2	5	1284	G
2	5	1287	G
2	5	1292	C
2	5	1293	G
2	5	1296	G
2	5	1301	C
2	5	1303	A
2	5	1304	C
2	5	1314	C
2	5	1319	U
2	5	1326	A2M
2	5	1330	A
2	5	1337	A
2	5	1354	A
2	5	1358	G
2	5	1359	G
2	5	1370	G
2	5	1371	A
2	5	1372	A
2	5	1377	G
2	5	1378	C
2	5	1379	C
2	5	1381	U
2	5	1387	A
2	5	1394	G
2	5	1397	A
2	5	1398	A
2	5	1406(C)	G
2	5	1412	G
2	5	1415	G
2	5	1419	G
2	5	1420	A
2	5	1421	G
2	5	1429	C
2	5	1436	C
2	5	1437	C
2	5	1438	U
2	5	1441	C

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Mol	Chain	Res	Type
2	5	1443	A
2	5	1445	U
2	5	1446	C
2	5	1448	G
2	5	1455	G
2	5	1456	B8Q
2	5	1457	G
2	5	1458	C
2	5	1462	A
2	5	1475	G
2	5	1477	C
2	5	1482	G
2	5	1483	C
2	5	1490	G
2	5	1493	G
2	5	1497	A
2	5	1498	G
2	5	1501	C
2	5	1502	G
2	5	1514	U
2	5	1516	G
2	5	1518	A
2	5	1523	A
2	5	1534	A2M
2	5	1535	C
2	5	1546	C
2	5	1547	A
2	5	1549	G
2	5	1563	A
2	5	1566	C
2	5	1574	B9B
2	5	1578	U
2	5	1582	PSU
2	5	1583	A
2	5	1591	U
2	5	1596	U
2	5	1602	U
2	5	1609	U
2	5	1612	G
2	5	1613	A
2	5	1624	G
2	5	1625	OMG

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Mol	Chain	Res	Type
2	5	1626	G
2	5	1631	A
2	5	1633	G
2	5	1634	A
2	5	1638	A
2	5	1640	C
2	5	1641	G
2	5	1649	U
2	5	1650	A
2	5	1654	G
2	5	1658	G
2	5	1661	C
2	5	1671	U
2	5	1676	C
2	5	1677	PSU
2	5	1678	C
2	5	1679	A
2	5	1691	G
2	5	1726	U
2	5	1734	G
2	5	1741	G
2	5	1742	A
2	5	1748	U
2	5	1750	G
2	5	1751	A
2	5	1753	G
2	5	1755	C
2	5	1756	U
2	5	1757	U
2	5	1761	G
2	5	1768	C
2	5	1772	C
2	5	1773	U
2	5	1774	C
2	5	1776	A
2	5	1777	C
2	5	1781	U
2	5	1787	A
2	5	1797	E7G
2	5	1803	G
2	5	1804	A
2	5	1805	A

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Mol	Chain	Res	Type
2	5	1806	G
2	5	1819	G
2	5	1821	G
2	5	1822	U
2	5	1828	C
2	5	1833	G
2	5	1835	G
2	5	1836	G
2	5	1837	A
2	5	1840	G
2	5	1842	G
2	5	1843	A
2	5	1848	C
2	5	1850	A
2	5	1855	G
2	5	1869	G
2	5	1881	C
2	5	1888	A
2	5	1897	A
2	5	1898	C
2	5	1918	U
2	5	1920	C
2	5	1921	C
2	5	1922	G
2	5	1923	A
2	5	1930	U
2	5	1931	C
2	5	1932	A
2	5	1935	C
2	5	1938	C
2	5	1940	G
2	5	1951	G
2	5	1956	A
2	5	1957	U
2	5	1958	A
2	5	1960	A
2	5	1961	G
2	5	1962	A
2	5	1964	A
2	5	1967	A
2	5	1971	U
2	5	1972	G

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Mol	Chain	Res	Type
2	5	1974	U
2	5	1975	G
2	5	1978	C
2	5	1980	U
2	5	1983	A
2	5	1984	A
2	5	1987	C
2	5	1991	A
2	5	1992	U
2	5	1993	C
2	5	1996	C
2	5	1997	U
2	5	1999	A
2	5	2001	G
2	5	2002	A
2	5	2003	G
2	5	2004	U
2	5	2007	G
2	5	2008	U
2	5	2011	C
2	5	2022	C
2	5	2025	A
2	5	2026	A
2	5	2029	A
2	5	2030	A
2	5	2033	A
2	5	2046	G
2	5	2047	A
2	5	2048	U
2	5	2052	G
2	5	2055	G
2	5	2056	G
2	5	2062	C
2	5	2064	G
2	5	2068	C
2	5	2069	A
2	5	2070	U
2	5	2084	U
2	5	2085	G
2	5	2090	U
2	5	2092	G
2	5	2093	G

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Mol	Chain	Res	Type
2	5	2094	C
2	5	2097	A
2	5	2098	G
2	5	2099	C
2	5	2100	G
2	5	2102	G
2	5	2104	A
2	5	2105	A
2	5	2106	G
2	5	2108	G
2	5	2259	G
2	5	2260	C
2	5	2267	U
2	5	2268	A
2	5	2269	C
2	5	2270	G
2	5	2275	G
2	5	2289	C
2	5	2294	G
2	5	2300	A
2	5	2301	G
2	5	2307	A
2	5	2313	A
2	5	2314	G
2	5	2316	G
2	5	2319	C
2	5	2333	G
2	5	2335	C
2	5	2347	A
2	5	2348	G
2	5	2351	C
2	5	2355	G
2	5	2357	G
2	5	2360	A
2	5	2364	OMG
2	5	2365	OMC
2	5	2380	B8W
2	5	2395	A
2	5	2396	A
2	5	2408	U
2	5	2410	C
2	5	2417	A

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Mol	Chain	Res	Type
2	5	2422	OMC
2	5	2424	OMG
2	5	2425	U
2	5	2433	G
2	5	2441	C
2	5	2447	U
2	5	2450	G
2	5	2453	A
2	5	2471	G
2	5	2475	G
2	5	2487	G
2	5	2488	C
2	5	2489	C
2	5	2490	U
2	5	2491	C
2	5	2495	U
2	5	2503	G
2	5	2504	C
2	5	2505	C
2	5	2506	G
2	5	2513	A
2	5	2520	C
2	5	2529	A
2	5	2530	U
2	5	2537	A
2	5	2544	G
2	5	2546	G
2	5	2547	G
2	5	2553	A
2	5	2554	U
2	5	2560	C
2	5	2566	G
2	5	2568	C
2	5	2570	U
2	5	2571	C
2	5	2572	C
2	5	2575	U
2	5	2583	C
2	5	2586	G
2	5	2587	A
2	5	2588	C
2	5	2589	C

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Mol	Chain	Res	Type
2	5	2600	A
2	5	2601	A
2	5	2611	A
2	5	2616	C
2	5	2618	G
2	5	2620	G
2	5	2627	C
2	5	2638	G
2	5	2639	U
2	5	2649	G
2	5	2653	C
2	5	2661	U
2	5	2662	G
2	5	2663	G
2	5	2668	G
2	5	2669	C
2	5	2670	C
2	5	2673	G
2	5	2676	A
2	5	2680	G
2	5	2686	G
2	5	2687	U
2	5	2695	A
2	5	2696	A
2	5	2707	U
2	5	2708	U
2	5	2709	C
2	5	2710	C
2	5	2711	G
2	5	2714	G
2	5	2715	G
2	5	2716	C
2	5	2724	G
2	5	2725	A
2	5	2726	G
2	5	2740	U
2	5	2741	U
2	5	2744	A
2	5	2754	B9B
2	5	2763	U
2	5	2764	A
2	5	2769	U

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Mol	Chain	Res	Type
2	5	2787	A
2	5	2788	U
2	5	2789	A
2	5	2790	U
2	5	2794	C
2	5	2798	A
2	5	2803	U
2	5	2814	C
2	5	2826	U
2	5	2827	G
2	5	2829	U
2	5	2837	U
2	5	2838	G
2	5	2842	G
2	5	2855	G
2	5	2856	C
2	5	2867	C
2	5	2875	C
2	5	2879	A
2	5	2884	G
2	5	2892	C
2	5	3598	C
2	5	3603	G
2	5	3604	A
2	5	3605	C
2	5	3606	U
2	5	3625	G
2	5	3626	G
2	5	3635	A
2	5	3646	A
2	5	3650	C
2	5	3657	U
2	5	3662	A
2	5	3664	G
2	5	3673	C
2	5	3679	U
2	5	3680	U
2	5	3689	G
2	5	3691	G
2	5	3692	A
2	5	3698	G
2	5	3711	A

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Mol	Chain	Res	Type
2	5	3712	A
2	5	3714	G
2	5	3729	PSU
2	5	3740	G
2	5	3753	G
2	5	3756	A
2	5	3759	A
2	5	3762	B8H
2	5	3763	A
2	5	3764	PSU
2	5	3766	A
2	5	3773	U
2	5	3774	A
2	5	3776	G
2	5	3777	G
2	5	3784	A
2	5	3785	A2M
2	5	3786	U
2	5	3787	G
2	5	3790	U
2	5	3792	OMG
2	5	3802	U
2	5	3810	C
2	5	3811	G
2	5	3812	C
2	5	3813	A
2	5	3814	U
2	5	3817	A
2	5	3819	G
2	5	3824	A
2	5	3838	U
2	5	3839	G
2	5	3840	U
2	5	3867	A2M
2	5	3876	A
2	5	3877	A
2	5	3878	C
2	5	3879	G
2	5	3889	G
2	5	3892	U
2	5	3897	B8K
2	5	3898	G

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Mol	Chain	Res	Type
2	5	3899	BGH
2	5	3901	A
2	5	3902	A
2	5	3904	G
2	5	3905	A
2	5	3906	A
2	5	3907	G
2	5	3908	A
2	5	3915	U
2	5	3916	G
2	5	3927	U
2	5	3938	G
2	5	3939	G
2	5	3946	G
2	5	3947	A
2	5	3948	C
2	5	3955	A
2	5	3956	G
2	5	3957	U
2	5	3962	A
2	5	3970	G
2	5	3972	A
2	5	3973	G
2	5	3974	G
2	5	3975	C
2	5	4042	G
2	5	4043	G
2	5	4047	A
2	5	4050	A
2	5	4051	C
2	5	4053	A
2	5	4054	C
2	5	4055	U
2	5	4056	A
2	5	4061	G
2	5	4062	A
2	5	4066	U
2	5	4073	A
2	5	4075	U
2	5	4076	G
2	5	4085	A
2	5	4086	G

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Mol	Chain	Res	Type
2	5	4088	C
2	5	4095	G
2	5	4096	C
2	5	4097	G
2	5	4100	C
2	5	4116	C
2	5	4119	C
2	5	4120	U
2	5	4121	G
2	5	4125	C
2	5	4127	A
2	5	4151	G
2	5	4155	C
2	5	4157	A
2	5	4158	C
2	5	4162	C
2	5	4163	U
2	5	4164	C
2	5	4170	A
2	5	4171	C
2	5	4172	A
2	5	4173	G
2	5	4183	G
2	5	4184	G
2	5	4191	G
2	5	4194	I4U
2	5	4197	G
2	5	4212	A
2	5	4215	C
2	5	4225	G
2	5	4228	G
2	5	4229	U
2	5	4232	U
2	5	4233	A
2	5	4238	G
2	5	4241	C
2	5	4242	U
2	5	4251	A
2	5	4254	G
2	5	4255	A
2	5	4265	U
2	5	4266	G

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Mol	Chain	Res	Type
2	5	4268	A
2	5	4271	A
2	5	4273	A
2	5	4281	A
2	5	4282	A
2	5	4291	G
2	5	4293	PSU
2	5	4304	A
2	5	4305	G
2	5	4306	OMU
2	5	4308	C
2	5	4313	A
2	5	4314	C
2	5	4317	A
2	5	4318	C
2	5	4319	C
2	5	4326	G
2	5	4330	G
2	5	4332	C
2	5	4348	A
2	5	4349	C
2	5	4354	U
2	5	4355	E6G
2	5	4360	U
2	5	4364	G
2	5	4368	G
2	5	4371	MHG
2	5	4373	G
2	5	4376	A
2	5	4377	G
2	5	4378	A
2	5	4380	A
2	5	4387	C
2	5	4391	G
2	5	4394	A
2	5	4395	U
2	5	4398	C
2	5	4401	G
2	5	4415	1MA
2	5	4419	U
2	5	4422	A
2	5	4426	C

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Mol	Chain	Res	Type
2	5	4440	G
2	5	4448	G
2	5	4449	A
2	5	4450	PSU
2	5	4464	A
2	5	4475	G
2	5	4476	C
2	5	4482	U
2	5	4488	A
2	5	4494	OMG
2	5	4500	PSU
2	5	4502	C
2	5	4510	A
2	5	4512	U
2	5	4513	A
2	5	4515	G
2	5	4518	A
2	5	4519	C
2	5	4520	G
2	5	4522	G
2	5	4523	A2M
2	5	4524	G
2	5	4548	A
2	5	4549	G
2	5	4560	C
2	5	4567	G
2	5	4570	G
2	5	4573	G
2	5	4574	U
2	5	4575	G
2	5	4582	C
2	5	4584	A
2	5	4586	G
2	5	4587	G
2	5	4589	A
2	5	4590	A
2	5	4599	A
2	5	4608	G
2	5	4624	A
2	5	4627	U
2	5	4629	U
2	5	4633	G

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Mol	Chain	Res	Type
2	5	4635	A
2	5	4636	PSU
2	5	4637	OMG
2	5	4639	G
2	5	4656	A
2	5	4657	U
2	5	4661	G
2	5	4664	A
2	5	4670	C
2	5	4672	A
2	5	4677	U
2	5	4691	A
2	5	4694	G
2	5	4695	C
2	5	4700	A
2	5	4702	G
2	5	4707	A
2	5	4709	U
2	5	4719	G
2	5	4720	C
2	5	4722	G
2	5	4736	C
2	5	4745	G
2	5	4750	G
2	5	4751	G
2	5	4754	G
2	5	4756	C
2	5	4757	C
2	5	4759	C
2	5	4761	G
2	5	4765	G
2	5	4771	C
2	5	4772	C
2	5	4867	G
2	5	4868	G
2	5	4870	OMG
2	5	4872	2MG
2	5	4875	G
2	5	4877	G
2	5	4878	C
2	5	4881	U
2	5	4882	U

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Mol	Chain	Res	Type
2	5	4883	C
2	5	4885	U
2	5	4887	C
2	5	4895	C
2	5	4903	G
2	5	4906	C
2	5	4910	A
2	5	4912	G
2	5	4914	G
2	5	4915	G
2	5	4918	C
2	5	4919	G
2	5	4920	C
2	5	4921	C
2	5	4925	U
2	5	4926	C
2	5	4927	G
2	5	4928	C
2	5	4929	C
2	5	4931	G
2	5	4934	A
2	5	4937	C
2	5	4938	A
2	5	4940	C
2	5	4943	A
2	5	4944	C
2	5	4947	U
2	5	4948	C
2	5	4949	G
2	5	4950	U
2	5	4951	G
2	5	4955	A
2	5	4956	A
2	5	4959	U
2	5	4960	G
2	5	4964	C
2	5	4965	U
2	5	4966	A
2	5	4967	A
2	5	4975	G
2	5	4976	U
2	5	4985	U

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Mol	Chain	Res	Type
2	5	4988	U
2	5	4990	C
2	5	4991	U
2	5	4993	G
2	5	4999	G
2	5	5006	U
2	5	5014	A
2	5	5017	G
2	5	5040	U
2	5	5041	G
2	5	5047	C
2	5	5049	G
2	5	5050	C
2	5	5053	U
2	5	5054	C
2	5	5058	A
2	5	5061	A
2	5	5062	G
2	5	5069	U
3	7	7	G
3	7	13	A
3	7	22	A
3	7	25	G
3	7	33	U
3	7	53	U
3	7	54	A
3	7	64	G
3	7	76	U
3	7	97	G
3	7	100	A
3	7	102	U
3	7	110	G
3	7	120	U
4	8	2	G
4	8	34	U
4	8	35	C
4	8	39	G
4	8	49	G
4	8	59	A
4	8	62	A
4	8	63	U
4	8	64	U

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Mol	Chain	Res	Type
4	8	75	G
4	8	78	G
4	8	86	U
4	8	87	G
4	8	94	G
4	8	99	U
4	8	103	A
4	8	105	C
4	8	109	C
4	8	110	U
4	8	111	U
4	8	114	G
4	8	123	U
4	8	125	C
4	8	126	C
4	8	127	U
4	8	137	A
4	8	147	G
49	9	2	A
49	9	3	C
49	9	17	C
49	9	23	G
49	9	25	A
49	9	26	U
49	9	33	G
49	9	41	G
49	9	44	U
49	9	45	A
49	9	46	A
49	9	47	G
49	9	56	G
49	9	58	C
49	9	62	G
49	9	65	C
49	9	67	C
49	9	68	A
49	9	70	G
49	9	71	G
49	9	73	C
49	9	74	G
49	9	77	A
49	9	79	A

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Mol	Chain	Res	Type
49	9	103	A
49	9	104	A
49	9	110	U
49	9	111	A
49	9	113	G
49	9	115	U
49	9	116	OMU
49	9	120	U
49	9	121	OMU
49	9	122	G
49	9	124	U
49	9	126	G
49	9	127	C
49	9	129	C
49	9	130	G
49	9	141	A
49	9	143	U
49	9	147	A
49	9	154	U
49	9	155	G
49	9	158	A
49	9	159	A2M
49	9	162	C
49	9	163	U
49	9	166	A2M
49	9	167	G
49	9	168	C
49	9	170	A
49	9	175	A
49	9	180	G
49	9	182	C
49	9	183	G
49	9	184	G
49	9	188	C
49	9	189	U
49	9	190	G
49	9	192	C
49	9	202	G
49	9	206	G
49	9	215	G
49	9	289	G
49	9	290	U

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Mol	Chain	Res	Type
49	9	294	U
49	9	307	G
49	9	308	G
49	9	309	G
49	9	312	G
49	9	318	A
49	9	319	C
49	9	320	G
49	9	332	G
49	9	339	A
49	9	340	C
49	9	343	A
49	9	347	G
49	9	350	C
49	9	351	G
49	9	357	C
49	9	360	A
49	9	364	A
49	9	367	U
49	9	368	U
49	9	369	C
49	9	381	C
49	9	385	G
49	9	400	C
49	9	408	A
49	9	409	C
49	9	417	C
49	9	418	A
49	9	419	G
49	9	435	A
49	9	438	G
49	9	441	C
49	9	448	A
49	9	449	A
49	9	450	C
49	9	455	A
49	9	465	A
49	9	466	G
49	9	471	G
49	9	472	C
49	9	473	A
49	9	474	G

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Mol	Chain	Res	Type
49	9	482	G
49	9	487	U
49	9	492	C
49	9	507	G
49	9	508	A
49	9	530	U
49	9	531	A
49	9	532	C
49	9	533	A
49	9	536	A
49	9	537	C
49	9	542	U
49	9	546	G
49	9	547	G
49	9	548	C
49	9	549	C
49	9	550	C
49	9	551	U
49	9	554	A
49	9	555	A
49	9	556	U
49	9	559	G
49	9	560	A
49	9	562	U
49	9	563	G
49	9	564	A
49	9	568	E3C
49	9	569	A
49	9	573	U
49	9	576	A
49	9	583	A
49	9	587	A
49	9	588	G
49	9	589	G
49	9	590	A
49	9	591	U
49	9	594	A
49	9	603	C
49	9	604	A
49	9	606	G
49	9	607	U
49	9	608	C

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Mol	Chain	Res	Type
49	9	614	C
49	9	615	C
49	9	617	G
49	9	628	A
49	9	643	A
49	9	655	A
49	9	660	C
49	9	663	C
49	9	664	A
49	9	666	U
49	9	668	A2M
49	9	669	A
49	9	671	A
49	9	672	A
49	9	673	G
49	9	683	OMG
49	9	688	U
49	9	689	U
49	9	690	G
49	9	744	G
49	9	752	G
49	9	753	C
49	9	754	G
49	9	791	C
49	9	798	G
49	9	801	U
49	9	810	A
49	9	811	A
49	9	821	G
49	9	822	PSU
49	9	830	A
49	9	834	C
49	9	844	U
49	9	847	A
49	9	848	U
49	9	852	G
49	9	865	A
49	9	867	G
49	9	870	A
49	9	871	U
49	9	872	A
49	9	873	G

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Mol	Chain	Res	Type
49	9	875	A
49	9	878	G
49	9	887	U
49	9	888	U
49	9	890	U
49	9	893	U
49	9	901	G
49	9	913	A
49	9	914	U
49	9	920	A
49	9	933	G
49	9	934	G
49	9	943	U
49	9	971	G
49	9	985	G
49	9	988	C
49	9	990	A
49	9	992	A
49	9	996	A
49	9	999	G
49	9	1002	U
49	9	1017	U
49	9	1023	A
49	9	1041	G
49	9	1045	U
49	9	1058	A
49	9	1060	A
49	9	1062	A
49	9	1067	C
49	9	1071	G
49	9	1083	A
49	9	1085	C
49	9	1089	G
49	9	1099	G
49	9	1100	A
49	9	1109	C
49	9	1113	A
49	9	1115	U
49	9	1116	C
49	9	1117	C
49	9	1118	C
49	9	1121	G

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Mol	Chain	Res	Type
49	9	1123	C
49	9	1131	G
49	9	1133	A
49	9	1138	C
49	9	1149	A
49	9	1153	C
49	9	1154	U
49	9	1155	U
49	9	1161	U
49	9	1170	A
49	9	1173	A
49	9	1194	A
49	9	1195	A
49	9	1208	A
49	9	1211	G
49	9	1212	G
49	9	1215	C
49	9	1221	G
49	9	1223	A
49	9	1224	G
49	9	1242	U
49	9	1243	PSU
49	9	1247	C
49	9	1248	B8N
49	9	1251	A
49	9	1253	A
49	9	1254	C
49	9	1256	G
49	9	1257	G
49	9	1259	A
49	9	1264	C
49	9	1271	C
49	9	1274	G
49	9	1275	G
49	9	1282	A
49	9	1284	A
49	9	1285	G
49	9	1286	G
49	9	1293	A
49	9	1299	A
49	9	1301	A
49	9	1302	G

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Mol	Chain	Res	Type
49	9	1304	U
49	9	1307	U
49	9	1308	U
49	9	1314	U
49	9	1322	G
49	9	1333	U
49	9	1341	C
49	9	1342	U
49	9	1348	G
49	9	1363	C
49	9	1371	U
49	9	1372	U
49	9	1378	A
49	9	1382	A
49	9	1386	A
49	9	1394	G
49	9	1395	C
49	9	1396	A
49	9	1397	U
49	9	1401	A
49	9	1404	U
49	9	1406	G
49	9	1428	G
49	9	1429	G
49	9	1454	A
49	9	1462	U
49	9	1463	U
49	9	1466	G
49	9	1473	G
49	9	1475	G
49	9	1476	A
49	9	1477	U
49	9	1480	A
49	9	1489	A
49	9	1490	G
49	9	1494	U
49	9	1495	G
49	9	1498	A
49	9	1509	U
49	9	1510	G
49	9	1521	C
49	9	1522	A

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Mol	Chain	Res	Type
49	9	1523	C
49	9	1531	A
49	9	1533	A
49	9	1536	G
49	9	1546	G
49	9	1548	G
49	9	1552	G
49	9	1553	C
49	9	1554	C
49	9	1555	U
49	9	1557	C
49	9	1560	U
49	9	1570	G
49	9	1578	U
49	9	1580	A
49	9	1582	C
49	9	1584	G
49	9	1585	U
49	9	1586	U
49	9	1587	G
49	9	1588	A
49	9	1600	G
49	9	1601	A
49	9	1604	G
49	9	1606	G
49	9	1612	G
49	9	1618	C
49	9	1621	U
49	9	1623	A
49	9	1629	C
49	9	1633	A
49	9	1637	A
49	9	1638	G
49	9	1646	C
49	9	1648	G
49	9	1665	G
49	9	1671	G
49	9	1683	C
49	9	1686	G
49	9	1695	A
49	9	1698	C
49	9	1699	A

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Mol	Chain	Res	Type
49	9	1703	OMC
49	9	1721	U
49	9	1722	G
49	9	1726	G
49	9	1744	G
49	9	1751	C
49	9	1757	G
49	9	1760	G
49	9	1779	G
49	9	1780	G
49	9	1783	C
49	9	1784	G
49	9	1785	C
49	9	1819	A
49	9	1826	G
49	9	1829	G
49	9	1831	A
49	9	1835	A
49	9	1836	G
49	9	1838	U
49	9	1849	G
49	9	1851	MA6
49	9	1859	A
49	9	1861	G
49	9	1862	G
49	9	1863	A
49	9	1864	U
49	9	1865	C
49	9	1866	A
49	9	1867	U
49	9	1869	A

All (90) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	4	72	C
2	5	12	A
2	5	47	A
2	5	48	G
2	5	125	C
2	5	134	G
2	5	217	C

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Mol	Chain	Res	Type
2	5	233	U
2	5	245	C
2	5	265	C
2	5	266	C
2	5	275	C
2	5	385	A
2	5	406	C
2	5	449	C
2	5	485	C
2	5	492	U
2	5	504	G
2	5	684	G
2	5	696	C
2	5	930	G
2	5	959	G
2	5	1072	C
2	5	1174	G
2	5	1211	G
2	5	1236	C
2	5	1238	A
2	5	1291	G
2	5	1329	G
2	5	1370	G
2	5	1406(B)	C
2	5	1440	U
2	5	1445	U
2	5	1474	C
2	5	1625	OMG
2	5	1633	G
2	5	1804	A
2	5	1818	G
2	5	1979	A
2	5	1983	A
2	5	2046	G
2	5	2089	G
2	5	2266	C
2	5	2474	G
2	5	2502	A
2	5	2546	G
2	5	2587	A
2	5	2661	U
2	5	2695	A

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Mol	Chain	Res	Type
2	5	3603	G
2	5	3625	G
2	5	3697	U
2	5	3876	A
2	5	3888	G
2	5	3904	G
2	5	4053	A
2	5	4065	G
2	5	4075	U
2	5	4119	C
2	5	4232	U
2	5	4254	G
2	5	4378	A
2	5	4448	G
2	5	4699	U
2	5	4719	G
2	5	4884	G
2	5	4925	U
2	5	4936	G
2	5	4947	U
4	8	124	U
49	9	110	U
49	9	140	U
49	9	434	G
49	9	465	A
49	9	532	C
49	9	553	U
49	9	642	U
49	9	688	U
49	9	752	G
49	9	870	A
49	9	874	G
49	9	1137	U
49	9	1253	A
49	9	1394	G
49	9	1395	C
49	9	1489	A
49	9	1520	G
49	9	1637	A
49	9	1664	A
49	9	1665	G

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$
2	PSU	5	4403	2	18,21,22	0.99	1 (5%)	21,30,33	2.00	6 (28%)
49	OMC	9	517	49	19,22,23	2.86	7 (36%)	25,31,34	1.01	1 (4%)
2	OMG	5	1625	2,83	23,26,27	2.33	8 (34%)	32,38,41	1.93	8 (25%)
2	A2M	5	2363	2,83	22,25,26	3.98	13 (59%)	30,36,39	2.44	12 (40%)
2	PSU	5	4442	2	18,21,22	1.08	2 (11%)	21,30,33	2.08	5 (23%)
2	OMG	5	2364	2	23,26,27	2.37	8 (34%)	32,38,41	1.96	7 (21%)
2	A2M	5	1524	2	22,25,26	3.95	12 (54%)	30,36,39	2.65	14 (46%)
2	B9B	5	237	2	25,28,29	3.81	9 (36%)	35,40,43	2.64	14 (40%)
49	OMU	9	116	49	19,22,23	2.82	7 (36%)	25,31,34	1.87	5 (20%)
2	OMG	5	4494	2	23,26,27	2.43	9 (39%)	32,38,41	1.97	11 (34%)
2	OMC	5	4536	2	19,22,23	2.77	7 (36%)	25,31,34	1.02	1 (4%)
49	M7A	9	1806	49	19,25,26	1.62	2 (10%)	25,37,40	3.88	8 (32%)
49	PSU	9	1243	49	18,21,22	1.22	2 (11%)	21,30,33	1.43	4 (19%)
2	2MG	5	4872	2	23,26,27	2.84	9 (39%)	33,38,41	3.31	16 (48%)
2	B8W	5	4529	2,83	23,26,27	3.35	11 (47%)	33,38,41	5.90	22 (66%)
2	OMG	5	3792	2	23,26,27	2.41	8 (34%)	32,38,41	2.05	9 (28%)
2	B8K	5	3897	2	24,28,29	4.73	17 (70%)	29,42,45	2.73	14 (48%)
2	OMG	5	4196	2	23,26,27	2.37	8 (34%)	32,38,41	1.92	8 (25%)
2	1MA	5	4415	2	21,25,26	2.66	5 (23%)	30,37,40	1.80	5 (16%)
2	PSU	5	3729	2	18,21,22	1.08	2 (11%)	21,30,33	1.84	4 (19%)
2	A2M	5	2401	2,83	22,25,26	3.92	13 (59%)	30,36,39	2.36	9 (30%)
2	OMC	5	2861	2	19,22,23	2.85	7 (36%)	25,31,34	1.07	2 (8%)
2	A2M	5	1534	2,83	22,25,26	3.97	12 (54%)	30,36,39	2.48	13 (43%)
2	UR3	5	4597	2	19,22,23	2.62	6 (31%)	26,32,35	1.57	5 (19%)
2	2MG	5	1517	2	23,26,27	2.91	7 (30%)	33,38,41	2.60	9 (27%)
2	PSU	5	3764	2	18,21,22	1.03	1 (5%)	21,30,33	1.70	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	B8Q	9	1219	49,83	18,22,23	2.89	5 (27%)	21,32,35	2.63	7 (33%)
49	B8N	9	1248	49	25,29,30	3.08	7 (28%)	28,42,45	2.05	7 (25%)
2	OMG	5	1883	2	23,26,27	2.47	8 (34%)	32,38,41	2.06	9 (28%)
2	OMC	5	3701	2,83	19,22,23	2.77	7 (36%)	25,31,34	0.83	0
49	OMC	9	1710	49	19,22,23	2.93	7 (36%)	25,31,34	1.15	2 (8%)
2	PSU	5	2508	2	18,21,22	1.01	1 (5%)	21,30,33	1.69	4 (19%)
2	A2M	5	398	2	22,25,26	3.92	11 (50%)	30,36,39	2.35	10 (33%)
49	A2M	9	1031	49	22,25,26	3.94	12 (54%)	30,36,39	2.41	10 (33%)
2	A2M	5	1326	2	22,25,26	3.94	13 (59%)	30,36,39	2.32	9 (30%)
2	I4U	5	1659	2	20,24,25	4.95	13 (65%)	27,34,37	2.02	3 (11%)
2	E6G	5	4355	2	24,27,28	3.61	11 (45%)	34,39,42	2.64	13 (38%)
2	OMC	5	2422	2,83	19,22,23	2.91	7 (36%)	25,31,34	0.78	1 (4%)
2	MHG	5	4371	2	29,32,33	3.66	11 (37%)	34,46,49	2.46	12 (35%)
49	OMG	9	683	49	23,26,27	2.42	9 (39%)	32,38,41	1.99	9 (28%)
2	A2M	5	3723	2	22,25,26	3.97	12 (54%)	30,36,39	2.28	8 (26%)
2	A2M	5	1871	2,83	22,25,26	3.92	12 (54%)	30,36,39	2.42	10 (33%)
2	OMC	5	3909	2	19,22,23	2.83	7 (36%)	25,31,34	0.66	0
49	PSU	9	823	49	18,21,22	1.06	2 (11%)	21,30,33	1.82	4 (19%)
2	7MG	5	2522	2	23,26,27	3.17	10 (43%)	27,39,42	2.18	9 (33%)
2	PSU	5	1582	2	18,21,22	1.18	2 (11%)	21,30,33	1.94	4 (19%)
2	BGH	5	3899	2,83	25,29,30	4.11	15 (60%)	30,43,46	2.70	16 (53%)
2	B9B	5	2754	2,83	25,28,29	3.74	9 (36%)	35,40,43	2.46	10 (28%)
49	4AC	9	1337	49	21,24,25	3.14	10 (47%)	28,34,37	1.18	4 (14%)
2	UR3	5	4530	2	19,22,23	2.69	7 (36%)	26,32,35	1.67	6 (23%)
2	A2M	5	4571	2	22,25,26	3.93	11 (50%)	30,36,39	2.40	10 (33%)
2	B8K	5	4690	2	24,28,29	4.92	17 (70%)	29,42,45	2.80	13 (44%)
49	A2M	9	668	49,83	22,25,26	3.96	11 (50%)	30,36,39	2.40	13 (43%)
2	OMC	5	3887	2	19,22,23	2.74	7 (36%)	25,31,34	0.88	1 (4%)
2	PSU	5	4531	2	18,21,22	1.11	2 (11%)	21,30,33	2.01	5 (23%)
49	OMG	9	644	49	23,26,27	2.37	8 (34%)	32,38,41	1.95	8 (25%)
2	P7G	5	3880	2	24,28,29	3.54	10 (41%)	25,41,44	1.48	3 (12%)
49	MA6	9	1850	49	23,26,27	1.58	5 (21%)	33,38,41	2.86	11 (33%)
2	I4U	5	4194	2	20,24,25	4.96	13 (65%)	27,34,37	1.88	5 (18%)
2	5MU	5	4083	2	19,22,23	4.71	7 (36%)	27,32,35	3.76	11 (40%)
2	OMG	5	2773	2	23,26,27	2.39	9 (39%)	32,38,41	1.82	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	5	2365	2	19,22,23	2.88	7 (36%)	25,31,34	0.94	0
2	B8H	5	3762	2	19,22,23	6.84	6 (31%)	21,32,35	2.54	5 (23%)
49	OMU	9	121	49	19,22,23	2.89	7 (36%)	25,31,34	1.99	6 (24%)
2	OMG	5	2424	2	23,26,27	2.45	9 (39%)	32,38,41	1.89	8 (25%)
2	A2M	5	4523	2,83	22,25,26	3.92	12 (54%)	30,36,39	2.43	12 (40%)
2	B8H	5	1860	2	19,22,23	6.83	6 (31%)	21,32,35	2.45	5 (23%)
49	PSU	9	612	49	18,21,22	0.98	2 (11%)	21,30,33	1.79	5 (23%)
2	B8H	5	4296	2	19,22,23	6.89	7 (36%)	21,32,35	2.62	5 (23%)
7	MLZ	C	333	7	8,9,10	0.87	0	4,9,11	0.78	0
2	PSU	5	4500	2	18,21,22	1.05	3 (16%)	21,30,33	2.07	6 (28%)
49	OMG	9	509	49,83	23,26,27	2.37	9 (39%)	32,38,41	1.81	7 (21%)
49	5MC	9	1374	49	19,22,23	3.73	8 (42%)	26,32,35	1.04	1 (3%)
49	A2M	9	166	49	22,25,26	3.92	10 (45%)	30,36,39	2.48	10 (33%)
2	OMG	5	1316	2	23,26,27	2.41	9 (39%)	32,38,41	1.97	10 (31%)
2	PSU	5	3715	2	18,21,22	1.03	1 (5%)	21,30,33	1.76	4 (19%)
49	5MU	9	814	49	19,22,23	4.84	7 (36%)	27,32,35	3.53	11 (40%)
2	M7A	5	4564	2	19,25,26	1.60	2 (10%)	25,37,40	4.04	7 (28%)
2	OMG	5	4870	2	23,26,27	2.42	9 (39%)	32,38,41	1.98	9 (28%)
2	2MG	5	729	2	23,26,27	2.90	7 (30%)	33,38,41	2.31	8 (24%)
2	P4U	5	1348	2,83	21,24,25	3.29	7 (33%)	28,33,36	1.87	3 (10%)
2	B9H	5	2786	2	21,25,26	2.91	3 (14%)	22,35,38	1.83	3 (13%)
49	PSU	9	119	49	18,21,22	0.97	1 (5%)	21,30,33	1.73	4 (19%)
49	PSU	9	1081	49	18,21,22	1.09	3 (16%)	21,30,33	1.78	4 (19%)
2	PSU	5	1677	2	18,21,22	1.19	3 (16%)	21,30,33	2.07	5 (23%)
49	MA6	9	1851	49	23,26,27	1.52	4 (17%)	33,38,41	2.73	12 (36%)
2	5MC	5	4447	2	19,22,23	3.85	8 (42%)	26,32,35	1.20	2 (7%)
49	OMC	9	174	49	19,22,23	2.90	7 (36%)	25,31,34	0.72	0
2	A2M	5	3785	2	22,25,26	3.87	13 (59%)	30,36,39	2.51	11 (36%)
2	OMC	5	3869	2	19,22,23	2.78	7 (36%)	25,31,34	0.81	0
49	UR3	9	1830	49	19,22,23	2.60	6 (31%)	26,32,35	1.88	5 (19%)
2	B8Q	5	1456	2	18,22,23	2.77	5 (27%)	21,32,35	1.95	5 (23%)
2	A2M	5	3718	2	22,25,26	3.97	13 (59%)	30,36,39	2.14	10 (33%)
2	6MZ	5	4220	2	22,25,26	2.94	7 (31%)	29,36,39	4.11	12 (41%)
49	A2M	9	159	49	22,25,26	3.94	11 (50%)	30,36,39	2.41	13 (43%)
2	B8W	5	2380	2	23,26,27	3.34	12 (52%)	33,38,41	5.70	19 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	5	2050	2	23,26,27	2.40	8 (34%)	32,38,41	1.83	8 (25%)
2	E7G	5	2297	2	24,27,28	3.15	11 (45%)	28,40,43	2.25	9 (32%)
2	7MG	5	4550	2	23,26,27	3.20	10 (43%)	27,39,42	2.16	11 (40%)
2	A2M	5	3825	2	22,25,26	3.93	11 (50%)	30,36,39	2.44	11 (36%)
2	5MC	5	3782	2	19,22,23	3.65	8 (42%)	26,32,35	1.13	2 (7%)
2	OMG	5	4623	2	23,26,27	2.39	9 (39%)	32,38,41	1.88	8 (25%)
2	UR3	5	1866	2	19,22,23	2.46	6 (31%)	26,32,35	1.56	5 (19%)
2	OMU	5	4306	2	19,22,23	2.69	7 (36%)	25,31,34	1.94	5 (20%)
2	PSU	5	4450	2,83	18,21,22	1.07	2 (11%)	21,30,33	2.24	6 (28%)
2	A2M	5	3867	2	22,25,26	3.98	11 (50%)	30,36,39	2.27	10 (33%)
2	PSU	5	4628	2	18,21,22	1.08	3 (16%)	21,30,33	2.25	5 (23%)
49	A2M	9	1678	49	22,25,26	3.97	12 (54%)	30,36,39	2.44	12 (40%)
2	PSU	5	4293	2	18,21,22	1.09	2 (11%)	21,30,33	1.89	4 (19%)
49	4AC	9	1842	49	21,24,25	3.07	10 (47%)	28,34,37	1.34	4 (14%)
49	A2M	9	27	49,83	22,25,26	3.97	13 (59%)	30,36,39	2.35	10 (33%)
2	B8T	5	4483	2	19,22,23	3.01	8 (42%)	25,31,34	1.15	2 (8%)
42	MLZ	m	72	42	8,9,10	0.79	0	4,9,11	0.85	0
2	OMC	5	2804	2	19,22,23	2.84	7 (36%)	25,31,34	0.91	1 (4%)
49	E3C	9	568	49	19,23,24	3.45	6 (31%)	21,33,36	2.81	6 (28%)
2	OMG	5	4370	2	23,26,27	2.41	8 (34%)	32,38,41	1.91	7 (21%)
2	B8W	5	4472	2	23,26,27	3.34	12 (52%)	33,38,41	5.35	22 (66%)
2	P7G	5	1909	2	24,28,29	3.70	10 (41%)	25,41,44	1.56	3 (12%)
2	B8W	5	4129	2	23,26,27	3.33	11 (47%)	33,38,41	5.43	21 (63%)
2	PSU	5	4636	2	18,21,22	1.14	2 (11%)	21,30,33	2.11	5 (23%)
49	PSU	9	822	49	18,21,22	1.04	1 (5%)	21,30,33	1.94	5 (23%)
2	OMG	5	4637	2	23,26,27	2.30	8 (34%)	32,38,41	1.92	8 (25%)
49	OMC	9	1703	49	19,22,23	2.95	7 (36%)	25,31,34	0.73	0
49	A2M	9	484	49	22,25,26	3.86	12 (54%)	30,36,39	2.40	11 (36%)
2	5MC	5	4335	2	19,22,23	3.82	8 (42%)	26,32,35	1.22	3 (11%)
2	OMG	5	373	2	23,26,27	2.41	9 (39%)	32,38,41	2.04	10 (31%)
2	OMU	5	4620	2	19,22,23	2.72	7 (36%)	25,31,34	2.05	6 (24%)
2	B8T	5	4671	2	19,22,23	3.05	8 (42%)	25,31,34	0.89	1 (4%)
2	B9B	5	1574	2	25,28,29	3.74	9 (36%)	35,40,43	2.41	15 (42%)
2	PSU	5	1683	2	18,21,22	1.22	2 (11%)	21,30,33	1.99	4 (19%)
2	E7G	5	1797	2	24,27,28	3.23	11 (45%)	28,40,43	2.31	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	B8W	5	4185	2	23,26,27	3.40	12 (52%)	33,38,41	5.48	22 (66%)
2	1MA	5	1322	2,83	21,25,26	2.49	5 (23%)	30,37,40	1.93	6 (20%)
49	6MZ	9	1832	49,83	22,25,26	3.04	5 (22%)	29,36,39	4.20	13 (44%)
4	OMU	8	14	4,2	19,22,23	2.83	7 (36%)	25,31,34	2.05	6 (24%)
2	OMG	5	1522	2	23,26,27	2.37	8 (34%)	32,38,41	1.98	8 (25%)
2	7MG	5	1605	2	23,26,27	3.23	10 (43%)	27,39,42	2.17	9 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	5	4403	2	-	2/7/25/26	0/2/2/2
49	OMC	9	517	49	-	1/9/27/28	0/2/2/2
2	OMG	5	1625	2,83	-	3/9/27/28	0/3/3/3
2	A2M	5	2363	2,83	-	0/9/27/28	0/3/3/3
2	PSU	5	4442	2	-	0/7/25/26	0/2/2/2
2	OMG	5	2364	2	-	2/9/27/28	0/3/3/3
2	A2M	5	1524	2	-	2/9/27/28	0/3/3/3
2	B9B	5	237	2	-	5/11/29/30	0/3/3/3
49	OMU	9	116	49	-	2/9/27/28	0/2/2/2
2	OMG	5	4494	2	-	3/9/27/28	0/3/3/3
2	OMC	5	4536	2	-	0/9/27/28	0/2/2/2
49	M7A	9	1806	49	-	0/7/37/38	0/3/3/3
49	PSU	9	1243	49	-	2/7/25/26	0/2/2/2
2	2MG	5	4872	2	-	2/9/27/28	0/3/3/3
2	B8W	5	4529	2,83	-	3/9/27/28	0/3/3/3
2	OMG	5	3792	2	-	2/9/27/28	0/3/3/3
2	B8K	5	3897	2	-	3/11/41/42	0/3/3/3
2	OMG	5	4196	2	-	0/9/27/28	0/3/3/3
2	1MA	5	4415	2	-	2/7/25/26	0/3/3/3
2	PSU	5	3729	2	-	2/7/25/26	0/2/2/2
2	A2M	5	2401	2,83	-	0/9/27/28	0/3/3/3
2	OMC	5	2861	2	-	1/9/27/28	0/2/2/2
2	A2M	5	1534	2,83	-	1/9/27/28	0/3/3/3
2	UR3	5	4597	2	-	0/7/25/26	0/2/2/2
2	2MG	5	1517	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	5	3764	2	-	1/7/25/26	0/2/2/2
49	B8Q	9	1219	49,83	-	1/7/42/43	0/2/2/2
49	B8N	9	1248	49	-	4/16/34/35	0/2/2/2
2	OMG	5	1883	2	-	0/9/27/28	0/3/3/3
2	OMC	5	3701	2,83	-	5/9/27/28	0/2/2/2
49	OMC	9	1710	49	-	0/9/27/28	0/2/2/2
2	PSU	5	2508	2	-	0/7/25/26	0/2/2/2
2	A2M	5	398	2	-	2/9/27/28	0/3/3/3
49	A2M	9	1031	49	-	0/9/27/28	0/3/3/3
2	A2M	5	1326	2	-	0/9/27/28	0/3/3/3
2	I4U	5	1659	2	-	2/9/29/30	0/2/2/2
2	E6G	5	4355	2	-	4/10/28/29	0/3/3/3
2	OMC	5	2422	2,83	-	0/9/27/28	0/2/2/2
2	MHG	5	4371	2	-	8/16/46/47	0/3/3/3
49	OMG	9	683	49	-	2/9/27/28	0/3/3/3
2	A2M	5	3723	2	-	0/9/27/28	0/3/3/3
2	A2M	5	1871	2,83	-	0/9/27/28	0/3/3/3
2	OMC	5	3909	2	-	0/9/27/28	0/2/2/2
49	PSU	9	823	49	-	0/7/25/26	0/2/2/2
2	7MG	5	2522	2	-	0/7/37/38	0/3/3/3
2	PSU	5	1582	2	-	2/7/25/26	0/2/2/2
2	BGH	5	3899	2,83	-	3/13/43/44	0/3/3/3
2	B9B	5	2754	2,83	-	4/11/29/30	0/3/3/3
49	4AC	9	1337	49	-	1/11/29/30	0/2/2/2
2	UR3	5	4530	2	-	1/7/25/26	0/2/2/2
2	A2M	5	4571	2	-	0/9/27/28	0/3/3/3
2	B8K	5	4690	2	-	0/11/41/42	0/3/3/3
49	A2M	9	668	49,83	-	3/9/27/28	0/3/3/3
2	OMC	5	3887	2	-	1/9/27/28	0/2/2/2
2	PSU	5	4531	2	-	0/7/25/26	0/2/2/2
49	OMG	9	644	49	-	1/9/27/28	0/3/3/3
2	P7G	5	3880	2	-	3/10/40/41	0/3/3/3
49	MA6	9	1850	49	-	0/11/29/30	0/3/3/3
2	I4U	5	4194	2	-	3/9/29/30	0/2/2/2
2	5MU	5	4083	2	-	0/7/25/26	0/2/2/2
2	OMG	5	2773	2	-	0/9/27/28	0/3/3/3
2	OMC	5	2365	2	-	2/9/27/28	0/2/2/2
2	B8H	5	3762	2	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	OMU	9	121	49	-	2/9/27/28	0/2/2/2
2	OMG	5	2424	2	-	2/9/27/28	0/3/3/3
2	A2M	5	4523	2,83	-	2/9/27/28	0/3/3/3
2	B8H	5	1860	2	-	0/7/25/26	0/2/2/2
49	PSU	9	612	49	-	0/7/25/26	0/2/2/2
2	B8H	5	4296	2	-	0/7/25/26	0/2/2/2
7	MLZ	C	333	7	-	2/7/8/10	-
2	PSU	5	4500	2	-	3/7/25/26	0/2/2/2
49	OMG	9	509	49,83	-	1/9/27/28	0/3/3/3
49	5MC	9	1374	49	-	0/7/25/26	0/2/2/2
49	A2M	9	166	49	-	2/9/27/28	0/3/3/3
2	OMG	5	1316	2	-	0/9/27/28	0/3/3/3
2	PSU	5	3715	2	-	0/7/25/26	0/2/2/2
49	5MU	9	814	49	-	1/7/25/26	0/2/2/2
2	M7A	5	4564	2	-	0/7/37/38	0/3/3/3
2	OMG	5	4870	2	-	3/9/27/28	0/3/3/3
2	2MG	5	729	2	-	2/9/27/28	0/3/3/3
2	P4U	5	1348	2,83	-	2/10/29/30	0/2/2/2
2	B9H	5	2786	2	-	2/12/47/48	0/2/2/2
49	PSU	9	119	49	-	1/7/25/26	0/2/2/2
49	PSU	9	1081	49	-	1/7/25/26	0/2/2/2
2	PSU	5	1677	2	-	0/7/25/26	0/2/2/2
49	MA6	9	1851	49	-	4/11/29/30	0/3/3/3
2	5MC	5	4447	2	-	4/7/25/26	0/2/2/2
49	OMC	9	174	49	-	0/9/27/28	0/2/2/2
2	A2M	5	3785	2	-	4/9/27/28	0/3/3/3
2	OMC	5	3869	2	-	0/9/27/28	0/2/2/2
49	UR3	9	1830	49	-	2/7/25/26	0/2/2/2
2	B8Q	5	1456	2	-	0/7/42/43	0/2/2/2
2	A2M	5	3718	2	-	0/9/27/28	0/3/3/3
2	6MZ	5	4220	2	-	2/9/27/28	0/3/3/3
49	A2M	9	159	49	-	3/9/27/28	0/3/3/3
2	B8W	5	2380	2	-	4/9/27/28	0/3/3/3
2	OMG	5	2050	2	-	0/9/27/28	0/3/3/3
2	E7G	5	2297	2	-	2/9/39/40	0/3/3/3
2	7MG	5	4550	2	-	0/7/37/38	0/3/3/3
2	A2M	5	3825	2	-	0/9/27/28	0/3/3/3
2	5MC	5	3782	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	5	4623	2	-	0/9/27/28	0/3/3/3
2	UR3	5	1866	2	-	1/7/25/26	0/2/2/2
2	OMU	5	4306	2	-	0/9/27/28	0/2/2/2
2	PSU	5	4450	2,83	-	2/7/25/26	0/2/2/2
2	A2M	5	3867	2	-	2/9/27/28	0/3/3/3
2	PSU	5	4628	2	-	0/7/25/26	0/2/2/2
49	A2M	9	1678	49	-	0/9/27/28	0/3/3/3
2	PSU	5	4293	2	-	1/7/25/26	0/2/2/2
49	4AC	9	1842	49	-	0/11/29/30	0/2/2/2
49	A2M	9	27	49,83	-	0/9/27/28	0/3/3/3
2	B8T	5	4483	2	-	0/7/27/28	0/2/2/2
42	MLZ	m	72	42	-	3/7/8/10	-
2	OMC	5	2804	2	-	0/9/27/28	0/2/2/2
49	E3C	9	568	49	-	6/9/44/45	0/2/2/2
2	OMG	5	4370	2	-	0/9/27/28	0/3/3/3
2	B8W	5	4472	2	-	2/9/27/28	0/3/3/3
2	P7G	5	1909	2	-	2/10/40/41	0/3/3/3
2	B8W	5	4129	2	-	3/9/27/28	0/3/3/3
2	PSU	5	4636	2	-	3/7/25/26	0/2/2/2
49	PSU	9	822	49	-	2/7/25/26	0/2/2/2
2	OMG	5	4637	2	-	2/9/27/28	0/3/3/3
49	OMC	9	1703	49	-	2/9/27/28	0/2/2/2
49	A2M	9	484	49	-	0/9/27/28	0/3/3/3
2	5MC	5	4335	2	-	0/7/25/26	0/2/2/2
2	OMG	5	373	2	-	1/9/27/28	0/3/3/3
2	OMU	5	4620	2	-	1/9/27/28	0/2/2/2
2	B8T	5	4671	2	-	0/7/27/28	0/2/2/2
2	B9B	5	1574	2	-	3/11/29/30	0/3/3/3
2	PSU	5	1683	2	-	0/7/25/26	0/2/2/2
2	E7G	5	1797	2	-	3/9/39/40	0/3/3/3
2	B8W	5	4185	2	-	4/9/27/28	0/3/3/3
2	1MA	5	1322	2,83	-	0/7/25/26	0/3/3/3
49	6MZ	9	1832	49,83	-	2/9/27/28	0/3/3/3
4	OMU	8	14	4,2	-	1/9/27/28	0/2/2/2
2	OMG	5	1522	2	-	0/9/27/28	0/3/3/3
2	7MG	5	1605	2	-	0/7/37/38	0/3/3/3

All (1048) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4296	B8H	C6-C5	-16.16	1.12	1.35
2	5	1860	B8H	C6-C5	-15.85	1.12	1.35
2	5	3762	B8H	C6-C5	-15.80	1.12	1.35
2	5	4296	B8H	C4-N3	-14.94	1.10	1.38
2	5	1860	B8H	C4-N3	-14.82	1.11	1.38
2	5	3762	B8H	C4-N3	-14.66	1.11	1.38
2	5	4296	B8H	C4-C5	13.95	1.83	1.44
2	5	3762	B8H	C4-C5	13.91	1.82	1.44
2	5	1860	B8H	C4-C5	13.58	1.82	1.44
2	5	3762	B8H	C6-N1	13.39	1.68	1.36
2	5	1860	B8H	C6-N1	13.36	1.68	1.36
2	5	4296	B8H	C6-N1	13.00	1.67	1.36
49	9	1832	6MZ	C6-N6	12.45	1.48	1.34
2	5	4690	B8K	C3'-C4'	-11.74	1.23	1.53
49	9	814	5MU	C2-N1	11.51	1.56	1.38
2	5	1659	I4U	C3'-C2'	-11.48	1.22	1.53
2	5	4194	I4U	C3'-C2'	-11.33	1.22	1.53
2	5	3897	B8K	C3'-C4'	-11.28	1.24	1.53
2	5	4220	6MZ	C6-N6	11.24	1.47	1.34
2	5	4083	5MU	C6-N1	10.60	1.56	1.38
2	5	4083	5MU	C2-N1	10.39	1.54	1.38
2	5	1659	I4U	C4-N3	10.39	1.44	1.31
2	5	1909	P7G	C8-N9	10.35	1.52	1.45
2	5	3899	BGH	C3'-C4'	-10.24	1.27	1.53
49	9	814	5MU	C6-N1	10.20	1.55	1.38
2	5	237	B9B	O4'-C1'	9.94	1.65	1.42
2	5	1348	P4U	C4-N3	9.89	1.44	1.31
2	5	4447	5MC	C6-C5	9.79	1.50	1.34
2	5	4194	I4U	C4-N3	9.79	1.44	1.31
2	5	2754	B9B	O4'-C1'	9.64	1.64	1.42
49	9	166	A2M	O4'-C1'	9.62	1.64	1.42
49	9	159	A2M	O4'-C1'	9.56	1.64	1.42
2	5	1574	B9B	O4'-C1'	9.52	1.64	1.42
2	5	3723	A2M	O4'-C1'	9.48	1.63	1.42
2	5	398	A2M	O4'-C1'	9.42	1.63	1.42
49	9	1031	A2M	O4'-C1'	9.42	1.63	1.42
2	5	4523	A2M	O4'-C1'	9.41	1.63	1.42
2	5	3880	P7G	C8-N9	9.40	1.52	1.45
2	5	4083	5MU	C4-C5	9.35	1.60	1.44
2	5	3899	BGH	O4'-C4'	9.34	1.65	1.45
2	5	4571	A2M	O4'-C1'	9.33	1.63	1.42
2	5	3718	A2M	O4'-C1'	9.31	1.63	1.42
2	5	4371	MHG	C8-N9	9.28	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	2363	A2M	O4'-C1'	9.28	1.63	1.42
49	9	1678	A2M	O4'-C1'	9.27	1.63	1.42
49	9	27	A2M	O4'-C1'	9.21	1.63	1.42
2	5	2401	A2M	O4'-C1'	9.20	1.63	1.42
49	9	1374	5MC	C6-C5	9.10	1.49	1.34
49	9	814	5MU	C4-C5	9.09	1.59	1.44
49	9	484	A2M	O4'-C1'	9.09	1.63	1.42
2	5	3867	A2M	O4'-C1'	9.05	1.62	1.42
2	5	1871	A2M	O4'-C1'	9.04	1.62	1.42
2	5	3825	A2M	O4'-C1'	9.03	1.62	1.42
2	5	1456	B8Q	C6-C5	9.02	1.52	1.33
2	5	1534	A2M	O4'-C1'	8.99	1.62	1.42
2	5	2786	B9H	C2-N3	8.94	1.48	1.37
2	5	4335	5MC	C6-C5	8.92	1.49	1.34
2	5	1524	A2M	O4'-C1'	8.92	1.62	1.42
2	5	1326	A2M	O4'-C1'	8.81	1.62	1.42
49	9	668	A2M	O4'-C1'	8.76	1.62	1.42
2	5	4690	B8K	C8-N9	8.73	1.51	1.45
49	9	1219	B8Q	C6-C5	8.72	1.51	1.33
2	5	3785	A2M	O4'-C1'	8.70	1.62	1.42
2	5	3867	A2M	C2'-C1'	-8.70	1.31	1.53
49	9	568	E3C	C2-N1	8.70	1.50	1.38
2	5	237	B9B	C2'-C1'	-8.66	1.26	1.53
2	5	4415	1MA	C2-N3	8.64	1.46	1.30
2	5	1574	B9B	C2'-C1'	-8.63	1.26	1.53
2	5	4194	I4U	O4'-C4'	-8.63	1.25	1.45
2	5	4355	E6G	O4'-C1'	8.59	1.61	1.42
49	9	814	5MU	C4-N3	-8.57	1.22	1.38
2	5	2754	B9B	C2'-C1'	-8.55	1.26	1.53
2	5	1534	A2M	C2'-C1'	-8.55	1.32	1.53
2	5	3825	A2M	C2'-C1'	-8.53	1.32	1.53
49	9	1248	B8N	C4-N3	-8.48	1.25	1.40
2	5	4690	B8K	C2'-C1'	-8.40	1.27	1.53
2	5	1326	A2M	C2'-C1'	-8.38	1.32	1.53
49	9	568	E3C	C2-N3	8.37	1.47	1.37
49	9	1678	A2M	C2'-C1'	-8.36	1.32	1.53
2	5	1524	A2M	C2'-C1'	-8.36	1.32	1.53
2	5	3785	A2M	C2'-C1'	-8.35	1.32	1.53
49	9	668	A2M	O4'-C4'	-8.35	1.26	1.45
2	5	3897	B8K	C2'-C1'	-8.34	1.27	1.53
2	5	2363	A2M	C2'-C1'	-8.32	1.32	1.53
2	5	3782	5MC	C6-C5	8.32	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	9	27	A2M	C2'-C1'	-8.30	1.32	1.53
2	5	2401	A2M	C2'-C1'	-8.29	1.32	1.53
2	5	1871	A2M	C2'-C1'	-8.28	1.32	1.53
49	9	668	A2M	C2'-C1'	-8.25	1.32	1.53
49	9	1031	A2M	C2'-C1'	-8.21	1.32	1.53
2	5	1909	P7G	C5-N7	8.21	1.45	1.35
2	5	4355	E6G	O4'-C4'	-8.19	1.26	1.45
2	5	3718	A2M	C2'-C1'	-8.16	1.33	1.53
2	5	4083	5MU	C4-N3	-8.16	1.23	1.38
2	5	398	A2M	C2'-C1'	-8.16	1.33	1.53
2	5	4571	A2M	C2'-C1'	-8.12	1.33	1.53
2	5	1322	1MA	C2-N3	8.10	1.45	1.30
2	5	4523	A2M	C2'-C1'	-8.08	1.33	1.53
2	5	3723	A2M	C2'-C1'	-8.06	1.33	1.53
2	5	4371	MHG	C2-N3	8.00	1.47	1.32
49	9	159	A2M	C2'-C1'	-7.94	1.33	1.53
2	5	1659	I4U	O4'-C4'	-7.93	1.27	1.45
49	9	166	A2M	C2'-C1'	-7.93	1.33	1.53
2	5	4371	MHG	C5-N7	7.78	1.45	1.35
49	9	484	A2M	C2'-C1'	-7.77	1.34	1.53
2	5	3867	A2M	O4'-C4'	-7.74	1.27	1.45
2	5	4355	E6G	C2'-C1'	-7.71	1.29	1.53
2	5	4523	A2M	O4'-C4'	-7.71	1.27	1.45
2	5	1524	A2M	O4'-C4'	-7.69	1.27	1.45
2	5	4129	B8W	O4'-C1'	7.67	1.59	1.42
2	5	1326	A2M	O4'-C4'	-7.67	1.27	1.45
2	5	3718	A2M	O4'-C4'	-7.66	1.28	1.45
2	5	2380	B8W	O4'-C1'	7.65	1.59	1.42
2	5	2363	A2M	O4'-C4'	-7.65	1.28	1.45
49	9	1678	A2M	O4'-C4'	-7.65	1.28	1.45
49	9	484	A2M	O4'-C4'	-7.65	1.28	1.45
2	5	3723	A2M	O4'-C4'	-7.62	1.28	1.45
2	5	2401	A2M	O4'-C4'	-7.61	1.28	1.45
2	5	3880	P7G	C5-N7	7.58	1.45	1.35
2	5	4571	A2M	O4'-C4'	-7.56	1.28	1.45
2	5	3825	A2M	O4'-C4'	-7.56	1.28	1.45
49	9	27	A2M	O4'-C4'	-7.55	1.28	1.45
2	5	4472	B8W	O4'-C1'	7.54	1.59	1.42
49	9	159	A2M	O4'-C4'	-7.53	1.28	1.45
2	5	1534	A2M	O4'-C4'	-7.50	1.28	1.45
2	5	4185	B8W	O4'-C1'	7.46	1.59	1.42
2	5	1871	A2M	O4'-C4'	-7.46	1.28	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1797	E7G	C5-N7	7.45	1.45	1.35
2	5	2786	B9H	C6-C5	7.42	1.48	1.33
2	5	4529	B8W	O4'-C1'	7.42	1.59	1.42
2	5	237	B9B	O4'-C4'	-7.42	1.28	1.45
2	5	3785	A2M	O4'-C4'	-7.42	1.28	1.45
2	5	3782	5MC	C4-N3	7.41	1.46	1.34
2	5	729	2MG	C2-N3	7.39	1.46	1.32
49	9	166	A2M	O4'-C4'	-7.39	1.28	1.45
2	5	398	A2M	O4'-C4'	-7.39	1.28	1.45
49	9	1031	A2M	O4'-C4'	-7.38	1.28	1.45
49	9	1248	B8N	C6-N1	7.30	1.54	1.36
2	5	2754	B9B	C2-N2	7.21	1.48	1.33
2	5	1574	B9B	O4'-C4'	-7.19	1.29	1.45
2	5	3897	B8K	O4'-C4'	7.19	1.61	1.45
2	5	237	B9B	C2-N2	7.18	1.48	1.33
2	5	4690	B8K	O4'-C4'	7.15	1.60	1.45
2	5	2754	B9B	O4'-C4'	-7.13	1.29	1.45
2	5	2297	E7G	C5-N7	7.07	1.44	1.35
49	9	1337	4AC	C4-N3	7.06	1.44	1.32
2	5	4530	UR3	C2-N1	7.06	1.48	1.38
2	5	1574	B9B	C2-N2	7.05	1.47	1.33
49	9	568	E3C	C6-C5	7.02	1.47	1.33
2	5	4185	B8W	C3'-C4'	-6.95	1.35	1.53
2	5	1517	2MG	C2-N3	6.94	1.45	1.32
2	5	4550	7MG	C5-N7	6.92	1.44	1.35
2	5	4550	7MG	C8-N9	6.90	1.50	1.45
2	5	1797	E7G	C8-N9	6.90	1.50	1.45
2	5	729	2MG	C4-N3	6.88	1.50	1.34
2	5	4529	B8W	C3'-C4'	-6.87	1.35	1.53
49	9	1830	UR3	C2-N1	6.81	1.47	1.38
2	5	4529	B8W	C2'-C1'	-6.78	1.32	1.53
2	5	4447	5MC	C4-N3	6.78	1.45	1.34
49	9	1374	5MC	C4-N3	6.78	1.45	1.34
2	5	4129	B8W	C2'-C1'	-6.76	1.32	1.53
49	9	121	OMU	C2-N3	6.76	1.49	1.38
2	5	4472	B8W	C2'-C1'	-6.76	1.32	1.53
2	5	4185	B8W	C2'-C1'	-6.73	1.32	1.53
2	5	4335	5MC	C4-N3	6.72	1.44	1.34
2	5	4129	B8W	C3'-C4'	-6.71	1.36	1.53
2	5	4597	UR3	C2-N1	6.71	1.47	1.38
2	5	1605	7MG	C5-N7	6.71	1.44	1.35
2	5	1517	2MG	C4-N3	6.70	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4472	B8W	C3'-C4'	-6.70	1.36	1.53
2	5	4671	B8T	C4-N3	6.70	1.44	1.32
4	8	14	OMU	C2-N3	6.66	1.49	1.38
2	5	2522	7MG	C5-N7	6.64	1.44	1.35
49	9	1842	4AC	C4-N3	6.64	1.44	1.32
49	9	1248	B8N	C4-C5	6.62	1.62	1.47
2	5	2380	B8W	C2'-C1'	-6.61	1.32	1.53
2	5	3897	B8K	C8-N9	6.61	1.50	1.45
2	5	1883	OMG	C4-N3	6.55	1.49	1.34
2	5	1517	2MG	C2-N2	6.53	1.47	1.33
2	5	4483	B8T	C4-N3	6.53	1.43	1.32
2	5	4335	5MC	C5-C4	6.53	1.49	1.44
2	5	4872	2MG	C2-N2	6.52	1.47	1.33
2	5	3867	A2M	C6-N6	6.52	1.50	1.34
49	9	166	A2M	C6-N6	6.52	1.50	1.34
2	5	398	A2M	C6-N6	6.48	1.50	1.34
2	5	4870	OMG	C4-N3	6.48	1.49	1.34
2	5	4571	A2M	C6-N6	6.47	1.50	1.34
2	5	3782	5MC	C2-N3	6.47	1.49	1.36
49	9	116	OMU	C2-N3	6.46	1.49	1.38
49	9	683	OMG	C4-N3	6.45	1.49	1.34
2	5	2380	B8W	C3'-C4'	-6.45	1.36	1.53
2	5	4523	A2M	C6-N6	6.44	1.50	1.34
49	9	159	A2M	C6-N6	6.44	1.50	1.34
2	5	3718	A2M	C6-N6	6.44	1.50	1.34
49	9	1678	A2M	C6-N6	6.42	1.50	1.34
2	5	3792	OMG	C4-N3	6.42	1.48	1.34
2	5	4620	OMU	C2-N3	6.41	1.49	1.38
49	9	27	A2M	C6-N6	6.39	1.50	1.34
49	9	668	A2M	C6-N6	6.39	1.50	1.34
2	5	1871	A2M	C6-N6	6.38	1.50	1.34
2	5	4370	OMG	C4-N3	6.37	1.48	1.34
2	5	373	OMG	C4-N3	6.37	1.48	1.34
4	8	14	OMU	C2-N1	6.36	1.48	1.38
2	5	1534	A2M	C6-N6	6.36	1.50	1.34
2	5	3723	A2M	C6-N6	6.35	1.50	1.34
2	5	1326	A2M	C6-N6	6.35	1.50	1.34
49	9	116	OMU	C2-N1	6.34	1.48	1.38
2	5	4371	MHG	C2-N1	6.32	1.46	1.36
2	5	2424	OMG	C4-N3	6.32	1.48	1.34
49	9	484	A2M	C6-N6	6.31	1.50	1.34
2	5	1605	7MG	C8-N9	6.31	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3825	A2M	C6-N6	6.31	1.50	1.34
2	5	2773	OMG	C4-N3	6.27	1.48	1.34
2	5	2522	7MG	C8-N9	6.27	1.49	1.45
49	9	1031	A2M	C6-N6	6.27	1.50	1.34
2	5	2363	A2M	C6-N6	6.26	1.50	1.34
49	9	1703	OMC	C2-N3	6.25	1.48	1.36
2	5	2401	A2M	C6-N6	6.25	1.50	1.34
49	9	1710	OMC	C2-N3	6.25	1.48	1.36
2	5	4494	OMG	C4-N3	6.25	1.48	1.34
2	5	4196	OMG	C4-N3	6.24	1.48	1.34
2	5	2297	E7G	C8-N9	6.23	1.49	1.45
2	5	2365	OMC	C6-C5	6.23	1.49	1.35
2	5	2422	OMC	C6-C5	6.21	1.49	1.35
49	9	1703	OMC	C6-C5	6.20	1.49	1.35
2	5	2422	OMC	C2-N3	6.20	1.48	1.36
2	5	2050	OMG	C4-N3	6.19	1.48	1.34
2	5	729	2MG	C2-N2	6.19	1.46	1.33
49	9	644	OMG	C4-N3	6.19	1.48	1.34
49	9	509	OMG	C4-N3	6.18	1.48	1.34
2	5	1524	A2M	C6-N6	6.16	1.50	1.34
2	5	4306	OMU	C2-N3	6.16	1.48	1.38
2	5	4483	B8T	C2-N3	6.16	1.48	1.36
49	9	174	OMC	C2-N3	6.15	1.48	1.36
2	5	2364	OMG	C4-N3	6.15	1.48	1.34
49	9	174	OMC	C6-C5	6.15	1.49	1.35
2	5	4371	MHG	C2-N2	6.14	1.46	1.33
2	5	2365	OMC	C2-N3	6.14	1.48	1.36
49	9	1710	OMC	C6-C5	6.13	1.49	1.35
2	5	4623	OMG	C4-N3	6.13	1.48	1.34
2	5	3785	A2M	C6-N6	6.13	1.49	1.34
2	5	2804	OMC	C6-C5	6.12	1.49	1.35
2	5	3909	OMC	C6-C5	6.11	1.49	1.35
2	5	3887	OMC	C6-C5	6.10	1.49	1.35
49	9	1374	5MC	C2-N3	6.10	1.48	1.36
2	5	1625	OMG	C4-N3	6.09	1.48	1.34
2	5	1659	I4U	C2-N3	6.09	1.48	1.36
2	5	1522	OMG	C4-N3	6.07	1.48	1.34
2	5	1866	UR3	C2-N1	6.07	1.46	1.38
49	9	121	OMU	C2-N1	6.05	1.47	1.38
2	5	4536	OMC	C6-C5	6.04	1.49	1.35
2	5	4637	OMG	C4-N3	6.04	1.48	1.34
2	5	4872	2MG	C2-N3	6.04	1.43	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4447	5MC	C2-N3	6.03	1.48	1.36
2	5	2804	OMC	C2-N3	6.03	1.48	1.36
2	5	1316	OMG	C4-N3	6.02	1.48	1.34
2	5	1348	P4U	C2-N3	6.01	1.48	1.36
49	9	517	OMC	C6-C5	6.01	1.49	1.35
2	5	237	B9B	O6-C6	6.01	1.43	1.34
2	5	4530	UR3	C6-C5	6.01	1.49	1.35
49	9	1842	4AC	C6-C5	6.00	1.49	1.35
49	9	517	OMC	C2-N3	6.00	1.48	1.36
2	5	1348	P4U	C6-C5	6.00	1.49	1.35
49	9	1337	4AC	C2-N3	5.99	1.48	1.36
2	5	3869	OMC	C6-C5	5.99	1.49	1.35
2	5	3701	OMC	C6-C5	5.98	1.48	1.35
2	5	4671	B8T	C2-N3	5.98	1.48	1.36
2	5	4335	5MC	C2-N3	5.96	1.48	1.36
2	5	4536	OMC	C2-N3	5.95	1.48	1.36
2	5	2861	OMC	C2-N3	5.93	1.48	1.36
2	5	4194	I4U	C1'-N1	-5.93	1.30	1.47
2	5	2861	OMC	C6-C5	5.93	1.48	1.35
49	9	1703	OMC	C4-N3	5.92	1.46	1.34
49	9	1337	4AC	C6-C5	5.90	1.48	1.35
2	5	1574	B9B	O6-C6	5.90	1.43	1.34
49	9	1219	B8Q	C2-N3	5.88	1.46	1.35
49	9	1830	UR3	C6-C5	5.88	1.48	1.35
2	5	3869	OMC	C2-N3	5.86	1.48	1.36
2	5	4415	1MA	C4-N3	5.85	1.47	1.35
2	5	4597	UR3	C6-C5	5.85	1.48	1.35
2	5	3701	OMC	C2-N3	5.85	1.48	1.36
2	5	3880	P7G	C4-N3	5.84	1.47	1.37
49	9	1842	4AC	C2-N3	5.83	1.47	1.36
2	5	2422	OMC	C4-N3	5.82	1.46	1.34
49	9	814	5MU	C6-C5	5.79	1.44	1.34
2	5	4671	B8T	C6-C5	5.77	1.48	1.35
49	9	174	OMC	C4-N3	5.75	1.45	1.34
49	9	1710	OMC	C4-N3	5.75	1.45	1.34
2	5	1605	7MG	C2-N3	5.74	1.47	1.33
2	5	3887	OMC	C2-N3	5.73	1.47	1.36
2	5	2786	B9H	C2-N1	5.73	1.46	1.38
2	5	2297	E7G	C2-N3	5.72	1.47	1.33
2	5	1909	P7G	C4-N3	5.71	1.47	1.37
2	5	3909	OMC	C2-N3	5.71	1.47	1.36
2	5	2365	OMC	C4-N3	5.68	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1866	UR3	C6-C5	5.66	1.48	1.35
2	5	2754	B9B	O6-C6	5.66	1.43	1.34
49	9	517	OMC	C4-N3	5.65	1.45	1.34
2	5	3909	OMC	C4-N3	5.64	1.45	1.34
2	5	2522	7MG	C2-N3	5.63	1.46	1.33
2	5	3701	OMC	C4-N3	5.62	1.45	1.34
2	5	4483	B8T	C6-C5	5.62	1.48	1.35
2	5	2861	OMC	C4-N3	5.61	1.45	1.34
2	5	3897	B8K	C4-N9	5.61	1.44	1.37
2	5	3762	B8H	C2-N3	5.60	1.47	1.38
2	5	2380	B8W	C2-N2	5.59	1.45	1.33
2	5	4620	OMU	C2-N1	5.58	1.47	1.38
2	5	2804	OMC	C4-N3	5.57	1.45	1.34
2	5	4355	E6G	C2-N2	5.54	1.44	1.33
2	5	1605	7MG	C4-N3	5.54	1.46	1.34
2	5	2522	7MG	C4-N3	5.53	1.46	1.34
2	5	1659	I4U	C6-C5	5.52	1.47	1.35
2	5	3897	B8K	C3'-C2'	5.52	1.68	1.53
2	5	1797	E7G	C2-N3	5.51	1.46	1.33
49	9	121	OMU	C6-C5	5.49	1.47	1.35
2	5	1909	P7G	C2-N1	5.49	1.46	1.33
2	5	3869	OMC	C4-N3	5.49	1.45	1.34
2	5	4872	2MG	C4-N3	5.45	1.46	1.34
49	9	1374	5MC	C5-C4	5.45	1.48	1.44
2	5	3880	P7G	C2-N1	5.45	1.46	1.33
2	5	4529	B8W	C2-N2	5.44	1.44	1.33
2	5	4194	I4U	C6-C5	5.43	1.47	1.35
2	5	4371	MHG	C4-N3	5.41	1.46	1.34
2	5	4870	OMG	C2-N3	5.40	1.46	1.33
49	9	116	OMU	C6-C5	5.39	1.47	1.35
2	5	3897	B8K	C2-N3	5.38	1.46	1.33
2	5	4690	B8K	C3'-C2'	5.38	1.68	1.53
2	5	4306	OMU	C6-C5	5.37	1.47	1.35
2	5	3899	BGH	C4-N3	5.32	1.46	1.34
2	5	4550	7MG	C4-N3	5.32	1.46	1.34
2	5	4194	I4U	C2-N3	5.30	1.46	1.36
2	5	3897	B8K	C4-N3	5.30	1.46	1.34
49	9	1248	B8N	C2-N1	5.29	1.54	1.39
2	5	4550	7MG	C2-N3	5.29	1.46	1.33
2	5	1860	B8H	C2-N3	5.28	1.47	1.38
2	5	4194	I4U	C3'-C4'	5.27	1.66	1.53
2	5	1322	1MA	C4-N3	5.26	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3880	P7G	C4-N9	5.25	1.43	1.35
2	5	4370	OMG	C2-N3	5.24	1.45	1.33
2	5	4690	B8K	C4-N3	5.24	1.46	1.34
2	5	4083	5MU	C6-C5	5.22	1.43	1.34
2	5	4620	OMU	C6-C5	5.22	1.47	1.35
2	5	1883	OMG	C2-N3	5.21	1.45	1.33
2	5	1456	B8Q	C2-N3	5.21	1.44	1.35
2	5	4296	B8H	C2-N3	5.21	1.47	1.38
2	5	3887	OMC	C4-N3	5.21	1.44	1.34
2	5	4306	OMU	C2-N1	5.20	1.46	1.38
49	9	644	OMG	C2-N3	5.20	1.45	1.33
2	5	4690	B8K	C2-N3	5.18	1.45	1.33
2	5	3792	OMG	C2-N3	5.15	1.45	1.33
2	5	4185	B8W	C2-N2	5.14	1.44	1.33
2	5	4129	B8W	C2-N2	5.13	1.44	1.33
2	5	1522	OMG	C2-N3	5.13	1.45	1.33
2	5	2424	OMG	C2-N3	5.11	1.45	1.33
2	5	3899	BGH	C2-N3	5.11	1.45	1.33
2	5	1659	I4U	C1'-N1	-5.11	1.33	1.47
2	5	2364	OMG	C2-N3	5.10	1.45	1.33
2	5	4196	OMG	C2-N3	5.10	1.45	1.33
2	5	4447	5MC	C5-C4	5.10	1.48	1.44
2	5	4494	OMG	C2-N3	5.09	1.45	1.33
2	5	1909	P7G	C4-N9	5.09	1.43	1.35
2	5	4472	B8W	C2-N2	5.09	1.44	1.33
2	5	4623	OMG	C2-N3	5.08	1.45	1.33
49	9	509	OMG	C2-N3	5.08	1.45	1.33
2	5	373	OMG	C2-N3	5.06	1.45	1.33
2	5	2050	OMG	C2-N3	5.04	1.45	1.33
49	9	683	OMG	C2-N3	5.03	1.45	1.33
2	5	4536	OMC	C4-N3	5.03	1.44	1.34
2	5	1316	OMG	C2-N3	4.99	1.45	1.33
49	9	1219	B8Q	C2-N1	4.98	1.45	1.38
2	5	3899	BGH	O4'-C1'	-4.96	1.30	1.42
2	5	1625	OMG	C2-N3	4.95	1.45	1.33
2	5	2773	OMG	C2-N3	4.95	1.45	1.33
2	5	4637	OMG	C2-N3	4.90	1.45	1.33
4	8	14	OMU	C6-C5	4.90	1.46	1.35
2	5	1797	E7G	C4-N3	4.83	1.45	1.34
2	5	2297	E7G	C4-N3	4.79	1.45	1.34
2	5	3782	5MC	C4-N4	4.78	1.46	1.34
2	5	3782	5MC	C5-C4	4.77	1.47	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	9	683	OMG	C2-N2	4.77	1.45	1.34
2	5	2424	OMG	C2-N2	4.76	1.45	1.34
2	5	4597	UR3	C2-N3	4.75	1.48	1.39
2	5	4335	5MC	C4-N4	4.74	1.46	1.34
2	5	3880	P7G	C2-N2	4.74	1.45	1.34
49	9	1374	5MC	C4-N4	4.74	1.46	1.34
2	5	1797	E7G	C4-N9	4.74	1.43	1.37
2	5	4690	B8K	C4-N9	4.73	1.43	1.37
2	5	4447	5MC	C4-N4	4.72	1.46	1.34
2	5	4371	MHG	C4-N9	4.72	1.43	1.37
2	5	1883	OMG	C2-N2	4.71	1.45	1.34
2	5	2297	E7G	C4-N9	4.71	1.43	1.37
2	5	3792	OMG	C2-N2	4.71	1.45	1.34
2	5	2522	7MG	C2-N2	4.69	1.45	1.34
2	5	373	OMG	C2-N2	4.69	1.45	1.34
2	5	1605	7MG	C2-N2	4.68	1.45	1.34
2	5	1605	7MG	C4-N9	4.68	1.43	1.37
2	5	4690	B8K	O4'-C1'	4.67	1.52	1.42
2	5	2364	OMG	C2-N2	4.65	1.45	1.34
2	5	4447	5MC	C6-N1	4.65	1.45	1.38
49	9	166	A2M	O3'-C3'	-4.64	1.31	1.43
2	5	4872	2MG	C2-N1	4.63	1.44	1.36
2	5	1316	OMG	C2-N2	4.62	1.45	1.34
2	5	1909	P7G	C2-N2	4.61	1.45	1.34
2	5	2773	OMG	C2-N2	4.60	1.44	1.34
2	5	4494	OMG	C2-N2	4.60	1.44	1.34
2	5	3899	BGH	O2'-C2'	-4.59	1.31	1.42
49	9	644	OMG	C2-N2	4.58	1.44	1.34
2	5	3897	B8K	C2-N2	4.57	1.44	1.34
2	5	4370	OMG	C2-N2	4.56	1.44	1.34
2	5	4550	7MG	C2-N2	4.56	1.44	1.34
2	5	1522	OMG	C2-N2	4.54	1.44	1.34
49	9	159	A2M	O3'-C3'	-4.54	1.31	1.43
2	5	4870	OMG	C2-N2	4.53	1.44	1.34
2	5	3899	BGH	C2-N2	4.52	1.44	1.34
2	5	2050	OMG	C2-N2	4.51	1.44	1.34
2	5	3718	A2M	O3'-C3'	-4.51	1.31	1.43
2	5	4690	B8K	C2-N2	4.50	1.44	1.34
2	5	398	A2M	O3'-C3'	-4.50	1.31	1.43
2	5	4623	OMG	C2-N2	4.49	1.44	1.34
2	5	3899	BGH	C8-N9	4.49	1.48	1.45
49	9	27	A2M	O3'-C3'	-4.48	1.31	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3723	A2M	O3'-C3'	-4.48	1.31	1.43
49	9	1806	M7A	C6-N6	4.48	1.45	1.34
2	5	4690	B8K	C71-N7	4.48	1.49	1.39
2	5	1326	A2M	O3'-C3'	-4.46	1.31	1.43
2	5	3867	A2M	O3'-C3'	-4.46	1.31	1.43
2	5	4530	UR3	C2-N3	4.45	1.47	1.39
49	9	1031	A2M	O3'-C3'	-4.44	1.32	1.43
2	5	3825	A2M	O3'-C3'	-4.44	1.32	1.43
49	9	509	OMG	C2-N2	4.43	1.44	1.34
49	9	1830	UR3	C2-N3	4.41	1.47	1.39
49	9	1337	4AC	C7-N4	4.40	1.46	1.37
2	5	1348	P4U	O4-C4	4.38	1.40	1.35
2	5	1524	A2M	O3'-C3'	-4.38	1.32	1.43
2	5	4196	OMG	C2-N2	4.38	1.44	1.34
2	5	1866	UR3	C2-N3	4.36	1.47	1.39
2	5	4564	M7A	C6-N6	4.36	1.45	1.34
49	9	1678	A2M	O3'-C3'	-4.35	1.32	1.43
2	5	1625	OMG	C2-N2	4.34	1.44	1.34
49	9	1248	B8N	C6-C5	4.34	1.41	1.35
2	5	1871	A2M	O3'-C3'	-4.31	1.32	1.43
2	5	4571	A2M	O3'-C3'	-4.31	1.32	1.43
2	5	1659	I4U	C3'-C4'	4.30	1.63	1.53
2	5	4529	B8W	O6-C6	4.28	1.41	1.35
49	9	668	A2M	O3'-C3'	-4.28	1.32	1.43
2	5	2363	A2M	O3'-C3'	-4.26	1.32	1.43
2	5	4671	B8T	C4-N4	4.25	1.44	1.36
49	9	484	A2M	O3'-C3'	-4.24	1.32	1.43
2	5	4637	OMG	C2-N2	4.23	1.44	1.34
49	9	1337	4AC	C4-N4	4.21	1.46	1.39
2	5	4690	B8K	C5-N7	4.21	1.48	1.39
2	5	4483	B8T	C4-N4	4.19	1.44	1.36
2	5	2401	A2M	O3'-C3'	-4.19	1.32	1.43
49	9	1842	4AC	C7-N4	4.18	1.45	1.37
2	5	4415	1MA	C2-N1	4.17	1.44	1.35
2	5	3897	B8K	C5-N7	4.14	1.47	1.39
2	5	2522	7MG	C4-N9	4.14	1.42	1.37
2	5	2297	E7G	C2-N2	4.14	1.43	1.34
49	9	1374	5MC	C2-N1	4.12	1.48	1.40
2	5	4335	5MC	C2-N1	4.11	1.48	1.40
2	5	1797	E7G	C2-N2	4.10	1.43	1.34
2	5	4335	5MC	C6-N1	4.09	1.45	1.38
2	5	4671	B8T	C2-N1	4.09	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4550	7MG	C4-N9	4.07	1.42	1.37
49	9	1710	OMC	C2-N1	4.07	1.48	1.40
2	5	1659	I4U	O4'-C1'	4.06	1.51	1.42
2	5	4447	5MC	C2-N1	4.06	1.48	1.40
49	9	1374	5MC	C6-N1	4.05	1.44	1.38
2	5	1534	A2M	O3'-C3'	-4.05	1.32	1.43
2	5	4220	6MZ	C5-C4	-4.05	1.31	1.39
49	9	1842	4AC	C4-N4	4.00	1.45	1.39
49	9	568	E3C	C4-N3	3.98	1.54	1.48
2	5	3897	B8K	O4'-C1'	3.96	1.51	1.42
49	9	1842	4AC	C2-N1	3.94	1.48	1.40
2	5	3899	BGH	C4-N9	3.92	1.42	1.37
49	9	1703	OMC	C4-N4	3.92	1.43	1.33
2	5	3897	B8K	C71-N7	3.92	1.48	1.39
2	5	237	B9B	O3'-C3'	-3.89	1.33	1.43
49	9	121	OMU	C4-N3	3.88	1.45	1.38
2	5	1524	A2M	C5-N7	-3.88	1.32	1.39
2	5	1326	A2M	C5-N7	-3.87	1.32	1.39
49	9	517	OMC	C2-N1	3.86	1.48	1.40
2	5	4523	A2M	O3'-C3'	-3.85	1.33	1.43
2	5	1517	2MG	C5-N7	-3.85	1.31	1.39
2	5	3782	5MC	C2-N1	3.84	1.48	1.40
2	5	1517	2MG	C2-N1	3.83	1.42	1.36
49	9	1806	M7A	C5-N7	3.83	1.48	1.39
4	8	14	OMU	C4-N3	3.83	1.45	1.38
49	9	1850	MA6	C6-N6	3.82	1.47	1.36
2	5	3782	5MC	C6-N1	3.82	1.44	1.38
49	9	174	OMC	C4-N4	3.82	1.43	1.33
49	9	1710	OMC	C4-N4	3.80	1.43	1.33
2	5	4483	B8T	C2-N1	3.80	1.48	1.40
49	9	116	OMU	C4-N3	3.79	1.45	1.38
2	5	3880	P7G	C2-N3	3.79	1.46	1.37
2	5	1534	A2M	C8-N9	-3.79	1.31	1.37
2	5	4129	B8W	O6-C6	3.78	1.40	1.35
2	5	729	2MG	C2-N1	3.78	1.42	1.36
2	5	2422	OMC	C4-N4	3.78	1.43	1.33
2	5	1534	A2M	C5-C4	-3.78	1.32	1.39
2	5	3723	A2M	O2'-C2'	3.77	1.51	1.42
2	5	2861	OMC	C4-N4	3.77	1.43	1.33
2	5	2804	OMC	C4-N4	3.76	1.43	1.33
2	5	4872	2MG	O6-C6	-3.75	1.16	1.23
2	5	3909	OMC	O2-C2	-3.73	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	9	1678	A2M	O2'-C2'	3.73	1.51	1.42
2	5	3785	A2M	C5-C4	-3.72	1.32	1.39
2	5	4564	M7A	C5-N7	3.71	1.47	1.39
2	5	2380	B8W	O4'-C4'	3.70	1.53	1.45
2	5	3869	OMC	C4-N4	3.70	1.42	1.33
2	5	3785	A2M	O3'-C3'	-3.69	1.33	1.43
2	5	1326	A2M	O2'-C2'	3.68	1.51	1.42
49	9	1851	MA6	C6-N6	3.68	1.47	1.36
2	5	3718	A2M	C5-N7	-3.66	1.32	1.39
2	5	2365	OMC	C4-N4	3.65	1.42	1.33
2	5	1348	P4U	C2-N1	3.65	1.47	1.40
2	5	1517	2MG	O6-C6	-3.65	1.16	1.23
2	5	4472	B8W	C5-C4	-3.65	1.32	1.39
2	5	4472	B8W	O6-C6	3.65	1.40	1.35
2	5	4185	B8W	O6-C6	3.65	1.40	1.35
2	5	3887	OMC	C4-N4	3.64	1.42	1.33
2	5	2297	E7G	C5-C6	3.64	1.52	1.43
2	5	4523	A2M	C5-C4	-3.64	1.32	1.39
2	5	1909	P7G	C2-N3	3.64	1.46	1.37
2	5	729	2MG	C5-N7	-3.64	1.31	1.39
2	5	4185	B8W	C5-C4	-3.63	1.32	1.39
2	5	4335	5MC	O2-C2	-3.63	1.16	1.23
2	5	1797	E7G	C5-C6	3.63	1.52	1.43
49	9	1337	4AC	C5-C4	3.62	1.49	1.41
2	5	1534	A2M	C5-N7	-3.61	1.32	1.39
49	9	1243	PSU	C6-C5	3.61	1.39	1.35
2	5	2365	OMC	C6-N1	3.61	1.46	1.38
2	5	3701	OMC	C4-N4	3.60	1.42	1.33
2	5	2380	B8W	C3'-C2'	3.60	1.63	1.53
2	5	1524	A2M	C5-C4	-3.60	1.32	1.39
2	5	398	A2M	C5-N7	-3.60	1.32	1.39
2	5	1683	PSU	C6-C5	3.60	1.39	1.35
2	5	4620	OMU	C4-N3	3.60	1.44	1.38
2	5	3897	B8K	C2-N1	3.59	1.46	1.37
49	9	27	A2M	C5-N7	-3.59	1.32	1.39
2	5	4371	MHG	C8-N7	3.58	1.52	1.45
2	5	3785	A2M	C5-N7	-3.57	1.32	1.39
2	5	4536	OMC	C4-N4	3.57	1.42	1.33
2	5	1871	A2M	C5-N7	-3.57	1.32	1.39
49	9	668	A2M	C5-C4	-3.57	1.32	1.39
2	5	2363	A2M	C5-C4	-3.57	1.32	1.39
49	9	1832	6MZ	C8-N9	-3.56	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4355	E6G	C5-C4	-3.55	1.32	1.39
49	9	517	OMC	C4-N4	3.55	1.42	1.33
49	9	174	OMC	C2-N1	3.55	1.47	1.40
2	5	3899	BGH	C5-C6	3.55	1.52	1.43
2	5	4529	B8W	O4'-C4'	3.55	1.52	1.45
2	5	2363	A2M	C5-N7	-3.53	1.32	1.39
2	5	4185	B8W	C3'-C2'	3.53	1.62	1.53
2	5	4690	B8K	C2-N1	3.53	1.46	1.37
2	5	1574	B9B	O3'-C3'	-3.52	1.34	1.43
2	5	1871	A2M	C5-C4	-3.52	1.32	1.39
2	5	1456	B8Q	C2-N1	3.52	1.43	1.38
2	5	1625	OMG	C5-N7	-3.52	1.32	1.39
49	9	1337	4AC	C2-N1	3.51	1.47	1.40
2	5	2754	B9B	O3'-C3'	-3.51	1.34	1.43
2	5	4690	B8K	O6-C6	-3.51	1.16	1.23
2	5	4447	5MC	O2-C2	-3.51	1.17	1.23
49	9	159	A2M	O2'-C2'	3.50	1.51	1.42
2	5	2861	OMC	C2-N1	3.50	1.47	1.40
49	9	1703	OMC	C2-N1	3.50	1.47	1.40
2	5	4194	I4U	C2-N1	3.49	1.47	1.40
2	5	2380	B8W	C5-C4	-3.49	1.32	1.39
2	5	3867	A2M	C5-C4	-3.49	1.32	1.39
2	5	2422	OMC	C6-N1	3.48	1.46	1.38
2	5	3909	OMC	C4-N4	3.48	1.42	1.33
2	5	1659	I4U	C2-N1	3.48	1.47	1.40
49	9	1031	A2M	C5-N7	-3.48	1.32	1.39
2	5	1797	E7G	C2-N1	3.47	1.46	1.37
49	9	27	A2M	O2'-C2'	3.47	1.51	1.42
2	5	2861	OMC	O2-C2	-3.47	1.17	1.23
2	5	4129	B8W	O4'-C4'	3.47	1.52	1.45
2	5	1605	7MG	C2-N1	3.47	1.46	1.37
2	5	729	2MG	O6-C6	-3.47	1.17	1.23
2	5	4623	OMG	C5-N7	-3.46	1.32	1.39
2	5	4194	I4U	O4'-C1'	3.46	1.50	1.42
2	5	1582	PSU	C6-C5	3.46	1.39	1.35
2	5	3825	A2M	C5-C4	-3.46	1.32	1.39
49	9	1703	OMC	C6-N1	3.46	1.46	1.38
49	9	484	A2M	O2'-C2'	3.46	1.51	1.42
2	5	2422	OMC	C2-N1	3.45	1.47	1.40
2	5	4536	OMC	C2-N1	3.45	1.47	1.40
2	5	2522	7MG	C5-C6	3.45	1.52	1.43
49	9	509	OMG	C5-N7	-3.45	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	9	517	OMC	C6-N1	3.44	1.46	1.38
49	9	166	A2M	O2'-C2'	3.44	1.51	1.42
2	5	4571	A2M	O2'-C2'	3.44	1.51	1.42
2	5	2804	OMC	C2-N1	3.44	1.47	1.40
2	5	2297	E7G	C8-N7	3.43	1.52	1.45
2	5	3718	A2M	O2'-C2'	3.43	1.51	1.42
2	5	4370	OMG	C5-N7	-3.43	1.32	1.39
2	5	2297	E7G	C2-N1	3.43	1.46	1.37
49	9	174	OMC	C6-N1	3.43	1.46	1.38
2	5	1605	7MG	C5-C6	3.42	1.52	1.43
2	5	3897	B8K	C5-C6	3.41	1.52	1.43
2	5	2401	A2M	C5-N7	-3.41	1.32	1.39
2	5	4196	OMG	C5-N7	-3.41	1.32	1.39
2	5	4371	MHG	C5-C6	3.40	1.52	1.43
2	5	4550	7MG	C5-C6	3.40	1.52	1.43
49	9	1031	A2M	C5-C4	-3.40	1.33	1.39
2	5	4355	E6G	C5-N7	-3.40	1.32	1.39
2	5	4472	B8W	O4'-C4'	3.39	1.52	1.45
2	5	2363	A2M	C8-N9	-3.39	1.31	1.37
2	5	1871	A2M	O2'-C2'	3.39	1.51	1.42
4	8	14	OMU	O4-C4	-3.38	1.17	1.24
2	5	3899	BGH	C5-N7	3.38	1.46	1.39
2	5	2401	A2M	C5-C4	-3.38	1.33	1.39
2	5	2363	A2M	O2'-C2'	3.38	1.51	1.42
2	5	3909	OMC	C6-N1	3.38	1.46	1.38
2	5	1326	A2M	C5-C4	-3.37	1.33	1.39
2	5	1883	OMG	C5-N7	-3.37	1.32	1.39
49	9	159	A2M	C5-N7	-3.37	1.32	1.39
2	5	2522	7MG	C2-N1	3.37	1.45	1.37
2	5	2050	OMG	C5-N7	-3.36	1.32	1.39
2	5	4523	A2M	C5-N7	-3.36	1.32	1.39
2	5	1797	E7G	C8-N7	3.35	1.51	1.45
49	9	1842	4AC	C5-C4	3.35	1.48	1.41
2	5	4536	OMC	O2-C2	-3.34	1.17	1.23
2	5	398	A2M	O2'-C2'	3.34	1.50	1.42
2	5	4129	B8W	C3'-C2'	3.34	1.62	1.53
2	5	373	OMG	C5-N7	-3.33	1.32	1.39
2	5	4129	B8W	C5-C4	-3.33	1.33	1.39
2	5	4355	E6G	O6-C6	3.33	1.39	1.34
2	5	3723	A2M	C5-C4	-3.33	1.33	1.39
2	5	4571	A2M	C5-C4	-3.33	1.33	1.39
2	5	3723	A2M	C5-N7	-3.33	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	9	1031	A2M	O2'-C2'	3.33	1.50	1.42
2	5	2773	OMG	C5-N7	-3.32	1.32	1.39
49	9	484	A2M	C5-C4	-3.32	1.33	1.39
2	5	4306	OMU	C4-N3	3.32	1.44	1.38
2	5	3867	A2M	O2'-C2'	3.31	1.50	1.42
49	9	27	A2M	C5-C4	-3.31	1.33	1.39
49	9	668	A2M	O2'-C2'	3.31	1.50	1.42
2	5	1524	A2M	O2'-C2'	3.31	1.50	1.42
2	5	3869	OMC	C2-N1	3.31	1.47	1.40
49	9	822	PSU	C6-C5	3.30	1.38	1.35
2	5	3792	OMG	C5-N7	-3.30	1.32	1.39
2	5	4185	B8W	O4'-C4'	3.30	1.52	1.45
49	9	1710	OMC	C6-N1	3.30	1.45	1.38
2	5	3899	BGH	O6-C6	-3.29	1.17	1.23
2	5	4355	E6G	O2'-C2'	3.29	1.51	1.43
49	9	644	OMG	C5-N7	-3.29	1.32	1.39
49	9	1850	MA6	C5-N7	-3.29	1.33	1.39
49	9	166	A2M	C5-N7	-3.28	1.33	1.39
2	5	1522	OMG	C5-N7	-3.28	1.32	1.39
2	5	4306	OMU	O2-C2	-3.28	1.17	1.23
2	5	4371	MHG	C6-N1	3.27	1.45	1.38
2	5	3825	A2M	O2'-C2'	3.27	1.50	1.42
2	5	1322	1MA	C5-C6	3.26	1.52	1.43
2	5	4306	OMU	O4-C4	-3.26	1.18	1.24
2	5	3701	OMC	C2-N1	3.26	1.46	1.40
2	5	1860	B8H	O4-C4	-3.25	1.17	1.23
2	5	398	A2M	C5-C4	-3.25	1.33	1.39
49	9	1678	A2M	C5-C4	-3.25	1.33	1.39
49	9	1851	MA6	C5-N7	-3.25	1.33	1.39
2	5	1909	P7G	C5-C4	3.24	1.44	1.36
2	5	3869	OMC	C6-N1	3.24	1.45	1.38
2	5	3785	A2M	O2'-C2'	3.24	1.50	1.42
2	5	3718	A2M	C5-C4	-3.24	1.33	1.39
2	5	2364	OMG	C5-N7	-3.24	1.32	1.39
2	5	4550	7MG	C2-N1	3.23	1.45	1.37
2	5	4494	OMG	C5-N7	-3.23	1.32	1.39
2	5	4194	I4U	O4-C41	-3.22	1.40	1.47
2	5	2861	OMC	C6-N1	3.22	1.45	1.38
2	5	4571	A2M	C5-N7	-3.21	1.33	1.39
2	5	4690	B8K	C5-C6	3.21	1.51	1.43
49	9	121	OMU	O4-C4	-3.21	1.18	1.24
2	5	4620	OMU	O4-C4	-3.21	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4671	B8T	C5-C4	3.20	1.48	1.41
49	9	166	A2M	C5-C4	-3.20	1.33	1.39
2	5	3867	A2M	C5-N7	-3.20	1.33	1.39
2	5	4355	E6G	O3'-C3'	-3.19	1.35	1.43
2	5	2365	OMC	O2-C2	-3.19	1.17	1.23
2	5	4870	OMG	C5-N7	-3.19	1.32	1.39
49	9	668	A2M	C5-N7	-3.17	1.33	1.39
2	5	4220	6MZ	C5-C6	-3.17	1.34	1.41
49	9	1703	OMC	O2-C2	-3.17	1.17	1.23
2	5	3764	PSU	C6-C5	3.16	1.38	1.35
2	5	3825	A2M	C5-N7	-3.16	1.33	1.39
2	5	1322	1MA	C2-N1	3.15	1.42	1.35
49	9	484	A2M	C5-N7	-3.15	1.33	1.39
2	5	3887	OMC	O2-C2	-3.15	1.17	1.23
2	5	3887	OMC	C6-N1	3.15	1.45	1.38
2	5	2804	OMC	O2-C2	-3.14	1.17	1.23
2	5	4523	A2M	O2'-C2'	3.14	1.50	1.42
2	5	3701	OMC	C6-N1	3.13	1.45	1.38
2	5	3899	BGH	C2-N1	3.12	1.45	1.37
2	5	2401	A2M	O2'-C2'	3.12	1.50	1.42
2	5	4194	I4U	O2'-C2'	3.12	1.50	1.43
2	5	4415	1MA	C5-C6	3.12	1.52	1.43
2	5	2804	OMC	C6-N1	3.11	1.45	1.38
2	5	3909	OMC	C2-N1	3.11	1.46	1.40
2	5	2365	OMC	C2-N1	3.10	1.46	1.40
2	5	1677	PSU	O4'-C1'	-3.10	1.39	1.43
2	5	4529	B8W	C3'-C2'	3.10	1.61	1.53
2	5	4536	OMC	C6-N1	3.10	1.45	1.38
2	5	1348	P4U	O2-C2	-3.10	1.17	1.23
49	9	1850	MA6	C8-N9	-3.09	1.32	1.37
2	5	4637	OMG	C5-N7	-3.09	1.32	1.39
49	9	1851	MA6	C5-C4	-3.09	1.33	1.39
49	9	823	PSU	C6-C5	3.09	1.38	1.35
2	5	1883	OMG	O6-C6	-3.08	1.17	1.23
2	5	2380	B8W	C5-N7	-3.08	1.33	1.39
2	5	3887	OMC	C2-N1	3.08	1.46	1.40
49	9	1678	A2M	C5-N7	-3.08	1.33	1.39
2	5	4185	B8W	C5-N7	-3.08	1.33	1.39
49	9	683	OMG	C5-N7	-3.08	1.32	1.39
2	5	3718	A2M	C8-N9	-3.07	1.32	1.37
2	5	1659	I4U	O4-C41	-3.07	1.40	1.47
49	9	119	PSU	C6-C5	3.07	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	9	517	OMC	O2-C2	-3.06	1.18	1.23
2	5	1524	A2M	C8-N9	-3.05	1.32	1.37
2	5	1871	A2M	C8-N9	-3.05	1.32	1.37
49	9	1374	5MC	O2-C2	-3.04	1.18	1.23
2	5	3880	P7G	C5-C4	3.04	1.44	1.36
49	9	1832	6MZ	C5-C4	-3.04	1.33	1.39
2	5	4872	2MG	C5-N7	-3.04	1.33	1.39
49	9	116	OMU	O4-C4	-3.04	1.18	1.24
49	9	159	A2M	C5-C4	-3.04	1.33	1.39
2	5	2422	OMC	O2-C2	-3.03	1.18	1.23
2	5	4194	I4U	O2-C2	-3.03	1.18	1.23
2	5	2424	OMG	C5-N7	-3.02	1.33	1.39
2	5	3762	B8H	O4-C4	-3.02	1.17	1.23
2	5	4483	B8T	O2-C2	-3.02	1.18	1.23
49	9	27	A2M	C8-N9	-3.02	1.32	1.37
2	5	2364	OMG	O6-C6	-3.01	1.17	1.23
2	5	4872	2MG	C4-N9	-3.01	1.30	1.38
2	5	4529	B8W	C5-C4	-3.01	1.33	1.39
49	9	1678	A2M	C8-N9	-2.99	1.32	1.37
2	5	4296	B8H	O4-C4	-2.98	1.17	1.23
2	5	4220	6MZ	C4-N9	-2.98	1.31	1.37
2	5	4472	B8W	C3'-C2'	2.98	1.61	1.53
2	5	4083	5MU	O2-C2	-2.98	1.17	1.23
2	5	3869	OMC	O2-C2	-2.98	1.18	1.23
2	5	3715	PSU	C6-C5	2.97	1.38	1.35
49	9	1710	OMC	O2-C2	-2.96	1.18	1.23
2	5	3825	A2M	C8-N9	-2.96	1.32	1.37
2	5	4483	B8T	C6-N1	2.95	1.45	1.38
2	5	2050	OMG	O6-C6	-2.95	1.18	1.23
2	5	2424	OMG	O6-C6	-2.95	1.18	1.23
49	9	159	A2M	C8-N9	-2.94	1.32	1.37
2	5	4185	B8W	C4-N9	-2.94	1.31	1.37
2	5	3782	5MC	O2-C2	-2.94	1.18	1.23
2	5	4083	5MU	O4-C4	-2.94	1.18	1.23
2	5	4671	B8T	O2-C2	-2.94	1.18	1.23
2	5	3729	PSU	C6-C5	2.94	1.38	1.35
49	9	1832	6MZ	C4-N9	-2.93	1.31	1.37
2	5	4293	PSU	C6-C5	2.92	1.38	1.35
2	5	1659	I4U	O2'-C2'	2.92	1.50	1.43
2	5	2380	B8W	O6-C6	2.92	1.39	1.35
2	5	1316	OMG	C5-N7	-2.92	1.33	1.39
2	5	3899	BGH	C71-N7	2.91	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1326	A2M	C8-N9	-2.91	1.32	1.37
49	9	814	5MU	O4-C4	-2.91	1.18	1.23
49	9	1851	MA6	C8-N9	-2.90	1.32	1.37
49	9	683	OMG	O6-C6	-2.90	1.18	1.23
49	9	1031	A2M	C8-N9	-2.90	1.32	1.37
2	5	4571	A2M	C8-N9	-2.90	1.32	1.37
2	5	4483	B8T	C5-C4	2.90	1.47	1.41
49	9	1850	MA6	C5-C4	-2.89	1.33	1.39
2	5	3792	OMG	O6-C6	-2.89	1.18	1.23
2	5	2522	7MG	C6-N1	2.88	1.44	1.38
49	9	668	A2M	C8-N9	-2.88	1.32	1.37
2	5	3897	B8K	O6-C6	-2.87	1.18	1.23
2	5	3897	B8K	C6-N1	2.87	1.44	1.38
49	9	174	OMC	O2-C2	-2.87	1.18	1.23
2	5	2401	A2M	C8-N9	-2.87	1.32	1.37
2	5	4636	PSU	C6-C5	2.87	1.38	1.35
49	9	1337	4AC	O2-C2	-2.86	1.18	1.23
2	5	4530	UR3	C6-N1	2.86	1.44	1.38
2	5	3867	A2M	C8-N9	-2.85	1.32	1.37
2	5	3785	A2M	C3'-C4'	2.85	1.60	1.53
49	9	1842	4AC	O2-C2	-2.85	1.18	1.23
2	5	2508	PSU	C6-C5	2.85	1.38	1.35
2	5	1659	I4U	O2-C2	-2.84	1.18	1.23
2	5	4472	B8W	C5-N7	-2.84	1.33	1.39
2	5	4196	OMG	O6-C6	-2.84	1.18	1.23
2	5	4550	7MG	C6-N1	2.83	1.44	1.38
2	5	1659	I4U	C6-N1	2.83	1.44	1.38
2	5	1534	A2M	O2'-C2'	2.83	1.49	1.42
2	5	1316	OMG	C4-N9	-2.83	1.30	1.38
2	5	4531	PSU	C6-C5	2.82	1.38	1.35
2	5	1456	B8Q	O2-C2	-2.82	1.17	1.22
2	5	4220	6MZ	C8-N9	-2.82	1.32	1.37
2	5	4620	OMU	O2-C2	-2.80	1.18	1.23
2	5	3723	A2M	C8-N9	-2.79	1.32	1.37
2	5	1316	OMG	O6-C6	-2.79	1.18	1.23
49	9	484	A2M	C8-N9	-2.79	1.32	1.37
2	5	1605	7MG	O6-C6	-2.78	1.18	1.23
2	5	4370	OMG	O6-C6	-2.78	1.18	1.23
2	5	4690	B8K	C6-N1	2.78	1.44	1.38
2	5	4494	OMG	C4-N9	-2.77	1.31	1.38
49	9	568	E3C	C6-N1	2.76	1.44	1.38
49	9	121	OMU	O2-C2	-2.76	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4494	OMG	O6-C6	-2.76	1.18	1.23
2	5	3701	OMC	O2-C2	-2.76	1.18	1.23
2	5	4442	PSU	C6-C5	2.75	1.38	1.35
2	5	4355	E6G	C5-C6	-2.75	1.36	1.41
2	5	1605	7MG	C6-N1	2.75	1.44	1.38
49	9	1337	4AC	C6-N1	2.75	1.44	1.38
2	5	4472	B8W	C4-N9	-2.75	1.32	1.37
49	9	814	5MU	O2-C2	-2.74	1.18	1.23
2	5	4597	UR3	C6-N1	2.74	1.44	1.38
2	5	4529	B8W	C5-N7	-2.73	1.34	1.39
2	5	3785	A2M	C8-N9	-2.73	1.32	1.37
2	5	2380	B8W	C5-C6	-2.73	1.36	1.41
2	5	1866	UR3	O4-C4	-2.73	1.17	1.23
2	5	4220	6MZ	C6-N1	-2.72	1.30	1.35
2	5	1574	B9B	C5-C4	-2.72	1.34	1.39
2	5	2754	B9B	C5-C4	-2.72	1.34	1.39
2	5	4129	B8W	C5-N7	-2.72	1.34	1.39
2	5	4671	B8T	C6-N1	2.71	1.44	1.38
2	5	1522	OMG	O6-C6	-2.71	1.18	1.23
2	5	4550	7MG	O6-C6	-2.69	1.18	1.23
2	5	1625	OMG	O6-C6	-2.69	1.18	1.23
49	9	1219	B8Q	O2-C2	-2.69	1.17	1.22
49	9	644	OMG	O6-C6	-2.69	1.18	1.23
2	5	4185	B8W	C5-C6	-2.67	1.36	1.41
49	9	1081	PSU	C6-C5	2.66	1.38	1.35
2	5	4623	OMG	O6-C6	-2.66	1.18	1.23
49	9	1842	4AC	C6-N1	2.65	1.44	1.38
49	9	509	OMG	O6-C6	-2.65	1.18	1.23
2	5	1797	E7G	C6-N1	2.64	1.43	1.38
49	9	166	A2M	C8-N9	-2.64	1.33	1.37
2	5	2424	OMG	C4-N9	-2.63	1.31	1.38
49	9	1830	UR3	C6-N1	2.63	1.44	1.38
2	5	398	A2M	C8-N9	-2.62	1.33	1.37
2	5	3880	P7G	O6-C6	-2.62	1.19	1.23
2	5	4472	B8W	C8-N9	-2.61	1.33	1.37
2	5	4403	PSU	C6-C5	2.61	1.38	1.35
2	5	2773	OMG	C2-N1	2.61	1.44	1.37
2	5	4637	OMG	O6-C6	-2.60	1.18	1.23
2	5	4872	2MG	C6-N1	2.60	1.43	1.38
2	5	4129	B8W	C8-N9	-2.59	1.33	1.37
2	5	2380	B8W	C8-N9	-2.59	1.33	1.37
2	5	1909	P7G	O6-C6	-2.58	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	2773	OMG	O6-C6	-2.58	1.18	1.23
2	5	4529	B8W	C8-N9	-2.58	1.33	1.37
2	5	2424	OMG	C2-N1	2.57	1.43	1.37
49	9	116	OMU	O2-C2	-2.57	1.18	1.23
2	5	2297	E7G	C6-N1	2.57	1.43	1.38
2	5	4870	OMG	C2-N1	2.57	1.43	1.37
49	9	612	PSU	C6-C5	2.56	1.38	1.35
2	5	2050	OMG	C4-N9	-2.56	1.31	1.38
2	5	237	B9B	C5-C4	-2.55	1.34	1.39
2	5	4500	PSU	C6-C5	2.54	1.38	1.35
49	9	1830	UR3	O2-C2	-2.54	1.17	1.22
49	9	509	OMG	C2-N1	2.54	1.43	1.37
2	5	4623	OMG	C2-N1	2.53	1.43	1.37
2	5	2754	B9B	O2'-C2'	2.53	1.49	1.43
2	5	373	OMG	O6-C6	-2.53	1.18	1.23
49	9	668	A2M	C4-N9	-2.51	1.32	1.37
2	5	3899	BGH	C6-N1	2.51	1.43	1.38
2	5	1574	B9B	O2'-C2'	2.50	1.49	1.43
4	8	14	OMU	O2-C2	-2.50	1.18	1.23
2	5	4523	A2M	C8-N9	-2.50	1.33	1.37
2	5	1348	P4U	C6-N1	2.49	1.44	1.38
2	5	4870	OMG	O6-C6	-2.49	1.18	1.23
2	5	4450	PSU	C4-C5	-2.49	1.37	1.44
2	5	2050	OMG	C2-N1	2.49	1.43	1.37
2	5	4637	OMG	C4-N9	-2.49	1.31	1.38
2	5	2522	7MG	O6-C6	-2.48	1.18	1.23
49	9	121	OMU	C6-N1	2.48	1.44	1.38
49	9	683	OMG	C2-N1	2.47	1.43	1.37
2	5	4371	MHG	O6-C6	-2.47	1.18	1.23
49	9	1830	UR3	O4-C4	-2.47	1.18	1.23
2	5	373	OMG	C4-N9	-2.46	1.31	1.38
2	5	4194	I4U	C6-N1	2.46	1.43	1.38
2	5	4129	B8W	C4-N9	-2.46	1.32	1.37
2	5	4628	PSU	C6-C5	2.45	1.38	1.35
49	9	644	OMG	C2-N1	2.44	1.43	1.37
2	5	4623	OMG	C4-N9	-2.44	1.31	1.38
2	5	3897	B8K	C5-C4	2.44	1.45	1.37
2	5	4185	B8W	C8-N9	-2.43	1.33	1.37
2	5	4494	OMG	C2-N1	2.43	1.43	1.37
2	5	1797	E7G	O6-C6	-2.43	1.19	1.23
2	5	4872	2MG	C5-C6	2.43	1.53	1.44
2	5	4597	UR3	O4-C4	-2.43	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	9	159	A2M	C5'-C4'	2.43	1.58	1.51
2	5	4530	UR3	O4-C4	-2.43	1.18	1.23
2	5	2773	OMG	C4-N9	-2.42	1.31	1.38
2	5	1866	UR3	C6-N1	2.42	1.43	1.38
2	5	4529	B8W	C4-N9	-2.41	1.32	1.37
2	5	4370	OMG	C2-N1	2.41	1.43	1.37
2	5	1316	OMG	C2-N1	2.40	1.43	1.37
2	5	4196	OMG	C4-N9	-2.39	1.32	1.38
2	5	4523	A2M	C4-N9	-2.39	1.32	1.37
2	5	1683	PSU	C4-C5	-2.39	1.37	1.44
49	9	509	OMG	C4-N9	-2.38	1.32	1.38
49	9	1832	6MZ	C6-N1	-2.38	1.31	1.35
49	9	27	A2M	C5'-C4'	2.38	1.58	1.51
2	5	1909	P7G	C8-N7	2.37	1.50	1.45
2	5	2364	OMG	C2-N1	2.36	1.43	1.37
2	5	1625	OMG	C4-N9	-2.35	1.32	1.38
2	5	3880	P7G	C8-N7	2.35	1.49	1.45
49	9	1081	PSU	O4'-C1'	-2.35	1.40	1.43
2	5	4220	6MZ	C5-N7	-2.34	1.34	1.39
2	5	1522	OMG	C4-N9	-2.34	1.32	1.38
49	9	1842	4AC	O7-C7	-2.33	1.18	1.23
2	5	4530	UR3	C4-N3	2.33	1.45	1.40
2	5	4415	1MA	C5-N7	-2.33	1.34	1.39
2	5	1866	UR3	O2-C2	-2.33	1.18	1.22
2	5	4636	PSU	C4-C5	-2.33	1.37	1.44
2	5	4637	OMG	C2-N1	2.33	1.43	1.37
2	5	4442	PSU	C4-C5	-2.33	1.37	1.44
2	5	2754	B9B	C5'-C4'	2.32	1.58	1.51
2	5	1322	1MA	C5-N7	-2.32	1.34	1.39
2	5	1677	PSU	C4-C5	-2.32	1.37	1.44
2	5	4196	OMG	C2-N1	2.31	1.43	1.37
2	5	4597	UR3	O2-C2	-2.31	1.18	1.22
2	5	2424	OMG	C5-C6	2.31	1.53	1.44
2	5	1316	OMG	C5-C6	2.31	1.53	1.44
49	9	1248	B8N	O4-C4	-2.31	1.18	1.23
2	5	4472	B8W	C5-C6	-2.31	1.37	1.41
49	9	644	OMG	C5-C6	2.30	1.53	1.44
2	5	3785	A2M	C4-N9	-2.30	1.32	1.37
2	5	1522	OMG	C2-N1	2.30	1.43	1.37
2	5	4355	E6G	C8-N9	-2.30	1.33	1.37
2	5	1883	OMG	C2-N1	2.29	1.43	1.37
2	5	1625	OMG	C2-N1	2.29	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	373	OMG	C2-N1	2.29	1.43	1.37
2	5	2297	E7G	O6-C6	-2.28	1.19	1.23
2	5	4530	UR3	O2-C2	-2.27	1.18	1.22
2	5	1522	OMG	C5-C6	2.27	1.52	1.44
2	5	1883	OMG	C4-N9	-2.27	1.32	1.38
2	5	4637	OMG	C5-C6	2.26	1.52	1.44
2	5	3792	OMG	C5-C6	2.26	1.52	1.44
2	5	3718	A2M	C5'-C4'	2.26	1.58	1.51
49	9	1031	A2M	C5'-C4'	2.26	1.58	1.51
2	5	4494	OMG	C6-N1	2.25	1.43	1.38
2	5	2363	A2M	C5'-C4'	2.25	1.58	1.51
2	5	4306	OMU	C6-N1	2.25	1.43	1.38
2	5	2364	OMG	C4-N9	-2.25	1.32	1.38
2	5	1534	A2M	C5'-C4'	2.25	1.58	1.51
2	5	1524	A2M	C5'-C4'	2.24	1.58	1.51
2	5	4450	PSU	C6-C5	2.24	1.37	1.35
2	5	3723	A2M	C3'-C4'	2.24	1.58	1.53
49	9	568	E3C	O2-C2	-2.24	1.18	1.22
49	9	683	OMG	C4-N9	-2.24	1.32	1.38
2	5	237	B9B	O2'-C2'	2.24	1.48	1.43
2	5	1316	OMG	C6-N1	2.24	1.43	1.38
2	5	4870	OMG	C5-C6	2.24	1.52	1.44
2	5	3718	A2M	C4-N9	-2.23	1.33	1.37
2	5	4531	PSU	C4-C5	-2.23	1.38	1.44
49	9	1678	A2M	C3'-C4'	2.23	1.58	1.53
2	5	2773	OMG	C6-N1	2.23	1.43	1.38
2	5	2773	OMG	C5-C6	2.22	1.52	1.44
49	9	668	A2M	C6-N1	-2.22	1.29	1.35
2	5	3792	OMG	C4-N9	-2.21	1.32	1.38
2	5	3792	OMG	C2-N1	2.21	1.43	1.37
2	5	729	2MG	C5-C6	2.21	1.52	1.44
2	5	1524	A2M	C6-N1	-2.20	1.29	1.35
2	5	2401	A2M	C5'-C4'	2.20	1.58	1.51
2	5	1677	PSU	C6-C5	2.20	1.37	1.35
2	5	4293	PSU	C4-C5	-2.20	1.38	1.44
2	5	3825	A2M	C4-N9	-2.19	1.33	1.37
49	9	683	OMG	C5-C6	2.19	1.52	1.44
49	9	644	OMG	C4-N9	-2.18	1.32	1.38
2	5	1534	A2M	C6-N1	-2.18	1.29	1.35
2	5	3867	A2M	C4-N9	-2.18	1.33	1.37
2	5	4623	OMG	C6-N1	2.18	1.42	1.38
49	9	484	A2M	C5'-C4'	2.17	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	9	1678	A2M	C5'-C4'	2.17	1.58	1.51
2	5	1883	OMG	C5-C6	2.16	1.52	1.44
2	5	4620	OMU	C6-N1	2.16	1.43	1.38
2	5	4523	A2M	C5'-C4'	2.16	1.58	1.51
2	5	1326	A2M	C4-N9	-2.15	1.33	1.37
2	5	3867	A2M	C5'-C4'	2.15	1.58	1.51
2	5	4571	A2M	C5'-C4'	2.15	1.58	1.51
49	9	484	A2M	C4-N9	-2.15	1.33	1.37
2	5	4500	PSU	C4-C5	-2.15	1.38	1.44
49	9	509	OMG	C5-C6	2.15	1.52	1.44
2	5	1574	B9B	C5'-C4'	2.14	1.58	1.51
2	5	4370	OMG	C5-C6	2.14	1.52	1.44
2	5	3723	A2M	C4-N9	-2.14	1.33	1.37
2	5	4628	PSU	O4'-C1'	-2.13	1.40	1.43
2	5	4870	OMG	C6-N1	2.13	1.42	1.38
49	9	1248	B8N	O2-C2	-2.13	1.18	1.22
49	9	1081	PSU	C4-C5	-2.12	1.38	1.44
49	9	116	OMU	C6-N1	2.12	1.43	1.38
2	5	4500	PSU	O4'-C1'	-2.12	1.40	1.43
2	5	2363	A2M	C4-N9	-2.12	1.33	1.37
2	5	2424	OMG	C6-N1	2.12	1.42	1.38
2	5	3785	A2M	C5'-C4'	2.12	1.57	1.51
2	5	1524	A2M	C3'-C4'	2.12	1.58	1.53
49	9	27	A2M	C4-N9	-2.12	1.33	1.37
2	5	4494	OMG	C5-C6	2.12	1.52	1.44
2	5	4623	OMG	C5-C6	2.12	1.52	1.44
2	5	3718	A2M	C6-N1	-2.11	1.29	1.35
2	5	398	A2M	C5'-C4'	2.11	1.57	1.51
2	5	3723	A2M	C5'-C4'	2.11	1.57	1.51
2	5	2401	A2M	C4-N9	-2.10	1.33	1.37
4	8	14	OMU	C6-N1	2.10	1.43	1.38
49	9	683	OMG	C6-N1	2.10	1.42	1.38
2	5	237	B9B	C5'-C4'	2.10	1.57	1.51
2	5	4370	OMG	C4-N9	-2.10	1.32	1.38
2	5	1625	OMG	C5-C6	2.09	1.52	1.44
2	5	2050	OMG	C5-C6	2.09	1.52	1.44
49	9	1850	MA6	C8-N7	2.09	1.35	1.31
2	5	4628	PSU	C4-C5	-2.09	1.38	1.44
49	9	612	PSU	O4'-C1'	-2.09	1.41	1.43
49	9	27	A2M	C3'-C4'	2.09	1.58	1.53
49	9	484	A2M	C3'-C4'	2.09	1.58	1.53
2	5	1517	2MG	C5-C6	2.08	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1326	A2M	C3'-C4'	2.08	1.58	1.53
49	9	1678	A2M	C4-N9	-2.08	1.33	1.37
49	9	159	A2M	C2-N3	2.08	1.37	1.33
49	9	1031	A2M	C3'-C4'	2.07	1.58	1.53
2	5	3825	A2M	C6-N1	-2.07	1.30	1.35
2	5	2380	B8W	C4-N9	-2.07	1.33	1.37
2	5	1534	A2M	C3'-C4'	2.07	1.58	1.53
2	5	373	OMG	C6-N1	2.07	1.42	1.38
49	9	1337	4AC	O7-C7	-2.07	1.18	1.23
2	5	398	A2M	C3'-C4'	2.07	1.58	1.53
49	9	27	A2M	C6-N1	-2.06	1.30	1.35
2	5	3785	A2M	C6-N1	-2.06	1.30	1.35
2	5	2363	A2M	C6-N1	-2.06	1.30	1.35
2	5	4196	OMG	C5-C6	2.06	1.52	1.44
2	5	2363	A2M	C3'-C4'	2.05	1.58	1.53
2	5	1871	A2M	C4-N9	-2.05	1.33	1.37
2	5	373	OMG	C5-C6	2.05	1.52	1.44
2	5	3729	PSU	C4-C5	-2.05	1.38	1.44
2	5	4690	B8K	C5-C4	2.05	1.44	1.37
2	5	1871	A2M	C5'-C4'	2.05	1.57	1.51
2	5	1456	B8Q	C4-N3	-2.05	1.45	1.48
2	5	1871	A2M	C6-N1	-2.05	1.30	1.35
49	9	1031	A2M	C6-N1	-2.05	1.30	1.35
2	5	2401	A2M	C3'-C4'	2.05	1.58	1.53
2	5	1326	A2M	C5'-C4'	2.04	1.57	1.51
2	5	3718	A2M	C3'-C4'	2.04	1.58	1.53
2	5	1326	A2M	C6-N1	-2.04	1.30	1.35
2	5	4870	OMG	C4-N9	-2.03	1.32	1.38
2	5	2401	A2M	C6-N1	-2.03	1.30	1.35
2	5	4296	B8H	O4'-C1'	-2.02	1.41	1.43
49	9	1243	PSU	O4'-C1'	-2.01	1.41	1.43
2	5	4571	A2M	C4-N9	-2.01	1.33	1.37
49	9	166	A2M	C5'-C4'	2.01	1.57	1.51
49	9	823	PSU	C4-C5	-2.01	1.38	1.44
2	5	2364	OMG	C5-C6	2.00	1.51	1.44
2	5	4523	A2M	C3'-C4'	2.00	1.58	1.53
2	5	1582	PSU	O4'-C1'	-2.00	1.41	1.43
49	9	509	OMG	C6-N1	2.00	1.42	1.38
49	9	1219	B8Q	C4-N3	-2.00	1.45	1.48

All (1011) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	2380	B8W	N2-C2-N3	19.07	145.81	117.22
2	5	4529	B8W	N2-C2-N3	18.80	145.41	117.22
2	5	4185	B8W	N2-C2-N3	18.44	144.87	117.22
2	5	4472	B8W	N2-C2-N3	18.00	144.22	117.22
2	5	4129	B8W	N2-C2-N3	17.96	144.15	117.22
2	5	2380	B8W	N2-C2-N1	-15.59	93.85	117.22
2	5	4529	B8W	N2-C2-N1	-15.35	94.21	117.22
2	5	4185	B8W	N2-C2-N1	-15.12	94.56	117.22
2	5	4472	B8W	N2-C2-N1	-14.67	95.23	117.22
2	5	4129	B8W	N2-C2-N1	-14.54	95.43	117.22
2	5	4564	M7A	C5-C6-N6	13.21	146.19	123.75
49	9	1832	6MZ	C4-N9-C8	13.17	119.57	105.74
49	9	1806	M7A	C5-C6-N6	12.48	144.96	123.75
2	5	4220	6MZ	C4-N9-C8	12.10	118.45	105.74
2	5	2380	B8W	C1'-N9-C8	-11.90	100.68	127.09
2	5	4083	5MU	C5-C4-N3	11.64	125.44	115.32
49	9	814	5MU	C5-C4-N3	11.46	125.29	115.32
2	5	4529	B8W	C1'-N9-C8	-11.15	102.36	127.09
2	5	4564	M7A	N6-C6-N1	-10.88	94.14	118.38
2	5	4129	B8W	C1'-N9-C8	-10.77	103.19	127.09
2	5	4472	B8W	C1'-N9-C8	-10.71	103.32	127.09
2	5	4185	B8W	C1'-N9-C8	-10.37	104.08	127.09
49	9	1806	M7A	N6-C6-N1	-10.32	95.39	118.38
2	5	2380	B8W	C4-N9-C1'	10.21	150.51	126.63
2	5	4872	2MG	N1-C2-N2	10.11	126.88	116.56
49	9	1832	6MZ	N9-C8-N7	-9.93	99.85	113.94
2	5	4529	B8W	C4-N9-C1'	9.63	149.16	126.63
2	5	4529	B8W	O6-C6-C5	9.63	128.78	117.17
2	5	4129	B8W	C4-N9-C1'	9.48	148.81	126.63
49	9	1850	MA6	N1-C6-N6	-9.21	105.64	116.86
2	5	4472	B8W	C4-N9-C1'	9.14	148.00	126.63
2	5	4220	6MZ	N9-C8-N7	-9.12	101.00	113.94
2	5	4220	6MZ	C5-C6-N1	9.10	127.92	118.15
49	9	814	5MU	C5-C6-N1	-8.67	113.90	123.31
2	5	4185	B8W	C4-N9-C1'	8.64	146.85	126.63
49	9	1851	MA6	N1-C6-N6	-8.26	106.79	116.86
2	5	1517	2MG	C2-N3-C4	8.21	122.27	112.00
2	5	4083	5MU	C5-C6-N1	-7.82	114.81	123.31
2	5	1659	I4U	O4-C4-C5	7.54	120.80	115.45
2	5	4194	I4U	O4-C4-C5	7.40	120.70	115.45
2	5	2754	B9B	C5-C4-N3	-7.38	119.41	127.18
2	5	4355	E6G	C5-C4-N3	-7.27	119.52	127.18
2	5	237	B9B	C5-C4-N3	-7.16	119.64	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4296	B8H	C4-N3-C2	-7.14	117.98	127.34
2	5	4220	6MZ	N3-C4-N9	7.10	139.24	127.17
49	9	1832	6MZ	C5-C6-N1	7.08	125.75	118.15
2	5	4872	2MG	C2-N3-C4	7.05	120.82	112.00
49	9	568	E3C	C1'-N1-C2	7.04	128.56	117.04
2	5	1348	P4U	O4-C4-C5	7.03	120.44	115.45
2	5	4529	B8W	C61-O6-C6	6.95	123.70	117.20
2	5	4296	B8H	N3-C2-N1	6.91	121.91	115.22
2	5	3762	B8H	C4-N3-C2	-6.90	118.30	127.34
2	5	1517	2MG	C5-C4-N3	-6.83	117.53	128.39
49	9	1219	B8Q	C1'-N1-C2	6.80	128.18	117.04
2	5	729	2MG	C5-C4-N3	-6.79	117.58	128.39
2	5	4129	B8W	O6-C6-C5	6.73	125.28	117.17
2	5	4564	M7A	N3-C4-N9	6.69	135.25	126.88
2	5	729	2MG	C2-N3-C4	6.68	120.35	112.00
2	5	3762	B8H	N3-C2-N1	6.57	121.58	115.22
2	5	1860	B8H	C4-N3-C2	-6.51	118.80	127.34
2	5	2380	B8W	C5-C4-N3	-6.49	120.34	127.18
2	5	1574	B9B	C5-C4-N3	-6.46	120.37	127.18
2	5	1797	E7G	C4-C5-N7	6.44	110.17	104.94
49	9	1850	MA6	C5-C6-N6	6.44	135.52	125.33
2	5	1871	A2M	N3-C2-N1	-6.43	118.85	128.58
2	5	4371	MHG	C2-N3-C4	6.31	119.89	112.00
4	8	14	OMU	C4-N3-C2	-6.30	118.78	126.61
2	5	4185	B8W	O6-C6-C5	6.28	124.75	117.17
2	5	4472	B8W	O6-C6-C5	6.23	124.68	117.17
2	5	1860	B8H	N3-C2-N1	6.22	121.24	115.22
2	5	2786	B9H	C31-N3-C2	6.20	124.91	117.29
2	5	3897	B8K	C72-C71-N7	6.19	127.94	118.80
2	5	4690	B8K	C5-C6-N1	6.14	121.75	110.94
2	5	4690	B8K	C72-C71-N7	6.11	127.81	118.80
2	5	4571	A2M	N3-C2-N1	-6.10	119.35	128.58
2	5	4355	E6G	C61-O6-C6	-6.10	111.52	117.57
2	5	4083	5MU	N3-C2-N1	6.07	122.80	114.89
49	9	1851	MA6	N1-C2-N3	-6.05	119.42	128.58
2	5	2401	A2M	N3-C2-N1	-6.04	119.44	128.58
49	9	1031	A2M	N3-C2-N1	-6.04	119.44	128.58
49	9	484	A2M	N3-C2-N1	-6.04	119.44	128.58
2	5	1524	A2M	N3-C2-N1	-6.03	119.46	128.58
49	9	1850	MA6	N1-C2-N3	-6.02	119.46	128.58
2	5	4620	OMU	C4-N3-C2	-6.02	119.14	126.61
2	5	2297	E7G	C4-C5-N7	6.00	109.81	104.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	3899	BGH	C5-C6-N1	5.99	121.49	110.94
2	5	3723	A2M	N3-C2-N1	-5.99	119.52	128.58
2	5	4306	OMU	C4-N3-C2	-5.96	119.21	126.61
2	5	4628	PSU	N1-C2-N3	5.95	121.44	115.17
2	5	1534	A2M	N3-C2-N1	-5.95	119.58	128.58
49	9	27	A2M	N3-C2-N1	-5.92	119.62	128.58
2	5	1326	A2M	N3-C2-N1	-5.91	119.63	128.58
2	5	4523	A2M	N3-C2-N1	-5.89	119.67	128.58
2	5	398	A2M	N3-C2-N1	-5.87	119.70	128.58
2	5	3825	A2M	N3-C2-N1	-5.86	119.71	128.58
49	9	166	A2M	N3-C2-N1	-5.86	119.72	128.58
2	5	4129	B8W	C5-C4-N3	-5.85	121.01	127.18
49	9	568	E3C	C4-N3-C2	-5.80	111.54	122.00
49	9	121	OMU	C4-N3-C2	-5.80	119.41	126.61
2	5	4564	M7A	N3-C2-N1	-5.80	119.81	128.58
2	5	4872	2MG	N2-C2-N3	-5.78	113.15	120.51
2	5	3792	OMG	C5-C4-N3	-5.77	119.20	128.39
2	5	3785	A2M	N3-C2-N1	-5.75	119.87	128.58
49	9	1832	6MZ	N3-C4-N9	5.75	136.94	127.17
2	5	2363	A2M	N3-C2-N1	-5.73	119.90	128.58
49	9	1806	M7A	N3-C2-N1	-5.71	119.94	128.58
2	5	3897	B8K	C4-C5-N7	5.71	109.55	104.93
49	9	116	OMU	C4-N3-C2	-5.71	119.53	126.61
2	5	4690	B8K	C4-C5-N7	5.70	109.54	104.93
49	9	1678	A2M	N3-C2-N1	-5.69	119.97	128.58
2	5	1524	A2M	C5-C4-N3	-5.68	118.90	126.72
2	5	4220	6MZ	N1-C2-N3	-5.63	120.07	128.58
49	9	1832	6MZ	N1-C2-N3	-5.63	120.07	128.58
49	9	1219	B8Q	O2-C2-N3	-5.59	115.11	122.95
49	9	166	A2M	C5-C4-N3	-5.56	119.06	126.72
2	5	4371	MHG	N1-C2-N2	5.54	122.21	116.56
2	5	398	A2M	C5-C4-N3	-5.53	119.10	126.72
49	9	568	E3C	O2-C2-N3	-5.53	115.03	122.10
2	5	4220	6MZ	C5-C4-N9	-5.52	99.80	105.81
2	5	4370	OMG	C5-C4-N3	-5.51	119.62	128.39
2	5	1322	1MA	N1-C2-N3	-5.50	119.46	126.00
49	9	1031	A2M	C5-C4-N3	-5.49	119.16	126.72
49	9	159	A2M	N3-C2-N1	-5.49	120.27	128.58
2	5	1322	1MA	C5-C4-N3	-5.48	119.21	127.27
2	5	4450	PSU	C4-N3-C2	-5.48	118.83	126.37
2	5	3867	A2M	N3-C2-N1	-5.48	120.29	128.58
2	5	4870	OMG	C5-C4-N3	-5.47	119.68	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4083	5MU	O4-C4-C5	-5.47	118.66	124.92
49	9	668	A2M	N3-C2-N1	-5.46	120.31	128.58
2	5	3897	B8K	C5-C6-N1	5.46	120.55	110.94
2	5	1883	OMG	C5-C4-N3	-5.40	119.80	128.39
49	9	644	OMG	C5-C4-N3	-5.38	119.83	128.39
2	5	1534	A2M	C5-C4-N3	-5.38	119.31	126.72
2	5	1625	OMG	C5-C4-N3	-5.37	119.84	128.39
2	5	1522	OMG	C5-C4-N3	-5.37	119.85	128.39
2	5	4450	PSU	N1-C2-N3	5.36	120.83	115.17
2	5	4636	PSU	C4-N3-C2	-5.36	118.99	126.37
2	5	4872	2MG	C1'-N9-C4	-5.35	110.68	126.49
2	5	2364	OMG	C5-C4-N3	-5.31	119.94	128.39
2	5	1677	PSU	C4-N3-C2	-5.31	119.06	126.37
2	5	4196	OMG	C5-C4-N3	-5.26	120.01	128.39
49	9	159	A2M	C5-C4-N3	-5.26	119.47	126.72
2	5	4636	PSU	N1-C2-N3	5.26	120.71	115.17
2	5	4403	PSU	N1-C2-N3	5.25	120.70	115.17
2	5	2363	A2M	C5-C4-N3	-5.24	119.51	126.72
2	5	4500	PSU	C4-N3-C2	-5.23	119.17	126.37
2	5	1605	7MG	C5-C6-N1	5.22	120.13	110.94
2	5	4529	B8W	O6-C6-N1	-5.22	112.02	118.96
2	5	4442	PSU	N1-C2-N3	5.22	120.67	115.17
2	5	237	B9B	O6-C6-C5	5.22	123.62	116.73
2	5	3899	BGH	C72-C71-N7	5.20	126.48	118.80
2	5	4872	2MG	C2-N1-C6	-5.20	118.27	124.55
49	9	683	OMG	C5-C4-N3	-5.19	120.12	128.39
2	5	4637	OMG	C5-C4-N3	-5.19	120.12	128.39
49	9	1248	B8N	C5-C4-N3	5.17	125.55	116.15
49	9	1851	MA6	C5-C6-N6	5.16	133.51	125.33
2	5	4472	B8W	C5-C4-N3	-5.16	121.74	127.18
2	5	3825	A2M	N6-C6-N1	-5.16	106.89	118.38
2	5	4529	B8W	C5-C4-N3	-5.16	121.75	127.18
49	9	27	A2M	C5-C4-N3	-5.14	119.64	126.72
2	5	4531	PSU	C4-N3-C2	-5.13	119.31	126.37
2	5	729	2MG	N9-C4-N3	5.12	136.20	125.95
2	5	4628	PSU	C4-N3-C2	-5.12	119.32	126.37
2	5	373	OMG	C5-C4-N3	-5.12	120.24	128.39
2	5	1909	P7G	C4-C5-N7	5.12	110.16	106.71
2	5	2297	E7G	C5-C6-N1	5.11	119.93	110.94
2	5	4415	1MA	C5-C4-N3	-5.10	119.77	127.27
2	5	4872	2MG	C1'-N9-C8	5.09	141.20	126.73
2	5	4083	5MU	C4-N3-C2	-5.08	120.67	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1797	E7G	C5-C6-N1	5.08	119.88	110.94
2	5	3880	P7G	C4-C5-N7	5.08	110.13	106.71
49	9	814	5MU	O4-C4-C5	-5.06	119.13	124.92
2	5	2401	A2M	C5-C4-N3	-5.06	119.75	126.72
2	5	1582	PSU	N1-C2-N3	5.05	120.49	115.17
2	5	4185	B8W	N9-C8-N7	-5.05	106.78	113.94
49	9	814	5MU	N3-C2-N1	5.04	121.46	114.89
2	5	4531	PSU	N1-C2-N3	5.04	120.48	115.17
2	5	3825	A2M	C5-C4-N3	-5.03	119.78	126.72
2	5	4355	E6G	C4-C5-C6	5.02	120.15	115.22
2	5	3718	A2M	N3-C2-N1	-5.02	120.99	128.58
2	5	1883	OMG	C2-N3-C4	5.01	120.93	112.30
49	9	484	A2M	N6-C6-N1	-5.01	107.22	118.38
2	5	4415	1MA	N1-C2-N3	-5.00	120.05	126.00
2	5	1871	A2M	C5-C4-N3	-5.00	119.83	126.72
2	5	4371	MHG	C5-C6-N1	4.99	119.73	110.94
2	5	4500	PSU	N1-C2-N3	4.98	120.42	115.17
2	5	4550	7MG	C5-C6-N1	4.98	119.70	110.94
2	5	4442	PSU	C4-N3-C2	-4.98	119.52	126.37
2	5	4571	A2M	C5-C4-N3	-4.98	119.86	126.72
49	9	683	OMG	C2-N3-C4	4.97	120.85	112.30
2	5	3792	OMG	C2-N3-C4	4.96	120.84	112.30
2	5	1524	A2M	N6-C6-N1	-4.96	107.33	118.38
2	5	1683	PSU	N1-C2-N3	4.94	120.38	115.17
2	5	4293	PSU	C4-N3-C2	-4.94	119.56	126.37
49	9	484	A2M	C5-C4-N3	-4.93	119.92	126.72
49	9	509	OMG	C5-C4-N3	-4.92	120.55	128.39
49	9	822	PSU	N1-C2-N3	4.92	120.36	115.17
2	5	3718	A2M	C5-C4-N3	-4.92	119.95	126.72
2	5	1534	A2M	N6-C6-N1	-4.92	107.43	118.38
2	5	1326	A2M	C5-C4-N3	-4.91	119.95	126.72
2	5	3785	A2M	C5-C4-N3	-4.91	119.95	126.72
2	5	1326	A2M	N6-C6-N1	-4.91	107.44	118.38
2	5	2050	OMG	C5-C4-N3	-4.91	120.58	128.39
2	5	2522	7MG	C5-C6-N1	4.91	119.58	110.94
49	9	1678	A2M	C5-C4-N3	-4.90	119.97	126.72
2	5	4530	UR3	C4-N3-C2	-4.90	120.64	124.58
2	5	4185	B8W	C5-C4-N3	-4.89	122.02	127.18
2	5	4403	PSU	C4-N3-C2	-4.89	119.63	126.37
49	9	1806	M7A	N3-C4-N9	4.88	132.98	126.88
49	9	668	A2M	N6-C6-N1	-4.88	107.52	118.38
2	5	3867	A2M	C5-C4-N3	-4.87	120.00	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1522	OMG	C2-N3-C4	4.87	120.70	112.30
49	9	1830	UR3	C4-N3-C2	-4.87	120.66	124.58
2	5	4623	OMG	C5-C4-N3	-4.87	120.63	128.39
49	9	1851	MA6	C5-C4-N3	-4.85	120.04	126.72
2	5	3899	BGH	C2-N3-C4	4.84	120.64	112.30
2	5	1677	PSU	N1-C2-N3	4.83	120.26	115.17
2	5	2363	A2M	N6-C6-N1	-4.81	107.67	118.38
2	5	4597	UR3	C4-N3-C2	-4.80	120.72	124.58
2	5	3723	A2M	C5-C4-N3	-4.77	120.15	126.72
49	9	1678	A2M	N6-C6-N1	-4.77	107.76	118.38
2	5	2401	A2M	N6-C6-N1	-4.75	107.81	118.38
2	5	4293	PSU	N1-C2-N3	4.75	120.17	115.17
2	5	4550	7MG	C2-N3-C4	4.74	120.46	112.30
2	5	373	OMG	C2-N3-C4	4.72	120.43	112.30
2	5	4083	5MU	C5M-C5-C4	4.72	123.82	118.78
2	5	237	B9B	N2-C2-N3	4.72	124.30	117.22
2	5	1517	2MG	N9-C4-N3	4.71	135.38	125.95
2	5	4494	OMG	C5-C4-N3	-4.71	120.89	128.39
49	9	1248	B8N	C4-N3-C2	-4.71	119.82	125.62
2	5	4355	E6G	N3-C4-N9	4.71	132.97	126.99
2	5	2754	B9B	N3-C4-N9	4.71	132.96	126.99
2	5	1582	PSU	C4-N3-C2	-4.70	119.89	126.37
2	5	1517	2MG	C2-N1-C6	-4.68	118.89	124.55
49	9	166	A2M	N6-C6-N1	-4.68	107.96	118.38
2	5	1316	OMG	C2-N3-C4	4.67	120.34	112.30
49	9	159	A2M	N6-C6-N1	-4.67	107.97	118.38
2	5	1683	PSU	C4-N3-C2	-4.66	119.96	126.37
2	5	3785	A2M	N6-C6-N1	-4.65	108.02	118.38
2	5	729	2MG	C2-N1-C6	-4.65	118.93	124.55
2	5	2364	OMG	C2-N3-C4	4.65	120.31	112.30
2	5	4529	B8W	N9-C8-N7	-4.65	107.34	113.94
2	5	4472	B8W	N9-C8-N7	-4.64	107.35	113.94
49	9	823	PSU	C4-N3-C2	-4.64	119.98	126.37
2	5	4571	A2M	N6-C6-N1	-4.63	108.06	118.38
2	5	3729	PSU	N1-C2-N3	4.63	120.05	115.17
2	5	4370	OMG	C2-N3-C4	4.63	120.27	112.30
49	9	822	PSU	C4-N3-C2	-4.62	120.01	126.37
2	5	2773	OMG	C5-C4-N3	-4.62	121.04	128.39
2	5	1348	P4U	C5-C4-N3	-4.61	118.09	124.86
2	5	4494	OMG	C2-N3-C4	4.61	120.24	112.30
2	5	4523	A2M	N6-C6-N1	-4.60	108.12	118.38
2	5	4523	A2M	C5-C4-N3	-4.60	120.38	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	3723	A2M	N6-C6-N1	-4.60	108.14	118.38
49	9	823	PSU	N1-C2-N3	4.60	120.02	115.17
2	5	1316	OMG	C5-C4-N3	-4.60	121.08	128.39
2	5	2424	OMG	C5-C4-N3	-4.59	121.08	128.39
2	5	398	A2M	N6-C6-N1	-4.58	108.18	118.38
49	9	1830	UR3	C1'-N1-C2	4.57	124.53	117.04
2	5	4306	OMU	N3-C2-N1	4.56	120.83	114.89
49	9	644	OMG	C2-N3-C4	4.56	120.15	112.30
49	9	27	A2M	N6-C6-N1	-4.56	108.23	118.38
2	5	2754	B9B	C4-C5-C6	4.55	119.69	115.22
49	9	1031	A2M	N6-C6-N1	-4.55	108.25	118.38
2	5	1456	B8Q	C31-N3-C4	4.54	122.63	114.76
49	9	612	PSU	C4-N3-C2	-4.54	120.12	126.37
2	5	2424	OMG	C2-N3-C4	4.54	120.11	112.30
2	5	237	B9B	N3-C4-N9	4.53	132.74	126.99
2	5	1871	A2M	N6-C6-N1	-4.53	108.30	118.38
2	5	4371	MHG	C4-C5-N7	4.53	108.61	104.94
49	9	1832	6MZ	C5-C4-N9	-4.53	100.88	105.81
2	5	3867	A2M	N6-C6-N1	-4.52	108.30	118.38
49	9	1219	B8Q	C6-N1-C2	-4.52	118.11	121.80
2	5	4637	OMG	C2-N3-C4	4.51	120.08	112.30
2	5	3715	PSU	N1-C2-N3	4.51	119.92	115.17
2	5	2754	B9B	N2-C2-N3	4.50	123.97	117.22
2	5	3715	PSU	C4-N3-C2	-4.49	120.18	126.37
49	9	1081	PSU	C4-N3-C2	-4.49	120.18	126.37
2	5	1797	E7G	C2-N3-C4	4.49	120.03	112.30
49	9	1832	6MZ	C5-N7-C8	4.49	110.51	103.45
2	5	2297	E7G	C2-N3-C4	4.49	120.03	112.30
2	5	2380	B8W	N9-C8-N7	-4.47	107.59	113.94
2	5	1659	I4U	C5-C4-N3	-4.47	118.30	124.86
2	5	3718	A2M	N6-C6-N1	-4.46	108.44	118.38
2	5	2380	B8W	O6-C6-C5	4.46	122.55	117.17
2	5	1605	7MG	C2-N3-C4	4.46	119.98	112.30
2	5	1625	OMG	C2-N3-C4	4.45	119.96	112.30
2	5	3729	PSU	C4-N3-C2	-4.44	120.26	126.37
2	5	4690	B8K	C2-N3-C4	4.43	119.93	112.30
2	5	4870	OMG	C2-N3-C4	4.42	119.92	112.30
49	9	1806	M7A	C4-N9-C1'	-4.41	116.36	126.63
49	9	668	A2M	N9-C8-N7	-4.41	107.69	113.94
49	9	814	5MU	C4-N3-C2	-4.40	121.57	127.34
2	5	1322	1MA	C2-N3-C4	4.40	121.16	112.53
2	5	2522	7MG	C2-N3-C4	4.40	119.88	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	9	1832	6MZ	C9-N6-C6	4.40	126.93	122.85
2	5	4129	B8W	N9-C8-N7	-4.38	107.72	113.94
2	5	1574	B9B	O6-C6-C5	4.37	122.51	116.73
2	5	4196	OMG	C2-N3-C4	4.36	119.82	112.30
2	5	2380	B8W	C4-C5-C6	4.36	119.50	115.22
49	9	612	PSU	N1-C2-N3	4.36	119.77	115.17
2	5	2380	B8W	N3-C4-N9	4.36	132.52	126.99
2	5	2508	PSU	C4-N3-C2	-4.36	120.37	126.37
49	9	119	PSU	N1-C2-N3	4.35	119.76	115.17
49	9	1832	6MZ	C1'-N9-C8	-4.35	117.44	127.09
2	5	3899	BGH	C4-C5-N7	4.35	108.45	104.93
4	8	14	OMU	C5-C4-N3	4.33	120.87	114.80
49	9	1081	PSU	N1-C2-N3	4.32	119.73	115.17
2	5	3785	A2M	N9-C8-N7	-4.30	107.83	113.94
2	5	237	B9B	N9-C8-N7	-4.27	107.88	113.94
49	9	1850	MA6	C5-C4-N3	-4.27	120.84	126.72
49	9	668	A2M	C5-C4-N3	-4.26	120.85	126.72
2	5	2773	OMG	C2-N3-C4	4.26	119.63	112.30
49	9	119	PSU	C4-N3-C2	-4.24	120.53	126.37
49	9	1678	A2M	N9-C8-N7	-4.23	107.93	113.94
2	5	1524	A2M	N9-C8-N7	-4.23	107.94	113.94
2	5	4220	6MZ	C5-C4-N3	-4.22	120.90	126.72
2	5	1517	2MG	N1-C2-N2	4.22	120.87	116.56
2	5	4690	B8K	C5-C4-N9	4.21	111.73	106.33
2	5	1456	B8Q	N3-C2-N1	4.21	123.02	117.16
2	5	4623	OMG	C2-N3-C4	4.21	119.55	112.30
2	5	1574	B9B	N9-C8-N7	-4.20	107.98	113.94
2	5	4083	5MU	C5M-C5-C6	-4.18	117.19	122.85
49	9	121	OMU	N3-C2-N1	4.18	120.34	114.89
2	5	2363	A2M	N9-C8-N7	-4.17	108.02	113.94
2	5	1456	B8Q	O2-C2-N3	-4.16	117.11	122.95
2	5	3764	PSU	N1-C2-N3	4.15	119.55	115.17
49	9	509	OMG	C2-N3-C4	4.14	119.42	112.30
2	5	4872	2MG	C5-C4-N3	-4.13	121.82	128.39
2	5	2508	PSU	N1-C2-N3	4.12	119.51	115.17
2	5	4550	7MG	C5-C4-N9	4.12	111.61	106.33
2	5	3897	B8K	C2-N3-C4	4.12	119.39	112.30
2	5	4620	OMU	N3-C2-N1	4.10	120.23	114.89
2	5	2050	OMG	C2-N3-C4	4.10	119.36	112.30
49	9	1248	B8N	C1'-C5-C4	4.09	123.82	117.61
2	5	4083	5MU	C6-N1-C2	-4.06	117.26	121.30
2	5	4571	A2M	N9-C8-N7	-4.06	108.18	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1605	7MG	C5-C4-N3	-4.06	120.51	128.13
2	5	2754	B9B	N9-C8-N7	-4.05	108.19	113.94
49	9	1850	MA6	N9-C8-N7	-4.04	108.20	113.94
2	5	4355	E6G	N9-C8-N7	-4.04	108.20	113.94
49	9	1031	A2M	N9-C8-N7	-4.02	108.23	113.94
2	5	3867	A2M	N9-C8-N7	-4.02	108.24	113.94
49	9	1830	UR3	C6-N1-C2	-3.99	118.54	121.80
2	5	3764	PSU	C4-N3-C2	-3.99	120.88	126.37
49	9	1850	MA6	C2-N1-C6	3.98	121.55	111.83
2	5	237	B9B	C4-C5-C6	3.97	119.12	115.22
2	5	2380	B8W	C61-O6-C6	-3.95	113.50	117.20
2	5	4083	5MU	O2-C2-N1	-3.95	117.65	122.80
2	5	2522	7MG	C5-C4-N3	-3.95	120.72	128.13
2	5	2522	7MG	C4-C5-N7	3.94	110.03	105.38
49	9	568	E3C	C6-N1-C2	-3.93	118.59	121.80
2	5	4371	MHG	C5-C4-N9	3.93	111.36	106.33
2	5	4628	PSU	O2-C2-N1	-3.93	118.74	122.79
49	9	116	OMU	N3-C2-N1	3.92	120.00	114.89
2	5	4415	1MA	C2-N3-C4	3.91	120.20	112.53
2	5	1909	P7G	N9-C8-N7	3.91	108.90	103.37
2	5	4129	B8W	O4'-C1'-N9	3.90	115.58	108.09
2	5	3825	A2M	N9-C8-N7	-3.89	108.42	113.94
2	5	4335	5MC	C5-C6-N1	-3.89	119.09	123.31
2	5	4185	B8W	O4'-C1'-N9	3.89	115.56	108.09
2	5	3899	BGH	C5-C4-N9	3.87	111.29	106.33
2	5	1574	B9B	N2-C2-N3	3.86	123.01	117.22
2	5	4523	A2M	N9-C8-N7	-3.86	108.46	113.94
2	5	3899	BGH	C2'-C1'-N9	-3.86	106.30	114.14
2	5	1866	UR3	C6-N1-C2	-3.85	118.65	121.80
2	5	2401	A2M	N9-C8-N7	-3.85	108.47	113.94
2	5	1574	B9B	C4-C5-C6	3.84	119.00	115.22
2	5	3723	A2M	N9-C8-N7	-3.84	108.49	113.94
49	9	568	E3C	C32-C31-N3	3.83	122.14	112.69
49	9	1851	MA6	N9-C8-N7	-3.83	108.50	113.94
49	9	484	A2M	N9-C8-N7	-3.82	108.51	113.94
49	9	1219	B8Q	C31-N3-C4	3.82	121.38	114.76
2	5	4450	PSU	C6-C5-C4	3.81	120.75	118.17
2	5	4690	B8K	N9-C8-N7	3.79	108.31	103.31
2	5	3825	A2M	C5-C6-N6	3.79	132.67	123.29
2	5	1883	OMG	N9-C4-N3	3.78	133.52	125.95
49	9	159	A2M	N9-C8-N7	-3.75	108.61	113.94
2	5	4550	7MG	C5-C4-N3	-3.75	121.09	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1524	A2M	C2-N3-C4	3.74	120.97	111.83
2	5	1574	B9B	N3-C4-N9	3.74	131.74	126.99
2	5	4355	E6G	N3-C2-N1	-3.74	119.76	125.48
2	5	4620	OMU	C5-C4-N3	3.73	120.03	114.80
49	9	568	E3C	C1'-N1-C6	-3.73	112.81	120.78
2	5	3762	B8H	O2-C2-N1	-3.72	119.02	122.78
49	9	668	A2M	C5-C6-N6	3.72	132.49	123.29
2	5	4185	B8W	C4-C5-C6	3.71	118.87	115.22
2	5	4870	OMG	N9-C4-N3	3.71	133.38	125.95
49	9	484	A2M	C5-C6-N6	3.70	132.44	123.29
2	5	1860	B8H	C5-C4-N3	3.69	124.68	116.55
49	9	1219	B8Q	N3-C2-N1	3.69	122.30	117.16
2	5	1860	B8H	O2-C2-N1	-3.69	119.05	122.78
2	5	4371	MHG	C5-C4-N3	-3.68	121.23	128.13
49	9	1851	MA6	C2-N3-C4	3.68	120.81	111.83
2	5	237	B9B	N3-C2-N1	-3.67	119.85	125.48
2	5	4628	PSU	C6-N1-C2	-3.67	119.28	122.69
2	5	1316	OMG	N9-C8-N7	-3.67	106.60	113.40
49	9	1851	MA6	C4-C5-C6	3.66	119.69	115.91
2	5	3897	B8K	N9-C8-N7	3.65	108.13	103.31
2	5	1326	A2M	N9-C8-N7	-3.65	108.76	113.94
49	9	121	OMU	C5-C4-N3	3.65	119.91	114.80
49	9	1031	A2M	C2-N3-C4	3.65	120.74	111.83
49	9	166	A2M	C2-N3-C4	3.65	120.74	111.83
2	5	4129	B8W	C4-C5-C6	3.65	118.80	115.22
49	9	27	A2M	N9-C8-N7	-3.64	108.77	113.94
49	9	166	A2M	N9-C8-N7	-3.64	108.77	113.94
2	5	4296	B8H	O2-C2-N1	-3.63	119.11	122.78
2	5	398	A2M	C2-N3-C4	3.62	120.68	111.83
2	5	1524	A2M	N3-C4-N9	3.62	133.33	127.17
2	5	2297	E7G	C5-C4-N3	-3.62	121.33	128.13
2	5	4690	B8K	C6-C5-C4	-3.62	116.03	122.40
49	9	1248	B8N	N3-C2-N1	3.62	121.14	116.72
2	5	1871	A2M	N9-C8-N7	-3.61	108.81	113.94
2	5	4371	MHG	C2-N1-C6	-3.61	120.19	124.55
2	5	1871	A2M	C2-N3-C4	3.60	120.61	111.83
2	5	4529	B8W	C2-N1-C6	3.57	120.92	115.96
49	9	116	OMU	C5-C4-N3	3.57	119.80	114.80
2	5	3792	OMG	N9-C4-N3	3.57	133.09	125.95
2	5	1605	7MG	C4-C5-N7	3.56	109.59	105.38
2	5	1326	A2M	C5-C6-N6	3.56	132.10	123.29
2	5	4597	UR3	C5-C4-N3	3.56	119.72	115.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1534	A2M	C2-N3-C4	3.55	120.51	111.83
2	5	3825	A2M	C2-N3-C4	3.55	120.50	111.83
49	9	484	A2M	C2-N3-C4	3.55	120.49	111.83
49	9	1678	A2M	C5-C6-N6	3.55	132.06	123.29
2	5	2401	A2M	C2-N3-C4	3.55	120.49	111.83
2	5	4494	OMG	N9-C8-N7	-3.54	106.84	113.40
2	5	1534	A2M	N9-C8-N7	-3.53	108.93	113.94
49	9	1850	MA6	C4-C5-C6	3.53	119.56	115.91
2	5	4571	A2M	C2-N3-C4	3.53	120.44	111.83
2	5	1524	A2M	C5-C6-N6	3.52	132.00	123.29
2	5	2363	A2M	C2-N3-C4	3.52	120.42	111.83
2	5	4529	B8W	C5-N7-C8	3.51	108.97	103.45
2	5	4564	M7A	C2-N3-C4	3.51	120.41	111.83
2	5	4196	OMG	N9-C4-N3	3.51	132.98	125.95
2	5	2363	A2M	C5-C6-N6	3.51	131.97	123.29
2	5	2522	7MG	C5-C4-N9	3.50	110.82	106.33
2	5	3762	B8H	C5-C4-N3	3.50	124.26	116.55
2	5	4185	B8W	C61-O6-C6	3.50	120.48	117.20
2	5	4296	B8H	C5-C4-N3	3.50	124.25	116.55
2	5	373	OMG	N9-C4-N3	3.50	132.95	125.95
2	5	4529	B8W	C4-C5-C6	3.50	118.66	115.22
2	5	2786	B9H	C4-N3-C2	-3.49	115.71	122.00
49	9	1851	MA6	C2-N1-C6	3.49	120.36	111.83
2	5	4523	A2M	C2'-C1'-N9	-3.48	108.02	113.75
2	5	3718	A2M	C5-C6-N6	3.48	131.91	123.29
49	9	822	PSU	O2-C2-N1	-3.48	119.20	122.79
2	5	4872	2MG	CM2-N2-C2	-3.47	116.19	123.65
2	5	2522	7MG	N9-C8-N7	3.47	108.28	103.37
2	5	1797	E7G	C5-C4-N3	-3.46	121.63	128.13
2	5	4872	2MG	N9-C8-N7	-3.46	106.98	113.40
49	9	166	A2M	N3-C4-N9	3.46	133.06	127.17
2	5	1883	OMG	N9-C8-N7	-3.46	106.98	113.40
2	5	1534	A2M	C5-C6-N6	3.46	131.84	123.29
2	5	1866	UR3	C4-N3-C2	-3.45	121.80	124.58
2	5	3899	BGH	N9-C8-N7	3.45	107.86	103.31
2	5	4523	A2M	C2-N3-C4	3.44	120.24	111.83
2	5	2786	B9H	O2-C2-N1	-3.44	115.11	122.78
2	5	4620	OMU	O4-C4-C5	-3.44	119.23	125.16
2	5	1866	UR3	C5-C4-N3	3.44	119.56	115.04
49	9	1830	UR3	C5-C4-N3	3.43	119.56	115.04
4	8	14	OMU	O4-C4-C5	-3.43	119.25	125.16
49	9	166	A2M	C5-C6-N6	3.42	131.76	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4529	B8W	C4-C5-N7	-3.42	106.67	110.58
2	5	2380	B8W	C3'-C2'-C1'	3.42	107.93	101.46
2	5	1326	A2M	C2-N3-C4	3.42	120.18	111.83
49	9	1832	6MZ	C2-N3-C4	3.42	120.17	111.83
2	5	3785	A2M	C2-N3-C4	3.41	120.16	111.83
2	5	3785	A2M	C2'-C1'-N9	-3.41	108.14	113.75
2	5	4220	6MZ	C2-N3-C4	3.41	120.15	111.83
49	9	27	A2M	C2-N3-C4	3.41	120.15	111.83
49	9	644	OMG	C2-N1-C6	-3.41	118.94	125.11
2	5	4523	A2M	C5-C6-N6	3.40	131.71	123.29
2	5	2364	OMG	N9-C4-N3	3.40	132.75	125.95
2	5	4196	OMG	C2-N1-C6	-3.40	118.94	125.11
2	5	3723	A2M	C5-C6-N6	3.40	131.69	123.29
2	5	4472	B8W	C4-C5-C6	3.40	118.56	115.22
2	5	1871	A2M	C5-C6-N6	3.39	131.69	123.29
49	9	159	A2M	C2-N3-C4	3.39	120.11	111.83
2	5	1683	PSU	O2-C2-N1	-3.39	119.30	122.79
4	8	14	OMU	N3-C2-N1	3.39	119.30	114.89
2	5	4637	OMG	C2-N1-C6	-3.38	118.97	125.11
2	5	3867	A2M	C2-N3-C4	3.37	120.07	111.83
2	5	2364	OMG	C2-N1-C6	-3.37	119.00	125.11
2	5	1316	OMG	C2-N1-C6	-3.37	119.00	125.11
2	5	1883	OMG	C2-N1-C6	-3.37	119.00	125.11
49	9	159	A2M	C5-C6-N6	3.37	131.62	123.29
2	5	3723	A2M	C2-N3-C4	3.36	120.05	111.83
2	5	3899	BGH	C6-C5-C4	-3.36	116.49	122.40
2	5	3899	BGH	C5-C4-N3	-3.36	121.83	128.13
2	5	2380	B8W	N1-C2-N3	-3.36	120.33	125.48
49	9	1678	A2M	C2-N3-C4	3.36	120.03	111.83
2	5	398	A2M	N9-C8-N7	-3.36	109.17	113.94
2	5	4571	A2M	C5-C6-N6	3.36	131.59	123.29
49	9	1031	A2M	N3-C4-N9	3.35	132.87	127.17
49	9	27	A2M	C5-C6-N6	3.35	131.59	123.29
2	5	237	B9B	O6-C6-N1	-3.35	115.54	120.02
2	5	1574	B9B	N3-C2-N1	-3.35	120.35	125.48
2	5	2773	OMG	N9-C8-N7	-3.35	107.19	113.40
2	5	3792	OMG	C2-N1-C6	-3.35	119.04	125.11
49	9	1243	PSU	C6-N1-C2	-3.34	119.59	122.69
2	5	373	OMG	N9-C8-N7	-3.33	107.22	113.40
49	9	683	OMG	N9-C4-N3	3.33	132.62	125.95
2	5	3729	PSU	C6-N1-C2	-3.33	119.60	122.69
2	5	4529	B8W	N1-C2-N3	-3.33	120.38	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4306	OMU	C5-C4-N3	3.33	119.46	114.80
2	5	4530	UR3	C5-C4-N3	3.32	119.42	115.04
2	5	4637	OMG	N9-C8-N7	-3.32	107.24	113.40
49	9	1832	6MZ	C5-C4-N3	-3.31	122.15	126.72
2	5	4623	OMG	N9-C8-N7	-3.31	107.25	113.40
2	5	1522	OMG	C2-N1-C6	-3.31	119.11	125.11
49	9	1219	B8Q	C1'-N1-C6	-3.31	113.71	120.78
2	5	2050	OMG	N9-C8-N7	-3.31	107.27	113.40
2	5	4129	B8W	N1-C2-N3	-3.30	120.42	125.48
2	5	3867	A2M	C5-C6-N6	3.30	131.45	123.29
49	9	683	OMG	N9-C8-N7	-3.30	107.29	113.40
2	5	1605	7MG	C5-C4-N9	3.29	110.55	106.33
2	5	398	A2M	C5-C6-N6	3.29	131.43	123.29
2	5	4129	B8W	O6-C6-N1	-3.29	114.59	118.96
2	5	1683	PSU	C6-N1-C2	-3.27	119.65	122.69
2	5	2424	OMG	N9-C8-N7	-3.26	107.35	113.40
2	5	398	A2M	N3-C4-N9	3.26	132.71	127.17
2	5	1582	PSU	C6-N1-C2	-3.26	119.67	122.69
2	5	4472	B8W	O4'-C1'-N9	3.26	114.35	108.09
2	5	2754	B9B	N3-C2-N1	-3.26	120.49	125.48
2	5	1625	OMG	N9-C4-N3	3.25	132.45	125.95
2	5	4550	7MG	C4-C5-N7	3.24	109.21	105.38
49	9	1850	MA6	C2-N3-C4	3.24	119.74	111.83
2	5	2050	OMG	C2-N1-C6	-3.24	119.23	125.11
49	9	1337	4AC	C6-C5-C4	3.24	120.90	117.00
2	5	1866	UR3	C1'-N1-C2	3.24	122.34	117.04
49	9	1832	6MZ	C6-C5-N7	3.24	135.96	132.43
2	5	4447	5MC	C5-C6-N1	-3.23	119.80	123.31
2	5	4529	B8W	O4'-C1'-N9	3.22	114.28	108.09
2	5	4529	B8W	C5-C6-N1	-3.22	119.18	123.49
49	9	121	OMU	O4-C4-C5	-3.22	119.61	125.16
2	5	4472	B8W	N1-C2-N3	-3.22	120.55	125.48
2	5	4185	B8W	N1-C2-N3	-3.21	120.57	125.48
2	5	1883	OMG	C5-C6-N1	3.20	121.41	113.25
2	5	2401	A2M	C5-C6-N6	3.20	131.21	123.29
2	5	2364	OMG	N9-C8-N7	-3.20	107.47	113.40
2	5	2297	E7G	C5-C4-N9	3.20	110.43	106.33
2	5	4306	OMU	O2-C2-N1	-3.20	118.63	122.80
49	9	644	OMG	N9-C8-N7	-3.20	107.47	113.40
2	5	4129	B8W	C4-C5-N7	-3.20	106.93	110.58
2	5	4370	OMG	C2-N1-C6	-3.19	119.32	125.11
2	5	4220	6MZ	C5-N7-C8	3.19	108.47	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1625	OMG	C2-N1-C6	-3.19	119.32	125.11
2	5	1524	A2M	C2'-C1'-N9	-3.19	108.50	113.75
49	9	166	A2M	C5'-C4'-C3'	-3.19	103.74	115.21
49	9	644	OMG	N9-C4-N3	3.19	132.32	125.95
2	5	4370	OMG	N9-C4-N3	3.17	132.30	125.95
2	5	4450	PSU	O2-C2-N1	-3.17	119.52	122.79
2	5	1522	OMG	N9-C8-N7	-3.17	107.53	113.40
2	5	4185	B8W	C4-N9-C8	3.17	109.06	105.74
2	5	2401	A2M	N3-C4-N9	3.16	132.54	127.17
2	5	4185	B8W	O4'-C4'-C3'	-3.16	98.88	105.15
2	5	4442	PSU	C6-N1-C2	-3.16	119.76	122.69
2	5	1522	OMG	N9-C4-N3	3.16	132.26	125.95
49	9	159	A2M	N3-C4-N9	3.16	132.53	127.17
2	5	4623	OMG	N9-C4-N3	3.15	132.26	125.95
49	9	814	5MU	C1'-N1-C2	3.15	123.25	117.59
49	9	1806	M7A	C2-N3-C4	3.15	119.52	111.83
2	5	3785	A2M	C5-C6-N6	3.14	131.06	123.29
49	9	814	5MU	C6-N1-C2	-3.14	118.17	121.30
2	5	1534	A2M	N3-C4-N9	3.14	132.50	127.17
2	5	2754	B9B	O6-C6-C5	3.14	120.88	116.73
2	5	3897	B8K	C6-C5-C4	-3.14	116.88	122.40
2	5	4494	OMG	C2-N1-C6	-3.13	119.43	125.11
2	5	4185	B8W	C5-N7-C8	3.13	108.37	103.45
49	9	1248	B8N	C31-N3-C4	3.12	121.60	117.18
49	9	1243	PSU	N1-C2-N3	3.12	118.46	115.17
2	5	4129	B8W	C5-N7-C8	3.12	108.35	103.45
2	5	4623	OMG	C2-N1-C6	-3.12	119.45	125.11
2	5	2424	OMG	C2-N1-C6	-3.12	119.46	125.11
49	9	1031	A2M	C5-C6-N6	3.11	130.99	123.29
2	5	4442	PSU	O2-C2-N1	-3.11	119.58	122.79
49	9	27	A2M	N3-C4-N9	3.10	132.44	127.17
2	5	3764	PSU	C6-N1-C2	-3.10	119.82	122.69
2	5	3718	A2M	N9-C8-N7	-3.09	109.56	113.94
2	5	4185	B8W	C2-N1-C6	3.08	120.25	115.96
2	5	4220	6MZ	C1'-N9-C8	-3.08	120.27	127.09
2	5	4472	B8W	C5-N7-C8	3.08	108.28	103.45
49	9	668	A2M	C2-N3-C4	3.07	119.33	111.83
49	9	1710	OMC	O2-C2-N3	-3.07	117.50	122.33
2	5	4597	UR3	C6-N1-C2	-3.06	119.30	121.80
49	9	612	PSU	O2-C2-N1	-3.05	119.64	122.79
2	5	4530	UR3	C6-N1-C2	-3.05	119.31	121.80
2	5	4620	OMU	O2-C2-N1	-3.04	118.83	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4194	I4U	C5-C4-N3	-3.04	120.39	124.86
2	5	1534	A2M	O4'-C1'-C2'	-3.04	101.36	106.59
2	5	4529	B8W	C3'-C2'-C1'	3.04	107.21	101.46
49	9	1374	5MC	C5-C6-N1	-3.04	120.02	123.31
49	9	509	OMG	C2-N1-C6	-3.03	119.61	125.11
2	5	4872	2MG	C5-C6-N1	3.03	120.98	113.25
2	5	3792	OMG	N9-C8-N7	-3.03	107.78	113.40
2	5	4870	OMG	C2-N1-C6	-3.03	119.62	125.11
49	9	683	OMG	C2-N1-C6	-3.03	119.62	125.11
2	5	4870	OMG	N9-C8-N7	-3.02	107.80	113.40
2	5	3785	A2M	N3-C4-N9	3.02	132.30	127.17
49	9	509	OMG	N9-C4-N3	3.02	131.99	125.95
2	5	1517	2MG	C5-C6-N1	3.02	120.94	113.25
2	5	4371	MHG	C21-N2-C2	-3.01	117.17	123.65
2	5	2363	A2M	C5-N7-C8	3.00	108.17	103.45
2	5	237	B9B	C5-N7-C8	3.00	108.17	103.45
2	5	3718	A2M	C2-N3-C4	3.00	119.16	111.83
2	5	1797	E7G	C5-C4-N9	3.00	110.18	106.33
49	9	1842	4AC	C6-C5-C4	2.99	120.60	117.00
2	5	4571	A2M	N3-C4-N9	2.98	132.24	127.17
2	5	3897	B8K	C5-C4-N3	-2.97	122.55	128.13
49	9	1850	MA6	C5-N7-C8	2.97	108.12	103.45
4	8	14	OMU	C1'-N1-C2	2.97	122.93	117.59
2	5	1316	OMG	C5-C6-N1	2.97	120.80	113.25
2	5	2364	OMG	C5-C6-N1	2.96	120.80	113.25
49	9	1842	4AC	C5-C4-N3	-2.96	117.97	122.60
2	5	2050	OMG	N9-C4-N3	2.96	131.87	125.95
2	5	1871	A2M	N3-C4-N9	2.96	132.20	127.17
2	5	4403	PSU	C6-N1-C2	-2.96	119.95	122.69
2	5	3785	A2M	O4'-C1'-N9	2.95	113.76	108.09
2	5	4564	M7A	C5-C4-N3	-2.95	119.75	126.56
2	5	3792	OMG	C5-C6-N1	2.95	120.75	113.25
2	5	4371	MHG	C71-C72-C73	-2.94	106.27	114.13
49	9	1248	B8N	O4-C4-C5	-2.94	117.50	122.58
2	5	3897	B8K	C5-C4-N9	2.93	110.09	106.33
2	5	4129	B8W	C5-C4-N9	2.93	109.01	105.81
49	9	1806	M7A	C71-N7-C5	-2.93	111.23	123.44
2	5	1517	2MG	O6-C6-C5	-2.93	118.80	126.53
49	9	814	5MU	O2-C2-N3	-2.93	116.09	121.49
49	9	517	OMC	O2-C2-N3	-2.92	117.73	122.33
2	5	2380	B8W	C4-N9-C8	2.92	108.80	105.74
49	9	814	5MU	C5M-C5-C6	-2.92	118.90	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1871	A2M	C2'-C1'-N9	-2.92	108.95	113.75
2	5	4637	OMG	N9-C4-N3	2.91	131.77	125.95
2	5	1582	PSU	O2-C2-N1	-2.91	119.79	122.79
2	5	1322	1MA	N9-C8-N7	-2.91	108.01	113.40
2	5	237	B9B	C2-N1-C6	2.90	120.00	115.96
2	5	4083	5MU	C1'-N1-C6	2.90	125.92	121.15
2	5	2424	OMG	C5-C6-N1	2.90	120.63	113.25
49	9	683	OMG	C5-C6-N1	2.90	120.62	113.25
2	5	4196	OMG	N9-C8-N7	-2.89	108.05	113.40
2	5	2364	OMG	O6-C6-C5	-2.88	118.92	126.53
2	5	373	OMG	C2-N1-C6	-2.88	119.89	125.11
2	5	4500	PSU	C6-C5-C4	2.87	120.11	118.17
49	9	668	A2M	O4'-C1'-N9	-2.87	102.57	108.09
2	5	1524	A2M	C5-N7-C8	2.87	107.96	103.45
2	5	4494	OMG	C5-C6-N1	2.87	120.55	113.25
49	9	121	OMU	O2-C2-N1	-2.86	119.07	122.80
2	5	1883	OMG	O6-C6-C5	-2.86	118.98	126.53
2	5	4531	PSU	O2-C2-N1	-2.86	119.84	122.79
2	5	4185	B8W	C4'-O4'-C1'	-2.86	103.16	109.47
2	5	1625	OMG	N9-C8-N7	-2.85	108.11	113.40
2	5	4690	B8K	C5-C4-N3	-2.85	122.78	128.13
2	5	4494	OMG	O6-C6-C5	-2.85	119.01	126.53
2	5	4185	B8W	C5-C6-N1	-2.85	119.68	123.49
2	5	1605	7MG	C2-N1-C6	-2.85	119.95	125.11
2	5	4355	E6G	C2-N1-C6	2.85	119.92	115.96
2	5	1522	OMG	C5-C6-N1	2.84	120.49	113.25
2	5	4196	OMG	C5-C6-N1	2.84	120.47	113.25
49	9	1850	MA6	C4-C5-N7	-2.83	107.34	110.58
2	5	4472	B8W	O6-C6-N1	-2.83	115.20	118.96
2	5	4196	OMG	O6-C6-C5	-2.83	119.06	126.53
49	9	116	OMU	O4-C4-C5	-2.83	120.29	125.16
2	5	2773	OMG	C2-N1-C6	-2.82	119.99	125.11
49	9	1031	A2M	C5-N7-C8	2.82	107.88	103.45
2	5	3782	5MC	C5-C6-N1	-2.82	120.25	123.31
2	5	4690	B8K	C2-N1-C6	-2.81	120.02	125.11
49	9	1678	A2M	C2'-C1'-N9	2.81	118.38	113.75
2	5	3723	A2M	N3-C4-N9	2.80	131.93	127.17
49	9	644	OMG	C5-C6-N1	2.80	120.37	113.25
2	5	4415	1MA	N9-C8-N7	-2.79	108.22	113.40
49	9	1851	MA6	C5-N7-C8	2.79	107.84	103.45
2	5	3897	B8K	O4'-C1'-C2'	-2.79	100.64	106.62
2	5	4472	B8W	C4-N9-C8	2.79	108.67	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1326	A2M	N3-C4-N9	2.79	131.91	127.17
2	5	237	B9B	C3'-C2'-C1'	2.79	106.74	101.46
2	5	3867	A2M	N3-C4-N9	2.79	131.91	127.17
49	9	1850	MA6	C5-C4-N9	2.78	108.85	105.81
2	5	3880	P7G	N9-C8-N7	2.78	107.31	103.37
2	5	2363	A2M	N3-C4-N9	2.78	131.90	127.17
2	5	4872	2MG	O6-C6-C5	-2.78	119.19	126.53
2	5	4523	A2M	C5-C4-N9	2.78	108.84	105.81
2	5	1456	B8Q	C6-N1-C2	-2.77	119.54	121.80
49	9	1678	A2M	C5-N7-C8	2.77	107.80	103.45
2	5	2297	E7G	C2-N1-C6	-2.76	120.11	125.11
2	5	2380	B8W	C4'-O4'-C1'	-2.76	103.38	109.47
2	5	2363	A2M	C4-C5-N7	-2.76	107.43	110.58
2	5	4415	1MA	N9-C4-N3	2.75	133.17	126.90
2	5	1605	7MG	N9-C8-N7	2.75	107.27	103.37
2	5	4636	PSU	O2-C2-N1	-2.75	119.96	122.79
2	5	4637	OMG	C5-C6-N1	2.74	120.24	113.25
2	5	2380	B8W	C5-N7-C8	2.74	107.76	103.45
49	9	1678	A2M	N3-C4-N9	2.74	131.82	127.17
2	5	4530	UR3	C1'-N1-C2	2.73	121.51	117.04
2	5	4129	B8W	C2-N1-C6	2.72	119.75	115.96
2	5	4185	B8W	C2'-C1'-N9	-2.72	106.54	113.30
2	5	4523	A2M	O4'-C1'-N9	2.72	113.32	108.09
2	5	4355	E6G	C5-N7-C8	2.72	107.73	103.45
2	5	4370	OMG	C5-C6-N1	2.72	120.17	113.25
49	9	159	A2M	C5-N7-C8	2.71	107.71	103.45
2	5	3899	BGH	C2-N1-C6	-2.71	120.20	125.11
49	9	823	PSU	C6-N1-C2	-2.71	120.18	122.69
2	5	4472	B8W	C4-C5-N7	-2.70	107.49	110.58
2	5	373	OMG	C5-C6-N1	2.70	120.12	113.25
2	5	4472	B8W	C2-N1-C6	2.70	119.71	115.96
2	5	4690	B8K	O6-C6-C5	-2.69	121.01	127.62
49	9	509	OMG	N9-C8-N7	-2.69	108.40	113.40
2	5	4872	2MG	C6-C5-N7	2.69	135.19	130.29
2	5	3897	B8K	O3'-C3'-C4'	-2.69	103.35	111.08
2	5	4531	PSU	C6-C5-C4	2.68	119.98	118.17
2	5	373	OMG	O6-C6-C5	-2.67	119.47	126.53
2	5	729	2MG	C5-C6-N1	2.67	120.05	113.25
2	5	1574	B9B	O6-C6-N1	-2.67	116.46	120.02
49	9	822	PSU	C6-N1-C2	-2.67	120.22	122.69
2	5	1574	B9B	C5-N7-C8	2.66	107.63	103.45
2	5	2773	OMG	N9-C4-N3	2.65	131.26	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	3825	A2M	C5-C4-N9	2.65	108.70	105.81
2	5	1574	B9B	C4-N9-C1'	-2.65	120.43	126.63
2	5	2754	B9B	C5-N7-C8	2.65	107.62	103.45
2	5	4494	OMG	N9-C4-N3	2.65	131.24	125.95
49	9	1830	UR3	O2-C2-N3	-2.65	117.68	121.33
49	9	1806	M7A	C5-C4-N3	-2.64	120.45	126.56
2	5	4370	OMG	N9-C8-N7	-2.64	108.50	113.40
2	5	4483	B8T	C6-C5-C4	2.64	120.18	117.00
2	5	4472	B8W	C4'-O4'-C1'	-2.64	103.64	109.47
49	9	668	A2M	C4-N9-C8	2.64	108.51	105.74
49	9	1842	4AC	O2-C2-N3	-2.64	118.18	122.33
2	5	1625	OMG	O6-C6-C5	-2.63	119.58	126.53
49	9	683	OMG	O6-C6-C5	-2.63	119.58	126.53
2	5	237	B9B	C2-N3-C4	2.63	120.55	113.51
2	5	4623	OMG	O6-C6-C5	-2.63	119.59	126.53
2	5	3729	PSU	O2-C2-N1	-2.62	120.08	122.79
2	5	2050	OMG	C5-C6-N1	2.62	119.93	113.25
2	5	1659	I4U	C5'-C4'-C3'	-2.62	105.78	115.21
2	5	3718	A2M	N3-C4-N9	2.61	131.61	127.17
2	5	1348	P4U	O2-C2-N3	-2.61	118.21	122.33
2	5	3785	A2M	C5-N7-C8	2.60	107.54	103.45
2	5	4529	B8W	C4-N9-C8	2.60	108.47	105.74
49	9	509	OMG	O6-C6-C5	-2.60	119.67	126.53
2	5	1797	E7G	C2-N1-C6	-2.60	120.40	125.11
2	5	4636	PSU	C6-N1-C2	-2.60	120.28	122.69
2	5	1534	A2M	C2'-C3'-C4'	-2.60	96.41	101.99
2	5	2861	OMC	O2-C2-N3	-2.59	118.24	122.33
49	9	119	PSU	C6-N1-C2	-2.59	120.29	122.69
2	5	4185	B8W	O6-C6-N1	-2.59	115.51	118.96
2	5	4355	E6G	N2-C2-N1	2.59	121.11	117.22
2	5	1517	2MG	N1-C2-N3	-2.59	119.32	123.68
49	9	1081	PSU	C6-N1-C2	-2.58	120.30	122.69
2	5	3782	5MC	C1'-N1-C6	-2.58	116.91	121.15
2	5	2050	OMG	O6-C6-C5	-2.58	119.73	126.53
2	5	4129	B8W	C61-O6-C6	2.57	119.61	117.20
49	9	1337	4AC	C5-C4-N3	-2.57	118.58	122.60
2	5	3825	A2M	C5-N7-C8	2.57	107.49	103.45
49	9	484	A2M	N3-C4-N9	2.56	131.53	127.17
49	9	814	5MU	C5M-C5-C4	2.56	121.52	118.78
49	9	668	A2M	C4'-O4'-C1'	-2.56	103.81	109.47
2	5	4355	E6G	C2-N3-C4	2.56	120.37	113.51
2	5	1677	PSU	O2-C2-N1	-2.56	120.15	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	2380	B8W	C2-N1-C6	2.56	119.52	115.96
2	5	4623	OMG	C5-C6-N1	2.56	119.76	113.25
2	5	2522	7MG	C2-N1-C6	-2.56	120.47	125.11
2	5	1625	OMG	C5-C6-N1	2.56	119.76	113.25
2	5	2363	A2M	C5-C4-N9	2.56	108.60	105.81
2	5	3825	A2M	N3-C4-N9	2.55	131.51	127.17
2	5	3764	PSU	O2-C2-N1	-2.55	120.16	122.79
2	5	2380	B8W	O4'-C1'-N9	2.55	112.98	108.09
2	5	3899	BGH	C4'-O4'-C1'	-2.55	103.84	109.47
49	9	166	A2M	C5-N7-C8	2.54	107.44	103.45
49	9	668	A2M	C5-N7-C8	2.54	107.44	103.45
49	9	823	PSU	O2-C2-N1	-2.54	120.17	122.79
49	9	1851	MA6	C5-C4-N9	2.54	108.58	105.81
2	5	4564	M7A	C71-N7-C5	-2.54	112.86	123.44
2	5	1326	A2M	C5-N7-C8	2.54	107.44	103.45
2	5	1522	OMG	O6-C6-C5	-2.53	119.84	126.53
2	5	4872	2MG	C4-C5-N7	-2.53	106.66	110.67
2	5	4129	B8W	C5-C6-N1	-2.53	120.10	123.49
2	5	4472	B8W	C5-C6-N1	-2.53	120.11	123.49
2	5	1316	OMG	O6-C6-C5	-2.52	119.87	126.53
49	9	1243	PSU	C4-N3-C2	-2.52	122.89	126.37
2	5	4571	A2M	C5-N7-C8	2.52	107.41	103.45
2	5	4872	2MG	C5-C4-N9	2.52	110.17	105.66
49	9	1219	B8Q	C31-N3-C2	2.52	121.66	117.70
2	5	1322	1MA	N9-C4-N3	2.52	132.64	126.90
2	5	3792	OMG	O6-C6-C5	-2.52	119.88	126.53
2	5	373	OMG	CM2-O2'-C2'	-2.51	108.02	114.47
2	5	4536	OMC	O2-C2-N3	-2.51	118.37	122.33
49	9	509	OMG	C5-C6-N1	2.51	119.64	113.25
2	5	4296	B8H	O4-C4-N3	-2.51	115.40	120.11
2	5	4529	B8W	C5-C4-N9	2.50	108.54	105.81
2	5	4185	B8W	C4-C5-N7	-2.50	107.72	110.58
49	9	484	A2M	C5-C4-N9	2.50	108.54	105.81
2	5	3897	B8K	O4'-C1'-N9	-2.50	105.89	109.30
2	5	4870	OMG	O6-C6-C5	-2.50	119.92	126.53
49	9	1851	MA6	C4-C5-N7	-2.50	107.72	110.58
2	5	1797	E7G	O6-C6-C5	-2.50	121.49	127.62
2	5	4530	UR3	O2-C2-N3	-2.49	117.89	121.33
2	5	4870	OMG	C5-C6-N1	2.49	119.59	113.25
2	5	2754	B9B	C2-N3-C4	2.49	120.18	113.51
2	5	4523	A2M	C5-N7-C8	2.49	107.36	103.45
2	5	4483	B8T	O2-C2-N3	-2.49	118.41	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4597	UR3	C1'-N1-C2	2.49	121.11	117.04
2	5	2773	OMG	C5-C6-N1	2.48	119.57	113.25
49	9	1851	MA6	N3-C4-N9	2.48	131.39	127.17
2	5	1574	B9B	C4-N9-C8	2.48	108.34	105.74
2	5	4550	7MG	O6-C6-C5	-2.48	121.54	127.62
2	5	4870	OMG	C1'-N9-C8	-2.47	119.70	126.73
49	9	119	PSU	O2-C2-N1	-2.47	120.24	122.79
2	5	2773	OMG	O6-C6-C5	-2.47	120.01	126.53
2	5	1797	E7G	N9-C8-N7	2.47	106.87	103.37
49	9	484	A2M	C5-N7-C8	2.47	107.33	103.45
2	5	1517	2MG	N9-C8-N7	-2.47	108.83	113.40
2	5	3867	A2M	C5-N7-C8	2.46	107.32	103.45
2	5	1574	B9B	C2-N1-C6	2.45	119.36	115.96
2	5	4550	7MG	N9-C8-N7	2.45	106.84	103.37
49	9	814	5MU	O4-C4-N3	-2.44	115.53	120.11
2	5	2424	OMG	O6-C6-C5	-2.44	120.10	126.53
2	5	237	B9B	C4-N9-C8	2.44	108.30	105.74
2	5	3897	B8K	C2-N1-C6	-2.43	120.70	125.11
2	5	3723	A2M	C5-N7-C8	2.43	107.27	103.45
2	5	3825	A2M	C4-C5-N7	-2.42	107.81	110.58
2	5	4293	PSU	O2-C2-N1	-2.42	120.29	122.79
2	5	4500	PSU	O2-C2-N1	-2.42	120.29	122.79
2	5	4370	OMG	O6-C6-C5	-2.42	120.15	126.53
2	5	3718	A2M	C5-C4-N9	2.42	108.44	105.81
2	5	1316	OMG	N9-C4-N3	2.42	130.78	125.95
2	5	4371	MHG	O6-C6-C5	-2.41	121.70	127.62
2	5	4472	B8W	N3-C4-N9	2.41	130.05	126.99
2	5	1534	A2M	C5-N7-C8	2.41	107.24	103.45
2	5	1524	A2M	C4'-O4'-C1'	-2.41	104.15	109.47
49	9	1678	A2M	C4-C5-N7	-2.41	107.83	110.58
2	5	4355	E6G	C5-C6-N1	-2.40	120.27	123.49
2	5	4293	PSU	C6-N1-C2	-2.40	120.46	122.69
2	5	4671	B8T	C6-C5-C4	2.40	119.89	117.00
2	5	4472	B8W	C2'-C1'-N9	-2.39	107.36	113.30
2	5	3715	PSU	C6-N1-C2	-2.39	120.47	122.69
49	9	644	OMG	O6-C6-C5	-2.39	120.23	126.53
2	5	1797	E7G	C6-C5-C4	-2.39	118.20	122.40
2	5	4620	OMU	C2'-C1'-N1	-2.39	109.71	114.24
2	5	4129	B8W	C2-N3-C4	2.39	119.90	113.51
2	5	4550	7MG	C2-N1-C6	-2.39	120.78	125.11
2	5	1574	B9B	C2-N3-C4	2.38	119.89	113.51
2	5	4355	E6G	C6-C5-N7	-2.38	131.03	133.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	2424	OMG	N9-C4-N3	2.38	130.71	125.95
2	5	2861	OMC	C1'-N1-C2	2.38	123.69	118.44
2	5	1605	7MG	N9-C4-N3	2.37	128.94	125.46
2	5	4447	5MC	CM5-C5-C4	-2.37	116.61	120.51
2	5	2508	PSU	O2-C2-N1	-2.37	120.34	122.79
49	9	159	A2M	C2'-C1'-N9	-2.37	109.85	113.75
2	5	398	A2M	C5-N7-C8	2.36	107.17	103.45
2	5	4494	OMG	C2'-C1'-N9	-2.36	109.75	114.24
49	9	1678	A2M	C4-N9-C8	2.36	108.22	105.74
2	5	4529	B8W	C4'-O4'-C1'	-2.36	104.27	109.47
2	5	4129	B8W	N3-C4-N9	2.35	129.98	126.99
2	5	4196	OMG	C1'-N9-C8	-2.35	120.05	126.73
2	5	3880	P7G	N2-C2-N3	2.35	121.72	116.76
2	5	1316	OMG	C8-N7-C5	2.35	108.44	104.26
2	5	4335	5MC	C1'-N1-C6	-2.35	117.29	121.15
2	5	729	2MG	O6-C6-C5	-2.35	120.34	126.53
49	9	644	OMG	C8-N7-C5	2.34	108.44	104.26
2	5	3718	A2M	C6-C5-C4	2.34	120.38	117.18
2	5	3792	OMG	C1'-N9-C8	-2.34	120.08	126.73
2	5	3785	A2M	C4-N9-C8	2.34	108.19	105.74
2	5	4636	PSU	C6-C5-C4	2.34	119.75	118.17
49	9	27	A2M	C5-N7-C8	2.34	107.12	103.45
2	5	2522	7MG	O6-C6-C5	-2.34	121.89	127.62
2	5	2297	E7G	O6-C6-C5	-2.33	121.89	127.62
49	9	1337	4AC	O7-C7-CM7	-2.33	117.90	122.05
2	5	4531	PSU	C6-N1-C2	-2.33	120.53	122.69
2	5	2401	A2M	C5-N7-C8	2.33	107.11	103.45
2	5	4690	B8K	O4'-C4'-C3'	-2.32	100.54	105.15
49	9	612	PSU	C6-N1-C2	-2.32	120.54	122.69
2	5	4220	6MZ	C4-N9-C1'	-2.31	121.24	126.63
2	5	4637	OMG	O6-C6-C5	-2.30	120.45	126.53
2	5	3897	B8K	O6-C6-C5	-2.30	121.97	127.62
2	5	4185	B8W	N3-C4-N9	2.30	129.91	126.99
49	9	1832	6MZ	C4-C5-C6	-2.30	114.87	116.78
2	5	4355	E6G	O6-C6-N1	2.29	123.08	120.02
2	5	1625	OMG	C1'-N9-C8	-2.29	120.21	126.73
2	5	2773	OMG	C8-N7-C5	2.29	108.34	104.26
49	9	668	A2M	N3-C4-N9	2.29	131.06	127.17
2	5	4129	B8W	C3'-C2'-C1'	2.29	105.79	101.46
2	5	3762	B8H	O4-C4-N3	-2.28	115.82	120.11
2	5	1605	7MG	O6-C6-C5	-2.28	122.03	127.62
2	5	1860	B8H	O4-C4-N3	-2.28	115.83	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	9	1243	PSU	O2-C2-N1	-2.27	120.44	122.79
49	9	27	A2M	C2'-C1'-N9	-2.27	110.02	113.75
2	5	4571	A2M	C4-N9-C8	2.27	108.12	105.74
2	5	3899	BGH	O4'-C4'-C3'	-2.26	100.66	105.15
2	5	2380	B8W	C2-N3-C4	2.26	119.57	113.51
49	9	121	OMU	C2'-C1'-N1	-2.26	109.95	114.24
2	5	4371	MHG	N1-C2-N3	-2.26	119.87	123.68
2	5	2508	PSU	C6-N1-C2	-2.26	120.60	122.69
2	5	3887	OMC	O2-C2-N3	-2.25	118.78	122.33
2	5	4637	OMG	C8-N7-C5	2.24	108.26	104.26
2	5	4083	5MU	O4-C4-N3	-2.24	115.90	120.11
2	5	4550	7MG	N2-C2-N1	2.24	121.49	116.76
2	5	237	B9B	C4-C5-N7	-2.24	108.02	110.58
2	5	4220	6MZ	C9-N6-C6	-2.23	120.78	122.85
2	5	4403	PSU	O4'-C1'-C2'	2.23	108.24	105.15
2	5	4306	OMU	O4-C4-C5	-2.23	121.31	125.16
2	5	2363	A2M	C3'-C2'-C1'	2.22	107.06	102.81
2	5	3899	BGH	O6-C6-N1	-2.22	115.94	120.11
2	5	1871	A2M	C5-N7-C8	2.22	106.93	103.45
49	9	1842	4AC	O7-C7-CM7	-2.21	118.11	122.05
2	5	2754	B9B	C4-N9-C8	2.21	108.06	105.74
49	9	683	OMG	N1-C2-N3	-2.21	119.27	123.32
49	9	484	A2M	C4-C5-N7	-2.21	108.05	110.58
2	5	1677	PSU	C6-C5-C4	2.21	119.67	118.17
2	5	1316	OMG	N2-C2-N1	2.21	121.42	116.76
49	9	166	A2M	C6-C5-C4	2.21	120.19	117.18
2	5	3825	A2M	C5'-C4'-C3'	-2.21	107.27	115.21
2	5	4872	2MG	N1-C2-N3	-2.20	119.97	123.68
2	5	1677	PSU	C6-N1-C2	-2.20	120.65	122.69
2	5	4472	B8W	C5-C4-N9	2.19	108.20	105.81
49	9	1678	A2M	C5-C4-N9	2.19	108.20	105.81
4	8	14	OMU	C1'-N1-C6	-2.19	116.10	120.78
49	9	159	A2M	C5'-C4'-C3'	-2.18	107.35	115.21
2	5	4530	UR3	C3U-N3-C4	2.18	120.90	117.87
2	5	398	A2M	C5-C4-N9	2.18	108.19	105.81
2	5	4472	B8W	C3'-C2'-C1'	2.18	105.59	101.46
2	5	4335	5MC	CM5-C5-C6	-2.18	119.90	122.85
2	5	4623	OMG	C8-N7-C5	2.18	108.14	104.26
2	5	4550	7MG	C6-C5-C4	-2.18	118.57	122.40
2	5	729	2MG	N9-C8-N7	-2.18	109.37	113.40
49	9	159	A2M	C4-C5-N7	-2.18	108.09	110.58
2	5	1534	A2M	C5-C4-N9	2.17	108.18	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1456	B8Q	C1'-N1-C2	2.17	120.59	117.04
2	5	4472	B8W	C2-N3-C4	2.17	119.32	113.51
2	5	4450	PSU	C6-N1-C2	-2.17	120.68	122.69
2	5	3897	B8K	C3'-C2'-C1'	2.17	105.56	101.46
2	5	4872	2MG	C8-N7-C5	2.17	108.12	104.26
2	5	2297	E7G	N9-C8-N7	2.17	106.44	103.37
2	5	373	OMG	N1-C2-N3	-2.16	119.36	123.32
49	9	116	OMU	O2-C2-N1	-2.16	119.98	122.80
2	5	373	OMG	C2'-C1'-N9	-2.16	110.14	114.24
2	5	3899	BGH	N1-C2-N3	-2.16	119.37	123.32
2	5	2297	E7G	C6-C5-C4	-2.16	118.60	122.40
2	5	4442	PSU	C6-C5-C4	2.16	119.63	118.17
2	5	4523	A2M	C4-C5-N7	-2.16	108.12	110.58
2	5	4494	OMG	C8-N7-C5	2.16	108.10	104.26
49	9	1248	B8N	O4'-C1'-C2'	2.15	108.13	105.15
2	5	1524	A2M	C3'-C2'-C1'	2.15	106.93	102.81
2	5	1534	A2M	C6-C5-C4	2.15	120.11	117.18
2	5	4129	B8W	C4-N9-C8	2.15	107.99	105.74
2	5	4550	7MG	N1-C2-N3	-2.15	119.39	123.32
2	5	4529	B8W	N3-C4-N9	2.14	129.71	126.99
2	5	3867	A2M	C4-N9-C8	2.14	107.99	105.74
2	5	1871	A2M	C3'-C2'-C1'	2.14	106.91	102.81
2	5	1909	P7G	N2-C2-N3	2.14	121.27	116.76
49	9	159	A2M	C6-C5-C4	2.14	120.09	117.18
2	5	1524	A2M	C1'-N9-C8	-2.13	122.37	127.09
2	5	1326	A2M	C5-C4-N9	2.13	108.13	105.81
2	5	398	A2M	C6-C5-C4	2.13	120.08	117.18
2	5	1316	OMG	C4-C5-N7	-2.13	107.30	110.67
2	5	1883	OMG	N1-C2-N3	-2.13	119.43	123.32
2	5	4523	A2M	N3-C4-N9	2.12	130.78	127.17
2	5	1574	B9B	C4-C5-N7	-2.12	108.16	110.58
49	9	1031	A2M	C4-C5-N7	-2.11	108.16	110.58
49	9	27	A2M	C6-C5-C4	2.11	120.05	117.18
2	5	1524	A2M	C6-C5-C4	2.10	120.05	117.18
2	5	2401	A2M	C4-N9-C8	2.10	107.94	105.74
2	5	4690	B8K	C4'-O4'-C1'	-2.10	104.83	109.47
2	5	2804	OMC	O2-C2-N3	-2.10	119.02	122.33
2	5	1866	UR3	O2-C2-N3	-2.10	118.43	121.33
2	5	4597	UR3	C3U-N3-C2	2.10	120.99	117.33
2	5	4690	B8K	N1-C2-N3	-2.09	119.49	123.32
2	5	1524	A2M	C4-N9-C8	2.09	107.94	105.74
49	9	1031	A2M	C6-C5-C4	2.09	120.04	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1522	OMG	C8-N7-C5	2.09	107.98	104.26
2	5	4529	B8W	C2-N3-C4	2.09	119.11	113.51
2	5	4628	PSU	C6-C5-C4	2.09	119.58	118.17
49	9	668	A2M	C5-C4-N9	2.09	108.09	105.81
2	5	4870	OMG	C8-N7-C5	2.09	107.98	104.26
2	5	3867	A2M	C5-C4-N9	2.09	108.09	105.81
2	5	4403	PSU	O4-C4-N3	-2.08	116.19	120.11
2	5	729	2MG	C6-C5-C4	2.08	121.96	118.83
2	5	4450	PSU	C5-C6-N1	-2.08	119.25	122.14
49	9	683	OMG	C8-N7-C5	2.08	107.96	104.26
49	9	484	A2M	C3'-C2'-C1'	2.08	106.78	102.81
2	5	4494	OMG	N1-C2-N3	-2.08	119.52	123.32
2	5	4403	PSU	O2-C2-N1	-2.07	120.65	122.79
49	9	1337	4AC	N4-C4-N3	2.07	117.23	113.87
2	5	2424	OMG	C8-N7-C5	2.07	107.95	104.26
2	5	4185	B8W	C5-C4-N9	2.07	108.07	105.81
2	5	4194	I4U	C2'-C3'-C4'	2.07	106.61	102.61
2	5	2380	B8W	C5-C6-N1	-2.07	120.72	123.49
2	5	1534	A2M	C4-C5-N7	-2.06	108.22	110.58
2	5	3792	OMG	C8-N7-C5	2.06	107.94	104.26
2	5	4571	A2M	C2'-C1'-N9	-2.06	110.36	113.75
2	5	1574	B9B	C5'-C4'-C3'	-2.06	107.79	115.21
2	5	3899	BGH	O6-C6-C5	-2.06	122.57	127.62
2	5	3899	BGH	C5'-C4'-C3'	-2.05	107.82	115.21
2	5	4194	I4U	O4'-C1'-C2'	-2.05	102.22	106.62
49	9	612	PSU	O4'-C1'-C2'	2.05	107.99	105.15
49	9	1081	PSU	O4'-C1'-C2'	2.05	107.99	105.15
2	5	3718	A2M	C5-N7-C8	2.05	106.67	103.45
2	5	4494	OMG	N2-C2-N1	2.05	121.08	116.76
2	5	2050	OMG	C8-N7-C5	2.05	107.91	104.26
2	5	2522	7MG	N9-C4-N3	2.04	128.45	125.46
49	9	1710	OMC	C6-C5-C4	2.04	120.88	117.53
2	5	4500	PSU	O4'-C1'-C2'	2.04	107.98	105.15
49	9	822	PSU	O4'-C1'-C2'	2.04	107.98	105.15
2	5	4371	MHG	N2-C2-N3	-2.04	117.91	120.51
49	9	668	A2M	C4-C5-N7	-2.03	108.26	110.58
2	5	2363	A2M	C6-C5-C4	2.03	119.95	117.18
2	5	2422	OMC	O2-C2-N3	-2.02	119.14	122.33
2	5	4500	PSU	C6-N1-C2	-2.02	120.81	122.69
2	5	1883	OMG	C8-N7-C5	2.02	107.86	104.26
2	5	4194	I4U	C4'-O4'-C1'	-2.01	105.03	109.47
49	9	159	A2M	C5-C4-N9	2.01	108.00	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1322	1MA	C8-N7-C5	2.00	107.83	104.26
2	5	3715	PSU	O2-C2-N1	-2.00	120.72	122.79

There are no chirality outliers.

All (190) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	333	MLZ	N-CA-CB-CG
7	C	333	MLZ	C-CA-CB-CG
2	5	237	B9B	C5-C6-O6-C61
2	5	237	B9B	N1-C6-O6-C61
2	5	237	B9B	O4'-C4'-C5'-O5'
2	5	398	A2M	O4'-C4'-C5'-O5'
2	5	1348	P4U	N3-C4-O4-C41
2	5	1574	B9B	C5-C6-O6-C61
2	5	1574	B9B	N1-C6-O6-C61
2	5	1582	PSU	C3'-C4'-C5'-O5'
2	5	1582	PSU	O4'-C4'-C5'-O5'
2	5	2297	E7G	C72-C71-N7-C5
2	5	2364	OMG	O4'-C4'-C5'-O5'
2	5	2365	OMC	O4'-C4'-C5'-O5'
2	5	2380	B8W	C5-C6-O6-C61
2	5	2424	OMG	O4'-C4'-C5'-O5'
2	5	2786	B9H	C32-C31-N3-C2
2	5	3762	B8H	O4'-C4'-C5'-O5'
2	5	3792	OMG	O4'-C4'-C5'-O5'
2	5	3897	B8K	O4'-C4'-C5'-O5'
2	5	3899	BGH	C3'-C4'-C5'-O5'
2	5	3899	BGH	O4'-C4'-C5'-O5'
2	5	4129	B8W	C5-C6-O6-C61
2	5	4129	B8W	N1-C6-O6-C61
2	5	4185	B8W	C5-C6-O6-C61
2	5	4185	B8W	N1-C6-O6-C61
2	5	4185	B8W	O4'-C4'-C5'-O5'
2	5	4194	I4U	O4'-C4'-C5'-O5'
2	5	4220	6MZ	C5-C6-N6-C9
2	5	4220	6MZ	N1-C6-N6-C9
2	5	4355	E6G	C5-C6-O6-C61
2	5	4355	E6G	N1-C6-O6-C61
2	5	4403	PSU	O4'-C1'-C5-C4
2	5	4403	PSU	O4'-C1'-C5-C6
2	5	4447	5MC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
2	5	4472	B8W	C5-C6-O6-C61
2	5	4472	B8W	N1-C6-O6-C61
2	5	4500	PSU	O4'-C4'-C5'-O5'
2	5	4523	A2M	O4'-C4'-C5'-O5'
2	5	4529	B8W	C5-C6-O6-C61
2	5	4529	B8W	N1-C6-O6-C61
2	5	4636	PSU	O4'-C4'-C5'-O5'
2	5	4637	OMG	O4'-C4'-C5'-O5'
2	5	4870	OMG	O4'-C4'-C5'-O5'
2	5	4870	OMG	C3'-C4'-C5'-O5'
4	8	14	OMU	C1'-C2'-O2'-CM2
42	m	72	MLZ	CD-CE-NZ-CM
49	9	116	OMU	C3'-C4'-C5'-O5'
49	9	116	OMU	O4'-C4'-C5'-O5'
49	9	121	OMU	O4'-C4'-C5'-O5'
49	9	568	E3C	O4'-C1'-N1-C2
49	9	568	E3C	O4'-C1'-N1-C6
49	9	668	A2M	O4'-C4'-C5'-O5'
49	9	668	A2M	C3'-C4'-C5'-O5'
49	9	683	OMG	O4'-C4'-C5'-O5'
49	9	1248	B8N	O4'-C4'-C5'-O5'
49	9	1830	UR3	O4'-C1'-N1-C2
49	9	1832	6MZ	N1-C6-N6-C9
49	9	1851	MA6	O4'-C4'-C5'-O5'
49	9	1830	UR3	O4'-C1'-N1-C6
2	5	237	B9B	C3'-C4'-C5'-O5'
2	5	1625	OMG	C3'-C4'-C5'-O5'
2	5	1797	E7G	O4'-C4'-C5'-O5'
2	5	2364	OMG	C3'-C4'-C5'-O5'
2	5	2380	B8W	C3'-C4'-C5'-O5'
2	5	2380	B8W	O4'-C4'-C5'-O5'
2	5	2424	OMG	C3'-C4'-C5'-O5'
2	5	3729	PSU	O4'-C4'-C5'-O5'
2	5	3867	A2M	O4'-C4'-C5'-O5'
2	5	3867	A2M	C3'-C4'-C5'-O5'
2	5	3880	P7G	O4'-C4'-C5'-O5'
2	5	4415	1MA	C3'-C4'-C5'-O5'
2	5	4500	PSU	C3'-C4'-C5'-O5'
2	5	4636	PSU	C3'-C4'-C5'-O5'
2	5	4637	OMG	C3'-C4'-C5'-O5'
2	5	4872	2MG	O4'-C4'-C5'-O5'
49	9	159	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
49	9	159	A2M	C3'-C4'-C5'-O5'
49	9	166	A2M	C3'-C4'-C5'-O5'
49	9	683	OMG	C3'-C4'-C5'-O5'
49	9	1243	PSU	C3'-C4'-C5'-O5'
49	9	1243	PSU	O4'-C4'-C5'-O5'
49	9	1703	OMC	O4'-C4'-C5'-O5'
49	9	1851	MA6	C3'-C4'-C5'-O5'
2	5	237	B9B	O6-C61-C62-C63
2	5	2380	B8W	N1-C6-O6-C61
2	5	4447	5MC	C2'-C1'-N1-C2
2	5	729	2MG	O4'-C4'-C5'-O5'
2	5	3792	OMG	C3'-C4'-C5'-O5'
2	5	3897	B8K	C3'-C4'-C5'-O5'
2	5	4355	E6G	O4'-C4'-C5'-O5'
2	5	4371	MHG	C3'-C4'-C5'-O5'
2	5	4371	MHG	O4'-C4'-C5'-O5'
2	5	4450	PSU	C3'-C4'-C5'-O5'
2	5	4450	PSU	O4'-C4'-C5'-O5'
49	9	121	OMU	C3'-C4'-C5'-O5'
49	9	166	A2M	O4'-C4'-C5'-O5'
49	9	568	E3C	C3'-C4'-C5'-O5'
49	9	568	E3C	O4'-C4'-C5'-O5'
2	5	2754	B9B	N1-C6-O6-C61
2	5	3701	OMC	C2'-C1'-N1-C6
2	5	3701	OMC	C2'-C1'-N1-C2
2	5	398	A2M	C3'-C4'-C5'-O5'
2	5	2365	OMC	C3'-C4'-C5'-O5'
2	5	3762	B8H	C3'-C4'-C5'-O5'
2	5	3785	A2M	O4'-C4'-C5'-O5'
2	5	4194	I4U	C3'-C4'-C5'-O5'
2	5	4523	A2M	C3'-C4'-C5'-O5'
2	5	1348	P4U	O4-C41-C42-C43
2	5	3880	P7G	N7-C71-C72-C73
2	5	3785	A2M	C3'-C4'-C5'-O5'
2	5	3880	P7G	C3'-C4'-C5'-O5'
2	5	4415	1MA	O4'-C4'-C5'-O5'
2	5	4872	2MG	C3'-C4'-C5'-O5'
49	9	1248	B8N	C3'-C4'-C5'-O5'
2	5	4371	MHG	C2'-C1'-N9-C8
2	5	1625	OMG	O4'-C4'-C5'-O5'
2	5	1797	E7G	C3'-C4'-C5'-O5'
2	5	3729	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	5	4129	B8W	O4'-C4'-C5'-O5'
49	9	822	PSU	C3'-C4'-C5'-O5'
49	9	1703	OMC	C3'-C4'-C5'-O5'
2	5	2297	E7G	C72-C71-N7-C8
49	9	1851	MA6	C5-C6-N6-C9
2	5	729	2MG	C3'-C4'-C5'-O5'
2	5	2754	B9B	C5-C6-O6-C61
2	5	1909	P7G	C72-C71-N7-C8
2	5	4371	MHG	C75-C73-C74-C76
2	5	1574	B9B	O4'-C4'-C5'-O5'
49	9	568	E3C	C32-C31-N3-C2
2	5	4494	OMG	C3'-C4'-C5'-O5'
49	9	509	OMG	O4'-C4'-C5'-O5'
49	9	517	OMC	O4'-C4'-C5'-O5'
2	5	2754	B9B	C2'-C1'-N9-C8
2	5	3701	OMC	O4'-C1'-N1-C6
2	5	3701	OMC	O4'-C1'-N1-C2
49	9	822	PSU	O4'-C4'-C5'-O5'
49	9	1248	B8N	N3-C31-C32-C33
49	9	1832	6MZ	C5-C6-N6-C9
2	5	1866	UR3	O4'-C4'-C5'-O5'
2	5	4371	MHG	C72-C73-C74-C76
2	5	1534	A2M	C4'-C5'-O5'-P
2	5	4494	OMG	O4'-C4'-C5'-O5'
2	5	4447	5MC	O4'-C1'-N1-C6
2	5	3701	OMC	C3'-C2'-O2'-CM2
2	5	4447	5MC	O4'-C1'-N1-C2
2	5	1524	A2M	C3'-C4'-C5'-O5'
2	5	2786	B9H	C32-C31-N3-C4
2	5	1659	I4U	C42-C41-O4-C4
2	5	1659	I4U	C43-C41-O4-C4
2	5	1797	E7G	C72-C71-N7-C8
2	5	2754	B9B	C4'-C5'-O5'-P
2	5	3764	PSU	C4'-C5'-O5'-P
49	9	644	OMG	C4'-C5'-O5'-P
2	5	1625	OMG	C4'-C5'-O5'-P
49	9	1081	PSU	C4'-C5'-O5'-P
49	9	1248	B8N	N34-C33-C34-O35
2	5	3785	A2M	C3'-C2'-O2'-CM'
2	5	4494	OMG	C3'-C2'-O2'-CM2
2	5	3897	B8K	C4'-C5'-O5'-P
2	5	373	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	5	3887	OMC	C4'-C5'-O5'-P
2	5	4500	PSU	C4'-C5'-O5'-P
2	5	4870	OMG	C4'-C5'-O5'-P
49	9	159	A2M	C4'-C5'-O5'-P
2	5	2861	OMC	O4'-C4'-C5'-O5'
49	9	119	PSU	O4'-C4'-C5'-O5'
49	9	1337	4AC	O4'-C4'-C5'-O5'
2	5	4355	E6G	C62-C61-O6-C6
2	5	1909	P7G	C72-C71-N7-C5
2	5	4620	OMU	C1'-C2'-O2'-CM2
2	5	4185	B8W	C3'-C4'-C5'-O5'
2	5	4636	PSU	O4'-C1'-C5-C6
49	9	568	E3C	C32-C31-N3-C4
2	5	4371	MHG	C72-C71-N7-C8
2	5	4194	I4U	C43-C41-O4-C4
2	5	4529	B8W	O4'-C4'-C5'-O5'
49	9	668	A2M	C2'-C1'-N9-C8
42	m	72	MLZ	C-CA-CB-CG
2	5	4293	PSU	C3'-C4'-C5'-O5'
2	5	4530	UR3	C4'-C5'-O5'-P
2	5	3785	A2M	C2'-C1'-N9-C8
2	5	4371	MHG	O4'-C1'-N9-C8
2	5	3899	BGH	C4'-C5'-O5'-P
49	9	1851	MA6	C4'-C5'-O5'-P
2	5	1524	A2M	O4'-C1'-N9-C8
49	9	814	5MU	C2'-C1'-N1-C2
49	9	1219	B8Q	C2'-C1'-N1-C2
2	5	4371	MHG	C71-C72-C73-C75
42	m	72	MLZ	N-CA-CB-CG

There are no ring outliers.

54 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	1524	A2M	1	0
2	5	237	B9B	1	0
49	9	116	OMU	1	0
2	5	4494	OMG	1	0
2	5	3897	B8K	1	0
2	5	1517	2MG	1	0
2	5	1883	OMG	1	0
2	5	398	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	9	1031	A2M	1	0
2	5	1326	A2M	2	0
2	5	2422	OMC	1	0
2	5	3723	A2M	3	0
2	5	1871	A2M	1	0
2	5	2522	7MG	1	0
2	5	3899	BGH	1	0
2	5	2754	B9B	1	0
2	5	4571	A2M	1	0
49	9	1850	MA6	1	0
2	5	4194	I4U	1	0
2	5	2773	OMG	1	0
2	5	3762	B8H	6	0
2	5	4523	A2M	2	0
2	5	1860	B8H	6	0
2	5	4296	B8H	6	0
7	C	333	MLZ	1	0
2	5	4500	PSU	1	0
49	9	509	OMG	1	0
49	9	166	A2M	1	0
2	5	1316	OMG	1	0
49	9	814	5MU	1	0
2	5	729	2MG	1	0
49	9	174	OMC	1	0
2	5	3718	A2M	2	0
2	5	4220	6MZ	2	0
49	9	159	A2M	2	0
2	5	2380	B8W	1	0
2	5	3825	A2M	1	0
2	5	3782	5MC	1	0
2	5	1866	UR3	1	0
2	5	3867	A2M	1	0
49	9	1678	A2M	1	0
2	5	4293	PSU	1	0
49	9	1842	4AC	1	0
49	9	27	A2M	1	0
2	5	2804	OMC	1	0
2	5	4472	B8W	1	0
2	5	4129	B8W	1	0
2	5	373	OMG	1	0
2	5	4620	OMU	1	0
2	5	1574	B9B	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	1322	1MA	1	0
49	9	1832	6MZ	1	0
4	8	14	OMU	1	0
2	5	1605	7MG	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	5	43
49	9	18
4	8	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	40.50
1	5	1252:C	O3'	1271:G	P	34.93

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1219:G	O3'	1233:G	P	21.40
1	5	1405:C	O3'	1406:G	P	20.69
1	5	1406(C):G	O3'	1411:C	P	20.19
1	9	1761:U	O3'	1771:G	P	18.40
1	5	523:C	O3'	638:G	P	18.19
1	9	834:C	O3'	841:G	P	17.79
1	9	697:G	O3'	729:C	P	17.78
1	5	1411:C	O3'	1411(A):G	P	17.69
1	5	4138:C	O3'	4146:G	P	17.16
1	5	4777:C	O3'	4859:C	P	17.11
1	5	990:U	O3'	1064:G	P	16.99
1	5	4101:C	O3'	4107:G	P	16.88
1	9	756:C	O3'	788:G	P	16.83
1	9	323:C	O3'	329:G	P	16.82
1	9	1417:C	O3'	1423:C	P	16.68
1	9	130:G	O3'	140:U	P	15.74
1	5	760:G	O3'	904:C	P	15.14
1	5	1406:G	O3'	1406(A):G	P	14.91
1	5	1696:C	O3'	1720:C	P	14.63
1	5	3976:C	O3'	4039:G	P	14.13
1	5	922:C	O3'	922(A):G	P	13.77
1	5	5022:U	O3'	5028:G	P	13.62
1	5	1364:U	O3'	1368:A	P	13.07
1	5	2901:G	O3'	3597:G	P	13.00
1	8	79:G	O3'	85:U	P	12.92
1	5	182:G	O3'	189:G	P	12.56
1	5	738:C	O3'	738(A):C	P	11.67
1	5	921:C	O3'	922:C	P	11.50
1	5	4729:A	O3'	4735:G	P	10.11
1	5	922(B):C	O3'	923:C	P	9.34
1	9	225:G	O3'	287:U	P	8.80
1	5	1180:C	O3'	1183:C	P	8.52
1	5	935:A	O3'	935(A):G	P	7.84
1	5	738(A):C	O3'	739:G	P	7.74
1	9	745:C	O3'	749:U	P	7.40
1	5	512:U	O3'	515:C	P	6.60
1	5	4740:G	O3'	4743:G	P	6.40
1	5	935(A):G	O3'	936:C	P	6.35
1	5	500:G	O3'	504:G	P	6.23
1	5	1239:C	O3'	1244:G	P	6.23
1	5	737:C	O3'	738:C	P	6.16
1	9	736:C	O3'	743:U	P	6.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	480:C	O3'	481:G	P	5.96
1	5	481:G	O3'	481(A):C	P	5.75
1	9	1432:U	O3'	1438:A	P	4.96
1	9	322:C	O3'	323:C	P	4.84
1	9	309:G	O3'	310:C	P	4.48
1	9	304:C	O3'	305:U	P	4.44
1	9	798:G	O3'	799:U	P	4.43
1	5	934:C	O3'	935:A	P	4.09
1	5	170:C	O3'	171:U	P	3.98
1	5	4899:G	O3'	4902:C	P	3.80
1	5	1100:U	O3'	1168:G	P	3.77
1	5	1438:U	O3'	1440:U	P	3.66
1	9	902:G	O3'	903:A	P	3.55
1	5	751:G	O3'	752:G	P	3.34
1	9	903:A	O3'	904:A	P	3.34
1	9	1295:A	O3'	1296:U	P	3.23
1	5	5020:G	O3'	5021:C	P	3.20
1	5	267:G	O3'	268:G	P	3.16

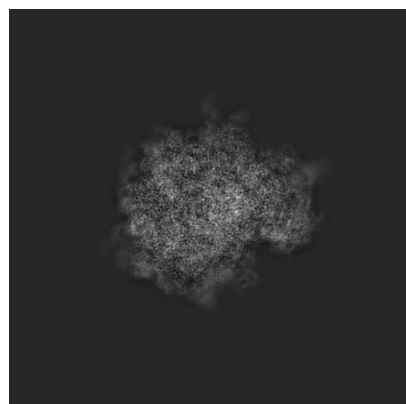
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9239. These allow visual inspection of the internal detail of the map and identification of artifacts.

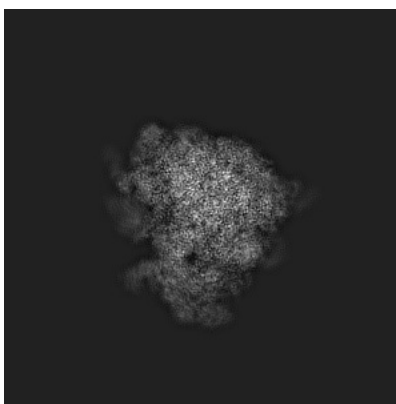
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

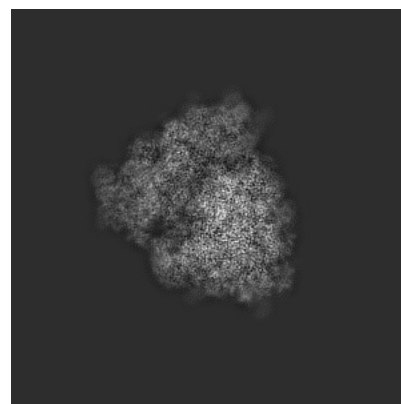
6.1.1 Primary map



X

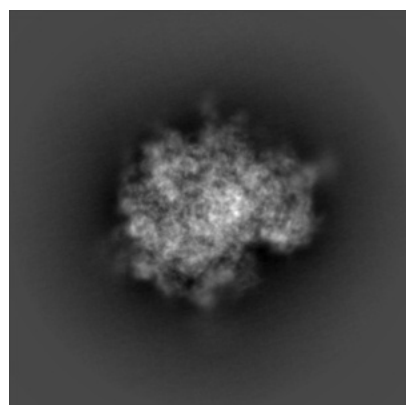


Y

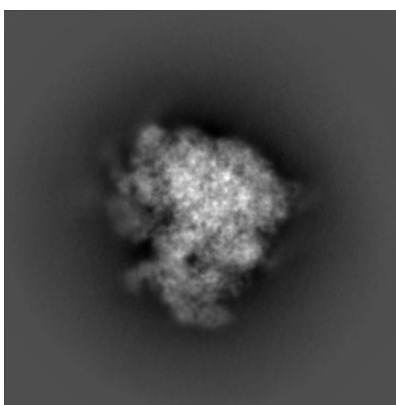


Z

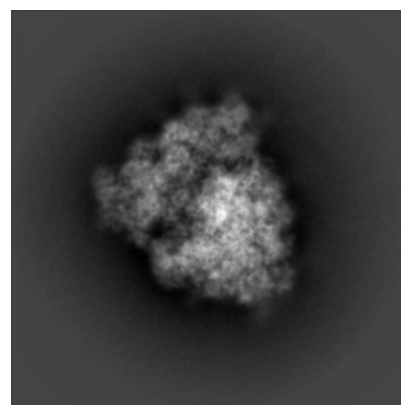
6.1.2 Raw map



X



Y

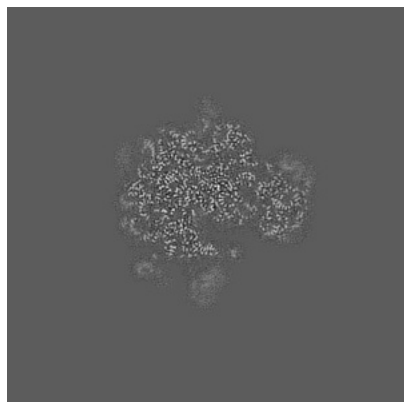


Z

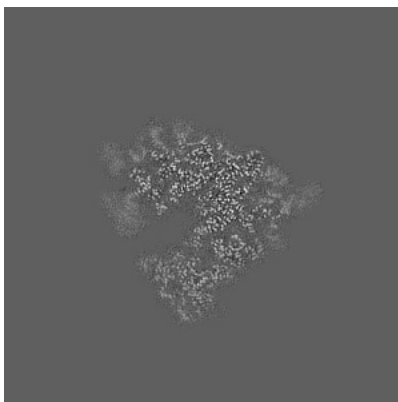
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

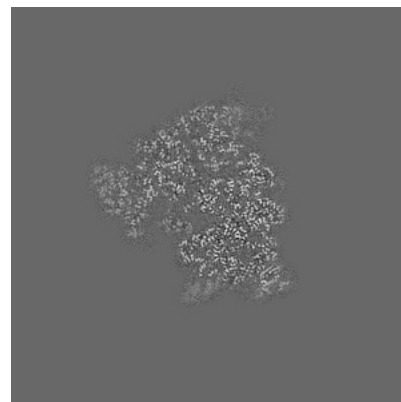
6.2.1 Primary map



X Index: 200

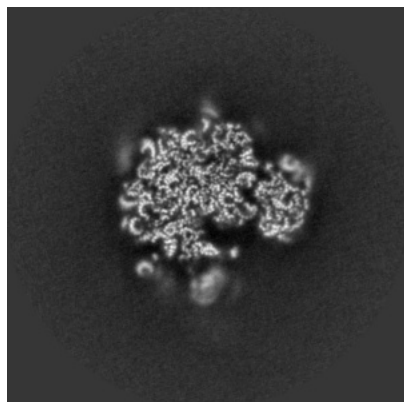


Y Index: 200

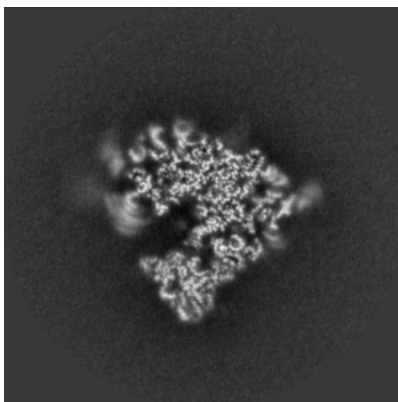


Z Index: 200

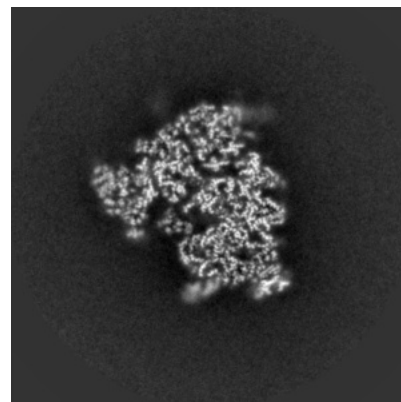
6.2.2 Raw map



X Index: 200



Y Index: 200

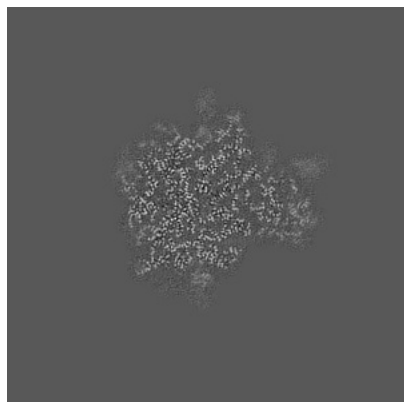


Z Index: 200

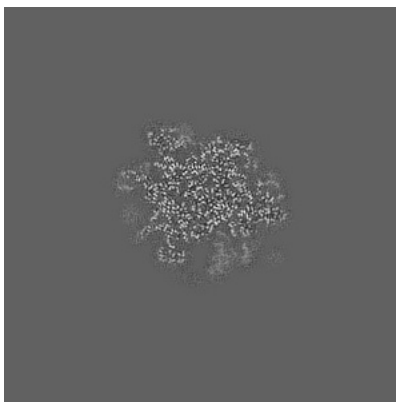
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

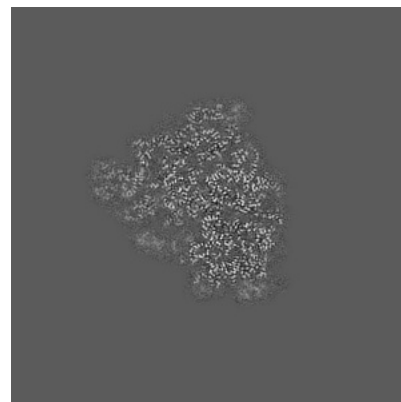
6.3.1 Primary map



X Index: 213

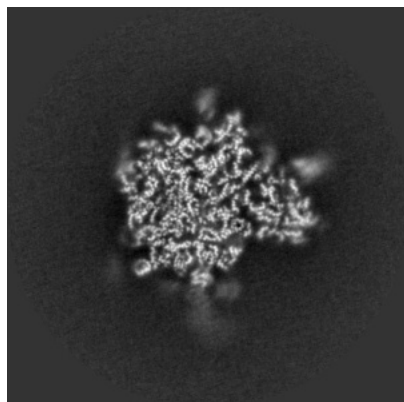


Y Index: 160

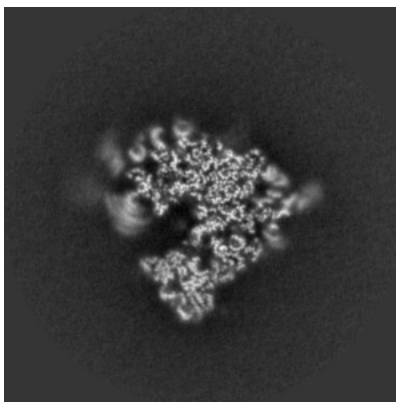


Z Index: 211

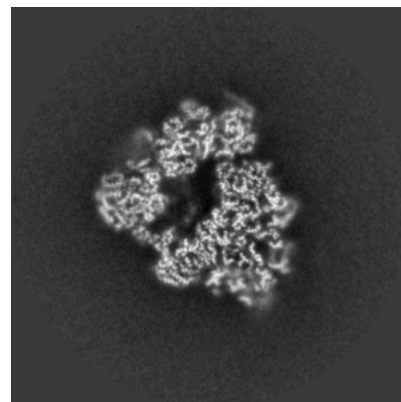
6.3.2 Raw map



X Index: 213



Y Index: 201

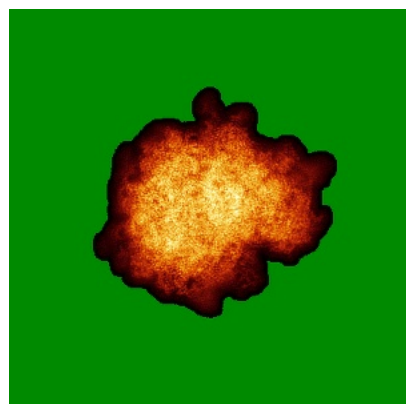


Z Index: 176

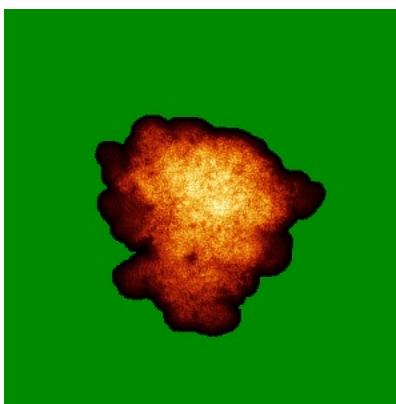
The images above show the largest variance slices of the map in three orthogonal directions.

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

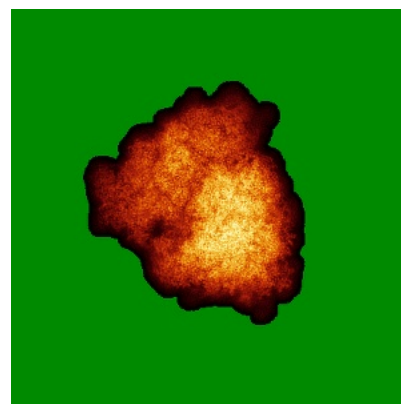
6.4.1 Primary map



X

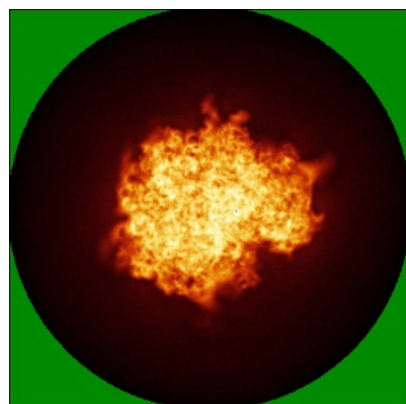


Y

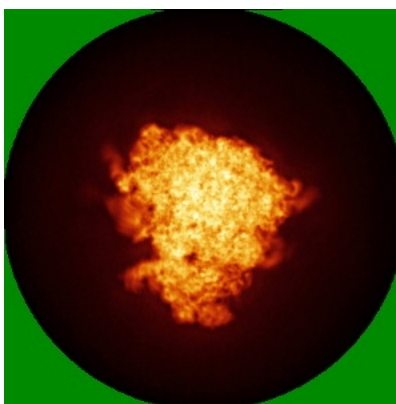


Z

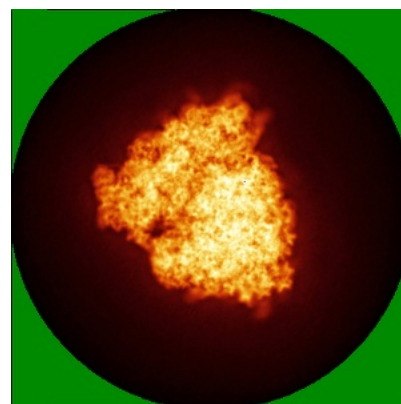
6.4.2 Raw map



X



Y

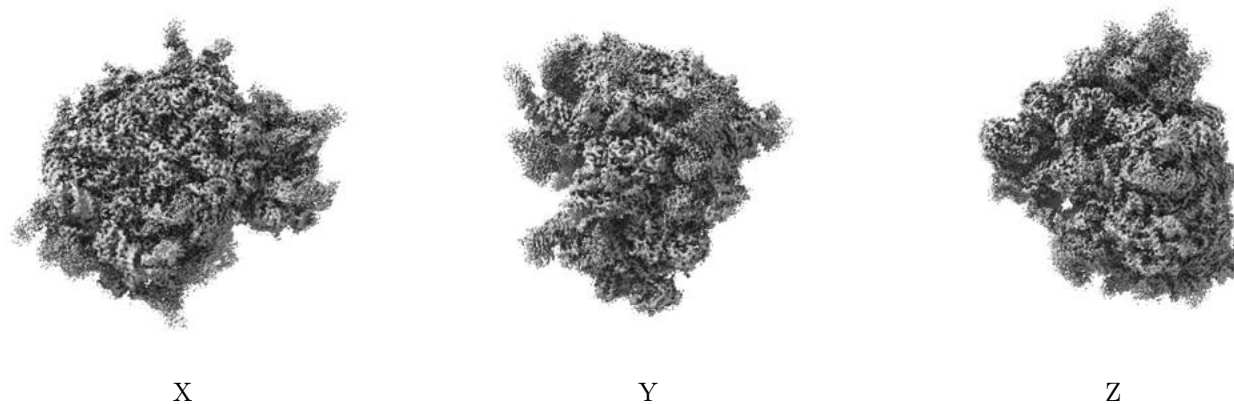


Z

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.

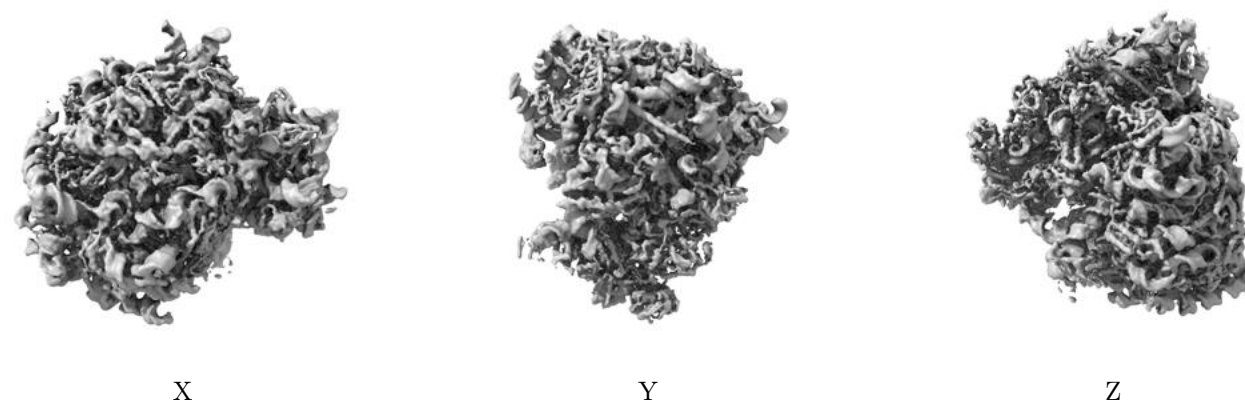
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

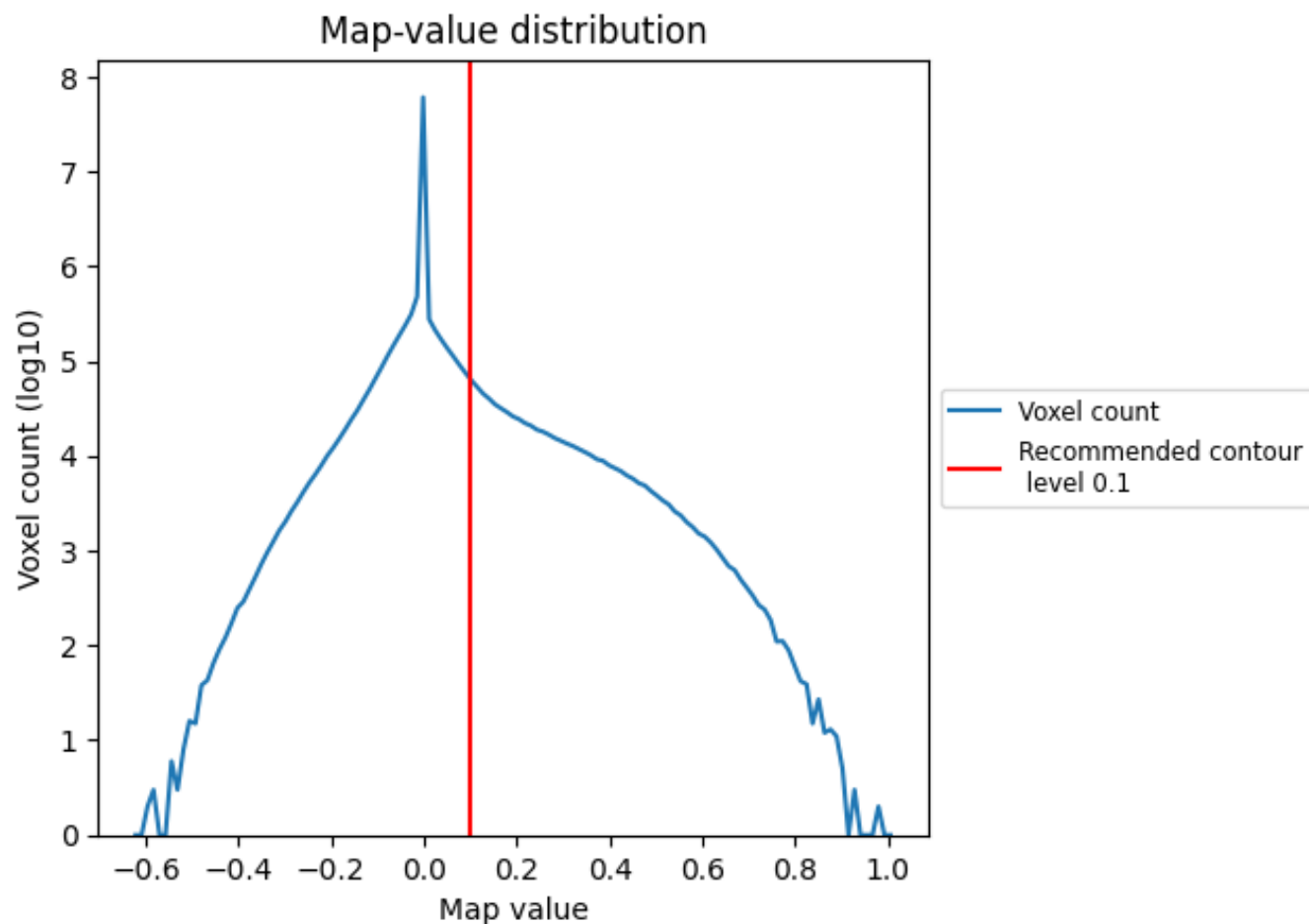
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

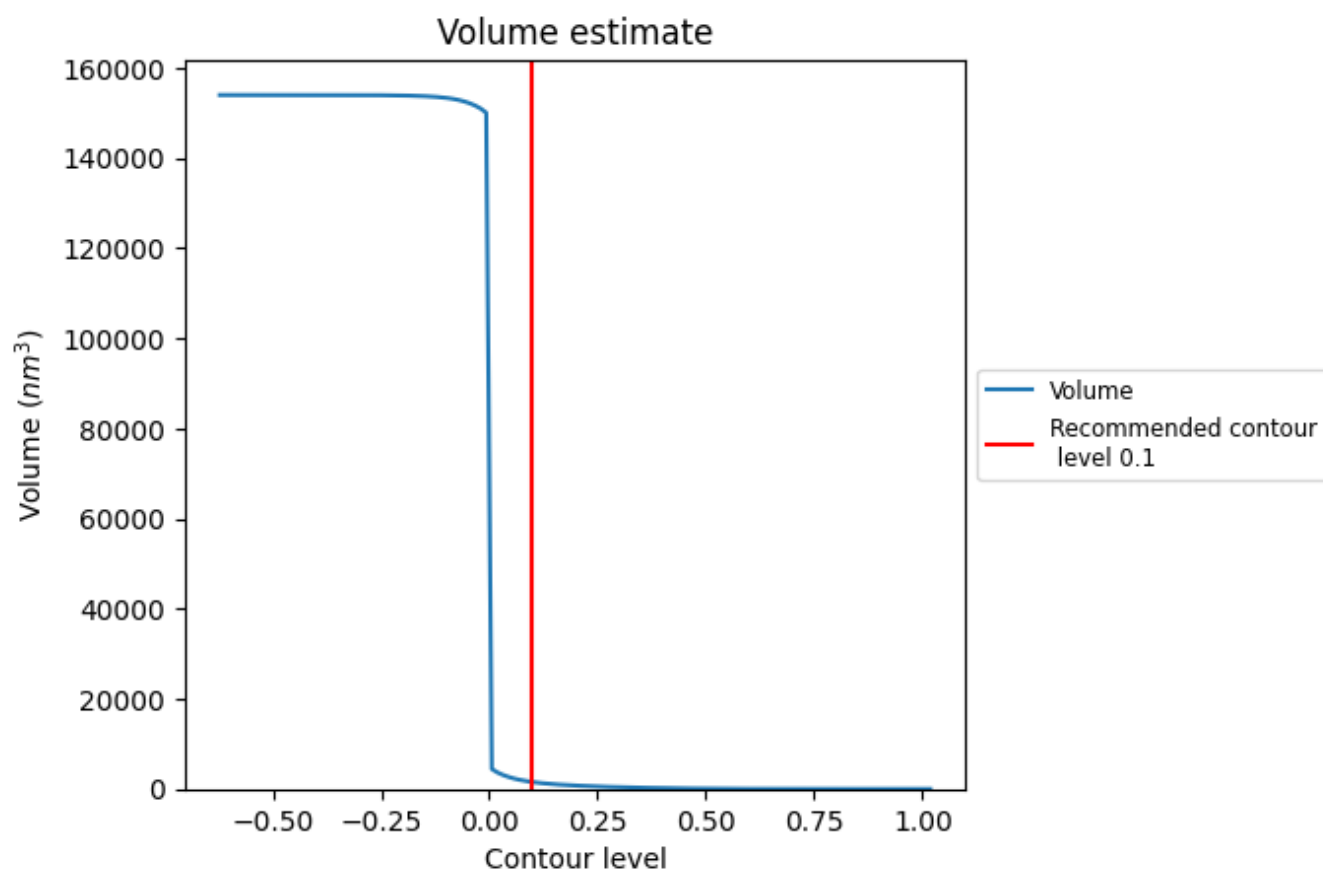
This section contains the results of statistical analysis of the map.

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.

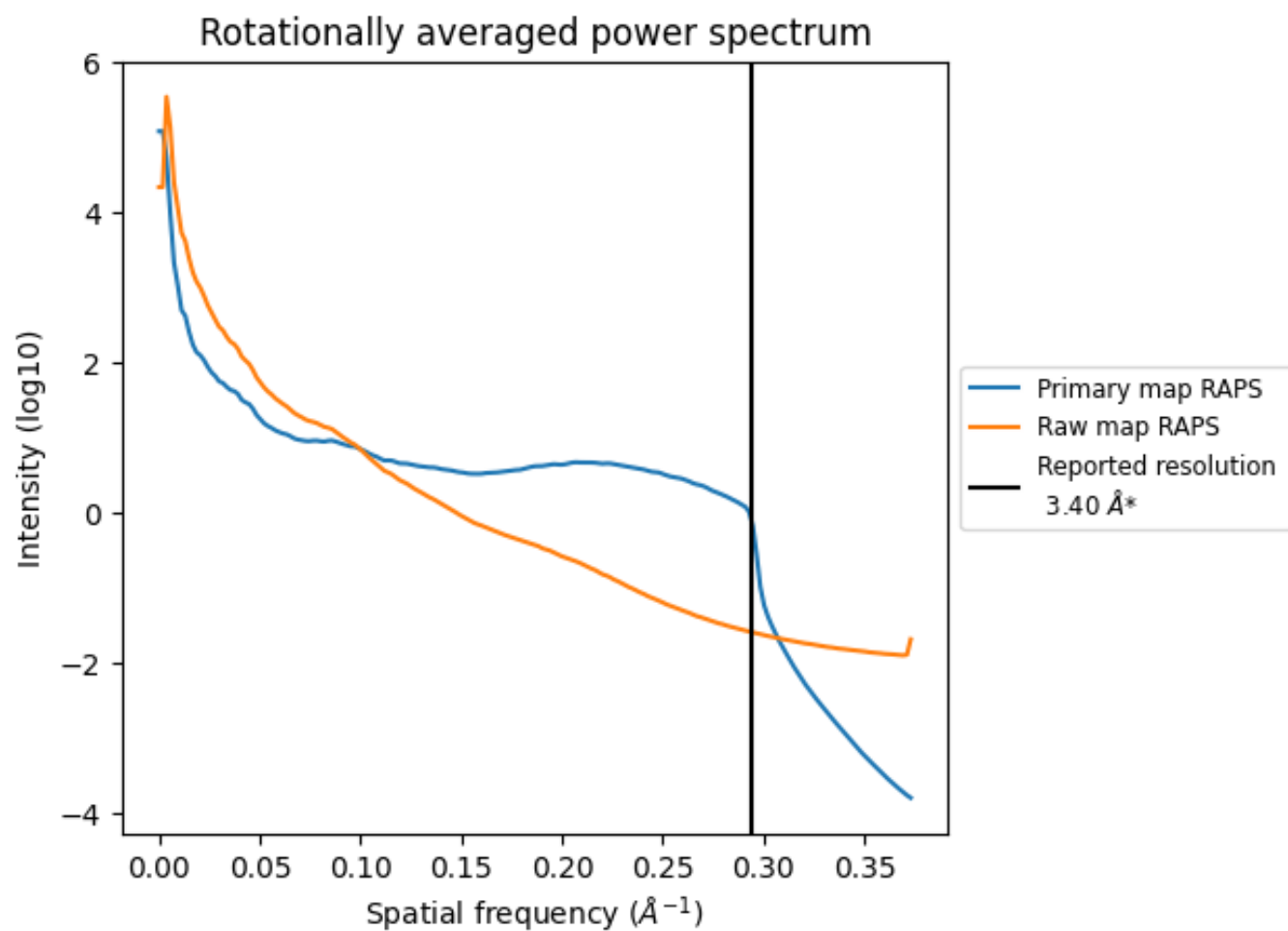
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1528 nm³; this corresponds to an approximate mass of 1381 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 ⓘ

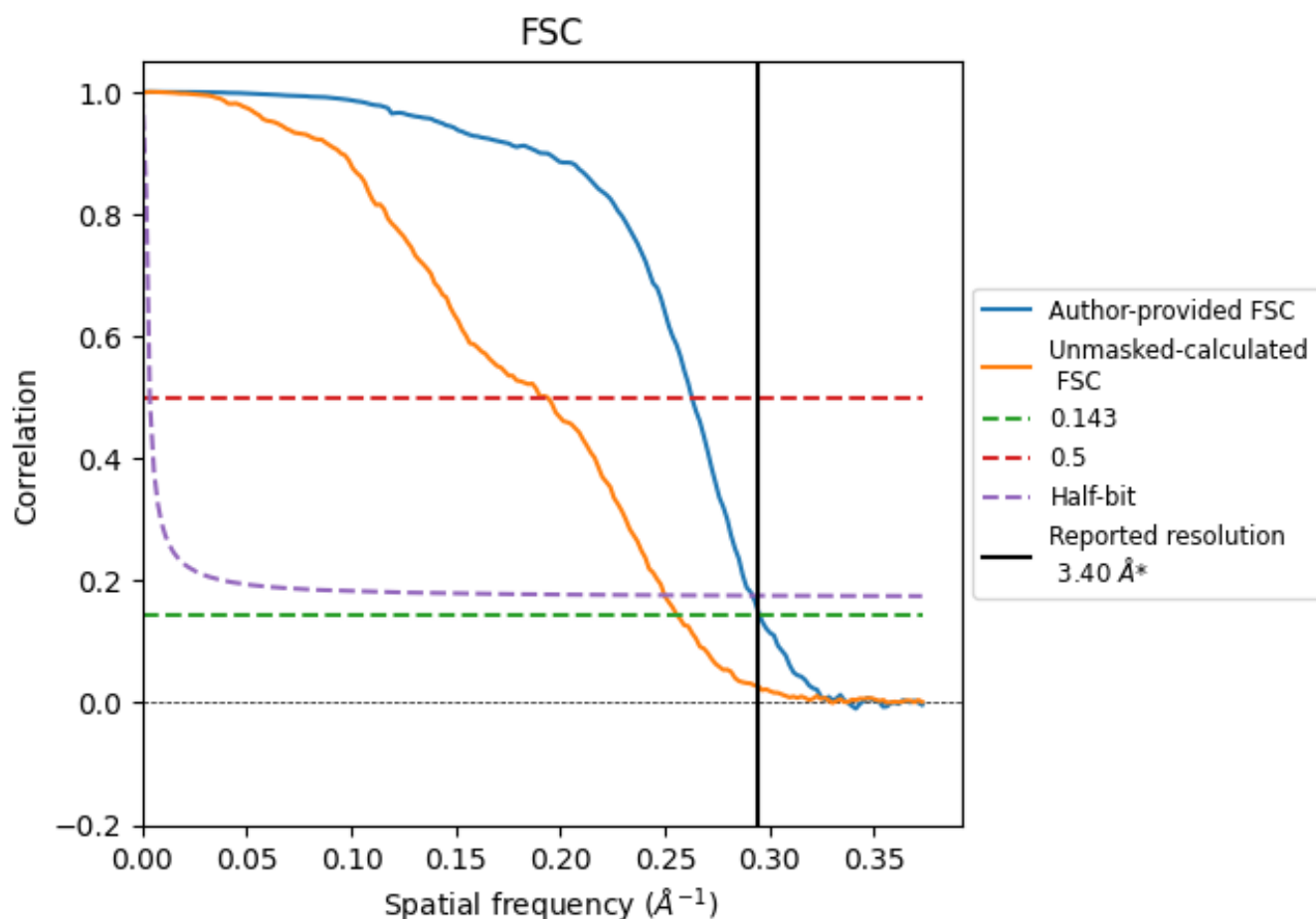


*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

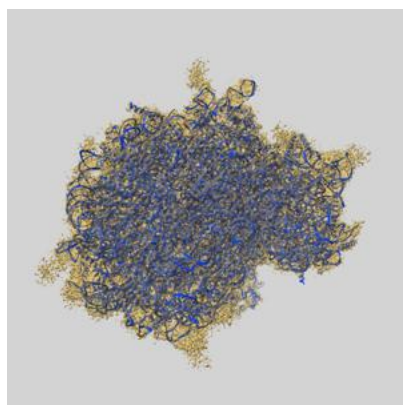
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.81	3.43
Unmasked-calculated*	3.91	5.16	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.4 by more than 10 %

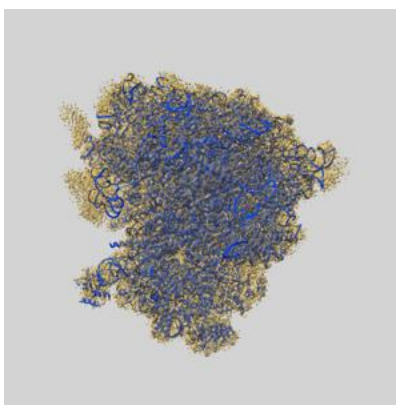
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9239 and PDB model 6MTC. Per-residue inclusion information can be found in section [3](#) on page [20](#).

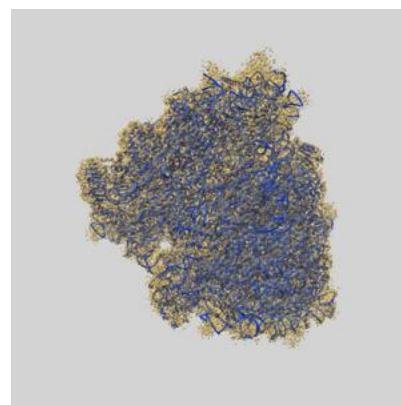
9.1 Map-model overlay [i](#)



X



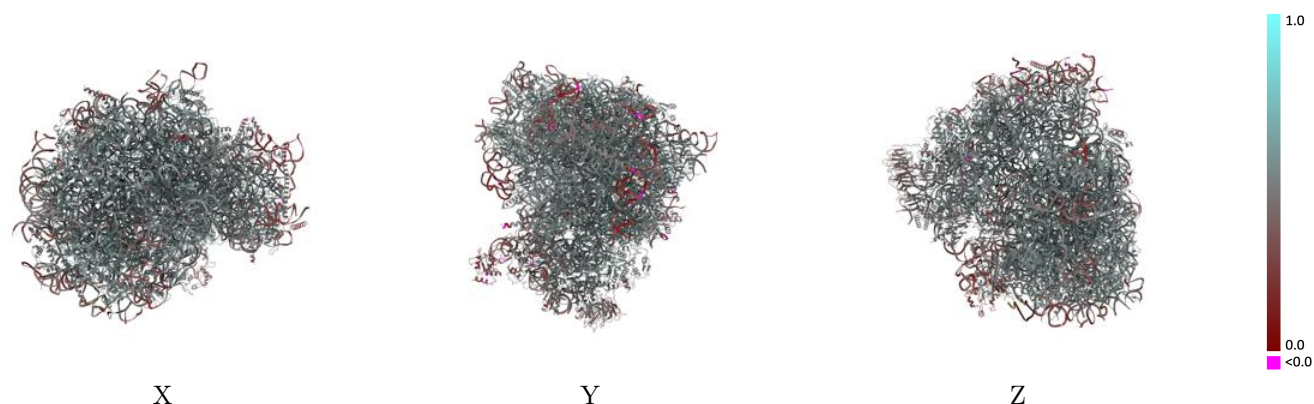
Y



Z

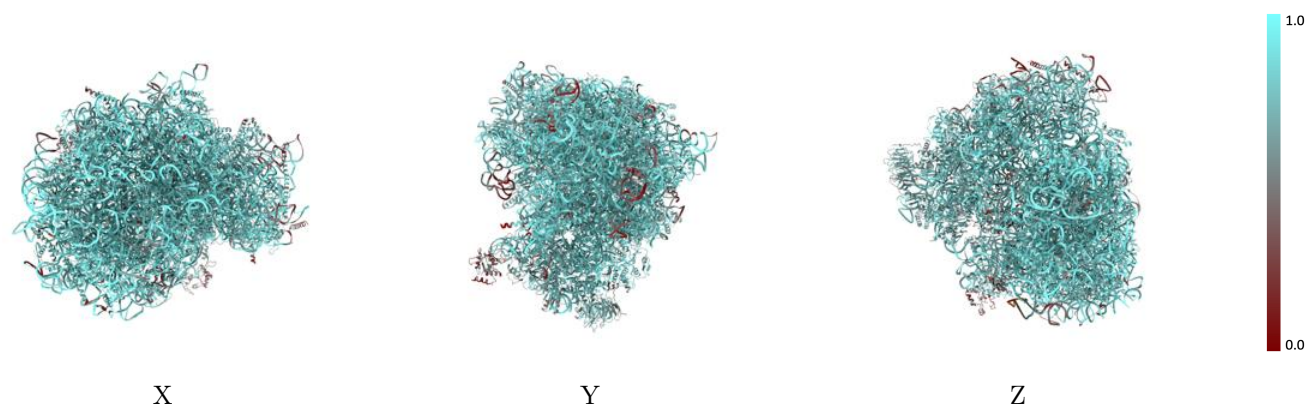
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



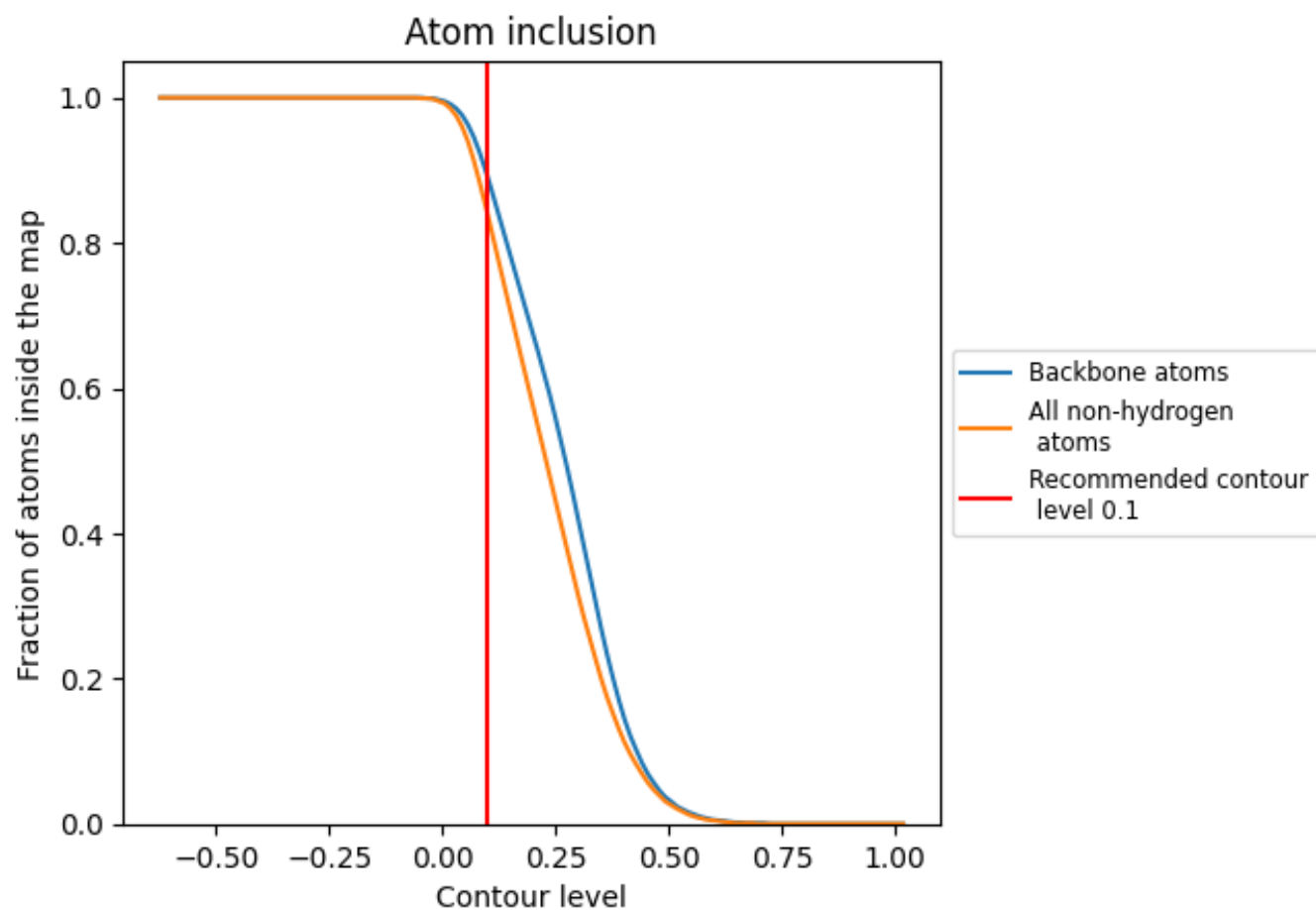
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.4970
4	 0.7290	 0.3350
5	 0.8830	 0.4920
7	 0.9390	 0.5210
8	 0.9060	 0.5060
9	 0.8690	 0.4760
A	 0.8870	 0.5620
AA	 0.8130	 0.5150
B	 0.8750	 0.5500
BB	 0.8030	 0.5210
C	 0.8650	 0.5490
CC	 0.8270	 0.5240
D	 0.8500	 0.5240
DD	 0.6920	 0.4640
E	 0.8410	 0.5280
EE	 0.8100	 0.5260
F	 0.8570	 0.5460
FF	 0.7740	 0.4930
G	 0.7970	 0.5110
GG	 0.7180	 0.4660
H	 0.8200	 0.5310
HH	 0.7300	 0.4720
I	 0.8510	 0.5440
II	 0.7890	 0.5150
J	 0.7900	 0.5020
JJ	 0.8080	 0.5050
KK	 0.6710	 0.4350
L	 0.8270	 0.5300
LL	 0.8150	 0.5350
M	 0.8470	 0.5280
MM	 0.3100	 0.2620
N	 0.8930	 0.5620
NN	 0.8410	 0.5300
O	 0.8540	 0.5430
OO	 0.8070	 0.5220



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Chain	Atom inclusion	Q-score
P	 0.8640	 0.5490
PP	 0.6710	 0.4330
Q	 0.8690	 0.5540
QQ	 0.7400	 0.4770
R	 0.8120	 0.5210
RR	 0.7500	 0.4860
S	 0.8660	 0.5520
SS	 0.7220	 0.4680
T	 0.8460	 0.5380
TT	 0.7430	 0.4740
U	 0.7830	 0.4850
UU	 0.6810	 0.4460
V	 0.8580	 0.5550
VV	 0.8020	 0.5250
W	 0.6940	 0.4530
WW	 0.8550	 0.5380
X	 0.8300	 0.5330
XX	 0.8230	 0.5300
Y	 0.8530	 0.5390
YY	 0.7810	 0.4960
Z	 0.8610	 0.5320
ZZ	 0.7050	 0.4620
a	 0.8730	 0.5560
aa	 0.8330	 0.5420
b	 0.7490	 0.4890
bb	 0.7870	 0.5180
c	 0.8360	 0.5290
cc	 0.7380	 0.5060
d	 0.8310	 0.5300
dd	 0.8080	 0.4980
e	 0.8730	 0.5590
ee	 0.6950	 0.4890
f	 0.8910	 0.5620
ff	 0.3810	 0.3280
g	 0.8310	 0.5430
gg	 0.6390	 0.4170
h	 0.8260	 0.5280
i	 0.8350	 0.5250
j	 0.9020	 0.5550
k	 0.7680	 0.5130
l	 0.8430	 0.5460
m	 0.8540	 0.5360

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Chain	Atom inclusion	Q-score
n	 0.7940	 0.5270
o	 0.8530	 0.5500
p	 0.8390	 0.5540
r	 0.8840	 0.5490
u	 0.4540	 0.3420
v	 0.6270	 0.4620