



Full wwPDB EM Validation Report ⓘ

Oct 28, 2025 – 07:55 pm GMT

PDB ID : 9QF5 / pdb_00009qf5
EMDB ID : EMD-53099
Title : Structure of P. furiosus 70S ribosome grown at 102deg
Authors : Matzov, D.; Georgeson, J.; Westhof, E.; Schwartz, S.; Shalev-Benami, M.
Deposited on : 2025-03-11
Resolution : 2.84 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

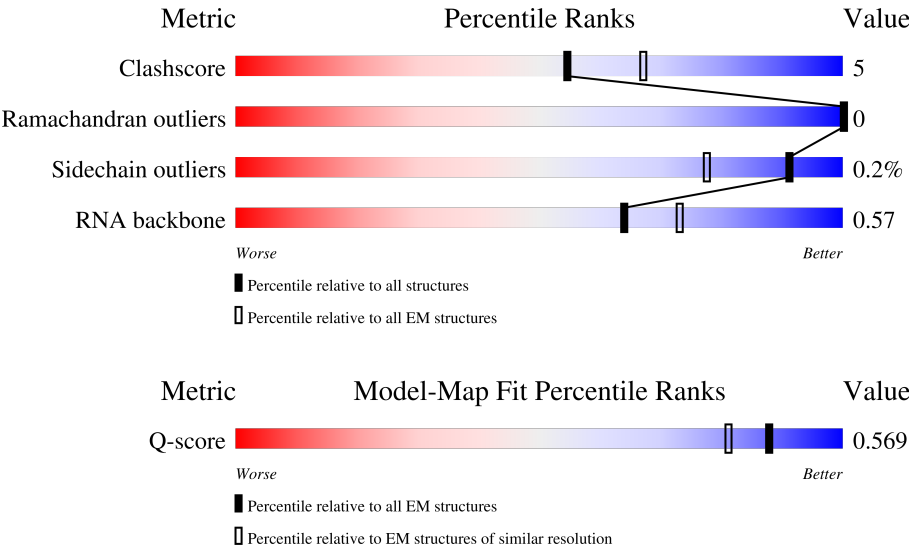
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	A1	1497	<div> <div>11%</div> <div>66%</div> <div>25%</div> <div>8%</div> </div>
2	Aa	202	<div> <div>38%</div> <div>87%</div> <div>10%</div> <div>•</div> </div>
3	Ab	210	<div> <div>74%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>


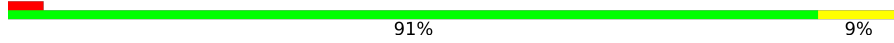

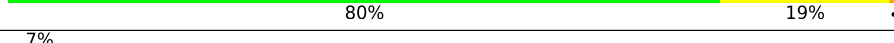
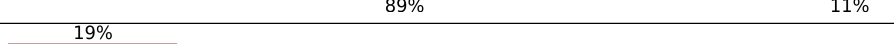
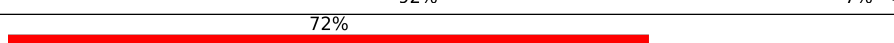


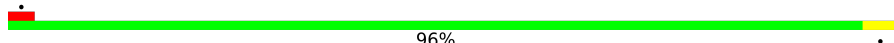



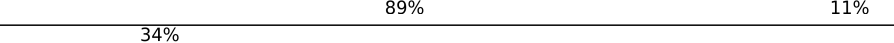

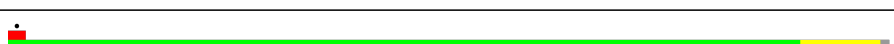


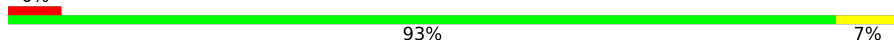

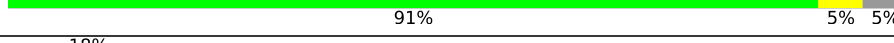

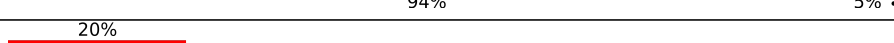
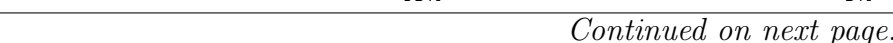


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Mol	Chain	Length	Quality of chain
4	Ac	198	
5	Ad	180	
6	Ae	243	
7	Af	236	
8	Ag	125	
9	Ah	215	
10	Ai	130	
11	Aj	127	
12	Ak	135	
13	Al	102	
14	Am	137	
15	An	147	
16	Ao	148	
17	Ap	56	
18	Aq	158	
19	Ar	113	
20	As	67	
21	At	132	
22	Au	150	
23	Av	99	
24	Aw	63	
25	Ax	71	
26	Ay	60	
27	B1	3051	
28	B2	125	

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Mol	Chain	Length	Quality of chain
29	BA	239	
30	BB	365	
31	BC	255	
32	BD	186	
33	BE	184	
34	BF	123	
34	BG	123	
35	BH	181	
36	BI	142	
37	BJ	141	
38	BK	83	
38	BL	83	
39	BM	147	
40	BN	194	
41	BO	203	
42	BP	120	
43	BQ	150	
44	BR	97	
45	BS	155	
46	BT	86	
47	BU	121	
48	BV	66	
49	BW	72	
50	BX	155	
51	BY	99	

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Mol	Chain	Length	Quality of chain
52	BZ	95	<p>9% 93% 6% .</p>
53	Ba	130	<p>87% 11% .</p>
54	Bb	89	<p>91% 7% .</p>
55	Bc	87	<p>91% 8% .</p>
56	Bd	62	<p>94% 5% .</p>
57	Be	83	<p>92% 6% .</p>
58	Bf	51	<p>92% 6% .</p>
59	Bg	51	<p>10% 82% 8% 10%</p>
60	Bh	37	<p>16% 81% 16% .</p>
61	Bi	94	<p>6% 90% 10%</p>
62	Bj	77	<p>25% 97% .</p>
63	Bk	64	<p>5% 86% 9% 5%</p>

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 164122 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 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	1490	Total	C	N	O	P	S	0	0
			32256	14418	5942	10405	1490	1		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	5	4AC	C	modified residue	GB 18980902
A1	41	4AC	C	modified residue	GB 18980902
A1	87	4AC	C	modified residue	GB 18980902
A1	141	4AC	C	modified residue	GB 18980902
A1	195	4AC	C	modified residue	GB 18980902
A1	216	4AC	C	modified residue	GB 18980902
A1	220	4AC	C	modified residue	GB 18980902
A1	231	4AC	C	modified residue	GB 18980902
A1	274	4AC	C	modified residue	GB 18980902
A1	291	4AC	C	modified residue	GB 18980902
A1	307	4AC	C	modified residue	GB 18980902
A1	367	4AC	C	modified residue	GB 18980902
A1	382	4AC	C	modified residue	GB 18980902
A1	405	4AC	C	modified residue	GB 18980902
A1	427	4AC	C	modified residue	GB 18980902
A1	444	4AC	C	modified residue	GB 18980902
A1	467	4AC	C	modified residue	GB 18980902
A1	499	4AC	C	modified residue	GB 18980902
A1	534	4AC	C	modified residue	GB 18980902
A1	540	4AC	C	modified residue	GB 18980902
A1	546	4AC	C	modified residue	GB 18980902
A1	578	4AC	C	modified residue	GB 18980902
A1	614	4AC	C	modified residue	GB 18980902
A1	624	4AC	C	modified residue	GB 18980902
A1	636	4AC	C	modified residue	GB 18980902
A1	691	4AC	C	modified residue	GB 18980902
A1	706	4AC	C	modified residue	GB 18980902
A1	719	4AC	C	modified residue	GB 18980902

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Chain	Residue	Modelled	Actual	Comment	Reference
A1	739	4AC	C	modified residue	GB 18980902
A1	761	4AC	C	modified residue	GB 18980902
A1	810	4AC	C	modified residue	GB 18980902
A1	816	4AC	C	modified residue	GB 18980902
A1	827	4AC	C	modified residue	GB 18980902
A1	836	4AC	C	modified residue	GB 18980902
A1	839	4AC	C	modified residue	GB 18980902
A1	856	4AC	C	modified residue	GB 18980902
A1	1016	4AC	C	modified residue	GB 18980902
A1	1029	4AC	C	modified residue	GB 18980902
A1	1067	4AC	C	modified residue	GB 18980902
A1	1092	4AC	C	modified residue	GB 18980902
A1	1135	4AC	C	modified residue	GB 18980902
A1	1181	4AC	C	modified residue	GB 18980902
A1	1221	4AC	C	modified residue	GB 18980902
A1	1227	4AC	C	modified residue	GB 18980902
A1	1254	4AC	C	modified residue	GB 18980902
A1	1288	4AC	C	modified residue	GB 18980902
A1	1314	4AC	C	modified residue	GB 18980902
A1	1467	4AC	C	modified residue	GB 18980902

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Aa	196	Total	C	N	O	S	0	0
			1572	1017	270	281	4		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ab	195	Total	C	N	O	S	0	0
			1529	979	282	265	3		

- Molecule 4 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ac	185	Total	C	N	O	S	0	0
			1520	983	265	267	5		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ad	173	Total	C	N	O	S	0	0
			1452	913	280	255	4		

- Molecule 6 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ae	242	Total	C	N	O	S	0	0
			1981	1280	356	340	5		

- Molecule 7 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Af	228	Total	C	N	O	S	0	0
			1800	1139	336	318	7		

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ag	124	Total	C	N	O	S	0	0
			975	618	179	177	1		

- Molecule 9 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ah	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		

- Molecule 10 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Ai	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		

- Molecule 11 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Aj	125	Total	C	N	O		0	0
			982	610	205	167			

- Molecule 12 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Ak	134	Total	C	N	O	S	0	0
			1058	663	201	189	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Al	99	Total	C	N	O	S	0	0
			798	494	155	146	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Am	128	Total	C	N	O	S	0	0
			963	597	192	172	2		

- Molecule 15 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	An	144	Total	C	N	O	S	0	0
			1124	715	215	191	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ao	137	Total	C	N	O	S	0	0
			1096	690	216	185	5		

- Molecule 17 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ap	54	Total	C	N	O	S	0	0
			441	279	92	65	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Aq	157	Total	C	N	O	S	0	0
			1302	829	249	220	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ar	107	Total	C	N	O	S	0	0
			877	560	165	149	3		

- Molecule 20 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	As	64	Total	C	N	O	S	0	0
			527	333	101	91	2		

- Molecule 21 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	At	122	Total	C	N	O	S	0	0
			991	635	185	165	6		

- Molecule 22 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Au	149	Total	C	N	O		0	0
			1221	790	219	212			

- Molecule 23 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Av	95	Total	C	N	O	S	0	0
			787	511	128	145	3		

- Molecule 24 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Aw	61	Total	C	N	O	S	0	0
			460	295	82	78	5		

- Molecule 25 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ax	64	Total	C	N	O		0	0
			508	311	101	96			

- Molecule 26 is a protein called Zn-ribbon RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ay	56	Total	C	N	O	S	0	0
			434	272	78	76	8		

- Molecule 27 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	B1	2931	Total	C	N	O	P	S	0	0
			63533	28393	11737	20471	2931	1		

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B2	125	Total	C	N	O	P	0	0
			2689	1198	494	872	125		

- Molecule 29 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BA	238	Total	C	N	O	S	0	0
			1825	1161	345	315	4		

- Molecule 30 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BB	364	Total	C	N	O	S	0	0
			2900	1862	525	499	14		

- Molecule 31 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BC	255	Total	C	N	O	S	0	0
			2026	1288	391	342	5		

- Molecule 32 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BD	184	Total	C	N	O	S	0	0
			1442	905	275	254	8		

- Molecule 33 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BE	183	Total	C	N	O	S	0	0
			1468	951	251	265	1		

- Molecule 34 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BF	122	Total	C	N	O	S	0	0
			931	594	154	180	3		
34	BG	121	Total	C	N	O	S	0	0
			921	588	152	178	3		

- Molecule 35 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BH	167	Total	C	N	O	S	0	0
			1367	868	261	232	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BI	142	Total	C	N	O	S	0	0
			1150	737	215	195	3		

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BJ	140	Total	C	N	O	S	0	0
			1062	660	214	185	3		

- Molecule 38 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BK	81	Total	C	N	O	S	0	0
			614	386	119	108	1		
38	BL	82	Total	C	N	O	S	0	0
			621	391	120	109	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BM	147	Total	C	N	O	S	0	0
			1154	727	227	195	5		

- Molecule 40 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BN	193	Total	C	N	O	S	0	0
			1587	1015	315	252	5		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BO	196	Total	C	N	O	S	0	0
			1560	996	294	269	1		

- Molecule 42 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BP	120	Total	C	N	O	S	0	0
			966	606	186	171	3		

- Molecule 43 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BQ	148	Total	C	N	O	S	0	0
			1238	783	252	199	4		

- Molecule 44 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BR	96	Total	C	N	O	S	0	0
			794	506	161	126	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BS	151	Total	C	N	O	S	0	0
			1204	770	228	202	4		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BT	86	Total	C	N	O	S	0	0
			696	449	120	126	1		

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BU	120	Total	C	N	O	S	0	0
			1003	635	194	170	4		

- Molecule 48 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BV	63	Total	C	N	O	S	0	0
			527	336	100	85	6		

- Molecule 49 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BW	67	Total	C	N	O	S	0	0
			545	338	107	96	4		

- Molecule 50 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BX	154	Total	C	N	O	S	0	0
			1235	783	234	212	6		

- Molecule 51 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BY	97	Total	C	N	O	S	0	0
			730	475	115	139	1		

- Molecule 52 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	BZ	94	Total	C	N	O	0	0
			746	487	138	121		

- Molecule 53 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Ba	127	Total	C	N	O	S	0	0
			1068	686	214	167	1		

- Molecule 54 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bb	87	Total	C	N	O	S	0	0
			725	454	156	104	11		

- Molecule 55 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Bc	86	Total	C	N	O	S	0	0
			677	429	131	116	1		

- Molecule 56 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bd	61	Total	C	N	O	S	0	0
			493	304	109	76	4		

- Molecule 57 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Be	81	Total	C	N	O	S	0	0
			606	378	126	97	5		

- Molecule 58 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Bf	50	Total	C	N	O	0	0
			437	279	97	61		

- Molecule 59 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bg	46	Total	C	N	O	S	0	0
			375	238	77	56	4		

- Molecule 60 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bh	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 61 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bi	94	Total	C	N	O	S	0	0
			787	499	161	122	5		

- Molecule 62 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bj	77	Total	C	N	O	S	0	0
			659	425	118	115	1		

- Molecule 63 is a protein called C2H2-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bk	61	Total	C	N	O	S	0	0
			508	327	102	76	3		

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
64	Af	1	Total	Zn	0
			1	1	
64	Ap	1	Total	Zn	0
			1	1	
64	Ar	1	Total	Zn	0
			1	1	
64	Aw	1	Total	Zn	0
			1	1	
64	Ay	2	Total	Zn	0
			2	2	
64	BV	1	Total	Zn	0
			1	1	
64	Bb	1	Total	Zn	0
			1	1	
64	Bd	1	Total	Zn	0
			1	1	
64	Be	1	Total	Zn	0
			1	1	
64	Bg	1	Total	Zn	0
			1	1	
64	Bi	1	Total	Zn	0
			1	1	
64	Bk	1	Total	Zn	0
			1	1	

- Molecule 65 is water.

Mol	Chain	Residues	Atoms		AltConf
65	A1	69	Total 69	O 69	0
65	Ac	1	Total 1	O 1	0
65	Ae	1	Total 1	O 1	0
65	Ah	1	Total 1	O 1	0
65	Aj	1	Total 1	O 1	0
65	Ak	1	Total 1	O 1	0
65	Aq	1	Total 1	O 1	0
65	B1	1221	Total 1221	O 1221	0
65	B2	9	Total 9	O 9	0
65	BA	16	Total 16	O 16	0
65	BB	12	Total 12	O 12	0
65	BC	14	Total 14	O 14	0
65	BE	2	Total 2	O 2	0
65	BH	7	Total 7	O 7	0
65	BI	5	Total 5	O 5	0
65	BJ	4	Total 4	O 4	0
65	BM	13	Total 13	O 13	0
65	BN	12	Total 12	O 12	0
65	BO	3	Total 3	O 3	0
65	BP	4	Total 4	O 4	0
65	BQ	4	Total 4	O 4	0

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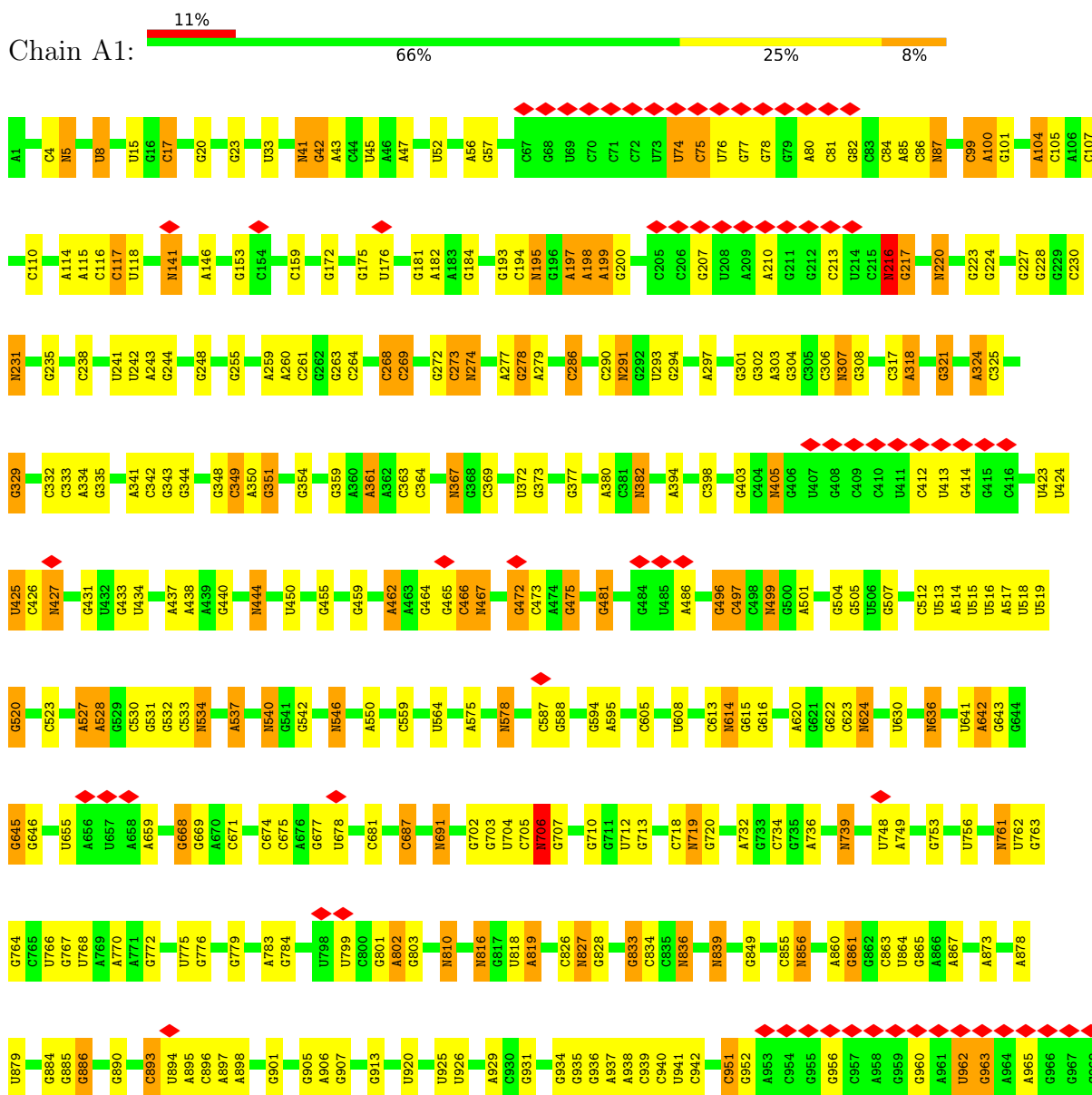
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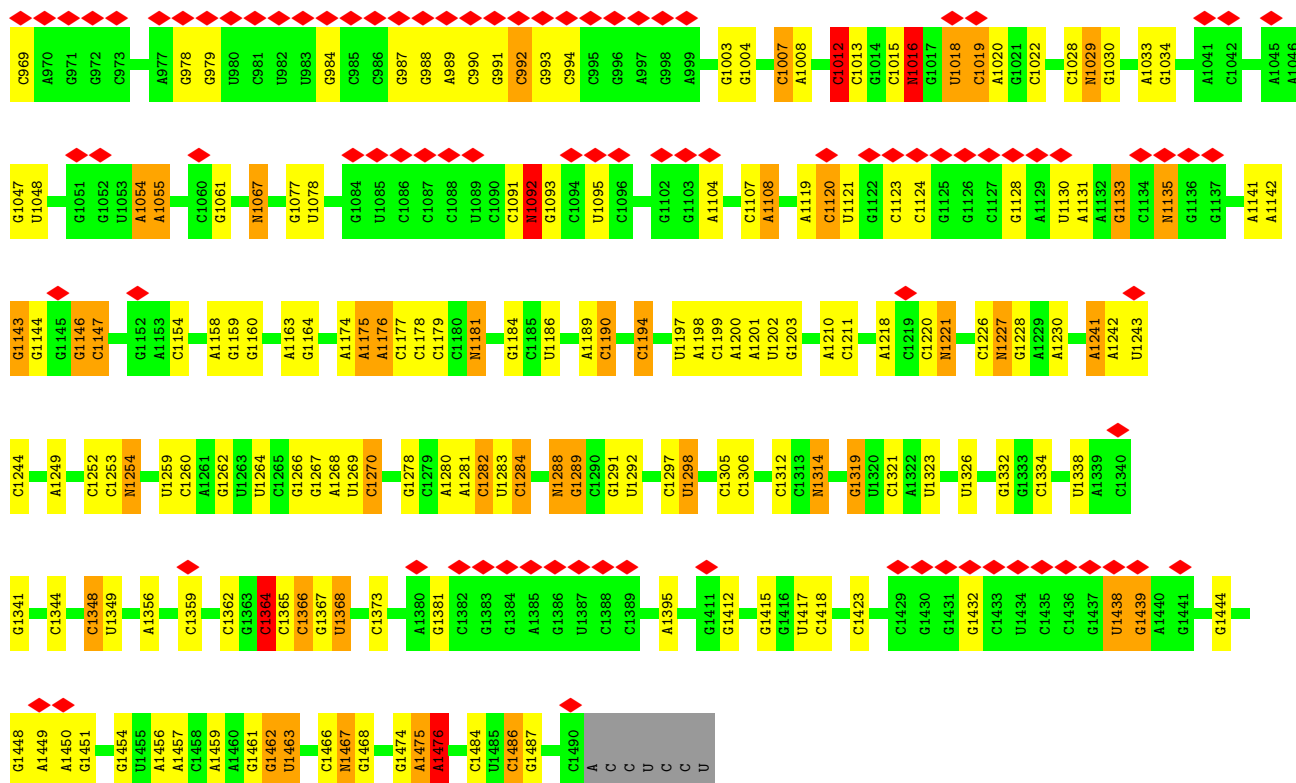
Mol	Chain	Residues	Atoms		AltConf
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65	BS	14	Total 14	O 14	0
65	BT	5	Total 5	O 5	0
65	BU	8	Total 8	O 8	0
65	BV	4	Total 4	O 4	0
65	BX	2	Total 2	O 2	0
65	BY	1	Total 1	O 1	0
65	BZ	3	Total 3	O 3	0
65	Ba	11	Total 11	O 11	0
65	Bb	7	Total 7	O 7	0
65	Bc	2	Total 2	O 2	0
65	Bd	7	Total 7	O 7	0
65	Be	2	Total 2	O 2	0
65	Bf	8	Total 8	O 8	0
65	Bg	1	Total 1	O 1	0
65	Bi	1	Total 1	O 1	0
65	Bj	1	Total 1	O 1	0
65	Bk	4	Total 4	O 4	0

3 Residue-property plots

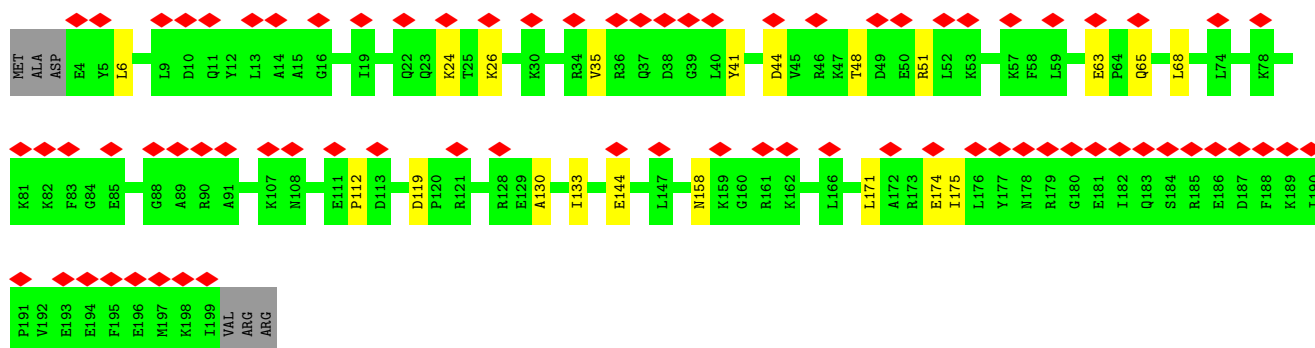
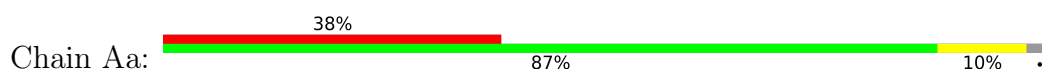
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

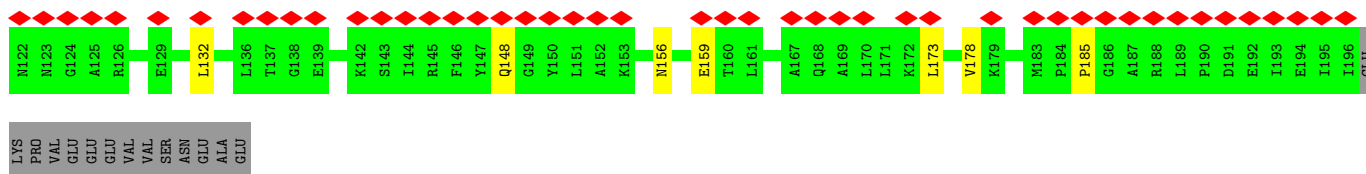
• Molecule 1: 16S rRNA



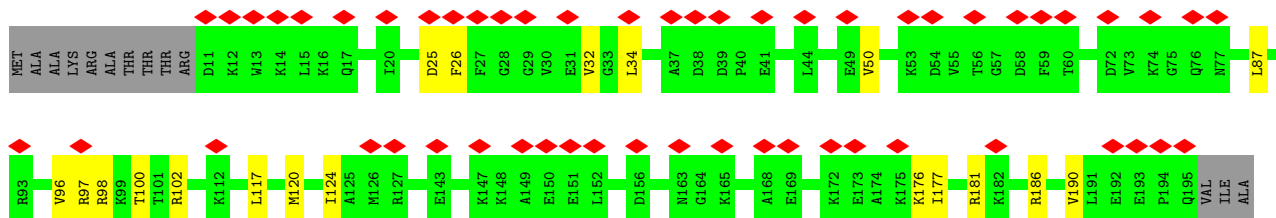
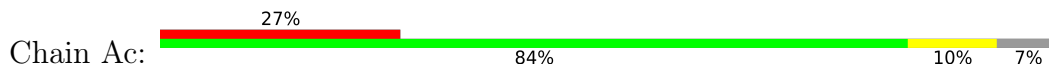


Chain Aa:

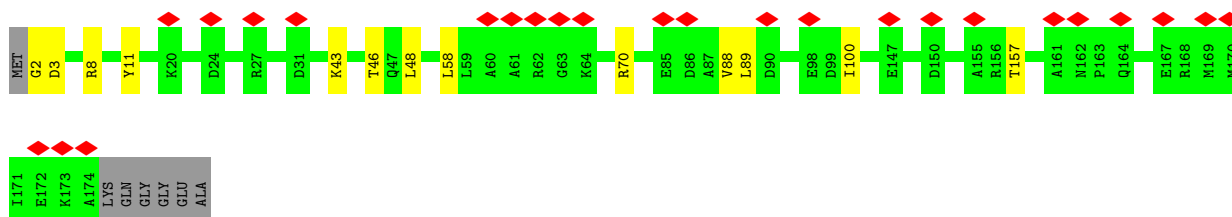
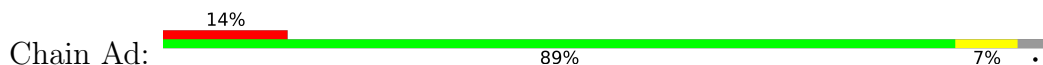




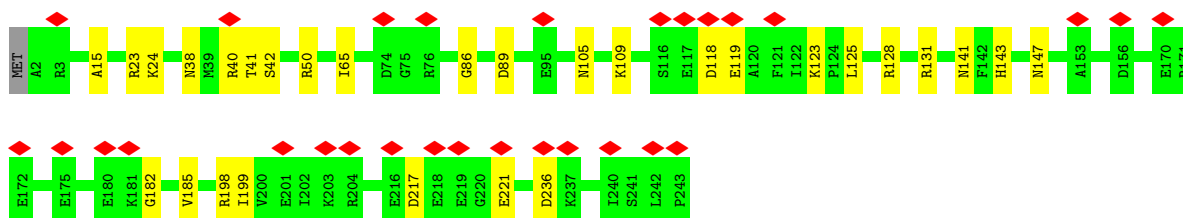
- Molecule 4: Small ribosomal subunit protein eS1



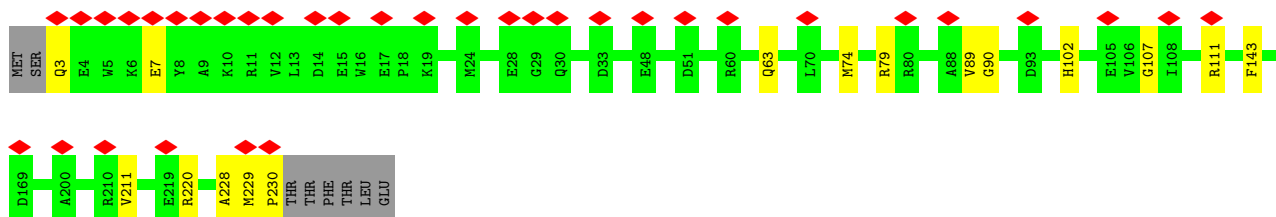
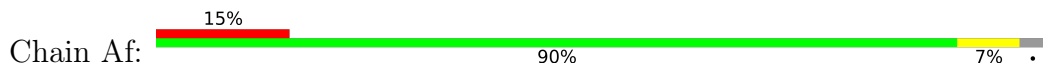
- Molecule 5: Small ribosomal subunit protein uS4



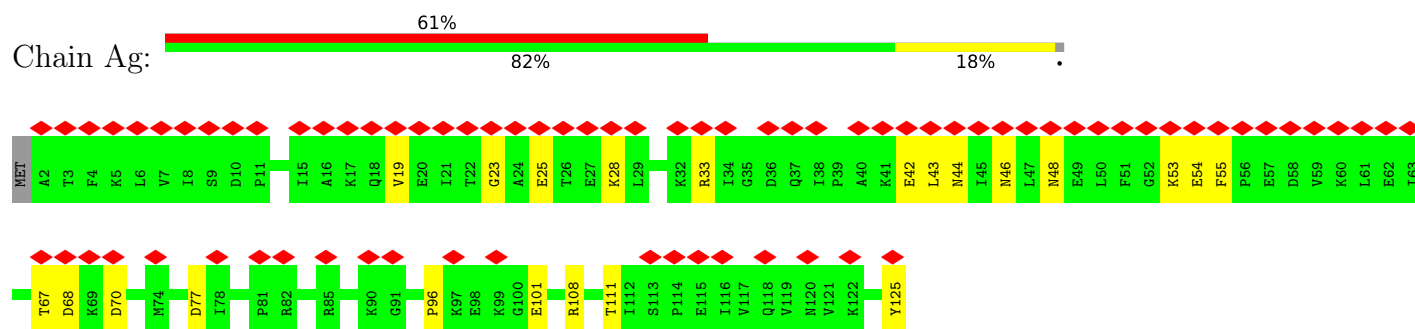
- Molecule 6: Small ribosomal subunit protein eS4



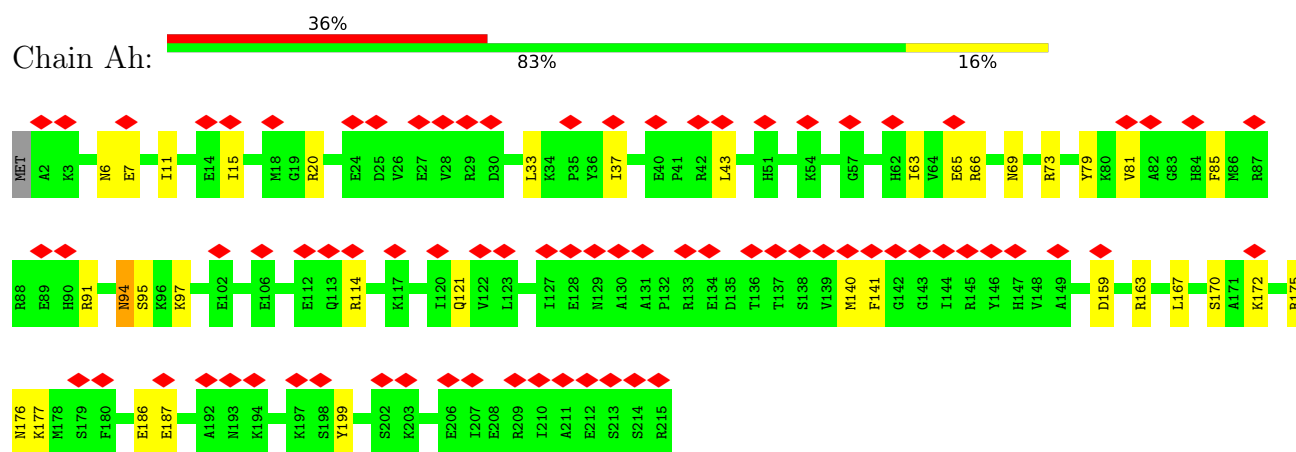
- Molecule 7: Small ribosomal subunit protein uS5



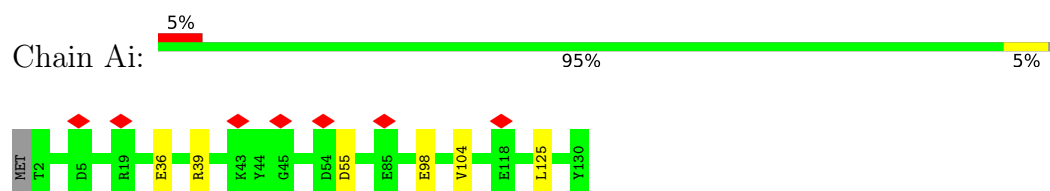
- Molecule 8: Small ribosomal subunit protein eS6



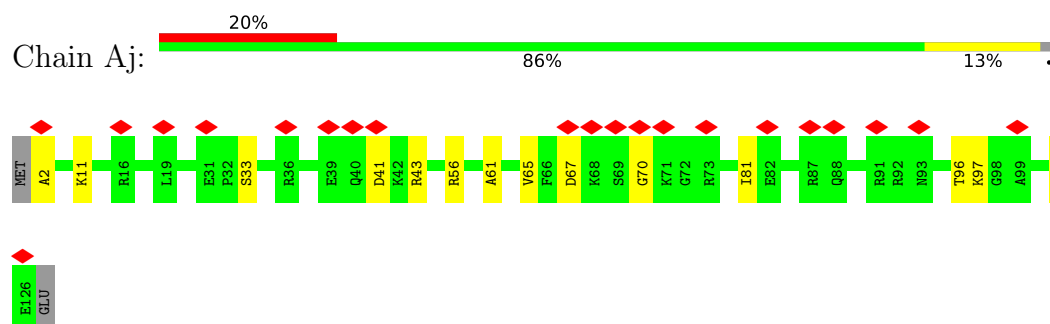
- Molecule 9: Small ribosomal subunit protein uS7



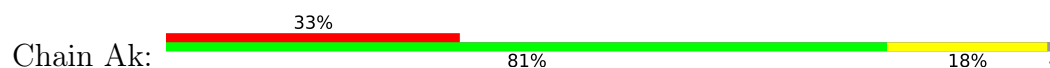
- Molecule 10: Small ribosomal subunit protein uS8

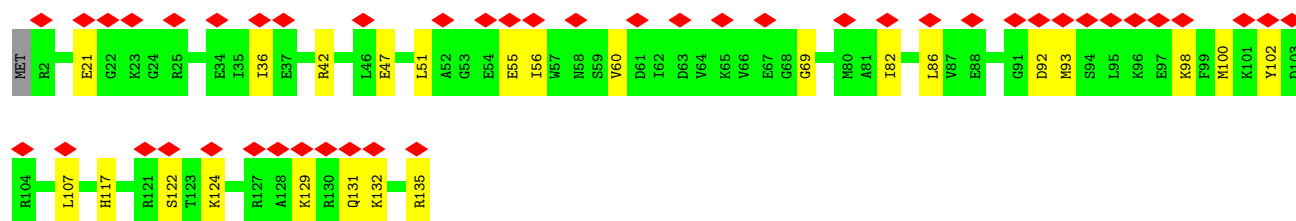


- Molecule 11: Small ribosomal subunit protein eS8

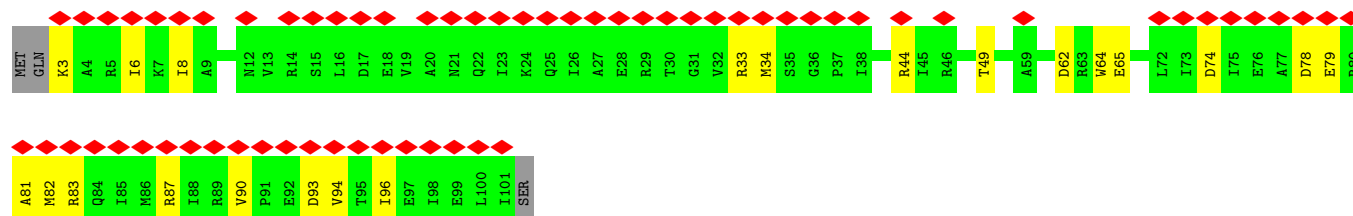
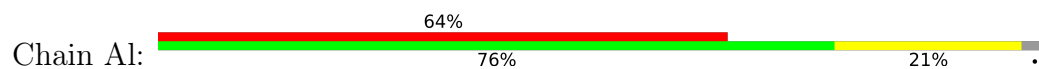


- Molecule 12: Small ribosomal subunit protein uS9

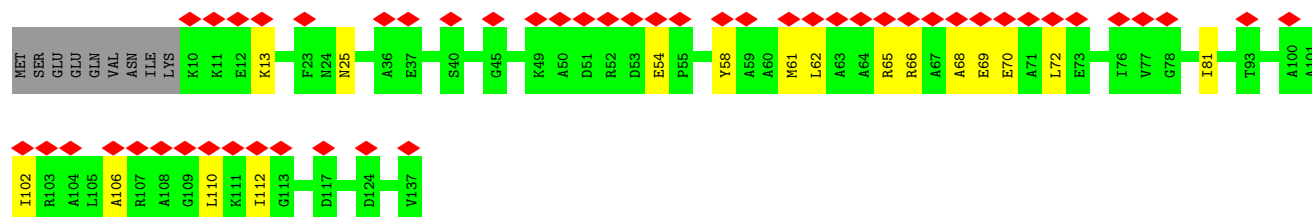
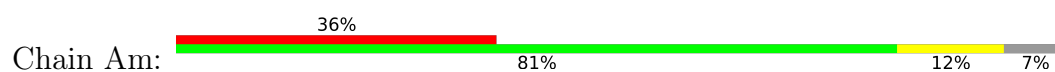




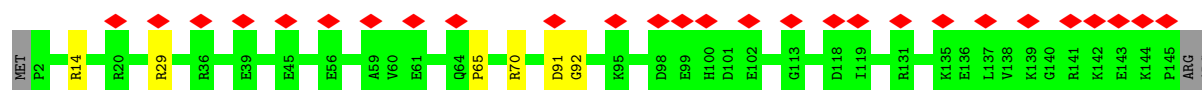
- Molecule 13: Small ribosomal subunit protein uS10



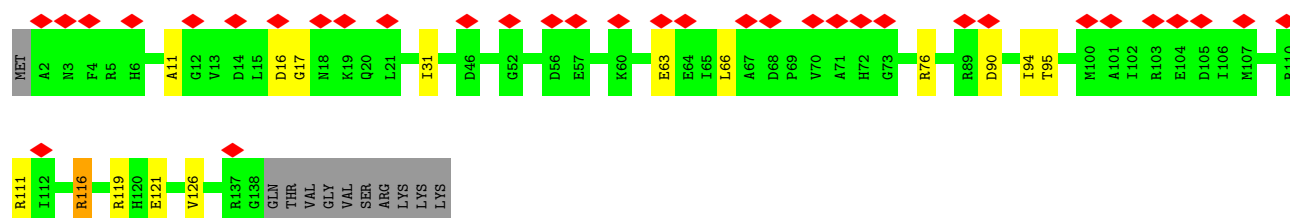
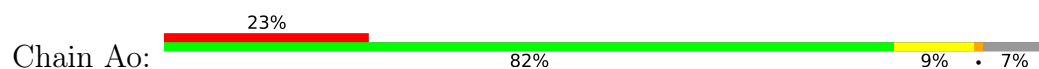
- Molecule 14: Small ribosomal subunit protein uS11



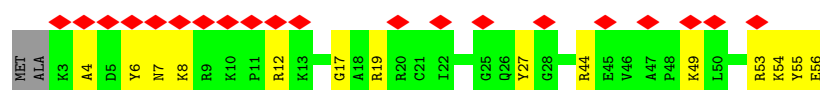
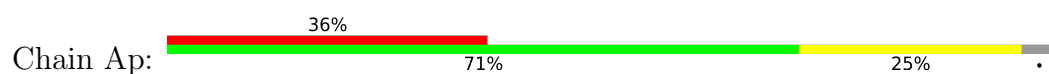
- Molecule 15: Small ribosomal subunit protein uS12



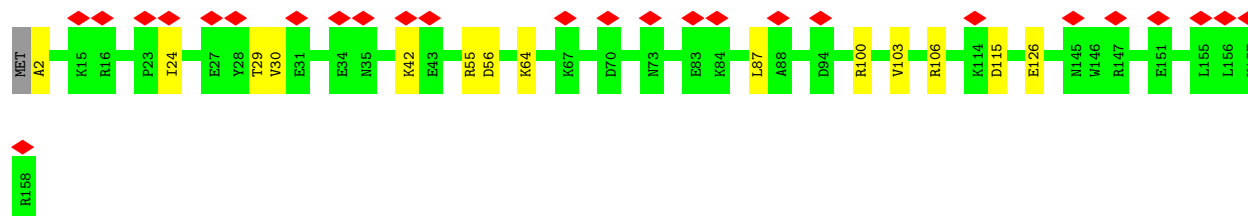
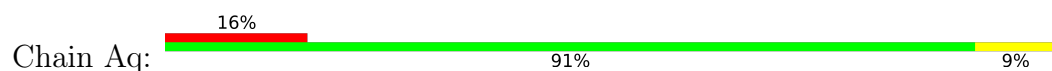
- Molecule 16: Small ribosomal subunit protein uS13



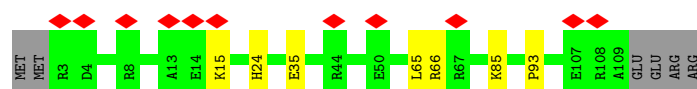
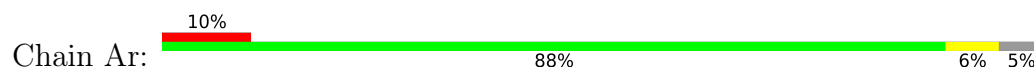
- Molecule 17: Small ribosomal subunit protein uS14



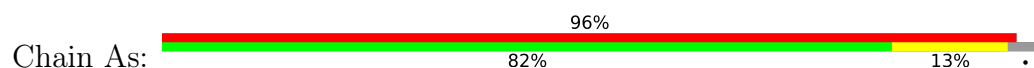
- Molecule 18: Small ribosomal subunit protein uS15



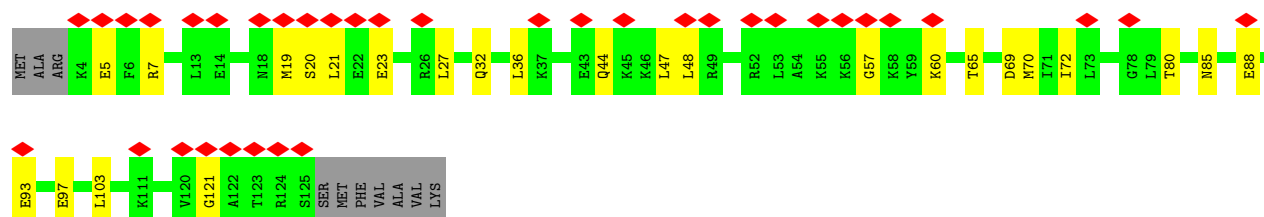
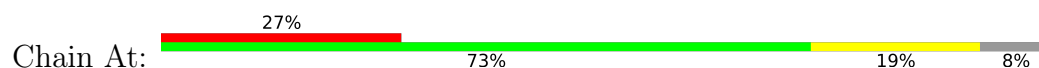
- Molecule 19: Small ribosomal subunit protein uS17



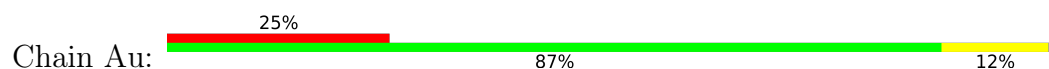
- Molecule 20: Small ribosomal subunit protein eS17

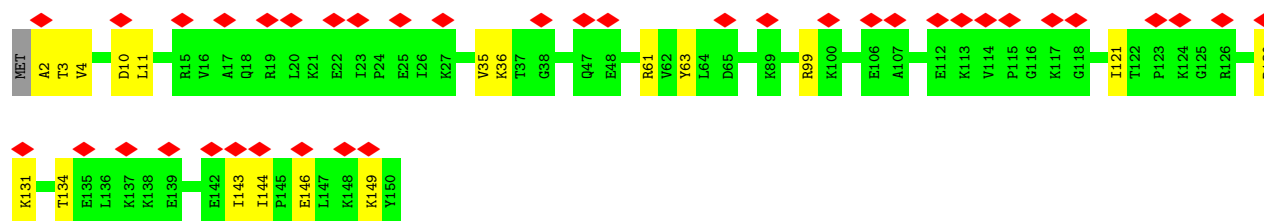


- Molecule 21: Small ribosomal subunit protein uS19

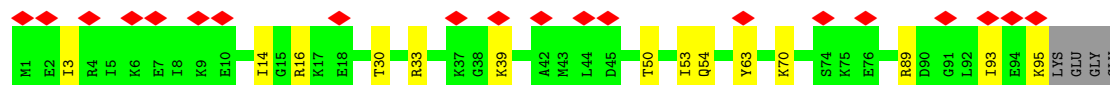
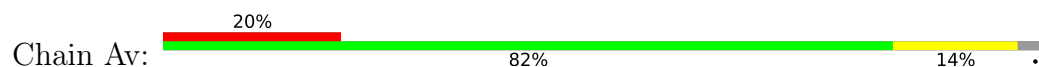


- Molecule 22: Small ribosomal subunit protein eS19

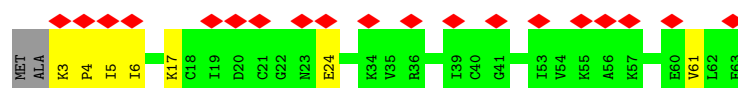
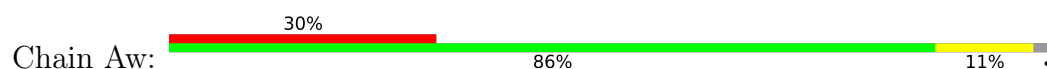




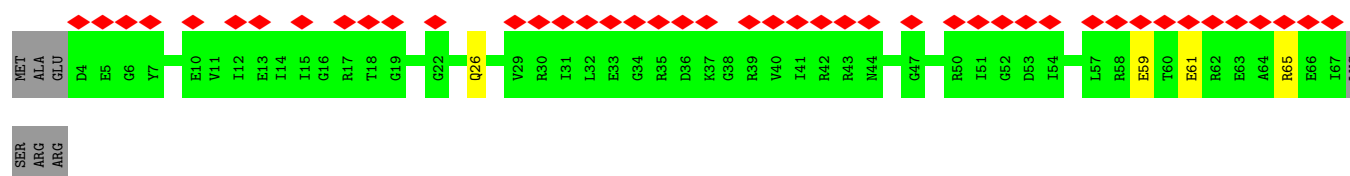
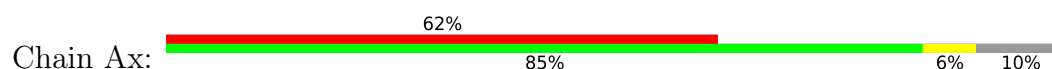
- Molecule 23: Small ribosomal subunit protein eS24



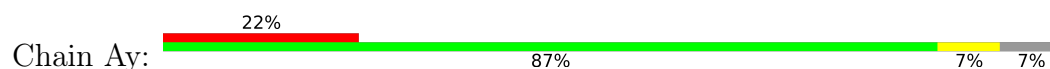
- Molecule 24: Small ribosomal subunit protein eS27



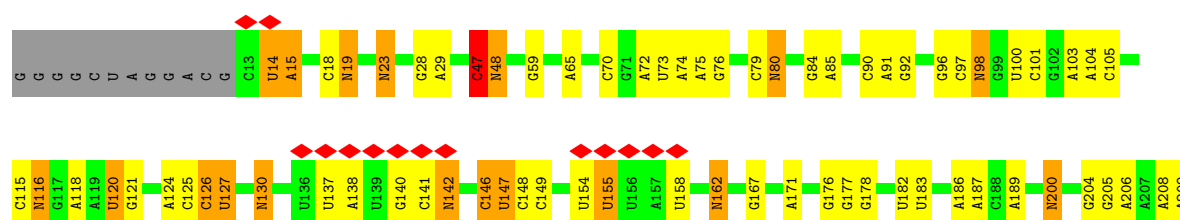
- Molecule 25: Small ribosomal subunit protein eS28



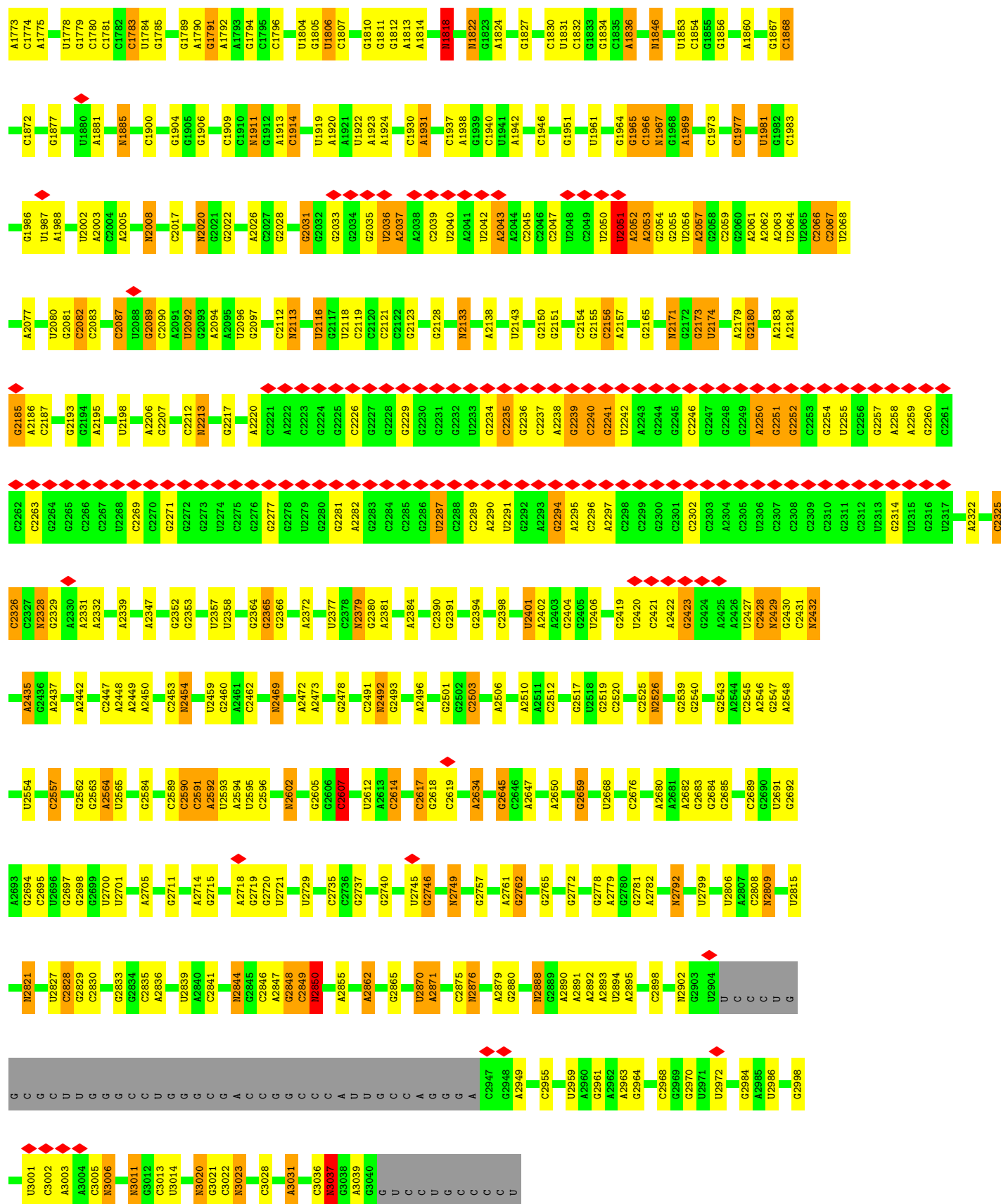
- Molecule 26: Zn-ribbon RNA-binding protein

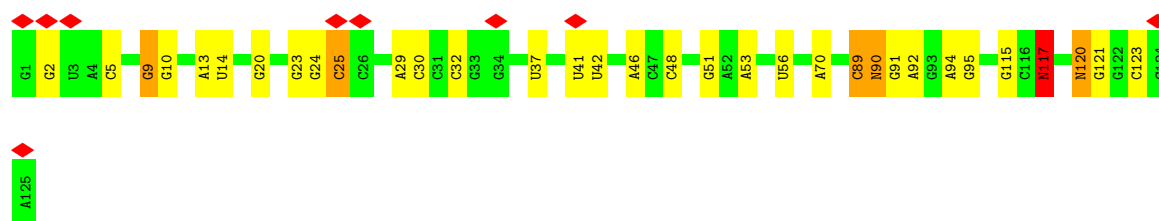
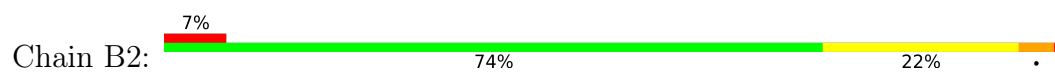


- Molecule 27: 23S rRNA





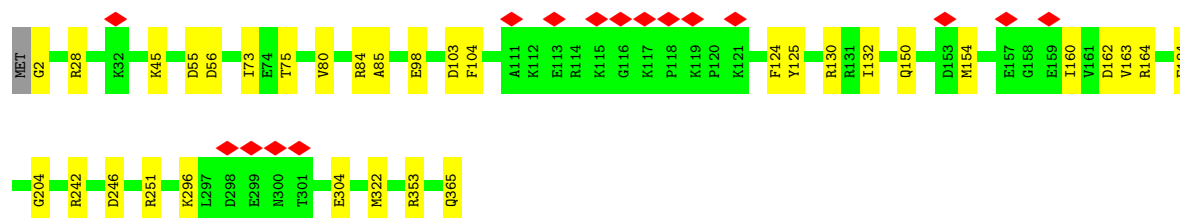




- Molecule 29: Large ribosomal subunit protein uL2



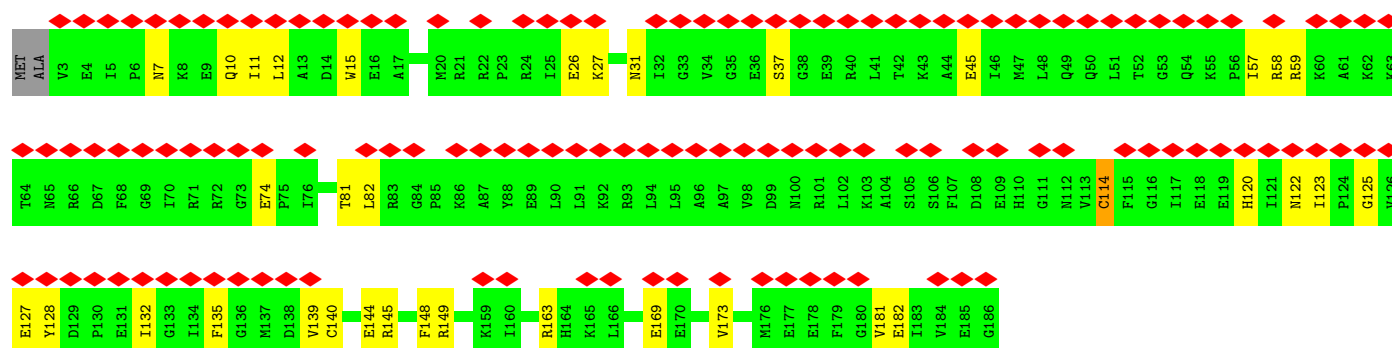
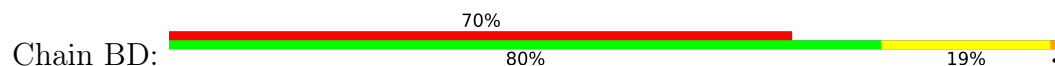
- Molecule 30: Large ribosomal subunit protein uL3



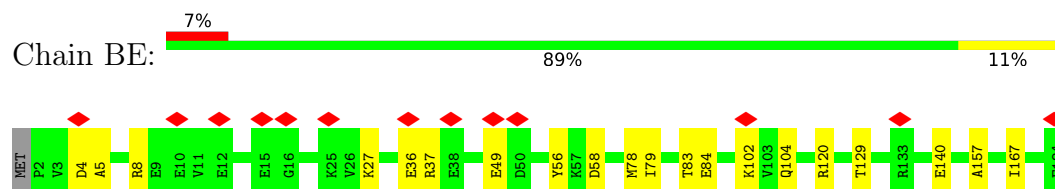
- Molecule 31: Large ribosomal subunit protein uL4



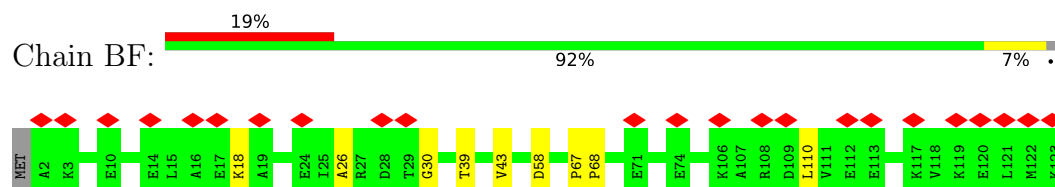
- Molecule 32: Large ribosomal subunit protein uL5



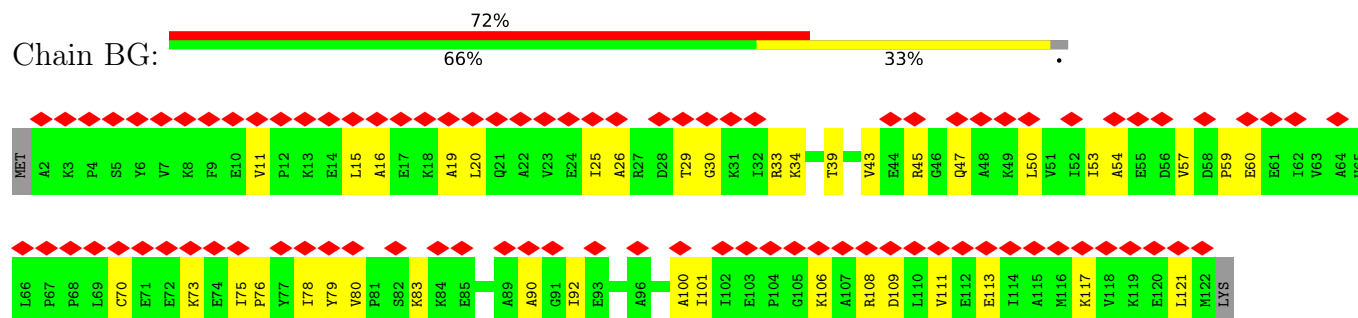
- Molecule 33: Large ribosomal subunit protein uL6



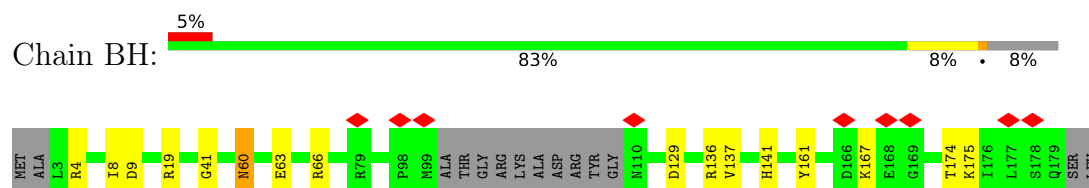
- Molecule 34: Large ribosomal subunit protein eL8



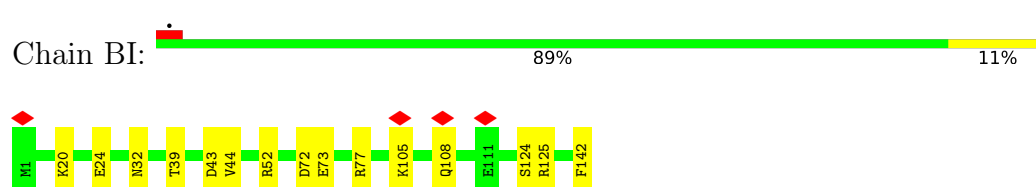
- Molecule 34: Large ribosomal subunit protein eL8



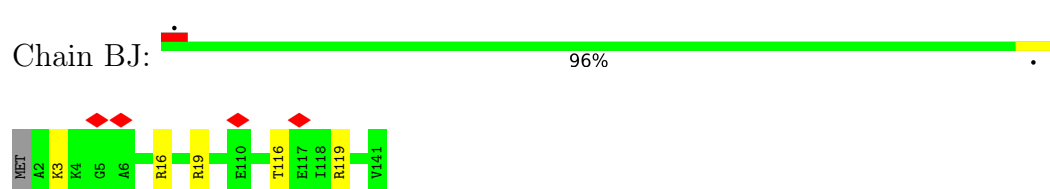
- Molecule 35: Large ribosomal subunit protein uL16



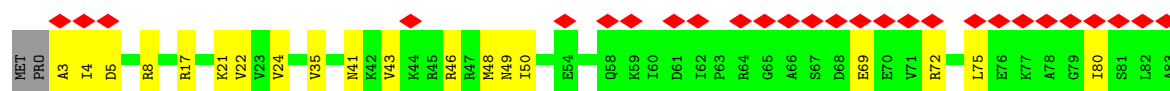
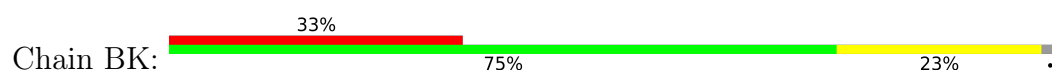
- Molecule 36: Large ribosomal subunit protein uL13



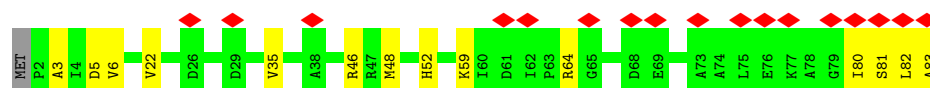
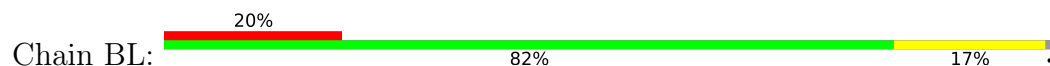
- Molecule 37: Large ribosomal subunit protein uL14



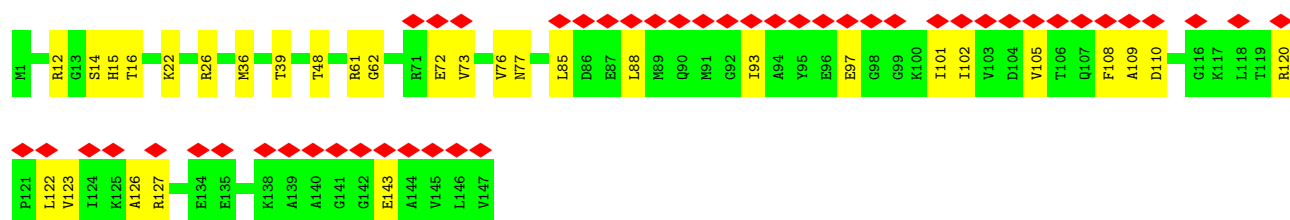
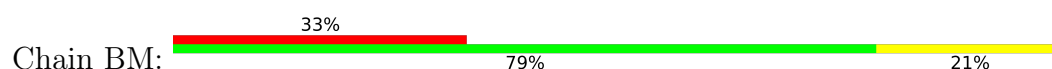
- Molecule 38: Large ribosomal subunit protein eL14



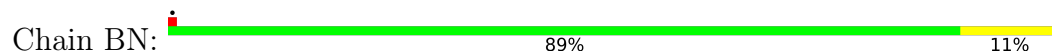
- Molecule 38: Large ribosomal subunit protein eL14



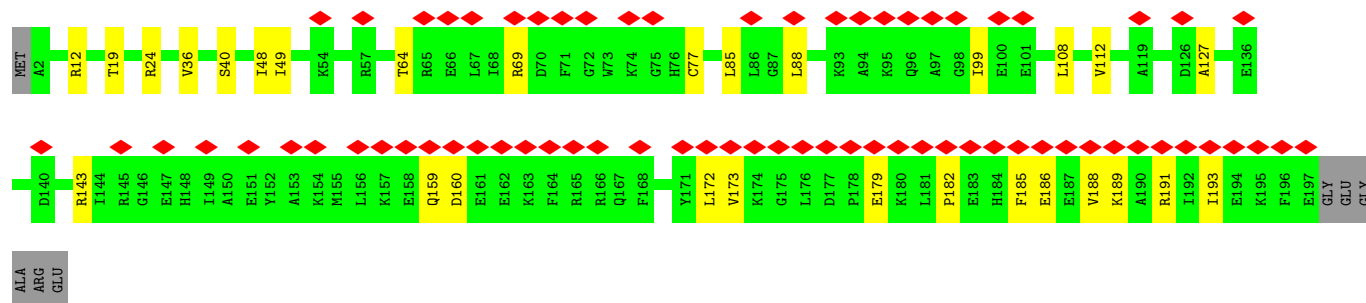
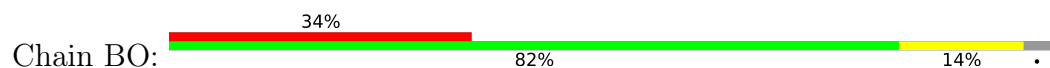
- Molecule 39: Large ribosomal subunit protein uL15



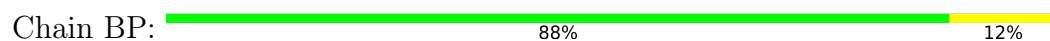
- Molecule 40: Large ribosomal subunit protein eL15



- Molecule 41: Large ribosomal subunit protein uL18

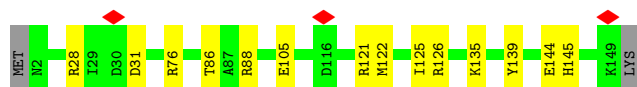


- Molecule 42: Large ribosomal subunit protein eL18





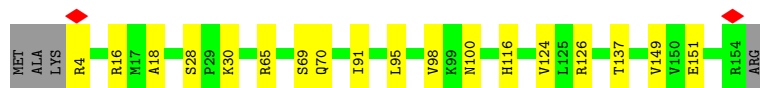
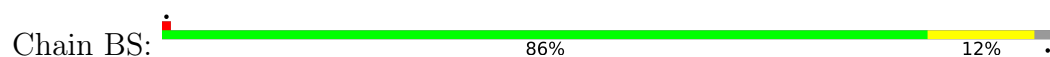
- Molecule 43: Large ribosomal subunit protein eL19



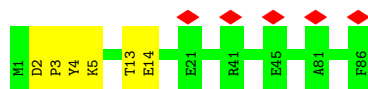
- Molecule 44: Large ribosomal subunit protein eL21



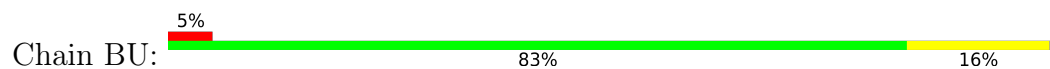
- Molecule 45: Large ribosomal subunit protein uL22



- Molecule 46: Large ribosomal subunit protein uL23



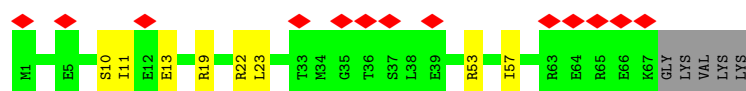
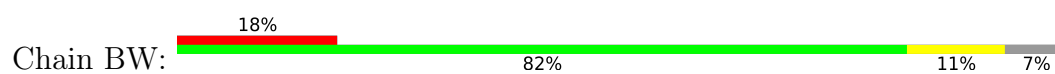
- Molecule 47: Large ribosomal subunit protein uL24



- Molecule 48: Large ribosomal subunit protein eL24



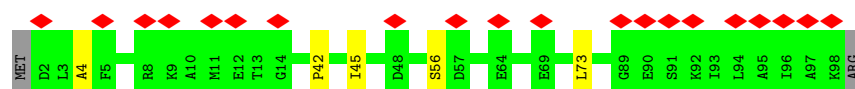
- Molecule 49: Large ribosomal subunit protein uL29



- Molecule 50: Large ribosomal subunit protein uL30



- Molecule 51: Large ribosomal subunit protein eL30



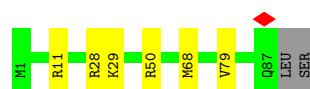
- Molecule 52: Large ribosomal subunit protein eL31



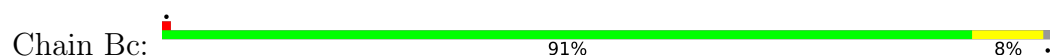
- Molecule 53: Large ribosomal subunit protein eL32



- Molecule 54: Large ribosomal subunit protein eL34

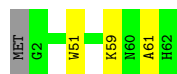


- Molecule 55: Large ribosomal subunit protein eL33



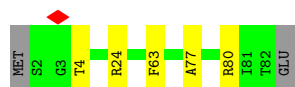
- Molecule 56: Large ribosomal subunit protein eL37

Chain Bd:  94% 5% .



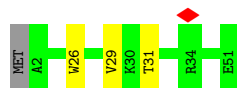
- Molecule 57: Large ribosomal subunit protein eL43

Chain Be:  92% 6% .




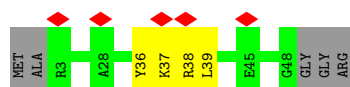
- Molecule 58: Large ribosomal subunit protein eL39

Chain Bf:  92% 6% .




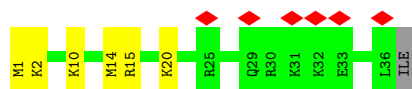
- Molecule 59: Large ribosomal subunit protein eL40

Chain Bg:  10% 82% 8% 10% .




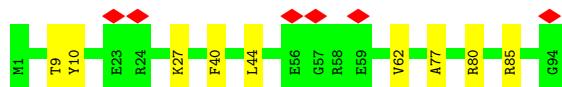
- Molecule 60: Small ribosomal subunit protein eS32

Chain Bh:  16% 81% 16% .



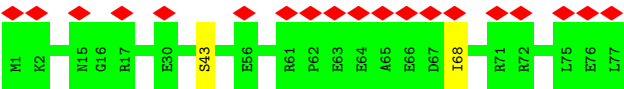
- Molecule 61: Large ribosomal subunit protein eL42

Chain Bi:  6% 90% 10% .

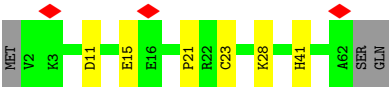
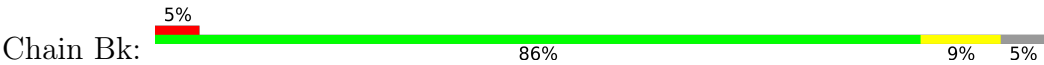


- Molecule 62: Large ribosomal subunit protein eL20

Chain Bj:  25% 97% .



• Molecule 63: C2H2-type domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37459	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.01	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.452	Depositor
Minimum map value	-1.201	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	443.52002, 443.52002, 443.52002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.99000007, 0.99000007, 0.99000007	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, A1I59, LHH, 5MC, OMG, 4AC, UR3, 4SU, OMU, 5MU, 2MG, MA6, A2M, G7M, ZN

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	A1	0.14	0/33307	0.23	0/51887
2	Aa	0.12	0/1603	0.27	0/2167
3	Ab	0.10	0/1551	0.25	0/2083
4	Ac	0.09	0/1546	0.23	0/2072
5	Ad	0.10	0/1476	0.22	0/1980
6	Ae	0.11	0/2030	0.25	0/2739
7	Af	0.20	0/1831	0.33	0/2468
8	Ag	0.11	0/990	0.27	0/1327
9	Ah	0.11	0/1765	0.27	0/2371
10	Ai	0.12	0/1049	0.26	0/1408
11	Aj	0.12	0/991	0.26	0/1322
12	Ak	0.12	0/1074	0.27	0/1438
13	Al	0.11	0/806	0.28	0/1083
14	Am	0.11	0/981	0.28	0/1320
15	An	0.10	0/1141	0.25	0/1518
16	Ao	0.14	0/1115	0.33	0/1500
17	Ap	0.38	0/450	0.66	1/594 (0.2%)
18	Aq	0.14	0/1330	0.30	0/1787
19	Ar	0.13	0/899	0.27	0/1215
20	As	0.09	0/533	0.25	0/708
21	At	0.10	0/1011	0.23	0/1351
22	Au	0.10	0/1251	0.24	0/1686
23	Av	0.11	0/803	0.27	0/1078
24	Aw	0.09	0/467	0.25	0/630
25	Ax	0.11	0/510	0.32	0/684
26	Ay	0.11	0/448	0.26	0/610
27	B1	0.16	0/65902	0.25	1/102618 (0.0%)
28	B2	0.10	0/2927	0.20	0/4559
29	BA	0.14	0/1870	0.29	0/2526
30	BB	0.16	0/2966	0.31	0/3989
31	BC	0.14	0/2068	0.30	0/2787
32	BD	0.25	0/1465	0.39	1/1962 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BE	0.13	0/1499	0.30	0/2022
34	BF	0.11	0/943	0.26	0/1271
34	BG	0.15	0/933	0.39	0/1260
35	BH	0.18	0/1396	0.34	0/1874
36	BI	0.17	0/1168	0.30	0/1561
37	BJ	0.15	0/1075	0.25	0/1448
38	BK	0.10	0/618	0.26	0/829
38	BL	0.12	0/626	0.27	0/840
39	BM	0.17	0/1175	0.34	0/1563
40	BN	0.13	0/1626	0.26	0/2169
41	BO	0.14	0/1598	0.29	0/2154
42	BP	0.14	0/980	0.29	0/1313
43	BQ	0.12	0/1254	0.25	0/1655
44	BR	0.15	0/815	0.29	0/1090
45	BS	0.16	0/1231	0.32	0/1658
46	BT	0.25	0/705	0.54	2/946 (0.2%)
47	BU	0.15	0/1019	0.27	0/1360
48	BV	0.12	0/542	0.25	0/724
49	BW	0.15	0/546	0.28	0/723
50	BX	0.14	0/1254	0.33	0/1677
51	BY	0.12	0/740	0.25	0/1000
52	BZ	0.14	0/760	0.34	0/1024
53	Ba	0.13	0/1093	0.27	0/1459
54	Bb	0.18	0/743	0.38	0/988
55	Bc	0.13	0/686	0.32	0/916
56	Bd	0.22	0/504	0.33	0/667
57	Be	0.13	0/615	0.30	0/820
58	Bf	0.15	0/445	0.26	0/593
59	Bg	0.10	0/384	0.25	0/509
60	Bh	0.18	0/349	0.45	0/451
61	Bi	0.13	0/805	0.24	0/1064
62	Bj	0.14	0/669	0.33	0/884
63	Bk	0.14	0/518	0.32	0/683
All	All	0.15	0/167470	0.27	5/246662 (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
12	Ak	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	BA	0	1
31	BC	0	1
45	BS	0	1
50	BX	0	1
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BT	5	LYS	N-CA-CB	-7.40	98.99	111.27
46	BT	5	LYS	CB-CA-C	6.64	121.59	110.44
27	B1	2051	U	C4'-C3'-O3'	5.38	121.08	113.00
32	BD	114	CYS	CA-CB-SG	5.22	126.42	114.40
17	Ap	4	ALA	N-CA-C	-5.11	106.63	112.92

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	Ak	135	ARG	Sidechain
29	BA	25	ARG	Sidechain
31	BC	128	ARG	Sidechain
45	BS	65	ARG	Sidechain
50	BX	123	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	32256	0	16364	265	0
2	Aa	1572	0	1629	13	0
3	Ab	1529	0	1618	18	0
4	Ac	1520	0	1603	14	0
5	Ad	1452	0	1521	11	0
6	Ae	1981	0	2051	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Af	1800	0	1851	11	0
8	Ag	975	0	1032	18	0
9	Ah	1728	0	1775	30	0
10	Ai	1028	0	1065	5	0
11	Aj	982	0	1066	11	0
12	Ak	1058	0	1105	15	0
13	Al	798	0	845	16	0
14	Am	963	0	994	12	0
15	An	1124	0	1217	5	0
16	Ao	1096	0	1132	9	0
17	Ap	441	0	456	12	0
18	Aq	1302	0	1380	10	0
19	Ar	877	0	898	5	0
20	As	527	0	559	6	0
21	At	991	0	1051	16	0
22	Au	1221	0	1263	15	0
23	Av	787	0	808	10	0
24	Aw	460	0	492	6	0
25	Ax	508	0	533	2	0
26	Ay	434	0	402	3	0
27	B1	63533	0	32139	575	0
28	B2	2689	0	1367	19	0
29	BA	1825	0	1891	15	0
30	BB	2900	0	3050	21	0
31	BC	2026	0	2137	20	0
32	BD	1442	0	1464	29	0
33	BE	1468	0	1507	11	0
34	BF	931	0	982	6	0
34	BG	921	0	969	29	0
35	BH	1367	0	1398	10	0
36	BI	1150	0	1240	9	0
37	BJ	1062	0	1127	4	0
38	BK	614	0	670	10	0
38	BL	621	0	678	10	0
39	BM	1154	0	1219	23	0
40	BN	1587	0	1683	17	0
41	BO	1560	0	1561	26	0
42	BP	966	0	1019	11	0
43	BQ	1238	0	1365	9	0
44	BR	794	0	836	5	0
45	BS	1204	0	1253	17	0
46	BT	696	0	754	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BU	1003	0	1074	15	0
48	BV	527	0	512	2	0
49	BW	545	0	593	6	0
50	BX	1235	0	1314	6	0
51	BY	730	0	768	4	0
52	BZ	746	0	803	4	0
53	Ba	1068	0	1157	10	0
54	Bb	725	0	789	5	0
55	Bc	677	0	731	6	0
56	Bd	493	0	502	2	0
57	Be	606	0	649	4	0
58	Bf	437	0	498	2	0
59	Bg	375	0	394	3	0
60	Bh	343	0	407	7	0
61	Bi	787	0	834	7	0
62	Bj	659	0	699	2	0
63	Bk	508	0	550	4	0
64	Af	1	0	0	0	0
64	Ap	1	0	0	0	0
64	Ar	1	0	0	0	0
64	Aw	1	0	0	0	0
64	Ay	2	0	0	0	0
64	BV	1	0	0	0	0
64	Bb	1	0	0	0	0
64	Bd	1	0	0	0	0
64	Be	1	0	0	0	0
64	Bg	1	0	0	0	0
64	Bi	1	0	0	0	0
64	Bk	1	0	0	0	0
65	A1	69	0	0	19	0
65	Ac	1	0	0	0	0
65	Ae	1	0	0	0	0
65	Ah	1	0	0	0	0
65	Aj	1	0	0	0	0
65	Ak	1	0	0	0	0
65	Aq	1	0	0	0	0
65	B1	1221	0	0	101	0
65	B2	9	0	0	0	0
65	BA	16	0	0	1	0
65	BB	12	0	0	1	0
65	BC	14	0	0	1	0
65	BE	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	BH	7	0	0	0	0
65	BI	5	0	0	0	0
65	BJ	4	0	0	0	0
65	BM	13	0	0	1	0
65	BN	12	0	0	0	0
65	BO	3	0	0	0	0
65	BP	4	0	0	0	0
65	BQ	4	0	0	0	0
65	BR	5	0	0	1	0
65	BS	14	0	0	3	0
65	BT	5	0	0	0	0
65	BU	8	0	0	0	0
65	BV	4	0	0	0	0
65	BX	2	0	0	1	0
65	BY	1	0	0	0	0
65	BZ	3	0	0	0	0
65	Ba	11	0	0	0	0
65	Bb	7	0	0	1	0
65	Bc	2	0	0	1	0
65	Bd	7	0	0	0	0
65	Be	2	0	0	0	0
65	Bf	8	0	0	0	0
65	Bg	1	0	0	0	0
65	Bi	1	0	0	0	0
65	Bj	1	0	0	0	0
65	Bk	4	0	0	0	0
All	All	164122	0	117293	1344	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 (1344) 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)
41:BO:85:LEU:HD11	41:BO:185:PHE:CE1	1.73	1.23
41:BO:85:LEU:CD1	41:BO:185:PHE:CE1	2.27	1.18
41:BO:85:LEU:CD1	41:BO:185:PHE:HE1	1.56	1.18
27:B1:85:A:OP2	47:BU:47:ARG:NH2	1.94	1.00
1:A1:302:G:HO2'	5:Ad:2:GLY:N	1.63	0.96
41:BO:85:LEU:HD11	41:BO:185:PHE:CD1	2.01	0.95
41:BO:85:LEU:HD12	41:BO:185:PHE:HE1	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:1360:4AC:HM73	27:B1:1374:4AC:HM73	1.55	0.88
27:B1:336:5MC:OP1	47:BU:25:LYS:NZ	2.07	0.87
27:B1:333:A:N1	27:B1:386:U:O2'	2.08	0.87
27:B1:942:C:OP1	27:B1:966:A:O2'	1.93	0.86
1:A1:1462:G:O2'	1:A1:1463:U:OP2	1.92	0.86
40:BN:56:LYS:NZ	40:BN:143:ASP:OD2	2.08	0.86
27:B1:2685:G:N7	30:BB:2:GLY:N	2.23	0.85
27:B1:154:U:O2'	27:B1:155:U:O2	1.94	0.85
1:A1:801:G:O2'	4:Ac:176:LYS:O	1.93	0.85
27:B1:1987:U:O2'	27:B1:1988:A:N7	2.09	0.85
1:A1:645:OMG:OP2	14:Am:25:ASN:ND2	2.09	0.84
1:A1:1334:C:O2	9:Ah:95:SER:OG	1.95	0.84
27:B1:2366:G:N7	65:B1:3151:HOH:O	2.10	0.84
27:B1:2052:A:O2'	27:B1:2053:A:O5'	1.95	0.83
20:As:47:ARG:NH1	20:As:48:ASN:OD1	2.10	0.83
1:A1:624:4AC:HM73	1:A1:691:4AC:HM73	1.61	0.82
27:B1:980:G:O2'	27:B1:981:G:O5'	1.95	0.82
1:A1:624:4AC:HM73	1:A1:691:4AC:CM7	2.09	0.81
27:B1:926:U:OP2	65:B1:3101:HOH:O	1.97	0.81
1:A1:472:G:N2	15:An:65:PRO:O	2.13	0.81
1:A1:197:A:O2'	1:A1:198:A:O5'	1.98	0.81
1:A1:335:G:OP2	37:BJ:119:ARG:NH2	2.13	0.81
1:A1:1211:C:O2'	12:Ak:69:GLY:O	1.97	0.81
1:A1:1241:A:O2'	1:A1:1243:U:OP2	1.97	0.81
27:B1:813:4AC:HM73	27:B1:933:4AC:CM7	2.10	0.81
27:B1:1569:A:N3	27:B1:1639:4AC:O2'	2.13	0.81
21:At:5:GLU:OE1	21:At:7:ARG:NH1	2.14	0.80
27:B1:178:G:OP2	65:B1:3106:HOH:O	2.00	0.80
27:B1:1885:4AC:OP2	43:BQ:76:ARG:NH1	2.15	0.80
1:A1:940:C:OP2	65:A1:1502:HOH:O	1.99	0.80
1:A1:1028:C:C4	1:A1:1029:4AC:HM73	2.17	0.80
27:B1:2862:A:OP2	65:B1:3105:HOH:O	1.99	0.80
27:B1:2254:G:O2'	27:B1:2282:A:N1	2.12	0.80
24:Aw:17:LYS:NZ	24:Aw:24:GLU:OE2	2.13	0.80
27:B1:2836:A:OP1	65:B1:3102:HOH:O	1.98	0.80
27:B1:879:G:OP1	65:B1:3108:HOH:O	2.00	0.79
27:B1:1118:C:OP1	65:B1:3103:HOH:O	1.99	0.79
1:A1:1266:G:OP2	65:A1:1501:HOH:O	1.98	0.79
27:B1:2503:C:OP2	65:B1:3112:HOH:O	2.01	0.79
3:Ab:19:GLU:OE2	17:Ap:49:LYS:NZ	2.15	0.79
27:B1:1690:G:N2	27:B1:1693:A:OP2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Aa:51:ARG:NH2	26:Ay:60:PRO:O	2.16	0.78
27:B1:1521:G:O2'	65:B1:3107:HOH:O	2.00	0.78
1:A1:74:U:O2'	1:A1:76:U:OP2	2.00	0.78
27:B1:885:C:OP2	65:B1:3104:HOH:O	1.99	0.78
1:A1:1462:G:OP1	65:A1:1504:HOH:O	2.02	0.78
27:B1:1412:G:OP2	65:B1:3109:HOH:O	2.00	0.78
27:B1:923:C:OP1	65:B1:3101:HOH:O	2.00	0.78
27:B1:1073:U:OP2	65:B1:3111:HOH:O	2.01	0.78
1:A1:939:C:O2	17:Ap:12:ARG:NH1	2.17	0.78
27:B1:821:C:OP1	65:B1:3113:HOH:O	2.02	0.78
27:B1:967:G:OP2	65:B1:3110:HOH:O	2.01	0.78
31:BC:71:GLU:OE2	65:BC:301:HOH:O	2.00	0.78
1:A1:1282:C:OP2	65:A1:1505:HOH:O	2.02	0.78
5:Ad:157:THR:OG1	23:Av:63:TYR:OH	2.01	0.78
27:B1:2198:U:OP1	65:B1:3116:HOH:O	2.02	0.78
28:B2:30:C:OP1	32:BD:149:ARG:NH1	2.16	0.78
1:A1:1199:C:OP2	9:Ah:91:ARG:NH1	2.18	0.77
16:Ao:11:ALA:N	16:Ao:63:GLU:OE2	2.17	0.77
27:B1:765:G:OP2	65:B1:3118:HOH:O	2.02	0.77
27:B1:2357:U:OP1	65:B1:3115:HOH:O	2.02	0.77
27:B1:2772:G:O4'	37:BJ:3:LYS:NZ	2.17	0.77
27:B1:1922:U:OP1	65:B1:3114:HOH:O	2.02	0.77
1:A1:514:A:OP1	65:A1:1506:HOH:O	2.03	0.77
1:A1:286:C:OP2	65:A1:1503:HOH:O	2.02	0.77
27:B1:1360:4AC:CM7	27:B1:1374:4AC:HM73	2.13	0.77
27:B1:660:U:OP1	65:B1:3117:HOH:O	2.02	0.77
27:B1:678:A:OP2	65:B1:3121:HOH:O	2.03	0.77
27:B1:479:4AC:O7	65:B1:3123:HOH:O	2.03	0.76
1:A1:1367:G:O2'	1:A1:1475:MA6:O2'	2.01	0.76
27:B1:1186:A:O2'	27:B1:1187:G:OP1	2.03	0.76
2:Aa:119:ASP:OD1	2:Aa:158:ASN:ND2	2.17	0.76
27:B1:187:A:OP1	65:B1:3122:HOH:O	2.03	0.76
27:B1:813:4AC:HM73	27:B1:933:4AC:HM71	1.66	0.76
27:B1:1068:G:OP2	65:B1:3120:HOH:O	2.03	0.76
27:B1:1919:U:OP2	27:B1:1924:A:N6	2.18	0.76
27:B1:1145:A:OP2	65:B1:3126:HOH:O	2.04	0.76
27:B1:2250:A:N6	27:B1:2287:U:OP1	2.19	0.76
27:B1:2829:G:OP2	65:B1:3124:HOH:O	2.03	0.76
27:B1:1771:A:OP1	65:B1:3119:HOH:O	2.02	0.76
21:At:57:GLY:O	21:At:60:LYS:NZ	2.19	0.75
1:A1:110:C:OP1	1:A1:559:C:O2'	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:662:G:O4'	27:B1:1119:A:N6	2.19	0.75
38:BL:6:VAL:O	38:BL:59:LYS:NZ	2.19	0.75
27:B1:1278:G:N2	65:B1:3177:HOH:O	2.20	0.75
27:B1:2123:G:HO2'	27:B1:2839:U:HO2'	1.30	0.75
1:A1:753:G:N2	65:A1:1515:HOH:O	2.20	0.75
27:B1:1392:C:OP1	65:B1:3121:HOH:O	2.05	0.75
1:A1:897:A:OP2	65:A1:1507:HOH:O	2.05	0.74
27:B1:1778:U:OP2	65:B1:3127:HOH:O	2.04	0.74
27:B1:1154:U:OP1	27:B1:1175:U:O2'	2.03	0.74
6:Ae:89:ASP:OD1	6:Ae:123:LYS:NZ	2.21	0.74
27:B1:1831:U:OP2	65:B1:3130:HOH:O	2.05	0.74
27:B1:2799:U:OP2	65:B1:3102:HOH:O	2.04	0.74
27:B1:1159:G:OP2	65:B1:3125:HOH:O	2.04	0.74
27:B1:666:C:OP1	65:B1:3132:HOH:O	2.05	0.74
27:B1:1476:G:OP1	65:B1:3129:HOH:O	2.05	0.74
27:B1:2564:A:OP1	65:B1:3133:HOH:O	2.05	0.74
1:A1:101:G:OP2	65:A1:1503:HOH:O	2.04	0.74
27:B1:183:U:OP2	65:B1:3128:HOH:O	2.04	0.74
1:A1:1146:G:O2'	1:A1:1147:C:OP1	2.06	0.74
1:A1:317:C:OP1	1:A1:1423:C:O2'	2.06	0.74
27:B1:1184:U:OP2	27:B1:1187:G:N2	2.20	0.74
27:B1:1417:G:OP2	65:B1:3134:HOH:O	2.06	0.74
27:B1:1459:C:OP2	65:B1:3129:HOH:O	2.06	0.73
1:A1:104:A:OP1	11:Aj:11:LYS:NZ	2.20	0.73
1:A1:462:A:N3	1:A1:497:C:O2'	2.21	0.73
27:B1:1522:G:OP2	65:B1:3135:HOH:O	2.06	0.73
27:B1:2659:OMG:OP2	65:B1:3131:HOH:O	2.05	0.73
27:B1:1791:G:O6	65:B1:3139:HOH:O	2.07	0.73
27:B1:1769:4AC:OP2	65:B1:3141:HOH:O	2.07	0.73
27:B1:836:G:OP1	43:BQ:86:THR:OG1	2.03	0.73
27:B1:1937:C:OP1	29:BA:233:ARG:NH1	2.22	0.73
1:A1:354:G:OP2	65:A1:1508:HOH:O	2.07	0.73
1:A1:1297:C:O2'	9:Ah:175:ARG:NH1	2.22	0.72
27:B1:913:G:O6	65:B1:3138:HOH:O	2.07	0.72
27:B1:208:A:OP2	65:B1:3136:HOH:O	2.06	0.72
1:A1:768:U:HO2'	1:A1:1468:G:HO2'	1.34	0.72
32:BD:114:CYS:CB	32:BD:140:CYS:HA	2.19	0.72
27:B1:539:G:N7	65:B1:3183:HOH:O	2.22	0.72
33:BE:129:THR:OG1	33:BE:140:GLU:OE2	2.07	0.72
27:B1:182:U:OP1	65:B1:3115:HOH:O	2.08	0.72
27:B1:209:A:N3	27:B1:224:U:O2'	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:2892:A:OP2	65:B1:3144:HOH:O	2.07	0.72
30:BB:251:ARG:O	65:BB:401:HOH:O	2.08	0.72
45:BS:69:SER:OG	65:BS:201:HOH:O	2.04	0.72
27:B1:493:A:OP1	65:B1:3140:HOH:O	2.07	0.71
27:B1:2380:G:OP1	65:B1:3143:HOH:O	2.07	0.71
27:B1:451:G:N7	40:BN:177:LYS:NZ	2.37	0.71
27:B1:2746:G:HO2'	27:B1:3039:A:HO2'	1.32	0.71
1:A1:207:G:O2'	1:A1:210:A:N6	2.23	0.71
1:A1:1186:U:O2'	1:A1:1284:C:OP1	2.08	0.71
1:A1:1259:U:O2'	9:Ah:177:LYS:NZ	2.16	0.71
16:Ao:121:GLU:OE1	27:B1:1026:A:O2'	2.08	0.71
23:Av:54:GLN:OE1	23:Av:70:LYS:NZ	2.24	0.71
27:B1:907:G:OP2	65:B1:3137:HOH:O	2.07	0.71
27:B1:1761:C:OP1	65:B1:3147:HOH:O	2.08	0.71
27:B1:1806:U:OP2	65:B1:3148:HOH:O	2.08	0.71
27:B1:2251:G:O2'	27:B1:2252:G:OP1	2.09	0.71
27:B1:251:G:OP2	65:B1:3149:HOH:O	2.09	0.70
27:B1:1522:G:OP1	65:B1:3145:HOH:O	2.08	0.70
1:A1:398:C:O2'	1:A1:575:A:N3	2.25	0.70
6:Ae:128:ARG:NH2	6:Ae:143:HIS:O	2.24	0.70
27:B1:1759:U:O4	65:B1:3146:HOH:O	2.08	0.70
34:BG:45:ARG:NE	34:BG:47:GLN:OE1	2.24	0.70
1:A1:1197:U:OP1	65:A1:1509:HOH:O	2.09	0.70
6:Ae:217:ASP:OD1	6:Ae:221:GLU:N	2.25	0.70
23:Av:33:ARG:NH2	23:Av:53:ILE:O	2.25	0.70
11:Aj:65:VAL:HG11	11:Aj:105:ILE:HD11	1.73	0.70
27:B1:413:G:N7	65:B1:3192:HOH:O	2.24	0.70
27:B1:1923:A:OP2	65:B1:3114:HOH:O	2.10	0.70
27:B1:3036:C:O2'	27:B1:3037:4AC:OP1	2.09	0.70
1:A1:1007:C:OP2	65:A1:1510:HOH:O	2.10	0.69
9:Ah:94:ASN:ND2	9:Ah:94:ASN:O	2.23	0.69
27:B1:1349:G:OP1	31:BC:172:ARG:NH2	2.25	0.69
4:Ac:120:MET:SD	4:Ac:186:ARG:NH2	2.65	0.69
6:Ae:141:ASN:ND2	6:Ae:147:ASN:OD1	2.25	0.69
19:Ar:35:GLU:OE1	19:Ar:85:LYS:NZ	2.24	0.69
9:Ah:73:ARG:NH2	9:Ah:79:TYR:OH	2.25	0.69
1:A1:1143:G:O2'	1:A1:1144:G:N7	2.24	0.69
27:B1:653:G:OP2	65:B1:3152:HOH:O	2.10	0.69
1:A1:348:G:OP2	1:A1:348:G:N2	2.16	0.69
44:BR:2:VAL:N	65:BR:101:HOH:O	2.24	0.69
3:Ab:13:ARG:NH1	3:Ab:73:PHE:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:963:C:OP1	65:B1:3155:HOH:O	2.11	0.69
1:A1:707:G:O6	18:Aq:64:LYS:NZ	2.26	0.68
27:B1:1572:G:OP1	65:B1:3154:HOH:O	2.11	0.68
1:A1:613:C:H2'	1:A1:614:4AC:H6	1.76	0.68
1:A1:938:A:OP2	65:A1:1511:HOH:O	2.11	0.68
27:B1:1416:C:OP2	65:B1:3134:HOH:O	2.10	0.68
27:B1:2692:G:O2'	27:B1:2695:C:OP2	2.11	0.68
1:A1:766:U:O2'	1:A1:860:A:N1	2.25	0.68
6:Ae:65:ILE:HD11	23:Av:14:ILE:HG13	1.74	0.68
9:Ah:7:GLU:OE2	9:Ah:20:ARG:NH2	2.26	0.68
27:B1:1588:A:OP2	65:B1:3150:HOH:O	2.10	0.68
27:B1:2406:U:O2'	27:B1:2492:4AC:O2	2.12	0.68
27:B1:2855:A:OP2	65:B1:3156:HOH:O	2.12	0.68
27:B1:1414:A:N3	27:B1:2128:G:O2'	2.26	0.68
27:B1:2077:A:N3	27:B1:2676:C:O2'	2.27	0.68
27:B1:2364:G:O2'	27:B1:2612:U:OP1	2.10	0.68
1:A1:849:G:O2'	1:A1:865:G:O6	2.11	0.68
29:BA:54:ARG:O	29:BA:55:THR:OG1	2.11	0.68
33:BE:4:ASP:OD1	33:BE:5:ALA:N	2.26	0.68
27:B1:996:G:O2'	27:B1:1053:G:O6	2.11	0.67
27:B1:979:4AC:O2'	27:B1:980:G:OP1	2.12	0.67
27:B1:1478:4AC:O2'	27:B1:1479:G:OP1	2.13	0.67
27:B1:2404:G:OP1	65:B1:3112:HOH:O	2.12	0.67
1:A1:332:C:O2'	1:A1:1395:A:N3	2.28	0.67
1:A1:1305:C:OP1	12:Ak:132:LYS:NZ	2.22	0.67
9:Ah:172:LYS:NZ	9:Ah:187:GLU:OE1	2.27	0.67
27:B1:1758:G:OP2	65:B1:3158:HOH:O	2.13	0.67
1:A1:223:G:O2'	6:Ae:141:ASN:ND2	2.28	0.67
27:B1:968:G:OP2	65:B1:3153:HOH:O	2.11	0.67
27:B1:2089:G:O2'	27:B1:2092:U:OP2	2.10	0.67
28:B2:9:G:O3'	41:BO:24:ARG:NH1	2.28	0.67
59:Bg:36:TYR:OH	59:Bg:38:ARG:NH2	2.27	0.67
10:Ai:36:GLU:OE1	10:Ai:39:ARG:NH1	2.27	0.67
27:B1:415:G:OP2	40:BN:44:ARG:NH1	2.28	0.67
15:An:91:ASP:OD1	15:An:92:GLY:N	2.27	0.67
1:A1:349:C:O2'	1:A1:351:G:OP1	2.10	0.66
27:B1:212:A:OP1	65:B1:3157:HOH:O	2.12	0.66
27:B1:765:G:OP1	42:BP:51:LYS:NZ	2.28	0.66
47:BU:5:SER:O	47:BU:11:GLN:NE2	2.28	0.66
27:B1:1102:U:OP1	65:B1:3162:HOH:O	2.14	0.66
1:A1:100:A:OP1	65:A1:1503:HOH:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B2:20:G:OP2	32:BD:163:ARG:NH2	2.27	0.66
1:A1:1160:G:OP2	65:A1:1513:HOH:O	2.13	0.66
3:Ab:117:LEU:HD21	3:Ab:148:GLN:HG2	1.77	0.66
32:BD:114:CYS:HB3	32:BD:140:CYS:HA	1.77	0.66
27:B1:867:G:N7	65:B1:3203:HOH:O	2.28	0.66
1:A1:532:G:OP1	65:A1:1512:HOH:O	2.13	0.66
6:Ae:15:ALA:O	6:Ae:23:ARG:NH2	2.29	0.66
6:Ae:118:ASP:OD1	6:Ae:119:GLU:N	2.29	0.66
13:Al:44:ARG:NH1	13:Al:65:GLU:OE2	2.28	0.66
27:B1:1439:4AC:OP1	65:B1:3164:HOH:O	2.14	0.66
27:B1:589:U:O4	34:BG:83:LYS:NZ	2.28	0.65
27:B1:662:G:O6	65:B1:3133:HOH:O	2.10	0.65
49:BW:10:SER:N	49:BW:13:GLU:OE2	2.26	0.65
27:B1:362:G:O2'	27:B1:381:A:N3	2.28	0.65
27:B1:1696:G:O2'	27:B1:1697:G:OP1	2.13	0.65
28:B2:37:U:O4'	41:BO:143:ARG:NH1	2.30	0.65
6:Ae:40:ARG:HG3	6:Ae:41:THR:HG23	1.79	0.65
1:A1:427:4AC:HM73	1:A1:444:4AC:CM7	2.27	0.65
27:B1:1830:C:OP1	65:B1:3130:HOH:O	2.14	0.65
38:BK:24:VAL:HG12	38:BK:35:VAL:HG12	1.78	0.65
27:B1:2052:A:HO2'	27:B1:2053:A:C5'	2.08	0.65
27:B1:1570:A:HO2'	27:B1:1638:C:HO2'	1.45	0.65
13:Al:82:MET:SD	13:Al:83:ARG:NE	2.65	0.65
27:B1:1360:4AC:HM73	27:B1:1374:4AC:CM7	2.25	0.65
27:B1:1294:G:OP1	55:Bc:11:ARG:NH1	2.29	0.65
27:B1:1760:A:OP1	65:B1:3163:HOH:O	2.14	0.64
9:Ah:66:ARG:NH2	9:Ah:159:ASP:OD1	2.30	0.64
51:BY:4:ALA:HB2	51:BY:73:LEU:HD11	1.80	0.64
27:B1:1824:A:OP2	65:B1:3161:HOH:O	2.13	0.64
27:B1:2430:G:OP1	32:BD:27:LYS:NZ	2.23	0.64
39:BM:36:MET:O	39:BM:39:THR:HG23	1.98	0.64
53:Ba:80:GLU:OE1	53:Ba:97:ARG:NH1	2.31	0.64
1:A1:1364:LHH:O7	1:A1:1365:C:N4	2.30	0.64
41:BO:85:LEU:HD12	41:BO:185:PHE:CE1	2.18	0.64
47:BU:43:ASN:O	47:BU:119:ARG:NH1	2.30	0.64
1:A1:940:C:O2	17:Ap:17:GLY:N	2.31	0.64
27:B1:2364:G:OP1	27:B1:2390:C:O2'	2.12	0.63
1:A1:674:C:N3	4:Ac:102:ARG:NH1	2.46	0.63
27:B1:1836:A:OP2	65:B1:3166:HOH:O	2.15	0.63
1:A1:939:C:OP1	65:A1:1502:HOH:O	2.15	0.63
1:A1:1228:G:N7	22:Au:99:ARG:NH2	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1438:U:O2'	1:A1:1439:G:OP1	2.16	0.63
54:Bb:68:MET:HE1	54:Bb:79:VAL:HG11	1.80	0.63
38:BK:75:LEU:CD2	38:BK:80:ILE:HD11	2.28	0.63
27:B1:834:G:O2'	27:B1:1790:A:N3	2.26	0.63
27:B1:2235:C:H4'	27:B1:2271:G:H21	1.64	0.63
27:B1:2970:G:OP2	30:BB:130:ARG:NH2	2.31	0.63
39:BM:48:THR:O	65:BM:201:HOH:O	2.15	0.63
32:BD:7:ASN:OD1	32:BD:10:GLN:NE2	2.31	0.63
9:Ah:6:ASN:OD1	9:Ah:7:GLU:N	2.31	0.63
27:B1:2053:A:O2'	27:B1:2054:G:O5'	2.07	0.63
8:Ag:28:LYS:NZ	8:Ag:42:GLU:O	2.25	0.62
30:BB:242:ARG:NE	30:BB:246:ASP:OD2	2.30	0.62
39:BM:85:LEU:HD12	39:BM:88:LEU:HD12	1.81	0.62
1:A1:512:C:OP2	1:A1:513:U:O2'	2.15	0.62
20:As:29:GLU:N	20:As:29:GLU:OE1	2.32	0.62
27:B1:2955:C:O2	27:B1:3031:A:O2'	2.17	0.62
27:B1:84:G:O5'	47:BU:115:ILE:HD11	2.00	0.62
2:Aa:63:GLU:OE2	2:Aa:65:GLN:NE2	2.32	0.62
3:Ab:88:PRO:O	3:Ab:95:GLN:NE2	2.33	0.62
27:B1:1761:C:OP2	65:B1:3163:HOH:O	2.16	0.62
40:BN:162:LEU:O	40:BN:167:LYS:NZ	2.33	0.62
61:Bi:62:VAL:O	61:Bi:85:ARG:NH1	2.32	0.62
27:B1:262:A2M:H62	27:B1:299:G:H1'	1.64	0.62
1:A1:941:U:OP2	1:A1:942:C:O2'	2.13	0.62
1:A1:207:G:N2	1:A1:210:A:OP2	2.31	0.61
27:B1:933:4AC:OP2	31:BC:74:LYS:NZ	2.30	0.61
27:B1:1831:U:O4	65:B1:3165:HOH:O	2.15	0.61
32:BD:182:GLU:N	32:BD:182:GLU:OE1	2.33	0.61
46:BT:2:ASP:OD1	46:BT:3:PRO:HD2	1.99	0.61
27:B1:1712:C:OP1	54:Bb:11:ARG:NH2	2.34	0.61
27:B1:1900:C:O2	65:B1:3159:HOH:O	2.13	0.61
1:A1:516:U:OP2	15:An:29:ARG:NH2	2.33	0.61
29:BA:28:VAL:HG23	29:BA:28:VAL:O	2.00	0.61
1:A1:1028:C:C5	1:A1:1029:4AC:HM73	2.35	0.61
18:Aq:106:ARG:NH2	18:Aq:126:GLU:OE2	2.33	0.61
27:B1:485:4AC:HM72	47:BU:9:ARG:NH1	2.15	0.61
27:B1:2828:C:O2'	27:B1:2830:C:OP2	2.11	0.61
38:BK:21:LYS:O	38:BK:41:ASN:ND2	2.34	0.61
27:B1:1528:G:OP2	54:Bb:28:ARG:NH2	2.34	0.61
28:B2:23:G:O2'	28:B2:24:G:O4'	2.15	0.61
1:A1:941:U:H4'	17:Ap:27:TYR:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BD:114:CYS:HB2	32:BD:140:CYS:HA	1.82	0.61
27:B1:711:G:O2'	31:BC:42:ARG:NH2	2.33	0.61
30:BB:162:ASP:OD1	30:BB:163:VAL:N	2.33	0.61
36:BI:43:ASP:OD1	36:BI:44:VAL:N	2.33	0.61
2:Aa:171:LEU:O	2:Aa:175:ILE:HD12	2.01	0.60
1:A1:1194:OMC:OP1	12:Ak:131:GLN:NE2	2.33	0.60
27:B1:336:5MC:HM53	47:BU:1:MET:HB3	1.83	0.60
45:BS:4:ARG:N	65:BS:203:HOH:O	2.34	0.60
45:BS:16:ARG:NH1	45:BS:151:GLU:OE2	2.33	0.60
27:B1:28:G:O2'	27:B1:29:A:OP2	2.19	0.60
38:BL:3:ALA:N	51:BY:56:SER:OG	2.35	0.60
27:B1:490:G:O6	65:B1:3140:HOH:O	2.12	0.60
3:Ab:57:ARG:O	3:Ab:60:ARG:NE	2.29	0.60
42:BP:39:ARG:NH1	42:BP:120:GLU:OE2	2.34	0.60
1:A1:496:G:O2'	1:A1:497:C:OP1	2.19	0.60
8:Ag:53:LYS:NZ	8:Ag:125:TYR:OH	2.31	0.60
27:B1:510:A:OP2	31:BC:56:ARG:NH1	2.35	0.60
1:A1:1119:A:N7	1:A1:1142:A:N6	2.50	0.59
1:A1:431:G:O2'	23:Av:30:THR:O	2.19	0.59
27:B1:1626:A:H2'	27:B1:1627:A:C8	2.37	0.59
38:BL:46:ARG:NH1	38:BL:48:MET:SD	2.75	0.59
27:B1:840:A:OP1	57:Be:4:THR:OG1	2.12	0.59
2:Aa:44:ASP:O	2:Aa:48:THR:HG23	2.02	0.59
27:B1:2036:U:O2'	27:B1:2037:A:OP1	2.19	0.59
27:B1:369:U:O4	65:B1:3167:HOH:O	2.16	0.59
40:BN:101:GLU:OE2	40:BN:116:SER:OG	2.16	0.59
1:A1:1146:G:HO2'	1:A1:1147:C:P	2.24	0.59
1:A1:1227:4AC:OP2	22:Au:99:ARG:NH1	2.34	0.59
27:B1:1064:4AC:H5	27:B1:1064:4AC:CM7	2.33	0.59
27:B1:1142:C:OP2	27:B1:1143:A:O2'	2.20	0.59
1:A1:1178:C:O2	17:Ap:7:ASN:ND2	2.35	0.59
27:B1:1601:OMG:HN21	27:B1:1706:4AC:C2	2.16	0.59
31:BC:61:ILE:HD13	31:BC:67:MET:HE3	1.84	0.59
32:BD:37:SER:OG	32:BD:74:GLU:OE2	2.10	0.59
46:BT:13:THR:HG22	46:BT:14:GLU:N	2.18	0.58
27:B1:1486:A:OP2	65:B1:3146:HOH:O	2.17	0.58
47:BU:87:ASN:OD1	47:BU:88:GLY:N	2.36	0.58
27:B1:2782:A:N1	65:B1:3214:HOH:O	2.31	0.58
30:BB:84:ARG:NH2	30:BB:98:GLU:OE1	2.36	0.58
38:BK:69:GLU:OE1	38:BK:72:ARG:NH2	2.36	0.58
27:B1:1877:G:OP2	43:BQ:135:LYS:NZ	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BG:26:ALA:O	34:BG:30:GLY:N	2.35	0.58
4:Ac:97:ARG:O	4:Ac:100:THR:OG1	2.21	0.58
42:BP:18:LEU:CD1	42:BP:107:ILE:HD11	2.32	0.58
27:B1:79:C:H2'	27:B1:80:4AC:H6	1.85	0.58
1:A1:849:G:C8	60:Bh:2:LYS:HB2	2.38	0.58
51:BY:42:PRO:HG2	51:BY:45:ILE:HD12	1.85	0.58
1:A1:1438:U:HO2'	1:A1:1439:G:P	2.27	0.58
21:At:20:SER:OG	21:At:23:GLU:OE1	2.10	0.58
27:B1:115:C:O2'	27:B1:127:U:O2'	2.18	0.58
27:B1:1608:4AC:CM7	27:B1:1621:4AC:HM73	2.33	0.58
27:B1:2347:A:OP1	65:B1:3168:HOH:O	2.17	0.58
27:B1:1608:4AC:HM73	27:B1:1621:4AC:HM73	1.86	0.58
27:B1:2081:G:H3'	27:B1:2082:5MC:HM53	1.86	0.58
27:B1:1393:G:OP2	39:BM:12:ARG:NH1	2.36	0.57
1:A1:343:G:O2'	8:Ag:70:ASP:OD2	2.22	0.57
2:Aa:35:VAL:HG22	2:Aa:41:TYR:CE2	2.39	0.57
27:B1:177:G:OP1	40:BN:194:LYS:NZ	2.25	0.57
38:BL:22:VAL:HG21	38:BL:35:VAL:HG12	1.86	0.57
1:A1:329:OMG:HM21	8:Ag:101:GLU:OE1	2.03	0.57
1:A1:1033:A:OP1	7:Af:102:HIS:NE2	2.37	0.57
27:B1:418:C:H2'	27:B1:419:4AC:H6	1.85	0.57
27:B1:2419:G:H22	27:B1:2427:U:H3	1.52	0.57
33:BE:79:ILE:O	33:BE:83:THR:HG22	2.03	0.57
42:BP:18:LEU:HD12	42:BP:107:ILE:HD11	1.85	0.57
43:BQ:28:ARG:NH2	43:BQ:31:ASP:OD2	2.38	0.57
1:A1:199:A:N1	1:A1:217:G:O2'	2.38	0.57
27:B1:2325:C:O2'	27:B1:2326:C:OP1	2.21	0.57
27:B1:2746:G:O2'	27:B1:3039:A:O2'	2.07	0.57
30:BB:45:LYS:HA	30:BB:73:ILE:HG22	1.86	0.57
47:BU:16:TYR:O	47:BU:23:ARG:NH2	2.37	0.57
1:A1:372:U:OP1	6:Ae:50:ARG:NH1	2.38	0.57
7:Af:228:ALA:HB3	7:Af:230:PRO:HD2	1.87	0.57
4:Ac:25:ASP:OD1	4:Ac:26:PHE:N	2.38	0.57
27:B1:2835:C:O2'	30:BB:365:GLN:OXT	2.23	0.57
1:A1:1030:G:N2	1:A1:1033:A:OP2	2.30	0.57
27:B1:1049:C:OP1	35:BH:19:ARG:NH1	2.37	0.57
27:B1:2525:C:OP2	65:B1:3173:HOH:O	2.18	0.57
27:B1:2605:G:N3	27:B1:2607:OMC:N4	2.52	0.57
27:B1:2691:U:OP2	65:B1:3171:HOH:O	2.18	0.57
45:BS:124:VAL:O	45:BS:126:ARG:NH1	2.36	0.57
13:Al:78:ASP:OD1	13:Al:81:ALA:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BP:36:ARG:NH1	42:BP:120:GLU:OE1	2.38	0.56
7:Af:107:GLY:O	7:Af:111:ARG:NE	2.36	0.56
1:A1:1298:U:O2'	9:Ah:85:PHE:O	2.23	0.56
13:Al:87:ARG:HG3	13:Al:87:ARG:O	2.06	0.56
21:At:44:GLN:O	21:At:48:LEU:HD23	2.05	0.56
27:B1:148:C:OP1	40:BN:107:LYS:NZ	2.38	0.56
27:B1:2064:U:OP1	27:B1:2720:G:O2'	2.17	0.56
34:BG:34:LYS:HD3	34:BG:90:ALA:HB1	1.88	0.56
27:B1:2809:4AC:O2	27:B1:2986:U:O2'	2.23	0.56
27:B1:1404:4AC:OP1	45:BS:126:ARG:NH2	2.37	0.56
27:B1:1608:4AC:O7	27:B1:1608:4AC:H5	2.05	0.56
27:B1:2051:U:N3	27:B1:2053:A:OP2	2.38	0.56
1:A1:302:G:N3	5:Ad:2:GLY:N	2.53	0.56
27:B1:120:U:OP2	65:B1:3169:HOH:O	2.17	0.56
27:B1:658:U:O2'	39:BM:22:LYS:NZ	2.39	0.56
27:B1:1451:5MC:HM51	27:B1:1763:G:N3	2.19	0.56
27:B1:1608:4AC:HM73	27:B1:1621:4AC:CM7	2.36	0.56
34:BG:19:ALA:HB2	34:BG:78:ILE:HD13	1.86	0.56
27:B1:490:G:OP2	65:B1:3174:HOH:O	2.18	0.56
28:B2:25:C:O2	28:B2:123:C:O2'	2.23	0.56
1:A1:1029:4AC:H5	1:A1:1029:4AC:CM7	2.36	0.56
27:B1:2563:G:O4'	27:B1:2617:5MC:HM53	2.06	0.56
27:B1:2384:A:OP1	65:B1:3172:HOH:O	2.18	0.56
39:BM:110:ASP:OD1	39:BM:127:ARG:NH2	2.39	0.56
43:BQ:105:GLU:OE2	43:BQ:139:TYR:OH	2.16	0.56
43:BQ:121:ARG:O	43:BQ:125:ILE:HD12	2.06	0.56
1:A1:828:G:N7	65:A1:1519:HOH:O	2.33	0.55
27:B1:1514:G:O2'	27:B1:1951:G:O2'	2.23	0.55
32:BD:12:LEU:HA	32:BD:15:TRP:HE3	1.71	0.55
1:A1:318:A:OP1	11:Aj:2:ALA:N	2.40	0.55
25:Ax:59:GLU:OE1	25:Ax:61:GLU:N	2.39	0.55
27:B1:2165:G:OP1	36:BI:77:ARG:NH2	2.39	0.55
63:Bk:23:CYS:SG	63:Bk:41:HIS:CE1	2.99	0.55
35:BH:60:ASN:ND2	35:BH:60:ASN:H	2.05	0.55
1:A1:898:A:N3	1:A1:1338:U:O2'	2.32	0.55
1:A1:1230:A:O2'	1:A1:1289:G:OP1	2.12	0.55
21:At:47:LEU:HD11	21:At:65:THR:HG21	1.87	0.55
27:B1:979:4AC:HO2'	27:B1:980:G:P	2.29	0.55
27:B1:813:4AC:H5	27:B1:813:4AC:O7	2.06	0.55
27:B1:1783:OMC:OP1	65:B1:3175:HOH:O	2.18	0.55
3:Ab:12:VAL:O	3:Ab:16:LEU:HD23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Af:229:MET:N	7:Af:230:PRO:HD2	2.22	0.55
27:B1:1313:4AC:OP2	42:BP:20:LYS:NZ	2.39	0.55
27:B1:2493:G:N2	27:B1:2496:A:OP2	2.36	0.55
1:A1:615:G:H2'	1:A1:616:G:C8	2.42	0.55
9:Ah:11:ILE:HD12	22:Au:144:ILE:HD11	1.89	0.55
27:B1:1286:4AC:O7	27:B1:1286:4AC:H5	2.07	0.55
32:BD:45:GLU:OE2	32:BD:58:ARG:NE	2.40	0.55
34:BG:15:LEU:HD23	34:BG:78:ILE:HD11	1.88	0.55
7:Af:3:GLN:O	7:Af:7:GLU:OE1	2.25	0.54
27:B1:2066:C:N4	27:B1:2090:C:O4'	2.40	0.54
30:BB:296:LYS:O	30:BB:353:ARG:NH1	2.40	0.54
27:B1:146:C:O2'	27:B1:147:U:OP1	2.22	0.54
27:B1:311:C:O2'	27:B1:312:C:O5'	2.21	0.54
27:B1:2647:A:H4'	33:BE:167:ILE:HD13	1.88	0.54
34:BF:18:LYS:CG	34:BF:110:LEU:HD11	2.37	0.54
35:BH:60:ASN:H	35:BH:60:ASN:HD22	1.55	0.54
12:Ak:92:ASP:OD1	12:Ak:93:MET:N	2.40	0.54
29:BA:47:GLU:OE1	29:BA:60:ARG:NH1	2.39	0.54
48:BV:11:GLY:O	48:BV:54:LYS:NZ	2.33	0.54
13:Al:93:ASP:OD1	13:Al:94:VAL:HG23	2.08	0.54
27:B1:73:U:OP2	49:BW:22:ARG:NH2	2.40	0.54
52:BZ:18:ILE:HD12	52:BZ:30:ARG:HG3	1.88	0.54
55:Bc:15:GLU:OE1	65:Bc:101:HOH:O	2.18	0.54
2:Aa:68:LEU:CD1	2:Aa:112:PRO:HG3	2.37	0.54
10:Ai:55:ASP:HB3	24:Aw:6:ILE:HD12	1.89	0.54
27:B1:1374:4AC:O5'	27:B1:1374:4AC:H6	2.08	0.54
27:B1:2539:G:H21	61:Bi:27:LYS:NZ	2.06	0.54
34:BG:34:LYS:HE3	34:BG:92:ILE:HG23	1.90	0.54
2:Aa:6:LEU:HD22	2:Aa:174:GLU:OE2	2.08	0.54
27:B1:765:G:H22	27:B1:981:G:P	2.30	0.54
27:B1:1172:G:OP1	59:Bg:37:LYS:NZ	2.33	0.54
27:B1:1360:4AC:H5	27:B1:1360:4AC:O7	2.07	0.54
27:B1:1374:4AC:O7	27:B1:1374:4AC:H5	2.07	0.54
32:BD:114:CYS:HB2	32:BD:139:VAL:O	2.08	0.54
1:A1:434:U:OP2	23:Av:89:ARG:NH1	2.41	0.54
27:B1:167:G:OP2	27:B1:167:G:N2	2.33	0.54
27:B1:1696:G:O2'	27:B1:1697:G:P	2.66	0.54
27:B1:2185:G:O2'	27:B1:2187:C:N4	2.30	0.54
1:A1:423:U:O2'	1:A1:425:OMU:O4	2.22	0.54
9:Ah:94:ASN:HD22	9:Ah:94:ASN:C	2.07	0.54
30:BB:164:ARG:NH1	30:BB:184:GLU:OE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BG:108:ARG:O	34:BG:111:VAL:HG12	2.07	0.54
27:B1:2240:C:N4	27:B1:2241:G:O6	2.41	0.54
27:B1:2821:4AC:OP2	65:B1:3176:HOH:O	2.18	0.54
30:BB:304:GLU:N	30:BB:304:GLU:OE1	2.41	0.54
27:B1:1280:U:OP2	36:BI:39:THR:OG1	2.24	0.54
27:B1:1961:U:OP1	29:BA:167:ARG:NH2	2.41	0.54
27:B1:2251:G:O2'	27:B1:2252:G:P	2.66	0.54
1:A1:1022:C:O2'	1:A1:1154:C:O2	2.17	0.53
27:B1:1150:4AC:H5	27:B1:1150:4AC:O7	2.07	0.53
27:B1:2711:G:N2	27:B1:2714:A:OP2	2.37	0.53
8:Ag:48:ASN:OD1	8:Ag:55:PHE:N	2.41	0.53
27:B1:1370:G:N7	65:B1:3224:HOH:O	2.33	0.53
1:A1:564:U:P	6:Ae:24:LYS:HZ1	2.31	0.53
27:B1:255:A:N6	63:Bk:21:PRO:O	2.40	0.53
27:B1:1459:C:O2'	27:B1:1538:U:O2	2.20	0.53
27:B1:1601:OMG:N2	27:B1:1706:4AC:O2	2.41	0.53
27:B1:149:C:OP1	40:BN:38:ARG:NH1	2.41	0.53
27:B1:539:G:N1	27:B1:542:A:OP2	2.37	0.53
29:BA:112:GLU:OE2	29:BA:156:ARG:NH2	2.40	0.53
27:B1:516:G:N1	27:B1:519:A:OP2	2.36	0.53
12:Ak:117:HIS:ND1	12:Ak:122:SER:O	2.41	0.53
27:B1:868:C:H5'	27:B1:896:4AC:HM71	1.89	0.53
27:B1:1161:U:O2'	27:B1:1166:C:N4	2.42	0.53
27:B1:1313:4AC:O2'	27:B1:1314:G:O5'	2.24	0.53
52:BZ:8:GLU:HB3	52:BZ:73:LYS:HD2	1.91	0.53
3:Ab:35:ILE:HD13	3:Ab:44:VAL:HG23	1.91	0.53
27:B1:2325:C:HO2'	27:B1:2326:C:P	2.32	0.53
27:B1:1150:4AC:HM73	27:B1:1286:4AC:HM72	1.91	0.53
27:B1:1277:G:OP1	36:BI:52:ARG:NH2	2.37	0.53
27:B1:2067:5MC:OP2	27:B1:2068:U:O2'	2.07	0.53
27:B1:337:4AC:O7	27:B1:337:4AC:H5	2.09	0.53
27:B1:1269:A:N6	27:B1:2607:OMC:OP1	2.42	0.53
27:B1:2964:G:OP2	27:B1:2964:G:N2	2.35	0.53
34:BG:117:LYS:O	34:BG:121:LEU:HD23	2.09	0.53
27:B1:979:4AC:O7	27:B1:979:4AC:H5	2.08	0.53
27:B1:1181:G:O2'	27:B1:1182:C:P	2.68	0.53
27:B1:1409:G:N7	45:BS:28:SER:OG	2.32	0.53
27:B1:1621:4AC:O7	27:B1:1621:4AC:H5	2.08	0.53
27:B1:2112:C:H2'	27:B1:2113:4AC:H6	1.90	0.53
27:B1:2133:4AC:OP1	45:BS:70:GLN:NE2	2.43	0.53
27:B1:2241:G:N2	27:B1:2294:G:O6	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BG:20:LEU:HD21	34:BG:80:VAL:HG13	1.91	0.53
10:Ai:55:ASP:OD1	10:Ai:55:ASP:N	2.41	0.52
10:Ai:104:VAL:HG22	10:Ai:125:LEU:HD23	1.89	0.52
13:Al:6:ILE:HG23	13:Al:96:ILE:HD11	1.91	0.52
27:B1:1608:4AC:H6	27:B1:1608:4AC:O5'	2.09	0.52
1:A1:519:U:OP2	1:A1:520:G:O2'	2.28	0.52
12:Ak:51:LEU:O	12:Ak:98:LYS:NZ	2.23	0.52
13:Al:49:THR:OG1	13:Al:62:ASP:OD1	2.22	0.52
20:As:33:LYS:O	20:As:37:GLU:OE1	2.28	0.52
1:A1:528:A:OP2	65:A1:1514:HOH:O	2.19	0.52
1:A1:952:G:O6	1:A1:992:C:O2'	2.23	0.52
27:B1:1186:A:HO2'	27:B1:1187:G:P	2.29	0.52
31:BC:234:THR:O	31:BC:234:THR:HG22	2.08	0.52
1:A1:624:4AC:O7	1:A1:624:4AC:H5	2.10	0.52
32:BD:11:ILE:HG22	32:BD:15:TRP:CZ3	2.45	0.52
12:Ak:36:ILE:O	12:Ak:42:ARG:NH1	2.39	0.52
27:B1:1783:OMC:HM22	27:B1:1784:U:O4'	2.10	0.52
27:B1:1824:A:H61	27:B1:2121:C:H42	1.56	0.52
27:B1:2589:C:OP1	27:B1:2645:G:N2	2.41	0.52
38:BK:46:ARG:NH1	38:BK:48:MET:SD	2.82	0.52
41:BO:48:ILE:HG21	41:BO:99:ILE:CD1	2.40	0.52
1:A1:1367:G:H2'	1:A1:1368:OMU:H6	1.92	0.52
27:B1:2173:G:O2'	27:B1:2174:U:P	2.67	0.52
29:BA:219:ARG:O	29:BA:226:LYS:NZ	2.42	0.52
1:A1:306:C:H2'	1:A1:307:4AC:H6	1.92	0.52
17:Ap:55:TYR:O	17:Ap:56:GLU:C	2.52	0.52
27:B1:978:C:H2'	27:B1:979:4AC:H6	1.92	0.52
33:BE:120:ARG:NH1	33:BE:157:ALA:O	2.43	0.52
45:BS:100:ASN:C	45:BS:100:ASN:HD22	2.17	0.52
55:Bc:87:VAL:HG12	55:Bc:87:VAL:O	2.09	0.52
1:A1:496:G:O2'	1:A1:497:C:P	2.68	0.52
1:A1:705:C:N4	1:A1:706:4AC:O7	2.43	0.52
13:Al:93:ASP:OD1	13:Al:94:VAL:N	2.43	0.52
27:B1:1095:U:H4'	35:BH:8:ILE:HG23	1.91	0.52
27:B1:1568:C:O2'	38:BL:52:HIS:ND1	2.39	0.52
27:B1:3013:C:OP2	27:B1:3014:U:O2'	2.15	0.52
41:BO:85:LEU:CD1	41:BO:185:PHE:CD1	2.78	0.52
1:A1:23:G:O2'	1:A1:293:U:OP1	2.28	0.51
1:A1:1288:4AC:O2'	1:A1:1289:G:P	2.68	0.51
27:B1:1149:5MC:H2'	27:B1:1150:4AC:H6	1.92	0.51
1:A1:427:4AC:O7	1:A1:427:4AC:H5	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:1313:4AC:O2'	27:B1:1314:G:P	2.68	0.51
27:B1:1360:4AC:H6	27:B1:1360:4AC:O5'	2.09	0.51
27:B1:933:4AC:O7	27:B1:933:4AC:H5	2.10	0.51
27:B1:1024:C:O2'	27:B1:1029:G:N2	2.44	0.51
27:B1:311:C:O2'	27:B1:312:C:P	2.68	0.51
41:BO:179:GLU:N	41:BO:179:GLU:OE1	2.43	0.51
8:Ag:68:ASP:OD2	8:Ag:108:ARG:NE	2.38	0.51
22:Au:10:ASP:OD1	22:Au:11:LEU:N	2.44	0.51
24:Aw:5:ILE:O	24:Aw:6:ILE:HD13	2.09	0.51
1:A1:1438:U:O2'	1:A1:1439:G:P	2.69	0.51
1:A1:1454:G:H1'	1:A1:1475:MA6:H2	1.92	0.51
6:Ae:131:ARG:NH1	6:Ae:141:ASN:OD1	2.43	0.51
27:B1:2428:OMC:OP1	32:BD:59:ARG:NH2	2.43	0.51
30:BB:55:ASP:OD1	30:BB:56:ASP:N	2.43	0.51
35:BH:41:GLY:O	35:BH:136:ARG:NH2	2.44	0.51
34:BG:53:ILE:HG22	34:BG:54:ALA:H	1.75	0.51
1:A1:691:4AC:O7	1:A1:691:4AC:H5	2.10	0.51
1:A1:1077:G:N2	1:A1:1078:U:O4	2.41	0.51
27:B1:2449:A:N6	41:BO:19:THR:O	2.43	0.51
45:BS:100:ASN:ND2	45:BS:100:ASN:O	2.43	0.51
1:A1:243:A:C2	1:A1:279:A:C5	2.98	0.51
1:A1:1146:G:O2'	1:A1:1147:C:P	2.69	0.51
1:A1:1314:4AC:HM71	12:Ak:124:LYS:O	2.10	0.51
27:B1:146:C:HO2'	27:B1:147:U:P	2.33	0.51
27:B1:485:4AC:OP2	31:BC:187:ARG:NH2	2.42	0.51
27:B1:1478:4AC:O2'	27:B1:1479:G:P	2.69	0.51
40:BN:141:LYS:NZ	63:Bk:11:ASP:OD2	2.44	0.51
55:Bc:3:ILE:HG22	55:Bc:4:LYS:N	2.25	0.51
63:Bk:15:GLU:OE2	63:Bk:28:LYS:NZ	2.33	0.51
1:A1:515:U:H4'	1:A1:517:A:H62	1.76	0.51
1:A1:668:OMG:H2'	1:A1:669:G:C8	2.45	0.51
1:A1:925:U:H6	1:A1:925:U:H5'	1.76	0.51
1:A1:1091:C:O2'	22:Au:130:ASP:OD2	2.29	0.51
1:A1:1297:C:HO2'	9:Ah:175:ARG:NH1	2.08	0.51
1:A1:1128:G:N1	1:A1:1131:A:OP2	2.39	0.50
1:A1:1253:C:H2'	1:A1:1254:4AC:H6	1.93	0.50
14:Am:68:ALA:O	14:Am:72:LEU:HD23	2.11	0.50
27:B1:1418:U:OP2	65:B1:3134:HOH:O	2.19	0.50
1:A1:444:4AC:O7	1:A1:444:4AC:H5	2.11	0.50
1:A1:1466:C:OP1	60:Bh:10:LYS:NZ	2.34	0.50
27:B1:1739:A:O2'	27:B1:1742:C:O2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:427:4AC:HM73	1:A1:444:4AC:HM73	1.93	0.50
1:A1:1462:G:HO2'	1:A1:1463:U:P	2.25	0.50
28:B2:48:C:H4'	41:BO:112:VAL:HG21	1.93	0.50
27:B1:653:G:O2'	53:Ba:57:LYS:NZ	2.34	0.50
27:B1:2237:C:N4	27:B1:2291:U:O2'	2.41	0.50
1:A1:268:C:O2'	1:A1:269:C:P	2.69	0.50
1:A1:1280:A:O2'	21:At:69:ASP:OD2	2.29	0.50
9:Ah:172:LYS:O	9:Ah:176:ASN:ND2	2.44	0.50
23:Av:50:THR:HG22	23:Av:50:THR:O	2.11	0.50
27:B1:744:A:N6	27:B1:763:G:O2'	2.44	0.50
27:B1:1885:4AC:OP1	43:BQ:88:ARG:HD2	2.12	0.50
27:B1:2680:A:OP1	27:B1:2765:G:O2'	2.24	0.50
34:BG:57:VAL:HG12	34:BG:59:PRO:O	2.11	0.50
52:BZ:18:ILE:HD13	52:BZ:34:PHE:HB2	1.93	0.50
7:Af:143:PHE:CE2	7:Af:211:VAL:HG21	2.47	0.50
27:B1:1478:4AC:HO2'	27:B1:1479:G:P	2.33	0.50
27:B1:2961:G:O2'	27:B1:2963:A:OP2	2.26	0.50
28:B2:90:4AC:H5	28:B2:90:4AC:O7	2.12	0.50
12:Ak:82:ILE:O	12:Ak:86:LEU:HD13	2.11	0.50
32:BD:26:GLU:HB3	32:BD:144:GLU:HG2	1.94	0.50
34:BG:43:VAL:O	34:BG:73:LYS:NZ	2.42	0.50
27:B1:1368:A:O2'	27:B1:1369:A:P	2.70	0.50
27:B1:2206:A:OP1	40:BN:88:VAL:HG22	2.12	0.50
1:A1:893:C:O2'	1:A1:1306:C:OP2	2.30	0.50
1:A1:141:4AC:H5	1:A1:141:4AC:O7	2.12	0.49
27:B1:1322:4AC:H5	27:B1:1322:4AC:O7	2.12	0.49
50:BX:123:ARG:NH2	65:BX:201:HOH:O	2.44	0.49
1:A1:1314:4AC:O7	1:A1:1314:4AC:H5	2.12	0.49
14:Am:58:TYR:O	14:Am:61:MET:HG2	2.12	0.49
27:B1:1621:4AC:O5'	27:B1:1621:4AC:H6	2.12	0.49
41:BO:188:VAL:O	41:BO:191:ARG:HG2	2.12	0.49
1:A1:739:4AC:H5	1:A1:739:4AC:O7	2.12	0.49
1:A1:1254:4AC:H5	1:A1:1254:4AC:O7	2.13	0.49
4:Ac:87:LEU:HD13	4:Ac:186:ARG:HA	1.93	0.49
6:Ae:38:ASN:O	6:Ae:42:SER:OG	2.20	0.49
27:B1:982:A:H1'	27:B1:983:G:OP2	2.12	0.49
27:B1:1148:G:C5	27:B1:1149:5MC:CM5	2.95	0.49
27:B1:2212:C:H2'	27:B1:2213:4AC:H6	1.94	0.49
1:A1:1476:MA6:H5''	1:A1:1476:MA6:H8	1.93	0.49
27:B1:1734:4AC:O7	27:B1:1734:4AC:H5	2.12	0.49
27:B1:732:4AC:O7	27:B1:732:4AC:H5	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:1061:4AC:O7	27:B1:1061:4AC:H5	2.13	0.49
31:BC:133:ILE:HD12	31:BC:172:ARG:HD2	1.94	0.49
39:BM:97:GLU:HB3	39:BM:102:ILE:HD13	1.94	0.49
1:A1:1092:4AC:O7	1:A1:1092:4AC:H5	2.12	0.49
1:A1:1467:4AC:O7	1:A1:1467:4AC:H5	2.13	0.49
27:B1:1703:4AC:O7	27:B1:1703:4AC:H5	2.13	0.49
27:B1:1762:4AC:H5	27:B1:1762:4AC:O7	2.13	0.49
27:B1:1930:C:H2'	27:B1:1931:A:C8	2.48	0.49
27:B1:1973:C:O2'	27:B1:2094:A:N1	2.41	0.49
5:Ad:58:LEU:O	5:Ad:70:ARG:NH1	2.46	0.49
27:B1:1383:4AC:H5	27:B1:1383:4AC:O7	2.13	0.49
27:B1:3006:4AC:H5	27:B1:3006:4AC:O7	2.13	0.49
27:B1:3037:4AC:H5	27:B1:3037:4AC:O7	2.13	0.49
30:BB:75:THR:HG21	30:BB:322:MET:HE2	1.94	0.49
45:BS:100:ASN:C	45:BS:100:ASN:ND2	2.69	0.49
1:A1:546:4AC:H5	1:A1:546:4AC:O7	2.13	0.49
3:Ab:173:LEU:HD23	3:Ab:173:LEU:H	1.78	0.49
9:Ah:11:ILE:CD1	22:Au:144:ILE:HD11	2.43	0.49
27:B1:90:C:OP2	27:B1:91:A:O2'	2.21	0.49
27:B1:807:4AC:H5	27:B1:807:4AC:O7	2.13	0.49
27:B1:1374:4AC:OP2	53:Ba:104:HIS:ND1	2.46	0.49
1:A1:427:4AC:H6	1:A1:427:4AC:O5'	2.13	0.49
1:A1:864:U:OP2	60:Bh:2:LYS:NZ	2.38	0.49
1:A1:965:A:O2'	1:A1:991:G:OP1	2.30	0.49
1:A1:1093:G:N7	22:Au:2:ALA:N	2.61	0.49
1:A1:1202:U:O4	9:Ah:170:SER:OG	2.29	0.49
1:A1:1288:4AC:O2'	1:A1:1289:G:OP1	2.30	0.49
4:Ac:124:ILE:O	4:Ac:181:ARG:N	2.46	0.49
5:Ad:11:TYR:HA	5:Ad:46:THR:HG21	1.94	0.49
13:Al:90:VAL:HG13	13:Al:90:VAL:O	2.13	0.49
27:B1:2429:4AC:O7	27:B1:2429:4AC:H5	2.13	0.49
27:B1:2847:A:H2'	27:B1:2848:G:O4'	2.13	0.49
27:B1:3020:4AC:H5	27:B1:3020:4AC:O7	2.13	0.49
38:BK:17:ARG:HD3	38:BK:43:VAL:HG12	1.95	0.49
58:Bf:31:THR:HG22	58:Bf:31:THR:O	2.13	0.49
1:A1:761:4AC:H5	1:A1:761:4AC:O7	2.13	0.49
1:A1:836:4AC:O7	1:A1:836:4AC:H5	2.13	0.49
1:A1:839:4AC:H5	1:A1:839:4AC:O7	2.13	0.49
27:B1:80:4AC:H5	27:B1:80:4AC:O7	2.13	0.49
27:B1:378:4AC:O7	27:B1:378:4AC:H5	2.13	0.49
1:A1:216:4AC:O7	1:A1:216:4AC:H5	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:666:C:O2	27:B1:2156:C:O2'	2.30	0.48
27:B1:943:U:OP2	39:BM:26:ARG:NH1	2.43	0.48
27:B1:2054:G:N2	27:B1:2054:G:OP2	2.45	0.48
27:B1:2428:OMC:O4'	32:BD:31:ASN:ND2	2.46	0.48
32:BD:81:THR:C	32:BD:82:LEU:HD22	2.37	0.48
9:Ah:163:ARG:O	9:Ah:167:LEU:HD23	2.13	0.48
14:Am:58:TYR:CE2	14:Am:62:LEU:HD11	2.48	0.48
26:Ay:32:CYS:SG	26:Ay:33:GLY:N	2.86	0.48
27:B1:2052:A:C2'	27:B1:2053:A:O5'	2.61	0.48
27:B1:2469:4AC:O7	27:B1:2469:4AC:H5	2.13	0.48
28:B2:117:4AC:H5	28:B2:117:4AC:O7	2.14	0.48
29:BA:78:LEU:HD12	57:Be:63:PHE:HB3	1.95	0.48
52:BZ:18:ILE:HD11	52:BZ:31:ALA:HA	1.95	0.48
1:A1:467:4AC:O7	1:A1:467:4AC:H5	2.13	0.48
13:Al:8:ILE:HG22	13:Al:96:ILE:HD12	1.94	0.48
27:B1:142:4AC:O7	27:B1:142:4AC:H5	2.12	0.48
27:B1:2377:U:OP2	44:BR:4:LYS:NZ	2.42	0.48
27:B1:2634:A:OP2	65:B1:3178:HOH:O	2.20	0.48
27:B1:2749:4AC:H5	27:B1:2749:4AC:O7	2.13	0.48
35:BH:4:ARG:NH2	35:BH:9:ASP:OD1	2.47	0.48
38:BL:5:ASP:N	38:BL:5:ASP:OD1	2.47	0.48
1:A1:220:4AC:O7	1:A1:220:4AC:H5	2.13	0.48
1:A1:1016:4AC:H5	1:A1:1016:4AC:O7	2.13	0.48
39:BM:143:GLU:N	39:BM:143:GLU:OE1	2.45	0.48
1:A1:5:4AC:H5	1:A1:5:4AC:O7	2.13	0.48
1:A1:367:4AC:O7	1:A1:367:4AC:H5	2.13	0.48
1:A1:405:4AC:H5	1:A1:405:4AC:O7	2.14	0.48
9:Ah:65:GLU:OE2	9:Ah:97:LYS:NZ	2.46	0.48
13:Al:8:ILE:HG22	13:Al:96:ILE:CD1	2.43	0.48
26:Ay:34:GLU:N	26:Ay:34:GLU:OE1	2.46	0.48
27:B1:276:4AC:O7	27:B1:276:4AC:H5	2.14	0.48
27:B1:1743:4AC:H5	27:B1:1743:4AC:O7	2.13	0.48
27:B1:1818:4AC:O7	27:B1:1818:4AC:H5	2.13	0.48
27:B1:1911:4AC:H5	27:B1:1911:4AC:O7	2.13	0.48
27:B1:2113:4AC:O7	27:B1:2113:4AC:H5	2.13	0.48
32:BD:144:GLU:OE1	32:BD:145:ARG:O	2.32	0.48
34:BG:50:LEU:HD12	34:BG:76:PRO:O	2.13	0.48
35:BH:129:ASP:OD1	35:BH:161:TYR:OH	2.30	0.48
41:BO:108:LEU:HD23	41:BO:108:LEU:H	1.78	0.48
42:BP:22:SER:HB2	42:BP:30:TRP:HB2	1.95	0.48
42:BP:32:ASP:HA	42:BP:35:TRP:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BR:33:GLN:NE2	44:BR:90:PRO:O	2.46	0.48
1:A1:614:4AC:O7	1:A1:614:4AC:H5	2.13	0.48
1:A1:1135:4AC:H5	1:A1:1135:4AC:O7	2.13	0.48
5:Ad:48:LEU:HB2	5:Ad:100:ILE:HD12	1.95	0.48
27:B1:262:A2M:H2	27:B1:306:G:N3	2.29	0.48
27:B1:2036:U:O2'	27:B1:2037:A:P	2.72	0.48
27:B1:2053:A:HO2'	27:B1:2054:G:P	2.34	0.48
34:BG:60:GLU:OE1	34:BG:60:GLU:N	2.47	0.48
49:BW:53:ARG:O	49:BW:57:ILE:HD12	2.14	0.48
1:A1:1020:A:N1	1:A1:1061:G:O2'	2.38	0.48
1:A1:1221:4AC:H5	1:A1:1221:4AC:O7	2.13	0.48
4:Ac:32:VAL:HG13	4:Ac:50:VAL:HG11	1.96	0.48
17:Ap:6:TYR:O	17:Ap:7:ASN:C	2.56	0.48
21:At:19:MET:HE1	21:At:27:LEU:HD11	1.95	0.48
27:B1:599:4AC:H5	27:B1:599:4AC:O7	2.13	0.48
27:B1:953:4AC:H5	27:B1:953:4AC:O7	2.13	0.48
27:B1:1501:4AC:O7	27:B1:1501:4AC:H5	2.14	0.48
27:B1:1546:4AC:O7	27:B1:1546:4AC:H5	2.14	0.48
41:BO:189:LYS:O	41:BO:193:ILE:HG12	2.14	0.48
1:A1:107:C:OP1	1:A1:308:G:O2'	2.28	0.48
1:A1:499:4AC:O7	1:A1:499:4AC:H5	2.14	0.48
11:Aj:81:ILE:HD11	11:Aj:102:GLU:HB3	1.94	0.48
27:B1:126:C:H4'	27:B1:127:U:OP2	2.14	0.48
27:B1:146:C:O2'	27:B1:147:U:P	2.71	0.48
27:B1:485:4AC:O7	27:B1:485:4AC:H5	2.14	0.48
27:B1:2821:4AC:H5	27:B1:2821:4AC:O7	2.14	0.48
27:B1:3023:4AC:H5	27:B1:3023:4AC:O7	2.14	0.48
38:BL:6:VAL:HG21	38:BL:64:ARG:HD2	1.96	0.48
27:B1:392:4AC:H5	27:B1:392:4AC:O7	2.13	0.48
27:B1:2473:A:O2'	44:BR:79:ASP:OD2	2.31	0.48
27:B1:2762:G:OP2	27:B1:2846:C:O2'	2.31	0.48
28:B2:120:4AC:O7	28:B2:120:4AC:H5	2.14	0.48
40:BN:113:VAL:HG22	40:BN:132:MET:HE3	1.95	0.48
43:BQ:144:GLU:OE1	43:BQ:145:HIS:ND1	2.47	0.48
1:A1:268:C:O2'	1:A1:269:C:O5'	2.30	0.48
1:A1:636:4AC:H5	1:A1:636:4AC:O7	2.13	0.48
1:A1:810:4AC:O7	1:A1:810:4AC:H5	2.13	0.48
27:B1:98:4AC:O7	27:B1:98:4AC:H5	2.14	0.48
27:B1:271:4AC:O7	27:B1:271:4AC:H5	2.13	0.48
27:B1:419:4AC:H5	27:B1:419:4AC:O7	2.14	0.48
27:B1:580:4AC:H5	27:B1:580:4AC:O7	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:715:4AC:O7	27:B1:715:4AC:H5	2.14	0.48
27:B1:950:4AC:O7	27:B1:950:4AC:H5	2.13	0.48
27:B1:1052:4AC:H5	27:B1:1052:4AC:O7	2.14	0.48
27:B1:1664:4AC:H5	27:B1:1664:4AC:O7	2.13	0.48
27:B1:2844:4AC:O7	27:B1:2844:4AC:H5	2.14	0.48
27:B1:2850:4AC:O7	27:B1:2850:4AC:H5	2.13	0.48
39:BM:101:ILE:HG23	39:BM:122:LEU:HB2	1.96	0.48
1:A1:1179:C:H4'	17:Ap:8:LYS:O	2.14	0.47
1:A1:1288:4AC:H5	1:A1:1288:4AC:O7	2.13	0.47
27:B1:759:4AC:H5	27:B1:759:4AC:O7	2.14	0.47
27:B1:798:4AC:H5	27:B1:798:4AC:O7	2.14	0.47
27:B1:1001:G:H2'	27:B1:1002:C:C6	2.49	0.47
27:B1:1439:4AC:O7	27:B1:1439:4AC:H5	2.14	0.47
27:B1:2258:A:O2'	27:B1:2259:A:O5'	2.25	0.47
29:BA:171:PRO:HG3	57:Be:24:ARG:HE	1.77	0.47
31:BC:2:LYS:HB3	31:BC:15:GLU:OE2	2.14	0.47
1:A1:578:4AC:O7	1:A1:578:4AC:H5	2.14	0.47
7:Af:229:MET:O	7:Af:230:PRO:C	2.56	0.47
27:B1:19:4AC:O7	27:B1:19:4AC:H5	2.13	0.47
27:B1:130:4AC:H5	27:B1:130:4AC:O7	2.13	0.47
27:B1:859:G:O2'	27:B1:860:G:O5'	2.18	0.47
27:B1:2325:C:O2'	27:B1:2326:C:P	2.72	0.47
27:B1:2454:4AC:O7	27:B1:2454:4AC:H5	2.14	0.47
27:B1:2876:4AC:H5	27:B1:2876:4AC:O7	2.13	0.47
27:B1:3036:C:HO2'	27:B1:3037:4AC:P	2.36	0.47
39:BM:101:ILE:HG23	39:BM:101:ILE:O	2.14	0.47
45:BS:91:ILE:O	45:BS:95:LEU:HD13	2.14	0.47
1:A1:87:4AC:H5	1:A1:87:4AC:O7	2.14	0.47
1:A1:291:4AC:O7	1:A1:291:4AC:H5	2.13	0.47
1:A1:382:4AC:H5	1:A1:382:4AC:O7	2.14	0.47
1:A1:1415:G:N2	8:Ag:77:ASP:OD1	2.46	0.47
27:B1:1394:C:O2'	27:B1:1395:G:O5'	2.30	0.47
27:B1:1757:4AC:O7	27:B1:1757:4AC:H5	2.14	0.47
27:B1:3011:4AC:O7	27:B1:3011:4AC:H5	2.15	0.47
27:B1:3036:C:H2'	27:B1:3037:4AC:H6	1.96	0.47
28:B2:91:G:N2	28:B2:94:A:OP2	2.41	0.47
1:A1:84:C:H2'	1:A1:85:A:C8	2.49	0.47
1:A1:540:4AC:O7	1:A1:540:4AC:H5	2.14	0.47
1:A1:1210:A:OP2	22:Au:61:ARG:NH2	2.46	0.47
1:A1:1241:A:O2'	1:A1:1244:C:N4	2.47	0.47
2:Aa:68:LEU:HD12	2:Aa:112:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Aj:65:VAL:CG1	11:Aj:105:ILE:HD11	2.42	0.47
27:B1:227:4AC:H5	27:B1:227:4AC:O7	2.13	0.47
27:B1:1264:4AC:H5	27:B1:1264:4AC:O7	2.14	0.47
27:B1:2002:U:N3	27:B1:2005:A:OP2	2.47	0.47
33:BE:83:THR:HG23	33:BE:84:GLU:OE1	2.15	0.47
34:BG:16:ALA:O	34:BG:20:LEU:HD23	2.14	0.47
1:A1:231:4AC:H5	1:A1:231:4AC:O7	2.15	0.47
1:A1:277:A:H3'	1:A1:278:G:H5'	1.96	0.47
2:Aa:144:GLU:OE1	2:Aa:144:GLU:N	2.45	0.47
27:B1:243:4AC:H5	27:B1:243:4AC:O7	2.15	0.47
27:B1:1612:4AC:O7	27:B1:1612:4AC:H5	2.13	0.47
9:Ah:114:ARG:NH1	9:Ah:186:GLU:OE2	2.48	0.47
27:B1:609:4AC:O7	27:B1:609:4AC:H5	2.14	0.47
27:B1:896:4AC:H5	27:B1:896:4AC:O7	2.15	0.47
27:B1:1442:4AC:H5	27:B1:1442:4AC:O7	2.15	0.47
27:B1:1906:G:N7	65:B1:3232:HOH:O	2.35	0.47
27:B1:2184:A:OP1	31:BC:65:HIS:N	2.47	0.47
27:B1:2251:G:HO2'	27:B1:2252:G:P	2.34	0.47
27:B1:2792:4AC:H5	27:B1:2792:4AC:O7	2.15	0.47
1:A1:86:C:H2'	1:A1:87:4AC:H6	1.97	0.47
1:A1:719:4AC:O7	1:A1:719:4AC:H5	2.15	0.47
1:A1:827:4AC:O7	1:A1:827:4AC:H5	2.14	0.47
22:Au:144:ILE:HG23	22:Au:144:ILE:O	2.14	0.47
27:B1:721:4AC:O7	27:B1:721:4AC:H5	2.15	0.47
27:B1:980:G:HO2'	27:B1:981:G:P	2.31	0.47
27:B1:1063:C:C5	27:B1:1064:4AC:HM73	2.50	0.47
27:B1:1478:4AC:H5	27:B1:1478:4AC:O7	2.14	0.47
27:B1:1696:G:HO2'	27:B1:1697:G:P	2.34	0.47
27:B1:1751:4AC:O7	27:B1:1751:4AC:H5	2.14	0.47
27:B1:1846:4AC:H5	27:B1:1846:4AC:O7	2.15	0.47
27:B1:1867:G:H3'	27:B1:1868:5MC:HM53	1.97	0.47
27:B1:1931:A:H4'	29:BA:172:LEU:O	2.13	0.47
27:B1:2328:4AC:H5	27:B1:2328:4AC:O7	2.15	0.47
42:BP:7:THR:O	42:BP:7:THR:HG22	2.12	0.47
1:A1:784:G:OP1	2:Aa:26:LYS:NZ	2.45	0.47
1:A1:1260:C:OP2	9:Ah:177:LYS:NZ	2.47	0.47
27:B1:741:4AC:H5	27:B1:741:4AC:O7	2.14	0.47
27:B1:1435:4AC:O7	27:B1:1435:4AC:H5	2.14	0.47
27:B1:1706:4AC:H5	27:B1:1706:4AC:O7	2.14	0.47
44:BR:22:ARG:HG3	44:BR:22:ARG:O	2.15	0.47
59:Bg:38:ARG:C	59:Bg:39:LEU:HD12	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:361:A2M:O5'	1:A1:361:A2M:H8	2.15	0.47
1:A1:1067:4AC:O7	1:A1:1067:4AC:H5	2.14	0.47
1:A1:1133:G:H5'	20:As:4:ILE:HG22	1.96	0.47
9:Ah:15:ILE:HD13	9:Ah:43:LEU:HD23	1.96	0.47
27:B1:1286:4AC:O5'	27:B1:1286:4AC:H6	2.15	0.47
39:BM:105:VAL:O	39:BM:105:VAL:HG22	2.15	0.47
1:A1:41:4AC:H5	1:A1:41:4AC:O7	2.15	0.47
1:A1:1227:4AC:H5	1:A1:1227:4AC:O7	2.15	0.47
8:Ag:96:PRO:O	8:Ag:101:GLU:OE2	2.32	0.47
13:Al:64:TRP:CE3	17:Ap:54:LYS:HG3	2.50	0.47
27:B1:360:4AC:H5	27:B1:360:4AC:O7	2.15	0.47
27:B1:1769:4AC:H5	27:B1:1769:4AC:O7	2.15	0.47
27:B1:2213:4AC:O7	27:B1:2213:4AC:H5	2.15	0.47
47:BU:107:LEU:HD11	47:BU:116:ILE:HD12	1.96	0.47
1:A1:816:4AC:H5	1:A1:816:4AC:O7	2.15	0.46
1:A1:1321:C:O2'	1:A1:1323:U:OP2	2.29	0.46
27:B1:658:U:H2'	27:B1:659:C:C6	2.50	0.46
27:B1:2809:4AC:H5	27:B1:2809:4AC:O7	2.15	0.46
28:B2:9:G:OP1	41:BO:24:ARG:NE	2.48	0.46
46:BT:2:ASP:OD1	46:BT:3:PRO:CD	2.61	0.46
1:A1:534:4AC:O7	1:A1:534:4AC:H5	2.15	0.46
7:Af:220:ARG:NH1	10:Ai:98:GLU:O	2.47	0.46
27:B1:786:4AC:H5	27:B1:786:4AC:O7	2.15	0.46
27:B1:1313:4AC:O7	27:B1:1313:4AC:H5	2.15	0.46
27:B1:1639:4AC:HM73	27:B1:1664:4AC:CM7	2.45	0.46
34:BG:50:LEU:HB3	34:BG:101:ILE:CG2	2.45	0.46
1:A1:307:4AC:H5	1:A1:307:4AC:O7	2.14	0.46
14:Am:72:LEU:HD22	14:Am:110:LEU:HD21	1.98	0.46
27:B1:479:4AC:O7	27:B1:479:4AC:H5	2.15	0.46
27:B1:866:4AC:O7	27:B1:866:4AC:H5	2.14	0.46
27:B1:1551:4AC:H5	27:B1:1551:4AC:O7	2.16	0.46
27:B1:2329:G:N2	27:B1:2332:A:OP2	2.40	0.46
27:B1:2772:G:O2'	27:B1:2781:G:O6	2.31	0.46
30:BB:124:PHE:O	30:BB:125:TYR:HB2	2.15	0.46
1:A1:261:C:O2'	19:Ar:93:PRO:O	2.32	0.46
27:B1:200:4AC:O7	27:B1:200:4AC:H5	2.16	0.46
27:B1:688:4AC:O7	27:B1:688:4AC:H5	2.16	0.46
27:B1:1107:4AC:H5	27:B1:1107:4AC:O7	2.16	0.46
27:B1:2171:4AC:O7	27:B1:2171:4AC:H5	2.16	0.46
34:BF:26:ALA:O	34:BF:30:GLY:N	2.49	0.46
34:BF:58:ASP:OD1	34:BF:58:ASP:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:537:A:N6	1:A1:713:G:O2'	2.42	0.46
1:A1:691:4AC:O5'	1:A1:691:4AC:H6	2.16	0.46
21:At:72:ILE:HD11	21:At:103:LEU:HD13	1.97	0.46
27:B1:1290:4AC:O7	27:B1:1290:4AC:H5	2.16	0.46
27:B1:1872:C:N4	65:B1:3304:HOH:O	2.48	0.46
1:A1:1181:4AC:H5	1:A1:1181:4AC:O7	2.15	0.46
13:Al:3:LYS:NZ	13:Al:74:ASP:OD2	2.40	0.46
22:Au:146:GLU:O	22:Au:149:LYS:NZ	2.48	0.46
27:B1:1178:4AC:H5	27:B1:1178:4AC:O7	2.14	0.46
27:B1:1293:4AC:H5	27:B1:1293:4AC:O7	2.16	0.46
47:BU:1:MET:O	47:BU:1:MET:HG3	2.15	0.46
1:A1:706:4AC:O7	1:A1:706:4AC:H5	2.15	0.46
5:Ad:43:LYS:O	5:Ad:46:THR:HG22	2.16	0.46
6:Ae:236:ASP:OD1	6:Ae:236:ASP:N	2.49	0.46
27:B1:116:4AC:H5	27:B1:116:4AC:O7	2.16	0.46
27:B1:1649:4AC:H5	27:B1:1649:4AC:O7	2.15	0.46
27:B1:1822:4AC:O7	27:B1:1822:4AC:H5	2.15	0.46
27:B1:2432:4AC:H5	27:B1:2432:4AC:O7	2.15	0.46
1:A1:195:4AC:O7	1:A1:195:4AC:H5	2.15	0.46
21:At:21:LEU:HD11	21:At:36:LEU:HD22	1.98	0.46
27:B1:933:4AC:O5'	27:B1:933:4AC:H6	2.15	0.46
27:B1:2614:C:OP1	65:B1:3179:HOH:O	2.20	0.46
34:BG:25:ILE:O	34:BG:29:THR:OG1	2.19	0.46
1:A1:913:G:O2'	21:At:121:GLY:O	2.28	0.46
27:B1:2133:4AC:H5	27:B1:2133:4AC:O7	2.16	0.46
27:B1:2138:A:O2'	45:BS:137:THR:HG22	2.16	0.46
27:B1:2423:G:N3	27:B1:2423:G:H2'	2.31	0.46
27:B1:2492:4AC:O7	27:B1:2492:4AC:H5	2.16	0.46
12:Ak:100:MET:HE3	12:Ak:107:LEU:HD12	1.98	0.46
18:Aq:29:THR:HG22	18:Aq:30:VAL:H	1.80	0.46
27:B1:434:4AC:H5	27:B1:434:4AC:O7	2.15	0.46
27:B1:484:C:N4	27:B1:485:4AC:O7	2.48	0.46
27:B1:1505:4AC:H5	27:B1:1505:4AC:O7	2.16	0.46
27:B1:2020:4AC:O7	27:B1:2020:4AC:H5	2.15	0.46
27:B1:2428:OMC:OP1	32:BD:59:ARG:NE	2.47	0.46
27:B1:2888:4AC:OP2	30:BB:28:ARG:NH2	2.45	0.46
61:Bi:9:THR:HG22	61:Bi:10:TYR:N	2.31	0.46
1:A1:712:U:H2'	1:A1:713:G:O4'	2.16	0.45
3:Ab:90:LEU:HD11	3:Ab:185:PRO:HD3	1.97	0.45
12:Ak:47:GLU:OE2	12:Ak:102:TYR:OH	2.15	0.45
18:Aq:29:THR:HG22	18:Aq:30:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:1368:A:O2'	27:B1:1369:A:OP1	2.31	0.45
27:B1:2602:4AC:H5	27:B1:2602:4AC:O7	2.15	0.45
34:BG:70:CYS:HA	34:BG:75:ILE:HG22	1.97	0.45
1:A1:677:G:OP1	4:Ac:98:ARG:NH1	2.44	0.45
1:A1:856:4AC:H5	1:A1:856:4AC:O7	2.15	0.45
24:Aw:61:VAL:HG13	24:Aw:61:VAL:O	2.16	0.45
27:B1:23:4AC:H5	27:B1:23:4AC:O7	2.14	0.45
27:B1:726:G:N3	27:B1:774:U:O2'	2.49	0.45
27:B1:2526:4AC:O7	27:B1:2526:4AC:H5	2.16	0.45
29:BA:55:THR:OG1	65:BA:301:HOH:O	2.11	0.45
34:BG:113:GLU:OE2	34:BG:117:LYS:HD3	2.17	0.45
38:BL:82:LEU:HD12	38:BL:83:ALA:N	2.31	0.45
39:BM:105:VAL:HG11	39:BM:126:ALA:HB2	1.98	0.45
1:A1:293:U:OP1	5:Ad:8:ARG:NH2	2.50	0.45
7:Af:74:MET:SD	7:Af:79:ARG:HG2	2.57	0.45
11:Aj:67:ASP:OD1	11:Aj:67:ASP:N	2.49	0.45
21:At:20:SER:HG	21:At:23:GLU:CD	2.14	0.45
27:B1:566:A:H2'	27:B1:566:A:N3	2.31	0.45
34:BF:18:LYS:HG3	34:BF:110:LEU:HD11	1.98	0.45
3:Ab:99:LEU:O	3:Ab:103:LEU:HD23	2.17	0.45
6:Ae:86:GLY:N	6:Ae:89:ASP:OD2	2.43	0.45
8:Ag:23:GLY:O	8:Ag:25:GLU:N	2.48	0.45
18:Aq:100:ARG:O	18:Aq:103:VAL:HG22	2.17	0.45
22:Au:131:LYS:O	22:Au:134:THR:HG22	2.16	0.45
27:B1:1542:U:H2'	27:B1:1542:U:O2	2.17	0.45
31:BC:169:ASP:O	31:BC:172:ARG:HG2	2.15	0.45
1:A1:622:G:OP1	1:A1:687:5MC:O2'	2.30	0.45
27:B1:792:C:C2	27:B1:793:A:C8	3.04	0.45
27:B1:877:5MC:H3'	27:B1:878:U:H4'	1.99	0.45
27:B1:1386:4AC:O7	27:B1:1386:4AC:H5	2.15	0.45
27:B1:1569:A:O2'	27:B1:1639:4AC:H4'	2.16	0.45
27:B1:2185:G:N2	27:B1:2186:A:N1	2.55	0.45
27:B1:2584:G:OP2	27:B1:2592:A:N6	2.47	0.45
32:BD:120:HIS:HB3	32:BD:135:PHE:CD1	2.51	0.45
34:BG:53:ILE:HG22	34:BG:54:ALA:N	2.32	0.45
50:BX:154:MET:O	50:BX:155:LEU:HB2	2.15	0.45
1:A1:235:G:OP1	19:Ar:66:ARG:NH1	2.47	0.45
27:B1:2008:4AC:O7	27:B1:2008:4AC:H5	2.15	0.45
27:B1:2595:U:N3	27:B1:2596:C:C5	2.84	0.45
28:B2:10:G:O6	41:BO:12:ARG:NH1	2.50	0.45
1:A1:802:A:O2'	4:Ac:177:ILE:O	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Av:14:ILE:O	23:Av:16:ARG:N	2.49	0.45
27:B1:85:A:C2	27:B1:103:A:C5	3.04	0.45
27:B1:1067:4AC:H5	27:B1:1067:4AC:O7	2.15	0.45
27:B1:1128:4AC:H5	27:B1:1128:4AC:O7	2.15	0.45
1:A1:290:C:O2'	5:Ad:3:ASP:O	2.33	0.45
1:A1:1028:C:N4	1:A1:1029:4AC:HM73	2.32	0.45
1:A1:1141:A:H2'	1:A1:1142:A:O4'	2.17	0.45
11:Aj:41:ASP:OD1	11:Aj:61:ALA:N	2.47	0.45
13:Al:78:ASP:OD1	13:Al:78:ASP:N	2.49	0.45
27:B1:1601:OMG:HM23	27:B1:1601:OMG:H1'	1.76	0.45
27:B1:1761:C:O2'	27:B1:1767:A:N1	2.42	0.45
39:BM:73:VAL:O	39:BM:73:VAL:HG13	2.17	0.45
1:A1:642:A:N1	1:A1:655:U:O2'	2.44	0.45
14:Am:66:ARG:O	14:Am:70:GLU:OE1	2.35	0.45
18:Aq:55:ARG:NH1	18:Aq:56:ASP:OD1	2.50	0.45
21:At:48:LEU:CD2	21:At:70:MET:HE1	2.46	0.45
27:B1:1482:G:O3'	46:BT:13:THR:HG21	2.17	0.45
29:BA:90:PRO:O	29:BA:95:ASN:ND2	2.43	0.45
32:BD:125:GLY:C	32:BD:127:GLU:H	2.24	0.45
32:BD:169:GLU:O	32:BD:173:VAL:HG23	2.17	0.45
53:Ba:109:LYS:O	53:Ba:113:GLU:OE1	2.34	0.45
1:A1:321:G:N1	1:A1:324:A:OP2	2.47	0.45
1:A1:624:4AC:HM73	1:A1:691:4AC:HM71	1.93	0.45
1:A1:674:C:O2	4:Ac:96:VAL:HG11	2.17	0.45
1:A1:779:G:OP1	18:Aq:2:ALA:N	2.50	0.45
3:Ab:51:PRO:O	3:Ab:52:GLY:C	2.59	0.45
22:Au:3:THR:HG22	22:Au:4:VAL:N	2.32	0.45
27:B1:162:4AC:O7	27:B1:162:4AC:H5	2.17	0.45
27:B1:214:OMG:H2'	27:B1:215:C:O4'	2.16	0.45
31:BC:29:ASP:N	31:BC:29:ASP:OD1	2.49	0.45
56:Bd:59:LYS:HG3	56:Bd:61:ALA:HB2	1.98	0.45
60:Bh:14:MET:HG2	60:Bh:15:ARG:N	2.32	0.45
8:Ag:33:ARG:CG	8:Ag:111:THR:HG22	2.47	0.44
27:B1:14:U:O2'	27:B1:15:A:OP2	2.29	0.44
27:B1:1050:U:C4	27:B1:1052:4AC:HM72	2.52	0.44
33:BE:27:LYS:HG3	33:BE:36:GLU:OE2	2.16	0.44
36:BI:72:ASP:OD1	36:BI:73:GLU:N	2.50	0.44
1:A1:294:G:N2	1:A1:297:A:OP2	2.43	0.44
2:Aa:130:ALA:HA	2:Aa:133:ILE:HG22	1.98	0.44
9:Ah:140:MET:O	9:Ah:141:PHE:HD1	2.00	0.44
19:Ar:15:LYS:HD3	19:Ar:24:HIS:CD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:48:4AC:O7	27:B1:48:4AC:H5	2.17	0.44
27:B1:793:A:H2'	27:B1:794:C:C6	2.53	0.44
27:B1:920:OMG:H5'	27:B1:921:OMG:OP1	2.18	0.44
27:B1:1100:4AC:H5	27:B1:1100:4AC:O7	2.17	0.44
27:B1:1639:4AC:H5	27:B1:1639:4AC:O7	2.18	0.44
62:Bj:68:ILE:HD12	62:Bj:68:ILE:H	1.83	0.44
1:A1:75:C:O2	1:A1:75:C:O4'	2.35	0.44
1:A1:1291:G:C6	1:A1:1292:U:C5	3.05	0.44
1:A1:1366:AIH59:O2	1:A1:1476:MA6:O2'	2.18	0.44
27:B1:47:5MC:HM53	27:B1:204:G:H3'	2.00	0.44
27:B1:266:A:C2	27:B1:295:U:C2	3.05	0.44
27:B1:613:G:N2	27:B1:616:A:OP2	2.40	0.44
27:B1:1152:G:N3	62:Bj:43:SER:OG	2.50	0.44
27:B1:2421:C:OP2	27:B1:2422:A:O2'	2.26	0.44
33:BE:37:ARG:HB3	33:BE:78:MET:HE1	1.99	0.44
1:A1:1012:5MC:O3'	17:Ap:44:ARG:NH2	2.50	0.44
1:A1:1016:4AC:OP2	1:A1:1016:4AC:H6	2.17	0.44
1:A1:1367:G:H4'	60:Bh:14:MET:HE2	1.98	0.44
2:Aa:35:VAL:HG22	2:Aa:41:TYR:CD2	2.52	0.44
27:B1:2888:4AC:O7	27:B1:2888:4AC:H5	2.16	0.44
34:BG:15:LEU:CD2	34:BG:78:ILE:HD11	2.48	0.44
45:BS:30:LYS:NZ	65:BS:205:HOH:O	2.45	0.44
1:A1:878:A:C2	1:A1:879:U:C5	3.05	0.44
6:Ae:182:GLY:O	6:Ae:198:ARG:NH2	2.49	0.44
8:Ag:43:LEU:O	8:Ag:44:ASN:OD1	2.35	0.44
8:Ag:67:THR:OG1	8:Ag:68:ASP:N	2.50	0.44
27:B1:1885:4AC:O7	27:B1:1885:4AC:H5	2.17	0.44
32:BD:122:ASN:O	32:BD:123:ILE:C	2.60	0.44
36:BI:20:LYS:O	36:BI:24:GLU:HG2	2.18	0.44
41:BO:172:LEU:HD12	41:BO:173:VAL:N	2.33	0.44
53:Ba:91:GLU:OE1	53:Ba:117:ARG:NH2	2.50	0.44
1:A1:301:G:H2'	1:A1:302:G:O4'	2.18	0.44
3:Ab:121:MET:HE2	3:Ab:148:GLN:HG3	2.00	0.44
13:Al:33:ARG:HE	13:Al:34:MET:H	1.65	0.44
16:Ao:116:ARG:HG2	16:Ao:126:VAL:HB	2.00	0.44
27:B1:652:4AC:O7	27:B1:652:4AC:H5	2.16	0.44
27:B1:727:G:N2	27:B1:730:A:OP2	2.41	0.44
27:B1:2087:5MC:O2'	27:B1:2089:G:OP2	2.32	0.44
32:BD:181:VAL:HG12	32:BD:182:GLU:N	2.33	0.44
35:BH:137:VAL:HG21	35:BH:141:HIS:HB2	2.00	0.44
38:BK:3:ALA:O	38:BK:4:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:At:32:GLN:N	21:At:32:GLN:OE1	2.50	0.44
27:B1:662:G:C1'	27:B1:1119:A:N6	2.81	0.44
27:B1:1149:5MC:N4	27:B1:1150:4AC:C7	2.80	0.44
28:B2:29:A:OP2	41:BO:40:SER:OG	2.36	0.44
30:BB:73:ILE:HD11	30:BB:322:MET:HE3	1.99	0.44
39:BM:72:GLU:OE2	39:BM:73:VAL:N	2.50	0.44
6:Ae:185:VAL:HG11	6:Ae:199:ILE:HD11	1.98	0.44
27:B1:851:C:O2	27:B1:851:C:O4'	2.36	0.44
27:B1:2749:4AC:O2'	30:BB:132:ILE:O	2.35	0.44
45:BS:116:HIS:HB3	45:BS:149:VAL:CG1	2.47	0.44
1:A1:622:G:O2'	18:Aq:115:ASP:OD1	2.28	0.44
4:Ac:34:LEU:HD11	14:Am:13:LYS:HD3	2.00	0.44
27:B1:979:4AC:O2'	27:B1:980:G:P	2.76	0.44
27:B1:2865:G:OP1	27:B1:2865:G:N2	2.51	0.44
28:B2:14:U:OP2	28:B2:70:A:O2'	2.35	0.44
28:B2:89:C:H2'	28:B2:90:4AC:H6	1.98	0.44
32:BD:128:TYR:HB2	32:BD:132:ILE:CB	2.47	0.44
34:BF:39:THR:O	34:BF:43:VAL:HG23	2.18	0.44
41:BO:36:VAL:HG21	41:BO:49:ILE:HD12	2.00	0.44
41:BO:88:LEU:HD12	41:BO:127:ALA:HB2	1.99	0.44
41:BO:159:GLN:HG3	41:BO:160:ASP:N	2.33	0.44
50:BX:104:GLU:N	50:BX:104:GLU:OE1	2.51	0.44
1:A1:15:U:O2'	1:A1:527:A:N6	2.51	0.43
1:A1:1184:G:OP2	1:A1:1284:C:N4	2.47	0.43
12:Ak:21:GLU:OE1	12:Ak:21:GLU:N	2.47	0.43
16:Ao:16:ASP:OD1	16:Ao:17:GLY:N	2.50	0.43
27:B1:1810:G:O2'	27:B1:1811:G:H5'	2.18	0.43
27:B1:2173:G:O2'	27:B1:2174:U:O5'	2.36	0.43
38:BK:22:VAL:HG12	38:BK:43:VAL:HG21	2.00	0.43
38:BL:80:ILE:HG22	38:BL:81:SER:N	2.33	0.43
57:Be:77:ALA:O	57:Be:80:ARG:HG2	2.18	0.43
27:B1:239:C:OP2	27:B1:2512:C:O2'	2.21	0.43
34:BG:29:THR:HG21	34:BG:106:LYS:HD2	2.01	0.43
16:Ao:94:ILE:C	16:Ao:95:THR:HG1	2.26	0.43
27:B1:299:G:C2	27:B1:300:U:O4	2.71	0.43
27:B1:647:U:H2'	27:B1:648:G:H8	1.84	0.43
29:BA:48:ILE:HD12	29:BA:79:VAL:HG23	2.00	0.43
39:BM:16:THR:HG22	39:BM:16:THR:O	2.16	0.43
42:BP:29:ILE:HG23	42:BP:30:TRP:N	2.33	0.43
6:Ae:105:ASN:N	6:Ae:109:LYS:O	2.50	0.43
27:B1:176:G:O6	40:BN:187:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:720:G:N1	1:A1:767:G:O2'	2.38	0.43
1:A1:1321:C:OP1	17:Ap:19:ARG:NH2	2.52	0.43
27:B1:920:OMG:H4'	27:B1:921:OMG:O5'	2.18	0.43
27:B1:1359:C:N4	27:B1:1360:4AC:HM72	2.33	0.43
27:B1:1827:G:O2'	27:B1:2116:U:O4	2.32	0.43
27:B1:1967:4AC:H5	27:B1:1967:4AC:O7	2.18	0.43
27:B1:2379:4AC:O7	27:B1:2379:4AC:H5	2.18	0.43
31:BC:196:GLY:N	31:BC:216:GLY:O	2.46	0.43
53:Ba:48:SER:O	53:Ba:52:LEU:HD23	2.18	0.43
1:A1:272:G:C8	1:A1:273:5MC:HM53	2.54	0.43
1:A1:274:4AC:O7	1:A1:274:4AC:H5	2.17	0.43
1:A1:1415:G:H1'	8:Ag:77:ASP:OD2	2.18	0.43
9:Ah:33:LEU:O	9:Ah:37:ILE:HG12	2.19	0.43
21:At:80:THR:OG1	21:At:93:GLU:OE1	2.29	0.43
27:B1:1107:4AC:H6	27:B1:1107:4AC:O5'	2.18	0.43
27:B1:1150:4AC:CM7	27:B1:1286:4AC:CM7	2.96	0.43
31:BC:61:ILE:HD13	31:BC:67:MET:CE	2.46	0.43
32:BD:120:HIS:HB3	32:BD:135:PHE:CE1	2.54	0.43
39:BM:102:ILE:HA	39:BM:123:VAL:HG13	1.99	0.43
1:A1:1226:C:N4	1:A1:1227:4AC:O7	2.52	0.43
27:B1:1404:4AC:H5	27:B1:1404:4AC:O7	2.17	0.43
34:BG:11:VAL:HG21	34:BG:79:TYR:HB2	2.00	0.43
1:A1:99:C:H4'	1:A1:100:A:O5'	2.18	0.43
1:A1:475:G:N7	15:An:70:ARG:NH1	2.66	0.43
3:Ab:47:PHE:HB3	3:Ab:85:ILE:HD13	1.99	0.43
8:Ag:19:VAL:O	8:Ag:19:VAL:HG13	2.18	0.43
27:B1:598:C:H2'	27:B1:599:4AC:H6	2.01	0.43
3:Ab:132:LEU:HD22	3:Ab:178:VAL:HG12	1.99	0.43
8:Ag:33:ARG:HG2	8:Ag:111:THR:HG22	2.01	0.43
13:Al:79:GLU:O	13:Al:82:MET:HG3	2.18	0.43
27:B1:348:G:N1	27:B1:351:A:OP2	2.46	0.43
27:B1:1454:G:N2	27:B1:1457:U:C4	2.87	0.43
9:Ah:37:ILE:HG23	9:Ah:63:ILE:HD11	2.01	0.43
14:Am:81:ILE:HD12	14:Am:102:ILE:HG23	2.01	0.43
27:B1:608:C:N4	27:B1:622:G:N2	2.67	0.43
31:BC:7:ASP:HB3	31:BC:13:VAL:HG21	2.01	0.43
31:BC:234:THR:O	31:BC:234:THR:CG2	2.67	0.43
32:BD:11:ILE:O	32:BD:15:TRP:CE3	2.72	0.43
39:BM:61:ARG:HG3	39:BM:62:GLY:H	1.84	0.43
1:A1:333:C:C2	1:A1:334:A:C8	3.06	0.42
1:A1:905:G:C2	1:A1:906:A:C8	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1175:A:H2'	1:A1:1176:A:H5''	2.01	0.42
27:B1:1909:C:O2'	27:B1:2083:C:OP1	2.34	0.42
27:B1:1938:A:O2'	27:B1:1942:A:N3	2.41	0.42
27:B1:2870:U:H4'	27:B1:2871:A:OP1	2.19	0.42
39:BM:76:VAL:HG22	39:BM:77:ASN:N	2.34	0.42
5:Ad:88:VAL:HG12	5:Ad:89:LEU:N	2.33	0.42
8:Ag:54:GLU:HG3	8:Ag:54:GLU:O	2.19	0.42
9:Ah:65:GLU:OE2	9:Ah:69:ASN:ND2	2.48	0.42
27:B1:1063:C:C4	27:B1:1064:4AC:HM73	2.54	0.42
27:B1:1761:C:H2'	27:B1:1762:4AC:H6	2.01	0.42
27:B1:2701:U:O2	27:B1:2701:U:O4'	2.37	0.42
33:BE:102:LYS:NZ	33:BE:104:GLN:OE1	2.51	0.42
39:BM:88:LEU:HB3	39:BM:93:ILE:HB	2.01	0.42
54:Bb:28:ARG:NH1	65:Bb:201:HOH:O	2.52	0.42
61:Bi:9:THR:HG21	61:Bi:80:ARG:HD2	2.01	0.42
1:A1:304:G:N2	5:Ad:3:ASP:OD1	2.49	0.42
1:A1:1415:G:N3	8:Ag:77:ASP:OD2	2.52	0.42
12:Ak:55:GLU:OE1	12:Ak:55:GLU:N	2.39	0.42
27:B1:453:A:H2'	27:B1:454:OMU:H6	2.00	0.42
27:B1:1366:G:N2	27:B1:1368:A:H3'	2.34	0.42
27:B1:1769:4AC:H6	27:B1:1769:4AC:O5'	2.20	0.42
27:B1:1964:G:OP1	29:BA:10:ARG:NH2	2.52	0.42
27:B1:2357:U:H2'	27:B1:2358:U:C6	2.54	0.42
28:B2:42:U:H6	32:BD:57:ILE:HD11	1.85	0.42
34:BG:108:ARG:O	34:BG:111:VAL:N	2.52	0.42
36:BI:43:ASP:OD1	36:BI:44:VAL:HG13	2.19	0.42
1:A1:99:C:H1'	1:A1:100:A:OP2	2.19	0.42
3:Ab:156:ASN:HA	3:Ab:159:GLU:HG2	2.00	0.42
12:Ak:56:ILE:O	12:Ak:60:VAL:HG22	2.20	0.42
20:As:24:PHE:CD1	20:As:54:VAL:HG11	2.54	0.42
27:B1:347:U:H2'	27:B1:348:G:O4'	2.19	0.42
27:B1:1617:A:C2	27:B1:1618:G:H1'	2.54	0.42
27:B1:2833:G:OP1	48:BV:35:ARG:NH2	2.52	0.42
27:B1:2849:C:H2'	27:B1:2850:4AC:H6	2.02	0.42
29:BA:28:VAL:HG21	29:BA:72:ILE:HG13	2.01	0.42
30:BB:80:VAL:O	30:BB:204:GLY:N	2.44	0.42
1:A1:645:OMG:H2'	1:A1:646:G:C8	2.55	0.42
21:At:85:ASN:ND2	21:At:88:GLU:O	2.53	0.42
27:B1:1570:A:O2'	27:B1:1638:C:O2'	2.21	0.42
27:B1:2173:G:HO2'	27:B1:2174:U:P	2.41	0.42
36:BI:105:LYS:HA	36:BI:108:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BJ:116:THR:HG22	37:BJ:116:THR:O	2.19	0.42
46:BT:4:TYR:CE2	49:BW:23:LEU:HD21	2.55	0.42
18:Aq:42:LYS:HE2	18:Aq:87:LEU:HD21	2.02	0.42
27:B1:59:G:O2'	27:B1:74:A:N1	2.48	0.42
27:B1:1567:G:N2	27:B1:1570:A:OP2	2.49	0.42
27:B1:2792:4AC:H6	27:B1:2792:4AC:O5'	2.20	0.42
38:BK:5:ASP:OD2	38:BK:8:ARG:NH2	2.52	0.42
38:BL:22:VAL:CG2	38:BL:35:VAL:HG12	2.49	0.42
39:BM:105:VAL:HG22	39:BM:108:PHE:O	2.19	0.42
50:BX:99:LYS:HB3	50:BX:105:MET:SD	2.60	0.42
1:A1:1319:G:OP2	1:A1:1321:C:N4	2.52	0.42
16:Ao:111:ARG:NH1	21:At:97:GLU:OE1	2.52	0.42
27:B1:863:G:O2'	27:B1:899:G:H4'	2.20	0.42
27:B1:1149:5MC:OP2	65:B1:3181:HOH:O	2.21	0.42
27:B1:2435:A:N3	27:B1:2435:A:H2'	2.35	0.42
47:BU:41:VAL:HG13	47:BU:119:ARG:HD2	2.01	0.42
3:Ab:40:LEU:HD23	3:Ab:40:LEU:H	1.83	0.42
27:B1:662:G:H2'	27:B1:2154:C:C5	2.54	0.42
27:B1:1488:OMU:H6	27:B1:1488:OMU:O5'	2.20	0.42
27:B1:2037:A:H62	27:B1:2043:A:H2	1.65	0.42
27:B1:2431:C:H2'	27:B1:2432:4AC:H6	2.02	0.42
27:B1:2705:A:OP1	65:B1:3182:HOH:O	2.22	0.42
33:BE:8:ARG:NH2	33:BE:49:GLU:OE1	2.49	0.42
1:A1:272:G:H3'	1:A1:273:5MC:HM53	2.02	0.42
1:A1:1417:U:C2	1:A1:1418:C:C5	3.08	0.42
9:Ah:81:VAL:HG23	9:Ah:199:TYR:CZ	2.55	0.42
27:B1:336:5MC:HM53	47:BU:1:MET:CB	2.50	0.42
27:B1:1986:G:H2'	27:B1:1987:U:O4'	2.20	0.42
27:B1:2517:G:O2'	61:Bi:77:ALA:O	2.33	0.42
37:BJ:16:ARG:HH21	37:BJ:19:ARG:NH1	2.18	0.42
45:BS:95:LEU:O	45:BS:98:VAL:HG12	2.20	0.42
1:A1:884:G:C2	1:A1:886:G:C8	3.07	0.41
1:A1:1018:U:H4'	1:A1:1019:C:O5'	2.20	0.41
1:A1:1108:A:N3	1:A1:1108:A:H2'	2.35	0.41
17:Ap:53:ARG:HB2	17:Ap:55:TYR:CZ	2.55	0.41
27:B1:293:U:H4'	40:BN:3:MET:HE1	2.03	0.41
27:B1:632:G:OP1	53:Ba:4:LYS:HD2	2.19	0.41
27:B1:711:G:O2'	31:BC:42:ARG:NE	2.53	0.41
27:B1:933:4AC:O2'	56:Bd:51:TRP:O	2.29	0.41
27:B1:1321:C:H2'	27:B1:1322:4AC:H6	2.01	0.41
27:B1:1368:A:H4'	27:B1:1369:A:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:1794:G:O2'	27:B1:1900:C:O2'	2.31	0.41
27:B1:2207:G:OP1	40:BN:72:LYS:NZ	2.51	0.41
27:B1:2462:C:H4'	61:Bi:80:ARG:HG2	2.02	0.41
27:B1:3005:C:H2'	27:B1:3006:4AC:H6	2.02	0.41
40:BN:41:ARG:NH1	40:BN:53:TYR:OH	2.53	0.41
1:A1:175:G:H2'	1:A1:176:U:O4'	2.20	0.41
1:A1:1278:G:N1	1:A1:1281:A:OP2	2.52	0.41
1:A1:1306:C:OP1	12:Ak:129:LYS:NZ	2.48	0.41
14:Am:65:ARG:O	14:Am:69:GLU:HG2	2.20	0.41
27:B1:255:A:H4'	27:B1:256:G:OP1	2.20	0.41
27:B1:1550:C:H2'	27:B1:1551:4AC:H6	2.02	0.41
23:Av:3:ILE:HD12	23:Av:39:LYS:HD2	2.02	0.41
24:Aw:3:LYS:N	24:Aw:4:PRO:HD2	2.35	0.41
27:B1:1981:OMU:H6	27:B1:1981:OMU:O5'	2.20	0.41
43:BQ:122:MET:SD	43:BQ:126:ARG:NE	2.90	0.41
51:BY:42:PRO:CG	51:BY:45:ILE:HD12	2.50	0.41
1:A1:372:U:H2'	1:A1:373:G:O4'	2.20	0.41
7:Af:89:VAL:HG22	7:Af:90:GLY:H	1.86	0.41
23:Av:93:ILE:HG22	23:Av:95:LYS:H	1.85	0.41
27:B1:1369:A:OP1	53:Ba:40:TRP:HB3	2.20	0.41
27:B1:1541:A:O2'	27:B1:1543:U:C6	2.74	0.41
28:B2:32:C:C2	28:B2:51:G:N2	2.88	0.41
30:BB:85:ALA:HB1	30:BB:160:ILE:HD12	2.02	0.41
3:Ab:76:GLU:OE1	3:Ab:76:GLU:N	2.52	0.41
18:Aq:24:ILE:O	18:Aq:24:ILE:HG22	2.20	0.41
24:Aw:5:ILE:C	24:Aw:6:ILE:HD13	2.45	0.41
25:Ax:26:GLN:NE2	25:Ax:65:ARG:O	2.53	0.41
27:B1:314:U:O2	27:B1:314:U:O4'	2.39	0.41
27:B1:584:A:H3'	27:B1:585:G:C5'	2.49	0.41
27:B1:589:U:H3'	27:B1:590:G:H5'	2.03	0.41
27:B1:1977:5MC:O2'	27:B1:2052:A:N3	2.52	0.41
27:B1:2590:C:O2'	27:B1:2591:C:OP1	2.36	0.41
41:BO:182:PRO:O	41:BO:186:GLU:HG2	2.21	0.41
49:BW:19:ARG:O	49:BW:23:LEU:HD23	2.21	0.41
1:A1:504:G:C2	1:A1:505:G:C8	3.09	0.41
1:A1:849:G:H3'	60:Bh:1:MET:HE3	2.02	0.41
16:Ao:31:ILE:HD11	16:Ao:66:LEU:HD22	2.02	0.41
27:B1:453:A:H1'	27:B1:2005:A:C2	2.55	0.41
27:B1:794:C:C2	27:B1:795:G:C8	3.09	0.41
27:B1:1496:A:H2'	27:B1:1497:A:C8	2.56	0.41
27:B1:2035:G:C6	27:B1:2047:C:N4	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:2263:C:N4	27:B1:2277:G:O6	2.52	0.41
30:BB:103:ASP:OD1	30:BB:104:PHE:N	2.54	0.41
31:BC:111:ARG:NH2	31:BC:254:TYR:O	2.54	0.41
46:BT:13:THR:HG22	46:BT:14:GLU:H	1.84	0.41
50:BX:105:MET:HB2	50:BX:109:ASP:OD2	2.21	0.41
8:Ag:44:ASN:OD1	8:Ag:44:ASN:C	2.64	0.41
27:B1:527:LHH:O4'	45:BS:100:ASN:OD1	2.39	0.41
27:B1:1311:A:OP1	42:BP:23:ASN:ND2	2.40	0.41
27:B1:1853:U:H4'	27:B1:1854:C:OP2	2.21	0.41
27:B1:1931:A:C2	27:B1:1969:A:H4'	2.55	0.41
31:BC:208:VAL:HG23	31:BC:209:LEU:N	2.36	0.41
1:A1:377:G:N2	1:A1:380:A:OP2	2.47	0.41
1:A1:1119:A:H4'	1:A1:1120:C:O4'	2.21	0.41
1:A1:1226:C:H2'	1:A1:1227:4AC:H6	2.02	0.41
3:Ab:34:ASP:OD1	3:Ab:45:ILE:HG13	2.20	0.41
11:Aj:43:ARG:NH1	11:Aj:118:GLY:O	2.54	0.41
20:As:54:VAL:O	20:As:58:VAL:HG23	2.21	0.41
22:Au:143:ILE:H	22:Au:143:ILE:HD12	1.86	0.41
27:B1:491:C:N4	27:B1:494:A:OP2	2.42	0.41
27:B1:994:G:O2'	27:B1:995:G:H5'	2.21	0.41
27:B1:1026:A:H4'	27:B1:1027:A:OP1	2.20	0.41
27:B1:1127:C:O2'	53:Ba:62:SER:OG	2.26	0.41
27:B1:1594:C:H2'	27:B1:1595:G:H8	1.85	0.41
27:B1:1626:A:H2'	27:B1:1627:A:H8	1.80	0.41
27:B1:1689:C:N4	27:B1:1690:G:N7	2.68	0.41
27:B1:1824:A:H61	27:B1:2121:C:N4	2.19	0.41
27:B1:2031:G:O6	27:B1:2054:G:C2	2.74	0.41
27:B1:2491:C:H2'	27:B1:2492:4AC:H6	2.02	0.41
27:B1:2749:4AC:HM73	27:B1:2898:C:N4	2.35	0.41
34:BG:39:THR:HG23	34:BG:100:ALA:HB2	2.01	0.41
39:BM:108:PHE:O	39:BM:109:ALA:HB3	2.21	0.41
61:Bi:40:PHE:CZ	61:Bi:44:LEU:HD11	2.56	0.41
1:A1:433:G:N2	1:A1:438:A:N7	2.69	0.41
1:A1:1054:A:H1'	1:A1:1055:A:OP2	2.21	0.41
9:Ah:121:GLN:O	9:Ah:121:GLN:NE2	2.54	0.41
11:Aj:96:THR:HG22	11:Aj:97:LYS:N	2.36	0.41
27:B1:588:A:C6	34:BG:92:ILE:HG21	2.56	0.41
27:B1:987:G:C8	50:BX:25:MET:HE1	2.56	0.41
27:B1:1064:4AC:H5	27:B1:1064:4AC:HM73	2.02	0.41
27:B1:1158:U:OP2	65:B1:3125:HOH:O	2.22	0.41
27:B1:1930:C:C3'	27:B1:1931:A:C8	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:2143:U:O2	53:Ba:30:ARG:NH2	2.51	0.41
27:B1:2697:G:OP2	27:B1:2697:G:N2	2.48	0.41
30:BB:150:GLN:O	30:BB:154:MET:HG3	2.21	0.41
34:BF:67:PRO:HB2	34:BF:68:PRO:HD3	2.02	0.41
34:BG:108:ARG:O	34:BG:109:ASP:C	2.63	0.41
35:BH:63:GLU:OE2	35:BH:66:ARG:NH2	2.53	0.41
40:BN:88:VAL:HG23	40:BN:89:LYS:HG3	2.03	0.41
47:BU:52:VAL:CG1	47:BU:100:VAL:HB	2.51	0.41
47:BU:55:MET:HE2	47:BU:55:MET:HA	2.01	0.41
55:Bc:4:LYS:HE2	55:Bc:83:TYR:HB3	2.03	0.41
55:Bc:41:ARG:CZ	55:Bc:87:VAL:HG21	2.50	0.41
1:A1:42:G:OP2	1:A1:363:C:N4	2.45	0.41
1:A1:906:A:H2'	1:A1:907:G:C8	2.55	0.41
11:Aj:33:SER:HB3	11:Aj:56:ARG:HD3	2.02	0.41
14:Am:106:ALA:HB2	14:Am:112:ILE:CD1	2.50	0.41
16:Ao:119:ARG:HB2	16:Ao:126:VAL:HG12	2.03	0.41
27:B1:259:C:O2	27:B1:259:C:H2'	2.21	0.41
27:B1:365:A:N6	27:B1:380:U:O4'	2.54	0.41
27:B1:1181:G:O2'	27:B1:1182:C:O5'	2.39	0.41
27:B1:1608:4AC:HM72	27:B1:1621:4AC:HM73	2.03	0.41
27:B1:2186:A:C5	27:B1:2187:C:C6	3.09	0.41
27:B1:2195:A:OP1	65:B1:3180:HOH:O	2.21	0.41
27:B1:2239:G:N3	27:B1:2241:G:O2'	2.54	0.41
32:BD:144:GLU:HB2	32:BD:148:PHE:CD2	2.56	0.41
45:BS:18:ALA:O	45:BS:149:VAL:HG23	2.21	0.41
54:Bb:29:LYS:O	54:Bb:50:ARG:NH1	2.54	0.41
1:A1:1312:C:O2'	9:Ah:94:ASN:OD1	2.27	0.40
22:Au:63:TYR:HD2	22:Au:121:ILE:HD13	1.86	0.40
27:B1:752:U:H2'	27:B1:754:A:OP2	2.21	0.40
27:B1:1796:C:O2	27:B1:2815:U:O2'	2.39	0.40
27:B1:2720:G:C5	27:B1:2721:U:C5	3.09	0.40
41:BO:64:THR:HG21	41:BO:77:CYS:HB3	2.03	0.40
58:Bf:26:TRP:HA	58:Bf:29:VAL:HG22	2.03	0.40
1:A1:172:G:H21	11:Aj:70:GLY:HA3	1.87	0.40
1:A1:675:C:O2'	4:Ac:100:THR:O	2.36	0.40
1:A1:818:U:H2'	1:A1:819:A2M:H8	2.02	0.40
6:Ae:123:LYS:HE3	6:Ae:125:LEU:HD21	2.02	0.40
7:Af:63:GLN:HG2	7:Af:89:VAL:HG23	2.03	0.40
9:Ah:140:MET:O	9:Ah:141:PHE:CD1	2.74	0.40
14:Am:58:TYR:O	14:Am:62:LEU:HD13	2.21	0.40
27:B1:638:G:OP1	34:BG:33:ARG:NH2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BN:88:VAL:HG23	40:BN:89:LYS:N	2.36	0.40
46:BT:13:THR:CG2	46:BT:14:GLU:N	2.83	0.40
1:A1:382:4AC:H6	1:A1:382:4AC:O5'	2.21	0.40
1:A1:896:C:C2	1:A1:897:A:C8	3.10	0.40
14:Am:25:ASN:OD1	14:Am:54:GLU:HB3	2.21	0.40
22:Au:35:VAL:HG12	22:Au:36:LYS:O	2.22	0.40
33:BE:56:TYR:CE2	33:BE:58:ASP:OD1	2.74	0.40
38:BK:49:ASN:OD1	38:BK:50:ILE:N	2.54	0.40
49:BW:10:SER:OG	49:BW:11:ILE:N	2.54	0.40
1:A1:594:G:C2	1:A1:595:A:C5	3.09	0.40
1:A1:962:U:C4'	1:A1:963:G:OP2	2.70	0.40
1:A1:1468:G:OP1	60:Bh:20:LYS:NZ	2.40	0.40
16:Ao:76:ARG:NE	16:Ao:90:ASP:OD2	2.54	0.40
27:B1:104:A:C8	27:B1:105:C:C5	3.10	0.40
27:B1:1281:C:OP2	36:BI:124:SER:OG	2.24	0.40
1:A1:884:G:O2'	1:A1:886:G:OP1	2.35	0.40
1:A1:1123:C:C2	1:A1:1124:C:C5	3.10	0.40
4:Ac:117:LEU:CD2	4:Ac:190:VAL:HG22	2.52	0.40
15:An:14:ARG:NH2	19:Ar:65:LEU:O	2.55	0.40
27:B1:637:G:H2'	27:B1:638:G:O4'	2.21	0.40
27:B1:1306:C:H2'	27:B1:1307:A:H8	1.86	0.40
27:B1:2778:G:H2'	27:B1:2779:A:O4'	2.22	0.40
28:B2:123:C:OP1	41:BO:69:ARG:HD2	2.21	0.40
35:BH:174:THR:HG23	35:BH:175:LYS:N	2.37	0.40
39:BM:14:SER:O	39:BM:15:HIS:HB3	2.22	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	
2	Aa	194/202 (96%)	191 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ab	193/210 (92%)	191 (99%)	2 (1%)	0	100	100
4	Ac	183/198 (92%)	183 (100%)	0	0	100	100
5	Ad	171/180 (95%)	168 (98%)	3 (2%)	0	100	100
6	Ae	240/243 (99%)	232 (97%)	8 (3%)	0	100	100
7	Af	226/236 (96%)	215 (95%)	11 (5%)	0	100	100
8	Ag	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
9	Ah	212/215 (99%)	202 (95%)	10 (5%)	0	100	100
10	Ai	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
11	Aj	123/127 (97%)	120 (98%)	3 (2%)	0	100	100
12	Ak	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
13	Al	97/102 (95%)	94 (97%)	3 (3%)	0	100	100
14	Am	126/137 (92%)	122 (97%)	4 (3%)	0	100	100
15	An	142/147 (97%)	141 (99%)	1 (1%)	0	100	100
16	Ao	135/148 (91%)	131 (97%)	4 (3%)	0	100	100
17	Ap	52/56 (93%)	45 (86%)	7 (14%)	0	100	100
18	Aq	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
19	Ar	105/113 (93%)	104 (99%)	1 (1%)	0	100	100
20	As	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
21	At	120/132 (91%)	119 (99%)	1 (1%)	0	100	100
22	Au	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
23	Av	93/99 (94%)	89 (96%)	4 (4%)	0	100	100
24	Aw	59/63 (94%)	59 (100%)	0	0	100	100
25	Ax	62/71 (87%)	59 (95%)	3 (5%)	0	100	100
26	Ay	54/60 (90%)	53 (98%)	1 (2%)	0	100	100
29	BA	236/239 (99%)	226 (96%)	10 (4%)	0	100	100
30	BB	362/365 (99%)	351 (97%)	11 (3%)	0	100	100
31	BC	253/255 (99%)	247 (98%)	6 (2%)	0	100	100
32	BD	182/186 (98%)	167 (92%)	15 (8%)	0	100	100
33	BE	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
34	BF	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
34	BG	119/123 (97%)	116 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BH	163/181 (90%)	154 (94%)	9 (6%)	0	100	100
36	BI	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
37	BJ	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
38	BK	79/83 (95%)	71 (90%)	8 (10%)	0	100	100
38	BL	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
39	BM	145/147 (99%)	132 (91%)	13 (9%)	0	100	100
40	BN	191/194 (98%)	187 (98%)	4 (2%)	0	100	100
41	BO	194/203 (96%)	190 (98%)	4 (2%)	0	100	100
42	BP	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
43	BQ	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
44	BR	94/97 (97%)	93 (99%)	1 (1%)	0	100	100
45	BS	149/155 (96%)	145 (97%)	4 (3%)	0	100	100
46	BT	84/86 (98%)	84 (100%)	0	0	100	100
47	BU	118/121 (98%)	114 (97%)	4 (3%)	0	100	100
48	BV	61/66 (92%)	61 (100%)	0	0	100	100
49	BW	65/72 (90%)	65 (100%)	0	0	100	100
50	BX	152/155 (98%)	148 (97%)	4 (3%)	0	100	100
51	BY	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
52	BZ	92/95 (97%)	89 (97%)	3 (3%)	0	100	100
53	Ba	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
54	Bb	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
55	Bc	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
56	Bd	59/62 (95%)	55 (93%)	4 (7%)	0	100	100
57	Be	79/83 (95%)	72 (91%)	7 (9%)	0	100	100
58	Bf	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
59	Bg	44/51 (86%)	42 (96%)	2 (4%)	0	100	100
60	Bh	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
61	Bi	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
62	Bj	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
63	Bk	59/64 (92%)	58 (98%)	1 (2%)	0	100	100
All	All	7873/8194 (96%)	7633 (97%)	240 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	Aa	168/173 (97%)	167 (99%)	1 (1%)	84	92
3	Ab	152/167 (91%)	152 (100%)	0	100	100
4	Ac	162/171 (95%)	162 (100%)	0	100	100
5	Ad	156/160 (98%)	156 (100%)	0	100	100
6	Ae	212/213 (100%)	212 (100%)	0	100	100
7	Af	188/197 (95%)	188 (100%)	0	100	100
8	Ag	107/108 (99%)	106 (99%)	1 (1%)	75	88
9	Ah	183/184 (100%)	182 (100%)	1 (0%)	86	94
10	Ai	107/108 (99%)	107 (100%)	0	100	100
11	Aj	100/103 (97%)	100 (100%)	0	100	100
12	Ak	109/111 (98%)	109 (100%)	0	100	100
13	Al	88/91 (97%)	88 (100%)	0	100	100
14	Am	95/104 (91%)	95 (100%)	0	100	100
15	An	117/121 (97%)	117 (100%)	0	100	100
16	Ao	111/122 (91%)	110 (99%)	1 (1%)	75	88
17	Ap	43/46 (94%)	43 (100%)	0	100	100
18	Aq	142/143 (99%)	142 (100%)	0	100	100
19	Ar	96/102 (94%)	96 (100%)	0	100	100
20	As	57/61 (93%)	57 (100%)	0	100	100
21	At	105/114 (92%)	105 (100%)	0	100	100
22	Au	126/127 (99%)	126 (100%)	0	100	100
23	Av	85/89 (96%)	85 (100%)	0	100	100
24	Aw	52/54 (96%)	52 (100%)	0	100	100
25	Ax	54/60 (90%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	Ay	48/53 (91%)	48 (100%)	0	100	100
29	BA	187/189 (99%)	186 (100%)	1 (0%)	86	94
30	BB	310/312 (99%)	310 (100%)	0	100	100
31	BC	213/213 (100%)	212 (100%)	1 (0%)	86	94
32	BD	146/158 (92%)	146 (100%)	0	100	100
33	BE	155/156 (99%)	155 (100%)	0	100	100
34	BF	98/99 (99%)	98 (100%)	0	100	100
34	BG	97/99 (98%)	97 (100%)	0	100	100
35	BH	142/152 (93%)	140 (99%)	2 (1%)	62	82
36	BI	122/122 (100%)	119 (98%)	3 (2%)	42	68
37	BJ	107/108 (99%)	107 (100%)	0	100	100
38	BK	64/66 (97%)	64 (100%)	0	100	100
38	BL	65/66 (98%)	65 (100%)	0	100	100
39	BM	117/117 (100%)	116 (99%)	1 (1%)	75	88
40	BN	161/162 (99%)	161 (100%)	0	100	100
41	BO	157/169 (93%)	157 (100%)	0	100	100
42	BP	101/101 (100%)	101 (100%)	0	100	100
43	BQ	128/130 (98%)	128 (100%)	0	100	100
44	BR	86/87 (99%)	86 (100%)	0	100	100
45	BS	126/130 (97%)	126 (100%)	0	100	100
46	BT	77/77 (100%)	77 (100%)	0	100	100
47	BU	110/110 (100%)	110 (100%)	0	100	100
48	BV	53/56 (95%)	53 (100%)	0	100	100
49	BW	58/66 (88%)	58 (100%)	0	100	100
50	BX	132/133 (99%)	132 (100%)	0	100	100
51	BY	77/80 (96%)	77 (100%)	0	100	100
52	BZ	76/83 (92%)	76 (100%)	0	100	100
53	Ba	113/117 (97%)	113 (100%)	0	100	100
54	Bb	79/81 (98%)	79 (100%)	0	100	100
55	Bc	73/74 (99%)	73 (100%)	0	100	100
56	Bd	49/51 (96%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	Be	59/61 (97%)	59 (100%)	0	100	100
58	Bf	46/47 (98%)	46 (100%)	0	100	100
59	Bg	37/39 (95%)	37 (100%)	0	100	100
60	Bh	34/35 (97%)	34 (100%)	0	100	100
61	Bi	82/83 (99%)	82 (100%)	0	100	100
62	Bj	72/72 (100%)	72 (100%)	0	100	100
63	Bk	52/55 (94%)	52 (100%)	0	100	100
All	All	6724/6938 (97%)	6712 (100%)	12 (0%)	91	97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Aa	24	LYS
8	Ag	46	ASN
9	Ah	94	ASN
16	Ao	116	ARG
29	BA	25	ARG
31	BC	123	ASN
35	BH	60	ASN
35	BH	167	LYS
36	BI	32	ASN
36	BI	125	ARG
36	BI	142	PHE
39	BM	120	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	Ab	148	GLN
4	Ac	133	GLN
32	BD	120	HIS
40	BN	174	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1487/1497 (99%)	238 (16%)	14 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	B1	2928/3051 (95%)	421 (14%)	28 (0%)
28	B2	124/125 (99%)	15 (12%)	0
All	All	4539/4673 (97%)	674 (14%)	42 (0%)

All (674) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	4	C
1	A1	8	OMU
1	A1	17	5MC
1	A1	20	G
1	A1	33	U
1	A1	42	G
1	A1	43	A
1	A1	45	U
1	A1	47	A
1	A1	56	A
1	A1	57	G
1	A1	74	U
1	A1	75	C
1	A1	77	G
1	A1	78	G
1	A1	80	A
1	A1	81	C
1	A1	82	G
1	A1	100	A
1	A1	104	A
1	A1	105	C
1	A1	114	A
1	A1	115	A
1	A1	116	C
1	A1	118	U
1	A1	146	A
1	A1	159	C
1	A1	181	G
1	A1	182	A
1	A1	184	G
1	A1	193	G
1	A1	194	C
1	A1	197	A
1	A1	198	A
1	A1	199	A

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Mol	Chain	Res	Type
1	A1	200	G
1	A1	213	C
1	A1	216	4AC
1	A1	217	G
1	A1	224	G
1	A1	241	U
1	A1	242	U
1	A1	244	G
1	A1	248	G
1	A1	255	G
1	A1	259	A
1	A1	260	A
1	A1	263	G
1	A1	264	C
1	A1	268	C
1	A1	269	C
1	A1	278	G
1	A1	286	C
1	A1	303	A
1	A1	318	A
1	A1	321	G
1	A1	324	A
1	A1	325	C
1	A1	341	A
1	A1	342	C
1	A1	344	G
1	A1	349	C
1	A1	350	A
1	A1	351	G
1	A1	359	G
1	A1	364	C
1	A1	369	C
1	A1	394	A
1	A1	403	G
1	A1	412	C
1	A1	413	U
1	A1	414	G
1	A1	424	U
1	A1	437	A
1	A1	440	G
1	A1	450	U
1	A1	462	A

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Mol	Chain	Res	Type
1	A1	464	G
1	A1	465	G
1	A1	466	5MC
1	A1	472	G
1	A1	475	G
1	A1	481	G7M
1	A1	486	A
1	A1	497	C
1	A1	501	A
1	A1	518	U
1	A1	520	G
1	A1	527	A
1	A1	528	A
1	A1	530	C
1	A1	531	G
1	A1	537	A
1	A1	542	G
1	A1	550	A
1	A1	587	C
1	A1	588	G
1	A1	608	U
1	A1	620	A
1	A1	630	U
1	A1	641	U
1	A1	642	A
1	A1	643	G
1	A1	659	A
1	A1	671	C
1	A1	678	U
1	A1	702	G
1	A1	703	G
1	A1	704	U
1	A1	706	4AC
1	A1	710	G
1	A1	732	A
1	A1	734	C
1	A1	736	A
1	A1	748	U
1	A1	749	A
1	A1	764	G
1	A1	770	A
1	A1	772	G

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Mol	Chain	Res	Type
1	A1	776	G
1	A1	783	A
1	A1	799	U
1	A1	802	A
1	A1	803	G
1	A1	833	OMG
1	A1	861	OMG
1	A1	867	A
1	A1	873	A
1	A1	885	G
1	A1	886	G
1	A1	890	G
1	A1	893	C
1	A1	894	U
1	A1	895	A
1	A1	920	U
1	A1	926	5MU
1	A1	929	A
1	A1	931	G
1	A1	934	G
1	A1	935	G
1	A1	936	G
1	A1	937	A
1	A1	951	5MC
1	A1	956	G
1	A1	960	G
1	A1	962	U
1	A1	963	G
1	A1	969	C
1	A1	978	G
1	A1	979	G
1	A1	984	G
1	A1	987	G
1	A1	988	G
1	A1	989	A
1	A1	990	C
1	A1	992	C
1	A1	993	G
1	A1	994	C
1	A1	1007	C
1	A1	1008	A
1	A1	1012	5MC

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Mol	Chain	Res	Type
1	A1	1016	4AC
1	A1	1018	U
1	A1	1019	C
1	A1	1034	G
1	A1	1047	G
1	A1	1048	U
1	A1	1054	A
1	A1	1055	A
1	A1	1092	4AC
1	A1	1095	U
1	A1	1104	A
1	A1	1108	A
1	A1	1120	C
1	A1	1121	U
1	A1	1130	U
1	A1	1133	G
1	A1	1143	G
1	A1	1147	C
1	A1	1158	A
1	A1	1159	G
1	A1	1163	A
1	A1	1164	G
1	A1	1174	A
1	A1	1175	A
1	A1	1176	A
1	A1	1177	C
1	A1	1189	A
1	A1	1190	5MC
1	A1	1198	A
1	A1	1200	A
1	A1	1201	A
1	A1	1203	G
1	A1	1218	A
1	A1	1220	C
1	A1	1241	A
1	A1	1242	A
1	A1	1249	A
1	A1	1262	G
1	A1	1264	U
1	A1	1267	G
1	A1	1268	A
1	A1	1269	U

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Mol	Chain	Res	Type
1	A1	1270	OMC
1	A1	1282	C
1	A1	1283	U
1	A1	1284	C
1	A1	1289	G
1	A1	1298	U
1	A1	1319	G
1	A1	1326	U
1	A1	1332	G
1	A1	1341	G
1	A1	1344	C
1	A1	1348	5MC
1	A1	1349	U
1	A1	1356	A
1	A1	1359	C
1	A1	1364	LHH
1	A1	1373	C
1	A1	1381	G
1	A1	1412	G
1	A1	1432	G
1	A1	1439	G
1	A1	1444	G
1	A1	1448	G
1	A1	1449	A
1	A1	1450	A
1	A1	1451	G
1	A1	1456	A
1	A1	1459	A
1	A1	1461	G
1	A1	1462	G
1	A1	1463	U
1	A1	1474	G
1	A1	1476	MA6
1	A1	1486	5MC
1	A1	1487	G
27	B1	14	U
27	B1	15	A
27	B1	47	5MC
27	B1	65	A
27	B1	70	C
27	B1	72	A
27	B1	75	A

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Mol	Chain	Res	Type
27	B1	76	G
27	B1	92	G
27	B1	96	G
27	B1	100	U
27	B1	101	C
27	B1	118	A
27	B1	120	U
27	B1	121	G
27	B1	124	A
27	B1	125	C
27	B1	127	U
27	B1	137	U
27	B1	138	A
27	B1	140	G
27	B1	141	C
27	B1	147	U
27	B1	155	U
27	B1	158	U
27	B1	171	A
27	B1	186	A
27	B1	189	A
27	B1	205	G
27	B1	206	A
27	B1	212	A
27	B1	215	C
27	B1	218	A
27	B1	219	A
27	B1	220	G
27	B1	223	A
27	B1	238	G
27	B1	255	A
27	B1	256	G
27	B1	275	5MC
27	B1	276	4AC
27	B1	279	C
27	B1	294	G
27	B1	302	G
27	B1	304	A
27	B1	312	C
27	B1	316	U
27	B1	333	A
27	B1	335	G

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Mol	Chain	Res	Type
27	B1	342	U
27	B1	343	C
27	B1	346	C
27	B1	352	C
27	B1	362	G
27	B1	364	G
27	B1	370	G
27	B1	371	A
27	B1	392	4AC
27	B1	403	G
27	B1	408	A
27	B1	415	G
27	B1	431	A
27	B1	441	A
27	B1	451	G
27	B1	470	A
27	B1	497	A
27	B1	507	G
27	B1	521	G
27	B1	524	C
27	B1	543	A
27	B1	547	C
27	B1	567	G
27	B1	569	A
27	B1	570	G
27	B1	571	G
27	B1	575	C
27	B1	582	A
27	B1	585	G
27	B1	590	G
27	B1	617	C
27	B1	624	G
27	B1	641	LHH
27	B1	655	C
27	B1	667	A
27	B1	671	G
27	B1	678	A
27	B1	679	G
27	B1	695	A
27	B1	735	C
27	B1	737	U
27	B1	778	A

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Mol	Chain	Res	Type
27	B1	782	C
27	B1	788	G
27	B1	809	A
27	B1	810	A
27	B1	813	4AC
27	B1	820	U
27	B1	830	G
27	B1	843	C
27	B1	850	C
27	B1	852	G
27	B1	857	A2M
27	B1	860	G
27	B1	864	C
27	B1	878	U
27	B1	883	U
27	B1	888	U
27	B1	904	LHH
27	B1	911	G
27	B1	912	G
27	B1	918	A
27	B1	920	OMG
27	B1	921	OMG
27	B1	925	A
27	B1	928	G
27	B1	933	4AC
27	B1	941	G
27	B1	948	C
27	B1	958	C
27	B1	964	G
27	B1	966	A
27	B1	980	G
27	B1	981	G
27	B1	982	A
27	B1	983	G
27	B1	996	G
27	B1	1003	A
27	B1	1016	G
27	B1	1017	C
27	B1	1018	A
27	B1	1019	G
27	B1	1020	G
27	B1	1022	G

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Mol	Chain	Res	Type
27	B1	1024	C
27	B1	1027	A
27	B1	1028	A
27	B1	1030	C
27	B1	1031	C
27	B1	1033	C
27	B1	1047	A
27	B1	1049	C
27	B1	1084	G
27	B1	1085	G
27	B1	1110	G
27	B1	1119	A
27	B1	1120	A
27	B1	1125	G
27	B1	1126	A
27	B1	1127	C
27	B1	1137	G
27	B1	1146	G
27	B1	1147	U
27	B1	1148	G
27	B1	1167	A
27	B1	1173	U
27	B1	1174	G
27	B1	1178	4AC
27	B1	1182	C
27	B1	1186	A
27	B1	1187	G
27	B1	1249	C
27	B1	1250	G
27	B1	1251	A
27	B1	1252	G
27	B1	1274	C
27	B1	1275	G
27	B1	1278	G
27	B1	1314	G
27	B1	1315	A
27	B1	1316	U
27	B1	1317	U
27	B1	1326	A
27	B1	1328	C
27	B1	1369	A
27	B1	1370	G

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Mol	Chain	Res	Type
27	B1	1379	G
27	B1	1381	G
27	B1	1383	4AC
27	B1	1389	U
27	B1	1392	C
27	B1	1395	G
27	B1	1396	G
27	B1	1399	C
27	B1	1416	C
27	B1	1417	G
27	B1	1445	A
27	B1	1450	C
27	B1	1451	5MC
27	B1	1479	G
27	B1	1489	OMC
27	B1	1515	C
27	B1	1523	A
27	B1	1529	A
27	B1	1532	C
27	B1	1541	A
27	B1	1574	A
27	B1	1576	G
27	B1	1590	G
27	B1	1600	A
27	B1	1617	A
27	B1	1639	4AC
27	B1	1643	G
27	B1	1644	A
27	B1	1645	G
27	B1	1646	U
27	B1	1647	G
27	B1	1658	G
27	B1	1659	A
27	B1	1666	G
27	B1	1669	G
27	B1	1670	A
27	B1	1679	A
27	B1	1680	U
27	B1	1690	G
27	B1	1697	G
27	B1	1699	G
27	B1	1700	U

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Mol	Chain	Res	Type
27	B1	1701	U
27	B1	1703	4AC
27	B1	1708	A
27	B1	1710	C
27	B1	1715	G
27	B1	1721	G
27	B1	1723	G
27	B1	1724	A
27	B1	1725	A
27	B1	1735	G
27	B1	1742	C
27	B1	1747	C
27	B1	1749	C
27	B1	1755	A
27	B1	1767	A
27	B1	1773	A
27	B1	1774	C
27	B1	1775	A
27	B1	1779	G
27	B1	1780	C
27	B1	1781	C
27	B1	1785	G
27	B1	1789	G
27	B1	1791	G
27	B1	1792	A
27	B1	1804	U
27	B1	1805	G
27	B1	1806	U
27	B1	1807	C
27	B1	1812	G
27	B1	1813	A
27	B1	1814	A
27	B1	1818	4AC
27	B1	1834	G
27	B1	1836	A
27	B1	1856	G
27	B1	1860	A
27	B1	1881	A
27	B1	1904	G
27	B1	1913	A
27	B1	1920	A
27	B1	1931	A

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Mol	Chain	Res	Type
27	B1	1940	C
27	B1	1965	OMG
27	B1	1966	5MC
27	B1	1969	A
27	B1	2003	A
27	B1	2017	C
27	B1	2026	A
27	B1	2031	G
27	B1	2033	G
27	B1	2037	A
27	B1	2039	C
27	B1	2040	U
27	B1	2042	U
27	B1	2043	A
27	B1	2045	C
27	B1	2050	U
27	B1	2051	U
27	B1	2053	A
27	B1	2055	G
27	B1	2056	U
27	B1	2057	A2M
27	B1	2061	A
27	B1	2062	A
27	B1	2063	A
27	B1	2066	C
27	B1	2080	U
27	B1	2089	G
27	B1	2092	U
27	B1	2096	U
27	B1	2097	G
27	B1	2116	U
27	B1	2118	U
27	B1	2150	G
27	B1	2151	G
27	B1	2155	G
27	B1	2156	C
27	B1	2157	A
27	B1	2174	U
27	B1	2179	A
27	B1	2180	OMG
27	B1	2183	A
27	B1	2185	G

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Mol	Chain	Res	Type
27	B1	2193	G
27	B1	2217	G
27	B1	2220	A
27	B1	2226	C
27	B1	2229	G
27	B1	2234	G
27	B1	2235	C
27	B1	2236	G
27	B1	2238	A
27	B1	2239	G
27	B1	2240	C
27	B1	2241	G
27	B1	2242	U
27	B1	2246	C
27	B1	2250	A
27	B1	2252	G
27	B1	2255	U
27	B1	2257	G
27	B1	2260	G
27	B1	2269	C
27	B1	2281	G
27	B1	2287	U
27	B1	2289	C
27	B1	2290	A
27	B1	2294	G
27	B1	2295	A
27	B1	2296	C
27	B1	2297	A
27	B1	2302	C
27	B1	2314	G
27	B1	2322	A
27	B1	2326	C
27	B1	2331	A
27	B1	2339	A
27	B1	2352	G
27	B1	2353	G
27	B1	2365	OMG
27	B1	2372	A
27	B1	2381	A
27	B1	2394	G
27	B1	2398	C
27	B1	2401	OMU

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Mol	Chain	Res	Type
27	B1	2402	A
27	B1	2420	U
27	B1	2423	G
27	B1	2435	A
27	B1	2437	A
27	B1	2442	A
27	B1	2447	C
27	B1	2448	A
27	B1	2450	A
27	B1	2459	U
27	B1	2460	G
27	B1	2472	A
27	B1	2478	G
27	B1	2501	G
27	B1	2503	C
27	B1	2510	A
27	B1	2519	G
27	B1	2520	C
27	B1	2543	G
27	B1	2545	C
27	B1	2546	A
27	B1	2547	G
27	B1	2548	A
27	B1	2557	OMC
27	B1	2564	A
27	B1	2591	C
27	B1	2592	A
27	B1	2594	A
27	B1	2607	OMC
27	B1	2614	C
27	B1	2618	G
27	B1	2619	C
27	B1	2634	A
27	B1	2645	G
27	B1	2650	A
27	B1	2682	A
27	B1	2683	G
27	B1	2689	C
27	B1	2694	G
27	B1	2698	G
27	B1	2715	G
27	B1	2718	A

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Mol	Chain	Res	Type
27	B1	2719	G
27	B1	2729	U
27	B1	2737	G
27	B1	2745	U
27	B1	2746	G
27	B1	2761	A
27	B1	2762	G
27	B1	2806	U
27	B1	2827	U
27	B1	2828	C
27	B1	2841	C
27	B1	2848	G
27	B1	2849	C
27	B1	2850	4AC
27	B1	2862	A
27	B1	2871	A
27	B1	2879	A
27	B1	2880	G
27	B1	2890	A
27	B1	2891	A
27	B1	2893	A
27	B1	2894	U
27	B1	2895	A
27	B1	2902	4AC
27	B1	2949	A
27	B1	2959	U
27	B1	2972	U
27	B1	2998	G
27	B1	3001	U
27	B1	3002	C
27	B1	3003	A
27	B1	3021	G
27	B1	3022	C
27	B1	3028	C
27	B1	3031	A
27	B1	3037	4AC
28	B2	2	G
28	B2	5	C
28	B2	9	G
28	B2	13	A
28	B2	25	C
28	B2	41	U

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Mol	Chain	Res	Type
28	B2	46	A
28	B2	53	A
28	B2	56	U
28	B2	89	C
28	B2	92	A
28	B2	95	G
28	B2	115	G
28	B2	117	4AC
28	B2	121	G

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A1	99	C
1	A1	117	OMC
1	A1	197	A
1	A1	268	C
1	A1	496	G
1	A1	962	U
1	A1	1018	U
1	A1	1054	A
1	A1	1107	C
1	A1	1146	G
1	A1	1163	A
1	A1	1348	5MC
1	A1	1438	U
1	A1	1462	G
27	B1	100	U
27	B1	120	U
27	B1	126	C
27	B1	146	C
27	B1	311	C
27	B1	315	A
27	B1	342	U
27	B1	542	A
27	B1	841	OMG
27	B1	877	5MC
27	B1	920	OMG
27	B1	980	G
27	B1	982	A
27	B1	1181	G
27	B1	1186	A

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Mol	Chain	Res	Type
27	B1	1368	A
27	B1	1394	C
27	B1	1696	G
27	B1	1914	OMC
27	B1	1965	OMG
27	B1	2036	U
27	B1	2052	A
27	B1	2173	G
27	B1	2251	G
27	B1	2325	C
27	B1	2590	C
27	B1	2870	U
27	B1	2893	A

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

316 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
1	MA6	A1	1457	1	18,26,27	1.03	1 (5%)	19,38,41	4.46	3 (15%)
1	5MC	A1	273	1	18,22,23	3.15	7 (38%)	26,32,35	1.01	1 (3%)
1	OMC	A1	1252	1	19,22,23	3.11	8 (42%)	26,31,34	0.70	0
27	4AC	B1	1313	27	21,24,25	3.25	10 (47%)	29,34,37	1.08	4 (13%)
1	5MC	A1	1015	1	18,22,23	3.17	7 (38%)	26,32,35	0.99	2 (7%)
1	OMG	A1	455	1	18,26,27	2.59	8 (44%)	19,38,41	1.52	4 (21%)
27	4AC	B1	2020	27	21,24,25	3.25	9 (42%)	29,34,37	1.01	4 (13%)
1	4AC	A1	195	1	21,24,25	3.31	10 (47%)	29,34,37	1.10	4 (13%)
27	5MC	B1	1451	27	18,22,23	3.11	7 (38%)	26,32,35	1.05	2 (7%)
27	5MC	B1	275	27	18,22,23	3.18	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	1706	27	21,24,25	3.25	10 (47%)	29,34,37	1.06	4 (13%)
27	OMG	B1	2562	27	18,26,27	2.53	8 (44%)	19,38,41	1.54	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	A1	901	1	18,26,27	2.60	8 (44%)	19,38,41	1.53	4 (21%)
1	5MC	A1	1190	1	18,22,23	3.16	7 (38%)	26,32,35	0.97	2 (7%)
27	4AC	B1	2809	27	21,24,25	3.20	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	933	27	21,24,25	3.11	10 (47%)	29,34,37	1.38	4 (13%)
1	OMG	A1	459	1	18,26,27	2.57	8 (44%)	19,38,41	1.50	4 (21%)
27	4AC	B1	80	27	21,24,25	3.23	10 (47%)	29,34,37	1.03	4 (13%)
27	OMG	B1	808	27	18,26,27	2.54	8 (44%)	19,38,41	1.53	4 (21%)
27	A2M	B1	857	27	18,25,26	4.19	7 (38%)	18,36,39	2.26	4 (22%)
27	4AC	B1	1751	27	21,24,25	3.23	10 (47%)	29,34,37	1.03	4 (13%)
27	5MC	B1	1149	27	18,22,23	3.10	7 (38%)	26,32,35	0.99	2 (7%)
1	4AC	A1	231	1	21,24,25	3.23	10 (47%)	29,34,37	1.03	4 (13%)
1	5MC	A1	1486	1	18,22,23	3.15	7 (38%)	26,32,35	1.04	2 (7%)
27	4AC	B1	3037	27	21,24,25	3.27	10 (47%)	29,34,37	1.49	7 (24%)
27	4AC	B1	1293	27	21,24,25	3.23	10 (47%)	29,34,37	1.02	4 (13%)
27	OMG	B1	2740	27	18,26,27	2.58	8 (44%)	19,38,41	1.54	4 (21%)
27	5MC	B1	877	27	18,22,23	3.12	7 (38%)	26,32,35	1.02	2 (7%)
27	4AC	B1	1649	27	21,24,25	3.22	10 (47%)	29,34,37	1.04	4 (13%)
1	OMU	A1	762	1	19,22,23	3.26	7 (36%)	26,31,34	2.03	7 (26%)
27	4AC	B1	378	27	21,24,25	3.40	10 (47%)	29,34,37	1.20	4 (13%)
27	OMG	B1	2365	27	18,26,27	2.56	8 (44%)	19,38,41	1.50	4 (21%)
27	4AC	B1	813	27	21,24,25	3.26	10 (47%)	29,34,37	1.32	5 (17%)
27	4AC	B1	1762	27	21,24,25	3.20	10 (47%)	29,34,37	1.06	4 (13%)
27	5MC	B1	2082	27	18,22,23	3.11	7 (38%)	26,32,35	0.96	1 (3%)
27	4AC	B1	479	27	21,24,25	3.22	10 (47%)	29,34,37	1.01	3 (10%)
27	4AC	B1	1383	27	21,24,25	3.20	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	2171	27	21,24,25	3.20	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	1290	27	21,24,25	3.21	10 (47%)	29,34,37	1.03	4 (13%)
1	5MC	A1	1362	1	18,22,23	3.18	7 (38%)	26,32,35	1.02	2 (7%)
1	4AC	A1	1067	1	21,24,25	3.26	10 (47%)	29,34,37	1.07	4 (13%)
1	4AC	A1	827	1	21,24,25	3.25	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	1150	27	21,24,25	3.23	10 (47%)	29,34,37	1.26	5 (17%)
27	4AC	B1	896	27	21,24,25	3.25	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	392	27	21,24,25	3.25	10 (47%)	29,34,37	1.06	4 (13%)
1	5MC	A1	523	1	18,22,23	3.14	7 (38%)	26,32,35	0.97	2 (7%)
1	OMG	A1	833	1	18,26,27	2.58	8 (44%)	19,38,41	1.50	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	2133	27	21,24,25	3.19	10 (47%)	29,34,37	1.02	4 (13%)
1	4AC	A1	1314	1	21,24,25	3.26	10 (47%)	29,34,37	1.36	6 (20%)
27	4AC	B1	2469	27	21,24,25	3.21	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	715	27	21,24,25	3.24	10 (47%)	29,34,37	1.05	4 (13%)
28	4AC	B2	117	28	21,24,25	3.24	10 (47%)	29,34,37	1.01	4 (13%)
1	4AC	A1	636	1	21,24,25	3.27	10 (47%)	29,34,37	1.07	4 (13%)
27	OMC	B1	2808	27	19,22,23	3.09	8 (42%)	26,31,34	0.74	0
27	5MC	B1	2453	27	18,22,23	3.16	7 (38%)	26,32,35	0.97	2 (7%)
27	4AC	B1	1612	27	21,24,25	3.29	10 (47%)	29,34,37	1.06	4 (13%)
1	OMC	A1	834	1	19,22,23	3.09	8 (42%)	26,31,34	0.72	0
27	4AC	B1	1374	27	21,24,25	3.23	10 (47%)	29,34,37	1.20	5 (17%)
1	MA6	A1	1476	1	18,26,27	1.03	1 (5%)	19,38,41	4.36	3 (15%)
27	4AC	B1	599	27	21,24,25	3.22	10 (47%)	29,34,37	1.03	4 (13%)
27	OMC	B1	1783	27	19,22,23	3.08	8 (42%)	26,31,34	0.71	0
27	5MC	B1	97	27	18,22,23	3.14	7 (38%)	26,32,35	0.98	2 (7%)
1	OMC	A1	1194	1	19,22,23	3.12	8 (42%)	26,31,34	0.70	0
1	5MC	A1	230	1	18,22,23	3.14	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	48	27	21,24,25	3.18	10 (47%)	29,34,37	0.97	2 (6%)
27	OMG	B1	2028	27	18,26,27	2.54	8 (44%)	19,38,41	1.49	4 (21%)
1	OMG	A1	329	1	18,26,27	2.60	8 (44%)	19,38,41	1.58	4 (21%)
27	4AC	B1	1107	27	21,24,25	3.20	10 (47%)	29,34,37	1.00	4 (13%)
1	OMG	A1	1003	1	18,26,27	2.60	8 (44%)	19,38,41	1.51	4 (21%)
27	OMC	B1	1489	27	19,22,23	3.10	8 (42%)	26,31,34	0.69	0
27	4AC	B1	786	27	21,24,25	3.22	10 (47%)	29,34,37	1.03	4 (13%)
1	4AC	A1	87	1	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)
1	4AC	A1	1227	1	21,24,25	3.24	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1435	27	21,24,25	3.22	10 (47%)	29,34,37	1.06	4 (13%)
27	5MC	B1	1620	27	18,22,23	3.15	7 (38%)	26,32,35	0.96	1 (3%)
1	5MC	A1	826	1	18,22,23	3.16	7 (38%)	26,32,35	0.99	2 (7%)
1	4AC	A1	624	1	21,24,25	3.27	10 (47%)	29,34,37	1.16	4 (13%)
1	4AC	A1	691	1	21,24,25	3.21	10 (47%)	29,34,37	1.05	4 (13%)
27	OMC	B1	1832	27	19,22,23	3.12	8 (42%)	26,31,34	0.73	0
28	4AC	B2	90	28	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
27	OMG	B1	1601	27	18,26,27	2.56	8 (44%)	19,38,41	1.55	4 (21%)
27	5MC	B1	18	27	18,22,23	3.13	7 (38%)	26,32,35	1.01	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	3020	27	21,24,25	3.23	10 (47%)	29,34,37	1.03	4 (13%)
1	4AC	A1	836	1	21,24,25	3.25	10 (47%)	29,34,37	1.03	3 (10%)
27	4AC	B1	1639	27	21,24,25	3.27	9 (42%)	29,34,37	1.10	4 (13%)
27	4AC	B1	866	27	21,24,25	3.23	10 (47%)	29,34,37	1.02	4 (13%)
27	A2M	B1	2057	27	18,25,26	4.24	8 (44%)	18,36,39	2.27	4 (22%)
27	5MC	B1	932	27	18,22,23	3.11	7 (38%)	26,32,35	0.98	2 (7%)
1	4AC	A1	1181	1	21,24,25	3.23	10 (47%)	29,34,37	1.05	4 (13%)
27	OMC	B1	1099	27	19,22,23	3.07	8 (42%)	26,31,34	0.69	0
27	4AC	B1	2888	27	21,24,25	3.22	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	142	27	21,24,25	3.30	10 (47%)	29,34,37	1.07	4 (13%)
27	OMU	B1	2554	27	19,22,23	3.25	7 (36%)	26,31,34	1.69	5 (19%)
27	OMG	B1	921	27	18,26,27	2.53	8 (44%)	19,38,41	1.51	4 (21%)
27	OMU	B1	1981	27	19,22,23	3.28	7 (36%)	26,31,34	1.71	5 (19%)
27	4AC	B1	1551	27	21,24,25	3.21	10 (47%)	29,34,37	0.99	4 (13%)
27	OMC	B1	2735	27	19,22,23	3.09	8 (42%)	26,31,34	0.73	0
1	OMU	A1	8	1	19,22,23	3.27	7 (36%)	26,31,34	1.71	5 (19%)
27	4AC	B1	950	27	21,24,25	3.21	10 (47%)	29,34,37	1.02	4 (13%)
1	4AC	A1	719	1	21,24,25	3.23	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	1404	27	21,24,25	3.17	10 (47%)	29,34,37	1.21	6 (20%)
1	5MC	A1	533	1	18,22,23	3.14	7 (38%)	26,32,35	0.97	2 (7%)
1	LHH	A1	1364	1	22,25,26	2.94	5 (22%)	29,35,38	1.60	4 (13%)
27	OMG	B1	1557	27	18,26,27	2.58	8 (44%)	19,38,41	1.51	4 (21%)
1	LHH	A1	238	1	22,25,26	2.89	6 (27%)	29,35,38	1.51	3 (10%)
1	5MC	A1	863	1	18,22,23	3.15	7 (38%)	26,32,35	0.99	2 (7%)
1	4AC	A1	1016	1	21,24,25	3.27	10 (47%)	29,34,37	1.07	4 (13%)
1	4AC	A1	220	1	21,24,25	3.25	10 (47%)	29,34,37	1.06	4 (13%)
1	4AC	A1	1029	1	21,24,25	3.30	9 (42%)	29,34,37	1.48	5 (17%)
27	5MC	B1	2087	27	18,22,23	3.13	7 (38%)	26,32,35	0.99	2 (7%)
1	5MC	A1	1012	1	18,22,23	3.18	7 (38%)	26,32,35	1.00	2 (7%)
27	OMG	B1	1533	27	18,26,27	2.53	8 (44%)	19,38,41	1.46	4 (21%)
27	5MC	B1	1977	27	18,22,23	3.14	7 (38%)	26,32,35	0.97	2 (7%)
27	4SU	B1	2565	27	18,21,22	3.83	8 (44%)	26,30,33	2.22	5 (19%)
1	4AC	A1	367	1	21,24,25	3.25	10 (47%)	29,34,37	1.06	4 (13%)
27	LHH	B1	2968	27	22,25,26	2.85	5 (22%)	29,35,38	1.51	3 (10%)
27	OMC	B1	977	27	19,22,23	3.07	8 (42%)	26,31,34	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	1100	27	21,24,25	3.22	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	2844	27	21,24,25	3.20	10 (47%)	29,34,37	1.01	4 (13%)
27	LHH	B1	641	27	22,25,26	2.91	6 (27%)	29,35,38	1.37	2 (6%)
27	4AC	B1	1439	27	21,24,25	3.23	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	2492	27	21,24,25	3.20	10 (47%)	29,34,37	1.40	6 (20%)
27	OMG	B1	2984	27	18,26,27	2.57	8 (44%)	19,38,41	1.56	5 (26%)
27	4AC	B1	337	27	21,24,25	3.20	10 (47%)	29,34,37	1.11	2 (6%)
1	OMG	A1	228	1	18,26,27	2.56	8 (44%)	19,38,41	1.53	4 (21%)
27	4AC	B1	2902	27	21,24,25	0.39	0	29,34,37	0.58	0
1	4AC	A1	1254	1	21,24,25	3.25	10 (47%)	29,34,37	1.09	4 (13%)
27	4AC	B1	1734	27	21,24,25	3.26	9 (42%)	29,34,37	1.10	4 (13%)
27	4AC	B1	271	27	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)
1	5MC	A1	718	1	18,22,23	3.14	7 (38%)	26,32,35	0.98	1 (3%)
1	5MU	A1	926	1	19,22,23	0.24	0	28,32,35	0.33	0
27	LHH	B1	1365	27	22,25,26	2.89	6 (27%)	29,35,38	1.44	3 (10%)
27	4AC	B1	2454	27	21,24,25	3.25	10 (47%)	29,34,37	1.04	4 (13%)
27	5MC	B1	1966	27	18,22,23	3.11	7 (38%)	26,32,35	1.01	2 (7%)
1	4AC	A1	405	1	21,24,25	3.27	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	2526	27	21,24,25	3.23	10 (47%)	29,34,37	1.05	4 (13%)
1	5MC	A1	1484	1	18,22,23	3.12	7 (38%)	26,32,35	0.95	1 (3%)
27	A2M	B1	262	27	18,25,26	0.65	1 (5%)	18,36,39	0.82	1 (5%)
27	4AC	B1	2850	27	21,24,25	3.23	10 (47%)	29,34,37	1.07	4 (13%)
27	LHH	B1	904	27	22,25,26	2.92	6 (27%)	29,35,38	1.39	2 (6%)
1	4SU	A1	756	1	18,21,22	3.85	8 (44%)	26,30,33	2.19	5 (19%)
27	4AC	B1	1911	27	21,24,25	3.23	10 (47%)	29,34,37	1.02	3 (10%)
27	4AC	B1	1769	27	21,24,25	3.17	10 (47%)	29,34,37	1.03	3 (10%)
27	4AC	B1	116	27	21,24,25	3.19	10 (47%)	29,34,37	1.01	4 (13%)
27	4AC	B1	1064	27	21,24,25	3.25	10 (47%)	29,34,37	1.47	5 (17%)
27	4AC	B1	2379	27	21,24,25	3.18	10 (47%)	29,34,37	1.07	3 (10%)
1	4AC	A1	274	1	21,24,25	3.23	10 (47%)	29,34,37	1.03	4 (13%)
27	OMC	B1	2119	27	19,22,23	3.08	8 (42%)	26,31,34	0.73	0
1	5MC	A1	681	1	18,22,23	3.14	7 (38%)	26,32,35	1.00	2 (7%)
27	4AC	B1	1501	27	21,24,25	3.20	10 (47%)	29,34,37	1.01	4 (13%)
27	4AC	B1	1608	27	21,24,25	3.25	10 (47%)	29,34,37	1.26	5 (17%)
27	OMG	B1	2757	27	18,26,27	2.56	8 (44%)	19,38,41	1.58	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	1822	27	21,24,25	3.20	10 (47%)	29,34,37	1.24	6 (20%)
27	4AC	B1	360	27	21,24,25	3.25	10 (47%)	29,34,37	1.24	6 (20%)
1	A2M	A1	361	1	18,25,26	4.21	7 (38%)	18,36,39	2.30	4 (22%)
27	4AC	B1	276	27	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	2876	27	21,24,25	3.24	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1386	27	21,24,25	3.21	10 (47%)	29,34,37	1.00	3 (10%)
1	OMU	A1	425	1	19,22,23	3.24	7 (36%)	26,31,34	1.71	5 (19%)
1	4AC	A1	578	1	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
1	4AC	A1	427	1	21,24,25	3.31	9 (42%)	29,34,37	1.17	4 (13%)
27	OMG	B1	675	27	18,26,27	2.55	8 (44%)	19,38,41	1.55	5 (26%)
1	4AC	A1	706	1	21,24,25	3.24	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	3011	27	21,24,25	3.19	10 (47%)	29,34,37	1.01	4 (13%)
27	4AC	B1	721	27	21,24,25	3.23	10 (47%)	29,34,37	1.07	4 (13%)
27	OMU	B1	2668	27	19,22,23	3.26	7 (36%)	26,31,34	1.69	5 (19%)
1	4AC	A1	534	1	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	759	27	21,24,25	3.26	10 (47%)	29,34,37	1.07	4 (13%)
27	OMU	B1	454	27	19,22,23	3.28	7 (36%)	26,31,34	1.68	5 (19%)
1	OMU	A1	1368	1	19,22,23	3.26	7 (36%)	26,31,34	1.71	5 (19%)
1	4AC	A1	540	1	21,24,25	3.25	10 (47%)	29,34,37	1.05	4 (13%)
1	OMG	A1	153	1	18,26,27	2.60	8 (44%)	19,38,41	1.50	4 (21%)
27	OMG	B1	2180	27	18,26,27	2.55	8 (44%)	19,38,41	1.53	4 (21%)
27	4AC	B1	741	27	21,24,25	3.26	10 (47%)	29,34,37	1.09	4 (13%)
1	5MC	A1	1348	1	18,22,23	3.16	7 (38%)	26,32,35	1.44	4 (15%)
1	OMG	A1	763	1	18,26,27	2.58	8 (44%)	19,38,41	1.51	4 (21%)
27	OMC	B1	2059	27	19,22,23	3.11	8 (42%)	26,31,34	0.77	0
27	5MC	B1	359	27	18,22,23	3.13	7 (38%)	26,32,35	1.01	2 (7%)
1	4AC	A1	739	1	21,24,25	3.27	10 (47%)	29,34,37	1.08	4 (13%)
1	4AC	A1	1135	1	21,24,25	3.29	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	1546	27	21,24,25	3.22	10 (47%)	29,34,37	1.02	4 (13%)
27	OMG	B1	2659	27	18,26,27	2.57	8 (44%)	19,38,41	1.56	4 (21%)
1	OMC	A1	1270	1	19,22,23	3.11	8 (42%)	26,31,34	0.73	0
27	4AC	B1	23	27	21,24,25	3.21	10 (47%)	29,34,37	1.06	4 (13%)
27	OMU	B1	2401	27	19,22,23	3.28	7 (36%)	26,31,34	1.71	5 (19%)
27	4AC	B1	130	27	21,24,25	3.24	10 (47%)	29,34,37	1.43	6 (20%)
27	4AC	B1	2328	27	21,24,25	3.23	10 (47%)	29,34,37	1.01	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A1	1004	1	18,26,27	2.52	7 (38%)	16,38,41	1.41	3 (18%)
27	OMG	B1	2022	27	18,26,27	2.54	8 (44%)	19,38,41	1.46	4 (21%)
27	LHH	B1	1946	27	22,25,26	2.85	6 (27%)	29,35,38	1.34	3 (10%)
27	5MC	B1	2617	27	18,22,23	3.12	7 (38%)	26,32,35	1.05	2 (7%)
27	4AC	B1	1743	27	21,24,25	3.26	10 (47%)	29,34,37	1.06	4 (13%)
1	5MC	A1	466	1	18,22,23	3.17	7 (38%)	26,32,35	0.99	2 (7%)
1	4AC	A1	291	1	21,24,25	3.22	10 (47%)	29,34,37	1.23	6 (20%)
27	5MC	B1	1983	27	18,22,23	3.11	7 (38%)	26,32,35	0.92	1 (3%)
27	4AC	B1	2749	27	21,24,25	3.22	10 (47%)	29,34,37	1.31	6 (20%)
27	4AC	B1	1967	27	21,24,25	3.18	10 (47%)	29,34,37	0.99	2 (6%)
27	4AC	B1	485	27	21,24,25	3.20	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	243	27	21,24,25	3.23	10 (47%)	29,34,37	1.08	4 (13%)
27	OMG	B1	1965	27	18,26,27	2.57	8 (44%)	19,38,41	1.98	6 (31%)
27	4AC	B1	200	27	21,24,25	3.20	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	2213	27	21,24,25	3.19	10 (47%)	29,34,37	1.04	4 (13%)
27	OMU	B1	2593	27	19,22,23	3.26	7 (36%)	26,31,34	1.64	4 (15%)
1	G7M	A1	481	1	20,26,27	4.07	10 (50%)	17,39,42	0.97	1 (5%)
27	4AC	B1	2792	27	21,24,25	3.22	10 (47%)	29,34,37	1.04	4 (13%)
1	4AC	A1	307	1	21,24,25	3.22	10 (47%)	29,34,37	1.07	4 (13%)
1	4AC	A1	499	1	21,24,25	3.24	9 (42%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1505	27	21,24,25	3.19	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	1286	27	21,24,25	3.19	10 (47%)	29,34,37	1.14	4 (13%)
1	OMG	A1	645	1	18,26,27	2.58	8 (44%)	19,38,41	1.47	4 (21%)
27	4AC	B1	953	27	21,24,25	3.21	10 (47%)	29,34,37	1.04	4 (13%)
1	5MC	A1	951	1	18,22,23	3.15	7 (38%)	26,32,35	1.00	2 (7%)
27	4AC	B1	1178	27	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)
1	4AC	A1	467	1	21,24,25	3.28	10 (47%)	29,34,37	1.08	4 (13%)
27	OMG	B1	2540	27	18,26,27	2.56	8 (44%)	19,38,41	1.48	4 (21%)
27	4AC	B1	2429	27	21,24,25	3.26	10 (47%)	29,34,37	1.06	4 (13%)
1	OMC	A1	117	1	19,22,23	3.11	8 (42%)	26,31,34	0.93	1 (3%)
27	A2M	B1	880	27	18,25,26	4.14	6 (33%)	18,36,39	2.45	5 (27%)
27	4AC	B1	2432	27	21,24,25	3.23	10 (47%)	29,34,37	1.03	4 (13%)
27	5MC	B1	1868	27	18,22,23	3.12	7 (38%)	26,32,35	0.97	1 (3%)
1	4AC	A1	41	1	21,24,25	3.23	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	580	27	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	1128	27	21,24,25	3.18	10 (47%)	29,34,37	1.00	4 (13%)
27	OMC	B1	2428	27	19,22,23	3.15	8 (42%)	26,31,34	1.02	2 (7%)
1	OMG	A1	668	1	18,26,27	2.56	8 (44%)	19,38,41	1.49	4 (21%)
27	OMG	B1	920	27	18,26,27	2.57	8 (44%)	19,38,41	1.53	4 (21%)
27	5MC	B1	2067	27	18,22,23	3.15	7 (38%)	26,32,35	1.44	5 (19%)
27	4AC	B1	1703	27	21,24,25	3.26	10 (47%)	29,34,37	1.06	4 (13%)
27	OMC	B1	501	27	19,22,23	3.07	8 (42%)	26,31,34	0.74	0
27	4AC	B1	1264	27	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
1	4AC	A1	839	1	21,24,25	3.23	10 (47%)	29,34,37	1.06	4 (13%)
27	A2M	B1	506	27	18,25,26	4.20	7 (38%)	18,36,39	2.25	4 (22%)
27	4AC	B1	1067	27	21,24,25	3.23	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	2113	27	21,24,25	3.18	10 (47%)	29,34,37	1.26	6 (20%)
1	OMU	A1	52	1	19,22,23	3.29	7 (36%)	26,31,34	1.70	5 (19%)
1	4AC	A1	141	1	21,24,25	3.30	9 (42%)	29,34,37	1.12	4 (13%)
27	4AC	B1	98	27	21,24,25	3.21	10 (47%)	29,34,37	1.01	4 (13%)
27	4AC	B1	798	27	21,24,25	3.20	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	1052	27	21,24,25	3.23	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	1360	27	21,24,25	3.19	10 (47%)	29,34,37	1.13	3 (10%)
1	4AC	A1	1467	1	21,24,25	3.23	10 (47%)	29,34,37	1.42	6 (20%)
27	4AC	B1	162	27	21,24,25	3.22	10 (47%)	29,34,37	1.02	3 (10%)
27	LHH	B1	527	27	22,25,26	2.85	6 (27%)	29,35,38	1.52	3 (10%)
1	4AC	A1	546	1	21,24,25	3.27	10 (47%)	29,34,37	1.06	4 (13%)
1	4AC	A1	1221	1	21,24,25	3.27	10 (47%)	29,34,37	1.07	4 (13%)
27	4AC	B1	732	27	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	19	27	21,24,25	3.22	10 (47%)	29,34,37	1.03	4 (13%)
1	MA6	A1	1475	1	18,26,27	0.99	1 (5%)	19,38,41	4.48	3 (15%)
1	OMG	A1	507	1	18,26,27	2.58	8 (44%)	19,38,41	1.54	4 (21%)
27	5MC	B1	226	27	18,22,23	3.12	7 (38%)	26,32,35	0.97	2 (7%)
27	4AC	B1	979	27	21,24,25	3.24	10 (47%)	29,34,37	1.52	6 (20%)
27	4AC	B1	1818	27	21,24,25	3.21	10 (47%)	29,34,37	1.43	6 (20%)
1	4AC	A1	216	1	21,24,25	3.26	10 (47%)	29,34,37	1.45	6 (20%)
1	4AC	A1	1092	1	21,24,25	3.28	10 (47%)	29,34,37	1.07	4 (13%)
1	A1I59	A1	1366	1	22,27,28	2.56	6 (27%)	29,39,42	0.96	2 (6%)
1	4AC	A1	1288	1	21,24,25	3.25	10 (47%)	29,34,37	1.10	4 (13%)
27	4AC	B1	227	27	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	UR3	B1	2700	27	19,22,23	3.14	7 (36%)	26,32,35	1.37	3 (11%)
27	5MC	B1	47	27	18,22,23	3.12	7 (38%)	26,32,35	1.02	2 (7%)
27	OMG	B1	2684	27	18,26,27	2.56	8 (44%)	19,38,41	1.52	4 (21%)
27	4AC	B1	688	27	21,24,25	3.22	10 (47%)	29,34,37	1.07	4 (13%)
1	OMC	A1	426	1	19,22,23	3.13	8 (42%)	26,31,34	0.73	0
27	4AC	B1	3023	27	21,24,25	3.22	10 (47%)	29,34,37	1.01	4 (13%)
27	4AC	B1	652	27	21,24,25	3.23	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	419	27	21,24,25	3.19	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	1885	27	21,24,25	3.22	10 (47%)	29,34,37	0.99	4 (13%)
27	4AC	B1	1757	27	21,24,25	3.22	10 (47%)	29,34,37	1.05	4 (13%)
1	5MC	A1	855	1	18,22,23	3.15	7 (38%)	26,32,35	0.97	2 (7%)
27	4AC	B1	2008	27	21,24,25	3.21	10 (47%)	29,34,37	1.02	4 (13%)
1	5MC	A1	1013	1	18,22,23	3.17	7 (38%)	26,32,35	0.98	2 (7%)
1	5MC	A1	687	1	18,22,23	3.13	7 (38%)	26,32,35	0.97	1 (3%)
27	OMU	B1	1488	27	19,22,23	3.25	7 (36%)	26,31,34	1.79	7 (26%)
1	5MC	A1	17	1	18,22,23	3.14	7 (38%)	26,32,35	0.96	2 (7%)
27	4AC	B1	3006	27	21,24,25	3.26	10 (47%)	29,34,37	1.07	4 (13%)
27	4AC	B1	434	27	21,24,25	3.16	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	1061	27	21,24,25	3.24	10 (47%)	29,34,37	1.27	6 (20%)
27	OMG	B1	887	27	18,26,27	2.57	8 (44%)	19,38,41	1.58	5 (26%)
1	5MC	A1	605	1	18,22,23	3.15	7 (38%)	26,32,35	1.01	2 (7%)
1	4AC	A1	5	1	21,24,25	3.26	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	1478	27	21,24,25	3.24	10 (47%)	29,34,37	1.09	4 (13%)
27	A2M	B1	940	27	18,25,26	4.26	7 (38%)	18,36,39	2.26	4 (22%)
27	5MC	B1	336	27	18,22,23	3.08	7 (38%)	26,32,35	1.11	2 (7%)
27	4AC	B1	1442	27	21,24,25	3.20	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	2602	27	21,24,25	3.23	10 (47%)	29,34,37	1.02	4 (13%)
27	OMG	B1	2391	27	18,26,27	2.50	8 (44%)	19,38,41	1.54	5 (26%)
1	4AC	A1	382	1	21,24,25	3.24	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	344	27	21,24,25	0.41	0	29,34,37	0.53	0
1	4AC	A1	810	1	21,24,25	3.26	10 (47%)	29,34,37	1.07	4 (13%)
1	4AC	A1	816	1	21,24,25	3.25	10 (47%)	29,34,37	1.06	4 (13%)
1	5MC	A1	473	1	18,22,23	3.18	7 (38%)	26,32,35	1.02	2 (7%)
27	5MC	B1	2875	27	18,22,23	3.16	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	807	27	21,24,25	3.22	10 (47%)	29,34,37	1.05	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	1322	27	21,24,25	3.22	10 (47%)	29,34,37	1.04	4 (13%)
1	5MC	A1	623	1	18,22,23	3.15	7 (38%)	26,32,35	0.98	1 (3%)
27	OMC	B1	2557	27	19,22,23	3.08	8 (42%)	26,31,34	0.70	0
27	OMC	B1	2607	27	19,22,23	3.09	8 (42%)	26,31,34	0.69	0
27	4AC	B1	609	27	21,24,25	3.27	9 (42%)	29,34,37	1.07	4 (13%)
1	4AC	A1	614	1	21,24,25	3.22	10 (47%)	29,34,37	1.09	4 (13%)
27	5MC	B1	1648	27	18,22,23	3.15	7 (38%)	26,32,35	0.97	2 (7%)
1	OMU	A1	775	1	19,22,23	3.28	7 (36%)	26,31,34	1.81	6 (23%)
27	OMC	B1	1914	27	19,22,23	3.08	8 (42%)	26,31,34	1.32	2 (7%)
27	4AC	B1	1846	27	21,24,25	3.22	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	1621	27	21,24,25	3.23	10 (47%)	29,34,37	1.18	5 (17%)
1	A2M	A1	819	1	18,25,26	4.25	7 (38%)	18,36,39	2.28	4 (22%)
27	A2M	B1	2506	27	18,25,26	4.21	6 (33%)	18,36,39	2.27	4 (22%)
28	4AC	B2	120	28	21,24,25	3.26	10 (47%)	29,34,37	1.02	4 (13%)
27	OMG	B1	841	27	18,26,27	2.56	8 (44%)	19,38,41	1.97	6 (31%)
1	4AC	A1	856	1	21,24,25	3.23	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1664	27	21,24,25	3.23	10 (47%)	29,34,37	1.02	4 (13%)
1	OMG	A1	861	1	18,26,27	2.55	8 (44%)	19,38,41	1.53	4 (21%)
1	OMG	A1	227	1	18,26,27	2.55	8 (44%)	19,38,41	1.55	5 (26%)
27	LHH	B1	502	27	22,25,26	2.87	6 (27%)	29,35,38	1.39	3 (10%)
27	4AC	B1	2821	27	21,24,25	3.25	9 (42%)	29,34,37	1.01	4 (13%)
27	OMG	B1	214	27	18,26,27	2.56	8 (44%)	19,38,41	1.55	4 (21%)
1	4AC	A1	444	1	21,24,25	3.25	10 (47%)	29,34,37	1.06	4 (13%)
1	4AC	A1	761	1	21,24,25	3.26	10 (47%)	29,34,37	1.07	4 (13%)

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
1	MA6	A1	1457	1	-	3/7/29/30	0/3/3/3
1	5MC	A1	273	1	-	0/7/25/26	0/2/2/2
1	OMC	A1	1252	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	1313	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	1015	1	-	0/7/25/26	0/2/2/2
1	OMG	A1	455	1	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	2020	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	195	1	-	0/11/29/30	0/2/2/2
27	5MC	B1	1451	27	-	3/7/25/26	0/2/2/2
27	5MC	B1	275	27	-	2/7/25/26	0/2/2/2
27	4AC	B1	1706	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2562	27	-	0/5/27/28	0/3/3/3
1	OMG	A1	901	1	-	0/5/27/28	0/3/3/3
1	5MC	A1	1190	1	-	2/7/25/26	0/2/2/2
27	4AC	B1	2809	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	933	27	-	2/11/29/30	0/2/2/2
1	OMG	A1	459	1	-	1/5/27/28	0/3/3/3
27	4AC	B1	80	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	808	27	-	0/5/27/28	0/3/3/3
27	A2M	B1	857	27	-	1/5/27/28	0/3/3/3
27	4AC	B1	1751	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	1149	27	-	0/7/25/26	0/2/2/2
1	4AC	A1	231	1	-	0/11/29/30	0/2/2/2
1	5MC	A1	1486	1	-	4/7/25/26	0/2/2/2
27	4AC	B1	3037	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1293	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2740	27	-	0/5/27/28	0/3/3/3
27	5MC	B1	877	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1649	27	-	0/11/29/30	0/2/2/2
1	OMU	A1	762	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	378	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2365	27	-	2/5/27/28	0/3/3/3
27	4AC	B1	813	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1762	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	2082	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	479	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1383	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	2171	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1290	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	1362	1	-	2/7/25/26	0/2/2/2
1	4AC	A1	1067	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	827	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1150	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	896	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	392	27	-	2/11/29/30	0/2/2/2
1	5MC	A1	523	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A1	833	1	-	0/5/27/28	0/3/3/3
27	4AC	B1	2133	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1314	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	2469	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	715	27	-	2/11/29/30	0/2/2/2
28	4AC	B2	117	28	-	2/11/29/30	0/2/2/2
1	4AC	A1	636	1	-	0/11/29/30	0/2/2/2
27	OMC	B1	2808	27	-	0/9/27/28	0/2/2/2
27	5MC	B1	2453	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1612	27	-	3/11/29/30	0/2/2/2
1	OMC	A1	834	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	1374	27	-	0/11/29/30	0/2/2/2
1	MA6	A1	1476	1	-	1/7/29/30	0/3/3/3
27	4AC	B1	599	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	1783	27	-	0/9/27/28	0/2/2/2
27	5MC	B1	97	27	-	1/7/25/26	0/2/2/2
1	OMC	A1	1194	1	-	0/9/27/28	0/2/2/2
1	5MC	A1	230	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	48	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2028	27	-	0/5/27/28	0/3/3/3
1	OMG	A1	329	1	-	1/5/27/28	0/3/3/3
27	4AC	B1	1107	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	1003	1	-	0/5/27/28	0/3/3/3
27	OMC	B1	1489	27	-	2/9/27/28	0/2/2/2
27	4AC	B1	786	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	87	1	-	3/11/29/30	0/2/2/2
1	4AC	A1	1227	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1435	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	1620	27	-	0/7/25/26	0/2/2/2
1	5MC	A1	826	1	-	1/7/25/26	0/2/2/2
1	4AC	A1	624	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	691	1	-	0/11/29/30	0/2/2/2
27	OMC	B1	1832	27	-	0/9/27/28	0/2/2/2
28	4AC	B2	90	28	-	0/11/29/30	0/2/2/2
27	OMG	B1	1601	27	-	1/5/27/28	0/3/3/3
27	5MC	B1	18	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	3020	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	836	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1639	27	-	3/11/29/30	0/2/2/2
27	4AC	B1	866	27	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	A2M	B1	2057	27	-	2/5/27/28	0/3/3/3
27	5MC	B1	932	27	-	0/7/25/26	0/2/2/2
1	4AC	A1	1181	1	-	0/11/29/30	0/2/2/2
27	OMC	B1	1099	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	2888	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	142	27	-	0/11/29/30	0/2/2/2
27	OMU	B1	2554	27	-	0/9/27/28	0/2/2/2
27	OMG	B1	921	27	-	1/5/27/28	0/3/3/3
27	OMU	B1	1981	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	1551	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2735	27	-	0/9/27/28	0/2/2/2
1	OMU	A1	8	1	-	3/9/27/28	0/2/2/2
27	4AC	B1	950	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	719	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1404	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	533	1	-	2/7/25/26	0/2/2/2
1	LHH	A1	1364	1	-	4/13/31/32	0/2/2/2
27	OMG	B1	1557	27	-	0/5/27/28	0/3/3/3
1	LHH	A1	238	1	-	2/13/31/32	0/2/2/2
1	5MC	A1	863	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	1016	1	-	2/11/29/30	0/2/2/2
1	4AC	A1	220	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	1029	1	-	2/11/29/30	0/2/2/2
27	5MC	B1	2087	27	-	0/7/25/26	0/2/2/2
1	5MC	A1	1012	1	-	2/7/25/26	0/2/2/2
27	OMG	B1	1533	27	-	2/5/27/28	0/3/3/3
27	5MC	B1	1977	27	-	0/7/25/26	0/2/2/2
27	4SU	B1	2565	27	-	0/7/25/26	0/2/2/2
1	4AC	A1	367	1	-	0/11/29/30	0/2/2/2
27	LHH	B1	2968	27	-	2/13/31/32	0/2/2/2
27	OMC	B1	977	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	1100	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2844	27	-	0/11/29/30	0/2/2/2
27	LHH	B1	641	27	-	2/13/31/32	0/2/2/2
27	4AC	B1	1439	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2492	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2984	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	337	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	228	1	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	2902	27	-	4/11/29/30	0/2/2/2
1	4AC	A1	1254	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1734	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	271	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	718	1	-	1/7/25/26	0/2/2/2
1	5MU	A1	926	1	-	2/7/25/26	0/2/2/2
27	LHH	B1	1365	27	-	4/13/31/32	0/2/2/2
27	4AC	B1	2454	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	1966	27	-	2/7/25/26	0/2/2/2
1	4AC	A1	405	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	2526	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	1484	1	-	0/7/25/26	0/2/2/2
27	A2M	B1	262	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	2850	27	-	2/11/29/30	0/2/2/2
27	LHH	B1	904	27	-	2/13/31/32	0/2/2/2
1	4SU	A1	756	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	1911	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1769	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	116	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1064	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	2379	27	-	2/11/29/30	0/2/2/2
1	4AC	A1	274	1	-	0/11/29/30	0/2/2/2
27	OMC	B1	2119	27	-	0/9/27/28	0/2/2/2
1	5MC	A1	681	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	1501	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1608	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2757	27	-	1/5/27/28	0/3/3/3
27	4AC	B1	1822	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	360	27	-	0/11/29/30	0/2/2/2
1	A2M	A1	361	1	-	0/5/27/28	0/3/3/3
27	4AC	B1	276	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	2876	27	-	1/11/29/30	0/2/2/2
27	4AC	B1	1386	27	-	0/11/29/30	0/2/2/2
1	OMU	A1	425	1	-	1/9/27/28	0/2/2/2
1	4AC	A1	578	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	427	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	675	27	-	2/5/27/28	0/3/3/3
1	4AC	A1	706	1	-	2/11/29/30	0/2/2/2
27	4AC	B1	3011	27	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	721	27	-	0/11/29/30	0/2/2/2
27	OMU	B1	2668	27	-	0/9/27/28	0/2/2/2
1	4AC	A1	534	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	759	27	-	0/11/29/30	0/2/2/2
27	OMU	B1	454	27	-	0/9/27/28	0/2/2/2
1	OMU	A1	1368	1	-	0/9/27/28	0/2/2/2
1	4AC	A1	540	1	-	0/11/29/30	0/2/2/2
1	OMG	A1	153	1	-	0/5/27/28	0/3/3/3
27	OMG	B1	2180	27	-	2/5/27/28	0/3/3/3
27	4AC	B1	741	27	-	2/11/29/30	0/2/2/2
1	5MC	A1	1348	1	-	2/7/25/26	0/2/2/2
1	OMG	A1	763	1	-	3/5/27/28	0/3/3/3
27	OMC	B1	2059	27	-	0/9/27/28	0/2/2/2
27	5MC	B1	359	27	-	0/7/25/26	0/2/2/2
1	4AC	A1	739	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	1135	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1546	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2659	27	-	0/5/27/28	0/3/3/3
1	OMC	A1	1270	1	-	2/9/27/28	0/2/2/2
27	4AC	B1	23	27	-	0/11/29/30	0/2/2/2
27	OMU	B1	2401	27	-	4/9/27/28	0/2/2/2
27	4AC	B1	130	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2328	27	-	0/11/29/30	0/2/2/2
1	2MG	A1	1004	1	-	0/5/27/28	0/3/3/3
27	OMG	B1	2022	27	-	0/5/27/28	0/3/3/3
27	LHH	B1	1946	27	-	2/13/31/32	0/2/2/2
27	5MC	B1	2617	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1743	27	-	3/11/29/30	0/2/2/2
1	5MC	A1	466	1	-	2/7/25/26	0/2/2/2
1	4AC	A1	291	1	-	0/11/29/30	0/2/2/2
27	5MC	B1	1983	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	2749	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1967	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	485	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	243	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	1965	27	-	2/5/27/28	0/3/3/3
27	4AC	B1	200	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2213	27	-	0/11/29/30	0/2/2/2
27	OMU	B1	2593	27	-	0/9/27/28	0/2/2/2
1	G7M	A1	481	1	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	2792	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	307	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	499	1	-	1/11/29/30	0/2/2/2
27	4AC	B1	1505	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1286	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	645	1	-	0/5/27/28	0/3/3/3
27	4AC	B1	953	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	951	1	-	3/7/25/26	0/2/2/2
27	4AC	B1	1178	27	-	2/11/29/30	0/2/2/2
1	4AC	A1	467	1	-	2/11/29/30	0/2/2/2
27	OMG	B1	2540	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	2429	27	-	0/11/29/30	0/2/2/2
1	OMC	A1	117	1	-	0/9/27/28	0/2/2/2
27	A2M	B1	880	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	2432	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	1868	27	-	0/7/25/26	0/2/2/2
1	4AC	A1	41	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	580	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1128	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2428	27	-	0/9/27/28	0/2/2/2
1	OMG	A1	668	1	-	0/5/27/28	0/3/3/3
27	OMG	B1	920	27	-	1/5/27/28	0/3/3/3
27	5MC	B1	2067	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1703	27	-	2/11/29/30	0/2/2/2
27	OMC	B1	501	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	1264	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	839	1	-	1/11/29/30	0/2/2/2
27	A2M	B1	506	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	1067	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2113	27	-	0/11/29/30	0/2/2/2
1	OMU	A1	52	1	-	0/9/27/28	0/2/2/2
1	4AC	A1	141	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	98	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	798	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1052	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1360	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1467	1	-	2/11/29/30	0/2/2/2
27	4AC	B1	162	27	-	0/11/29/30	0/2/2/2
27	LHH	B1	527	27	-	2/13/31/32	0/2/2/2
1	4AC	A1	546	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	1221	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	732	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	19	27	-	0/11/29/30	0/2/2/2
1	MA6	A1	1475	1	-	0/7/29/30	0/3/3/3
1	OMG	A1	507	1	-	0/5/27/28	0/3/3/3
27	5MC	B1	226	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	979	27	-	4/11/29/30	0/2/2/2
27	4AC	B1	1818	27	-	2/11/29/30	0/2/2/2
1	4AC	A1	216	1	-	1/11/29/30	0/2/2/2
1	4AC	A1	1092	1	-	2/11/29/30	0/2/2/2
1	A1I59	A1	1366	1	-	5/11/33/34	0/2/2/2
1	4AC	A1	1288	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	227	27	-	0/11/29/30	0/2/2/2
27	UR3	B1	2700	27	-	2/7/25/26	0/2/2/2
27	5MC	B1	47	27	-	1/7/25/26	0/2/2/2
27	OMG	B1	2684	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	688	27	-	3/11/29/30	0/2/2/2
1	OMC	A1	426	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	3023	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	652	27	-	1/11/29/30	0/2/2/2
27	4AC	B1	419	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1885	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1757	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	855	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	2008	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	1013	1	-	0/7/25/26	0/2/2/2
1	5MC	A1	687	1	-	0/7/25/26	0/2/2/2
27	OMU	B1	1488	27	-	1/9/27/28	0/2/2/2
1	5MC	A1	17	1	-	2/7/25/26	0/2/2/2
27	4AC	B1	3006	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	434	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1061	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	887	27	-	2/5/27/28	0/3/3/3
1	5MC	A1	605	1	-	1/7/25/26	0/2/2/2
1	4AC	A1	5	1	-	2/11/29/30	0/2/2/2
27	4AC	B1	1478	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	940	27	-	0/5/27/28	0/3/3/3
27	5MC	B1	336	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1442	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2602	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2391	27	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	A1	382	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	344	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	810	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	816	1	-	0/11/29/30	0/2/2/2
1	5MC	A1	473	1	-	0/7/25/26	0/2/2/2
27	5MC	B1	2875	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	807	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1322	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	623	1	-	0/7/25/26	0/2/2/2
27	OMC	B1	2557	27	-	1/9/27/28	0/2/2/2
27	OMC	B1	2607	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	609	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	614	1	-	0/11/29/30	0/2/2/2
27	5MC	B1	1648	27	-	3/7/25/26	0/2/2/2
1	OMU	A1	775	1	-	5/9/27/28	0/2/2/2
27	OMC	B1	1914	27	-	4/9/27/28	0/2/2/2
27	4AC	B1	1846	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1621	27	-	0/11/29/30	0/2/2/2
1	A2M	A1	819	1	-	0/5/27/28	0/3/3/3
27	A2M	B1	2506	27	-	0/5/27/28	0/3/3/3
28	4AC	B2	120	28	-	0/11/29/30	0/2/2/2
27	OMG	B1	841	27	-	0/5/27/28	0/3/3/3
1	4AC	A1	856	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1664	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	861	1	-	2/5/27/28	0/3/3/3
1	OMG	A1	227	1	-	0/5/27/28	0/3/3/3
27	LHH	B1	502	27	-	2/13/31/32	0/2/2/2
27	4AC	B1	2821	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	214	27	-	0/5/27/28	0/3/3/3
1	4AC	A1	444	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	761	1	-	0/11/29/30	0/2/2/2

All (2714) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	940	A2M	O4'-C1'	15.32	1.62	1.41
1	A1	819	A2M	O4'-C1'	15.30	1.62	1.41
27	B1	2057	A2M	O4'-C1'	15.19	1.62	1.41
27	B1	857	A2M	O4'-C1'	15.07	1.62	1.41
1	A1	361	A2M	O4'-C1'	15.07	1.62	1.41
27	B1	506	A2M	O4'-C1'	15.06	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2506	A2M	O4'-C1'	15.04	1.62	1.41
27	B1	880	A2M	O4'-C1'	14.91	1.61	1.41
1	A1	481	G7M	C8-N7	10.10	1.51	1.33
1	A1	481	G7M	C8-N9	9.96	1.51	1.33
1	A1	238	LHH	O2-C2	8.94	1.40	1.23
27	B1	904	LHH	O2-C2	8.94	1.40	1.23
27	B1	641	LHH	O2-C2	8.91	1.40	1.23
1	A1	1364	LHH	O2-C2	8.91	1.40	1.23
27	B1	2968	LHH	O2-C2	8.88	1.40	1.23
27	B1	1365	LHH	O2-C2	8.88	1.40	1.23
27	B1	502	LHH	O2-C2	8.87	1.40	1.23
27	B1	527	LHH	O2-C2	8.83	1.40	1.23
27	B1	1946	LHH	O2-C2	8.78	1.39	1.23
1	A1	1366	A1I59	O2-C2	8.72	1.39	1.23
27	B1	2565	4SU	C4-N3	8.65	1.46	1.37
1	A1	756	4SU	C4-N3	8.61	1.46	1.37
27	B1	2700	UR3	C2-N1	8.31	1.50	1.38
1	A1	1012	5MC	C6-C5	7.94	1.47	1.34
27	B1	2453	5MC	C6-C5	7.94	1.47	1.34
27	B1	275	5MC	C6-C5	7.93	1.47	1.34
27	B1	1620	5MC	C6-C5	7.93	1.47	1.34
1	A1	623	5MC	C6-C5	7.92	1.47	1.34
27	B1	2875	5MC	C6-C5	7.91	1.47	1.34
1	A1	473	5MC	C6-C5	7.91	1.47	1.34
27	B1	1977	5MC	C6-C5	7.91	1.47	1.34
1	A1	230	5MC	C6-C5	7.90	1.47	1.34
1	A1	605	5MC	C6-C5	7.90	1.47	1.34
1	A1	826	5MC	C6-C5	7.89	1.47	1.34
1	A1	1348	5MC	C6-C5	7.89	1.47	1.34
1	A1	863	5MC	C6-C5	7.89	1.47	1.34
1	A1	1013	5MC	C6-C5	7.88	1.47	1.34
27	B1	2082	5MC	C6-C5	7.88	1.47	1.34
1	A1	52	OMU	C2-N3	7.88	1.52	1.38
27	B1	454	OMU	C2-N3	7.87	1.52	1.38
1	A1	533	5MC	C6-C5	7.87	1.47	1.34
27	B1	97	5MC	C6-C5	7.86	1.47	1.34
1	A1	1362	5MC	C6-C5	7.86	1.47	1.34
27	B1	1868	5MC	C6-C5	7.86	1.47	1.34
1	A1	1190	5MC	C6-C5	7.86	1.47	1.34
1	A1	718	5MC	C6-C5	7.86	1.47	1.34
1	A1	1484	5MC	C6-C5	7.86	1.47	1.34
1	A1	466	5MC	C6-C5	7.85	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	1015	5MC	C6-C5	7.84	1.47	1.34
27	B1	2067	5MC	C6-C5	7.84	1.47	1.34
1	A1	273	5MC	C6-C5	7.84	1.47	1.34
27	B1	1981	OMU	C2-N3	7.84	1.51	1.38
27	B1	1983	5MC	C6-C5	7.84	1.47	1.34
1	A1	951	5MC	C6-C5	7.83	1.47	1.34
1	A1	523	5MC	C6-C5	7.83	1.47	1.34
27	B1	359	5MC	C6-C5	7.83	1.47	1.34
1	A1	1368	OMU	C2-N3	7.83	1.51	1.38
27	B1	1648	5MC	C6-C5	7.83	1.47	1.34
1	A1	855	5MC	C6-C5	7.82	1.47	1.34
1	A1	762	OMU	C2-N3	7.82	1.51	1.38
1	A1	17	5MC	C6-C5	7.82	1.47	1.34
1	A1	1486	5MC	C6-C5	7.81	1.47	1.34
1	A1	687	5MC	C6-C5	7.81	1.47	1.34
27	B1	1488	OMU	C2-N3	7.80	1.51	1.38
1	A1	8	OMU	C2-N3	7.80	1.51	1.38
27	B1	47	5MC	C6-C5	7.80	1.47	1.34
27	B1	2401	OMU	C2-N3	7.80	1.51	1.38
27	B1	18	5MC	C6-C5	7.80	1.47	1.34
1	A1	681	5MC	C6-C5	7.79	1.47	1.34
27	B1	877	5MC	C6-C5	7.79	1.47	1.34
1	A1	775	OMU	C2-N3	7.79	1.51	1.38
27	B1	2087	5MC	C6-C5	7.79	1.47	1.34
27	B1	226	5MC	C6-C5	7.78	1.47	1.34
1	A1	425	OMU	C2-N3	7.78	1.51	1.38
27	B1	1149	5MC	C6-C5	7.78	1.47	1.34
27	B1	2593	OMU	C2-N3	7.77	1.51	1.38
27	B1	2617	5MC	C6-C5	7.76	1.47	1.34
27	B1	932	5MC	C6-C5	7.75	1.47	1.34
27	B1	1966	5MC	C6-C5	7.74	1.47	1.34
27	B1	2554	OMU	C2-N3	7.73	1.51	1.38
27	B1	2668	OMU	C2-N3	7.73	1.51	1.38
27	B1	1451	5MC	C6-C5	7.65	1.47	1.34
1	A1	775	OMU	C2-N1	7.64	1.50	1.38
27	B1	2401	OMU	C2-N1	7.62	1.50	1.38
1	A1	52	OMU	C2-N1	7.58	1.50	1.38
27	B1	454	OMU	C2-N1	7.58	1.50	1.38
27	B1	1981	OMU	C2-N1	7.58	1.50	1.38
27	B1	336	5MC	C6-C5	7.55	1.47	1.34
1	A1	762	OMU	C2-N1	7.55	1.50	1.38
1	A1	8	OMU	C2-N1	7.53	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2593	OMU	C2-N1	7.52	1.50	1.38
27	B1	2668	OMU	C2-N1	7.52	1.50	1.38
1	A1	1368	OMU	C2-N1	7.51	1.50	1.38
27	B1	1488	OMU	C2-N1	7.47	1.50	1.38
27	B1	2554	OMU	C2-N1	7.47	1.50	1.38
27	B1	378	4AC	C4-N3	7.41	1.45	1.32
1	A1	425	OMU	C2-N1	7.39	1.50	1.38
1	A1	756	4SU	C2-N1	7.38	1.50	1.38
1	A1	426	OMC	C2-N3	7.38	1.51	1.36
27	B1	2428	OMC	C2-N3	7.37	1.51	1.36
27	B1	1832	OMC	C2-N3	7.37	1.51	1.36
1	A1	117	OMC	C2-N3	7.35	1.51	1.36
1	A1	1194	OMC	C2-N3	7.34	1.51	1.36
1	A1	1252	OMC	C2-N3	7.32	1.51	1.36
1	A1	427	4AC	C4-N3	7.31	1.45	1.32
27	B1	2059	OMC	C2-N3	7.30	1.51	1.36
1	A1	834	OMC	C2-N3	7.30	1.51	1.36
1	A1	1270	OMC	C2-N3	7.30	1.51	1.36
27	B1	1489	OMC	C2-N3	7.30	1.51	1.36
27	B1	977	OMC	C2-N3	7.30	1.51	1.36
27	B1	1914	OMC	C2-N3	7.27	1.51	1.36
27	B1	2557	OMC	C2-N3	7.27	1.51	1.36
27	B1	2119	OMC	C2-N3	7.24	1.51	1.36
27	B1	501	OMC	C2-N3	7.24	1.51	1.36
27	B1	2735	OMC	C2-N3	7.23	1.51	1.36
27	B1	2607	OMC	C2-N3	7.23	1.51	1.36
27	B1	1608	4AC	C4-N3	7.22	1.45	1.32
27	B1	2808	OMC	C2-N3	7.22	1.51	1.36
27	B1	2565	4SU	C2-N1	7.21	1.50	1.38
27	B1	1099	OMC	C2-N3	7.20	1.51	1.36
27	B1	1783	OMC	C2-N3	7.20	1.51	1.36
1	A1	141	4AC	C4-N3	7.19	1.45	1.32
27	B1	979	4AC	C4-N3	7.18	1.45	1.32
1	A1	1135	4AC	C4-N3	7.17	1.45	1.32
1	A1	1092	4AC	C4-N3	7.16	1.45	1.32
1	A1	1314	4AC	C4-N3	7.15	1.45	1.32
1	A1	467	4AC	C4-N3	7.14	1.45	1.32
27	B1	3037	4AC	C4-N3	7.14	1.45	1.32
1	A1	5	4AC	C4-N3	7.12	1.45	1.32
27	B1	1612	4AC	C4-N3	7.12	1.45	1.32
1	A1	624	4AC	C4-N3	7.12	1.45	1.32
1	A1	636	4AC	C4-N3	7.12	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1621	4AC	C4-N3	7.12	1.45	1.32
27	B1	142	4AC	C4-N3	7.11	1.45	1.32
1	A1	195	4AC	C4-N3	7.11	1.45	1.32
1	A1	444	4AC	C4-N3	7.11	1.45	1.32
28	B2	90	4AC	C4-N3	7.10	1.45	1.32
1	A1	739	4AC	C4-N3	7.10	1.45	1.32
1	A1	761	4AC	C4-N3	7.10	1.45	1.32
1	A1	836	4AC	C4-N3	7.10	1.45	1.32
1	A1	546	4AC	C4-N3	7.10	1.45	1.32
1	A1	810	4AC	C4-N3	7.09	1.45	1.32
27	B1	813	4AC	C4-N3	7.09	1.45	1.32
27	B1	80	4AC	C4-N3	7.09	1.45	1.32
27	B1	609	4AC	C4-N3	7.08	1.45	1.32
27	B1	360	4AC	C4-N3	7.08	1.45	1.32
27	B1	2850	4AC	C4-N3	7.08	1.45	1.32
27	B1	1286	4AC	C4-N3	7.08	1.45	1.32
27	B1	1322	4AC	C4-N3	7.08	1.45	1.32
1	A1	1016	4AC	C4-N3	7.08	1.45	1.32
1	A1	1221	4AC	C4-N3	7.07	1.45	1.32
27	B1	1664	4AC	C4-N3	7.07	1.45	1.32
1	A1	382	4AC	C4-N3	7.07	1.45	1.32
1	A1	1029	4AC	C4-N3	7.07	1.45	1.32
27	B1	1703	4AC	C4-N3	7.06	1.45	1.32
1	A1	691	4AC	C4-N3	7.06	1.45	1.32
27	B1	2429	4AC	C4-N3	7.06	1.45	1.32
27	B1	2454	4AC	C4-N3	7.06	1.45	1.32
27	B1	1734	4AC	C4-N3	7.05	1.45	1.32
27	B1	392	4AC	C4-N3	7.05	1.45	1.32
1	A1	291	4AC	C4-N3	7.05	1.45	1.32
1	A1	405	4AC	C4-N3	7.05	1.45	1.32
1	A1	367	4AC	C4-N3	7.04	1.45	1.32
27	B1	896	4AC	C4-N3	7.04	1.45	1.32
27	B1	1762	4AC	C4-N3	7.04	1.45	1.32
1	A1	220	4AC	C4-N3	7.04	1.45	1.32
27	B1	1374	4AC	C4-N3	7.04	1.45	1.32
1	A1	540	4AC	C4-N3	7.04	1.45	1.32
1	A1	816	4AC	C4-N3	7.04	1.45	1.32
27	B1	950	4AC	C4-N3	7.04	1.45	1.32
27	B1	1478	4AC	C4-N3	7.04	1.45	1.32
1	A1	614	4AC	C4-N3	7.04	1.45	1.32
27	B1	1743	4AC	C4-N3	7.03	1.45	1.32
27	B1	227	4AC	C4-N3	7.03	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1911	4AC	C4-N3	7.03	1.45	1.32
28	B2	120	4AC	C4-N3	7.03	1.45	1.32
27	B1	276	4AC	C4-N3	7.03	1.45	1.32
27	B1	759	4AC	C4-N3	7.03	1.45	1.32
1	A1	1254	4AC	C4-N3	7.02	1.45	1.32
1	A1	216	4AC	C4-N3	7.02	1.45	1.32
27	B1	243	4AC	C4-N3	7.02	1.45	1.32
27	B1	1150	4AC	C4-N3	7.02	1.45	1.32
27	B1	271	4AC	C4-N3	7.02	1.45	1.32
28	B2	117	4AC	C4-N3	7.02	1.45	1.32
27	B1	1546	4AC	C4-N3	7.02	1.45	1.32
1	A1	499	4AC	C4-N3	7.02	1.45	1.32
1	A1	1467	4AC	C4-N3	7.02	1.45	1.32
27	B1	1846	4AC	C4-N3	7.02	1.45	1.32
27	B1	715	4AC	C4-N3	7.01	1.45	1.32
27	B1	2749	4AC	C4-N3	7.01	1.45	1.32
27	B1	2876	4AC	C4-N3	7.01	1.45	1.32
27	B1	2020	4AC	C4-N3	7.01	1.45	1.32
1	A1	534	4AC	C4-N3	7.00	1.45	1.32
27	B1	732	4AC	C4-N3	7.00	1.45	1.32
1	A1	1288	4AC	C4-N3	7.00	1.45	1.32
27	B1	1360	4AC	C4-N3	7.00	1.45	1.32
27	B1	1061	4AC	C4-N3	7.00	1.45	1.32
1	A1	578	4AC	C4-N3	7.00	1.45	1.32
27	B1	2602	4AC	C4-N3	7.00	1.45	1.32
27	B1	2792	4AC	C4-N3	7.00	1.45	1.32
27	B1	953	4AC	C4-N3	7.00	1.45	1.32
1	A1	706	4AC	C4-N3	7.00	1.45	1.32
27	B1	1064	4AC	C4-N3	6.99	1.45	1.32
27	B1	1313	4AC	C4-N3	6.99	1.45	1.32
27	B1	1501	4AC	C4-N3	6.99	1.45	1.32
27	B1	130	4AC	C4-N3	6.99	1.45	1.32
27	B1	741	4AC	C4-N3	6.99	1.45	1.32
27	B1	866	4AC	C4-N3	6.99	1.45	1.32
27	B1	3023	4AC	C4-N3	6.99	1.45	1.32
27	B1	2700	UR3	C6-C5	6.98	1.51	1.35
27	B1	3006	4AC	C4-N3	6.98	1.45	1.32
27	B1	3020	4AC	C4-N3	6.98	1.45	1.32
1	A1	839	4AC	C4-N3	6.98	1.45	1.32
27	B1	599	4AC	C4-N3	6.98	1.45	1.32
27	B1	1435	4AC	C4-N3	6.98	1.45	1.32
27	B1	1751	4AC	C4-N3	6.98	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	1067	4AC	C4-N3	6.98	1.44	1.32
27	B1	1178	4AC	C4-N3	6.98	1.44	1.32
27	B1	807	4AC	C4-N3	6.97	1.44	1.32
27	B1	2526	4AC	C4-N3	6.97	1.44	1.32
27	B1	652	4AC	C4-N3	6.97	1.44	1.32
1	A1	307	4AC	C4-N3	6.97	1.44	1.32
27	B1	580	4AC	C4-N3	6.97	1.44	1.32
27	B1	485	4AC	C4-N3	6.96	1.44	1.32
27	B1	2821	4AC	C4-N3	6.96	1.44	1.32
1	A1	827	4AC	C4-N3	6.96	1.44	1.32
27	B1	786	4AC	C4-N3	6.96	1.44	1.32
1	A1	856	4AC	C4-N3	6.96	1.44	1.32
27	B1	479	4AC	C4-N3	6.96	1.44	1.32
27	B1	1757	4AC	C4-N3	6.96	1.44	1.32
27	B1	19	4AC	C4-N3	6.95	1.44	1.32
27	B1	2469	4AC	C4-N3	6.95	1.44	1.32
27	B1	162	4AC	C4-N3	6.95	1.44	1.32
1	A1	87	4AC	C4-N3	6.95	1.44	1.32
1	A1	1227	4AC	C4-N3	6.94	1.44	1.32
27	B1	23	4AC	C4-N3	6.94	1.44	1.32
27	B1	1706	4AC	C4-N3	6.94	1.44	1.32
27	B1	2888	4AC	C4-N3	6.94	1.44	1.32
1	A1	231	4AC	C4-N3	6.93	1.44	1.32
27	B1	1551	4AC	C4-N3	6.93	1.44	1.32
27	B1	2328	4AC	C4-N3	6.93	1.44	1.32
27	B1	1383	4AC	C4-N3	6.93	1.44	1.32
27	B1	2844	4AC	C4-N3	6.93	1.44	1.32
27	B1	1052	4AC	C4-N3	6.92	1.44	1.32
27	B1	1067	4AC	C4-N3	6.92	1.44	1.32
27	B1	1386	4AC	C4-N3	6.92	1.44	1.32
27	B1	1439	4AC	C4-N3	6.92	1.44	1.32
27	B1	1293	4AC	C4-N3	6.92	1.44	1.32
27	B1	419	4AC	C4-N3	6.92	1.44	1.32
27	B1	200	4AC	C4-N3	6.92	1.44	1.32
27	B1	1264	4AC	C4-N3	6.92	1.44	1.32
27	B1	2809	4AC	C4-N3	6.91	1.44	1.32
1	A1	1181	4AC	C4-N3	6.91	1.44	1.32
27	B1	721	4AC	C4-N3	6.91	1.44	1.32
27	B1	688	4AC	C4-N3	6.90	1.44	1.32
27	B1	2432	4AC	C4-N3	6.90	1.44	1.32
27	B1	1290	4AC	C4-N3	6.90	1.44	1.32
27	B1	2113	4AC	C4-N3	6.90	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2492	4AC	C4-N3	6.90	1.44	1.32
27	B1	116	4AC	C4-N3	6.90	1.44	1.32
1	A1	719	4AC	C4-N3	6.90	1.44	1.32
27	B1	98	4AC	C4-N3	6.90	1.44	1.32
1	A1	41	4AC	C4-N3	6.89	1.44	1.32
27	B1	798	4AC	C4-N3	6.88	1.44	1.32
27	B1	1822	4AC	C4-N3	6.88	1.44	1.32
27	B1	3011	4AC	C4-N3	6.88	1.44	1.32
27	B1	2171	4AC	C4-N3	6.88	1.44	1.32
27	B1	1107	4AC	C4-N3	6.88	1.44	1.32
27	B1	1639	4AC	C4-N3	6.88	1.44	1.32
27	B1	48	4AC	C4-N3	6.87	1.44	1.32
27	B1	1885	4AC	C4-N3	6.86	1.44	1.32
27	B1	1505	4AC	C4-N3	6.86	1.44	1.32
27	B1	1818	4AC	C4-N3	6.85	1.44	1.32
1	A1	274	4AC	C4-N3	6.85	1.44	1.32
27	B1	1442	4AC	C4-N3	6.85	1.44	1.32
27	B1	1649	4AC	C4-N3	6.84	1.44	1.32
27	B1	2008	4AC	C4-N3	6.84	1.44	1.32
27	B1	933	4AC	C4-N3	6.83	1.44	1.32
27	B1	2213	4AC	C4-N3	6.82	1.44	1.32
27	B1	337	4AC	C4-N3	6.82	1.44	1.32
27	B1	1100	4AC	C4-N3	6.82	1.44	1.32
27	B1	2133	4AC	C4-N3	6.81	1.44	1.32
27	B1	434	4AC	C4-N3	6.79	1.44	1.32
27	B1	2379	4AC	C4-N3	6.79	1.44	1.32
27	B1	1128	4AC	C4-N3	6.78	1.44	1.32
27	B1	1769	4AC	C4-N3	6.74	1.44	1.32
27	B1	1404	4AC	C4-N3	6.74	1.44	1.32
27	B1	1967	4AC	C4-N3	6.73	1.44	1.32
1	A1	756	4SU	C2-N3	6.72	1.49	1.38
27	B1	2565	4SU	C2-N3	6.68	1.49	1.38
1	A1	1270	OMC	C6-C5	6.63	1.50	1.35
1	A1	834	OMC	C6-C5	6.63	1.50	1.35
27	B1	2428	OMC	C6-C5	6.62	1.50	1.35
1	A1	1364	LHH	C2-N3	6.62	1.49	1.36
27	B1	2059	OMC	C6-C5	6.62	1.50	1.35
27	B1	2808	OMC	C6-C5	6.60	1.50	1.35
1	A1	1252	OMC	C6-C5	6.60	1.50	1.35
1	A1	426	OMC	C6-C5	6.60	1.50	1.35
27	B1	1832	OMC	C6-C5	6.59	1.50	1.35
27	B1	2735	OMC	C6-C5	6.58	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	1194	OMC	C6-C5	6.58	1.50	1.35
27	B1	2119	OMC	C6-C5	6.58	1.50	1.35
27	B1	1914	OMC	C6-C5	6.57	1.50	1.35
1	A1	117	OMC	C6-C5	6.56	1.50	1.35
27	B1	2557	OMC	C6-C5	6.56	1.50	1.35
27	B1	1489	OMC	C6-C5	6.56	1.50	1.35
27	B1	501	OMC	C6-C5	6.54	1.50	1.35
27	B1	1783	OMC	C6-C5	6.54	1.50	1.35
27	B1	378	4AC	C2-N3	6.53	1.49	1.36
27	B1	2607	OMC	C6-C5	6.52	1.50	1.35
27	B1	1099	OMC	C6-C5	6.50	1.50	1.35
27	B1	977	OMC	C6-C5	6.50	1.50	1.35
27	B1	2506	A2M	O4'-C4'	-6.48	1.30	1.45
27	B1	904	LHH	C2-N3	6.46	1.49	1.36
1	A1	238	LHH	C2-N3	6.46	1.49	1.36
27	B1	2057	A2M	O4'-C4'	-6.45	1.30	1.45
27	B1	378	4AC	C6-C5	6.44	1.50	1.35
27	B1	527	LHH	C2-N3	6.44	1.49	1.36
1	A1	1227	4AC	C6-C5	6.43	1.50	1.35
1	A1	274	4AC	C6-C5	6.41	1.50	1.35
27	B1	1885	4AC	C6-C5	6.40	1.49	1.35
27	B1	506	A2M	O4'-C4'	-6.40	1.30	1.45
27	B1	1100	4AC	C6-C5	6.40	1.49	1.35
27	B1	1365	LHH	C2-N3	6.40	1.49	1.36
1	A1	361	A2M	O4'-C4'	-6.39	1.30	1.45
27	B1	1290	4AC	C6-C5	6.39	1.49	1.35
27	B1	1313	4AC	C6-C5	6.39	1.49	1.35
1	A1	1029	4AC	C6-C5	6.39	1.49	1.35
27	B1	2379	4AC	C6-C5	6.38	1.49	1.35
27	B1	1639	4AC	C6-C5	6.38	1.49	1.35
27	B1	641	LHH	C2-N3	6.38	1.49	1.36
1	A1	195	4AC	C6-C5	6.37	1.49	1.35
27	B1	2888	4AC	C6-C5	6.37	1.49	1.35
27	B1	652	4AC	C6-C5	6.37	1.49	1.35
27	B1	1967	4AC	C6-C5	6.36	1.49	1.35
1	A1	719	4AC	C6-C5	6.36	1.49	1.35
27	B1	2432	4AC	C6-C5	6.36	1.49	1.35
27	B1	162	4AC	C6-C5	6.35	1.49	1.35
27	B1	1649	4AC	C6-C5	6.35	1.49	1.35
1	A1	534	4AC	C6-C5	6.35	1.49	1.35
1	A1	856	4AC	C6-C5	6.35	1.49	1.35
27	B1	360	4AC	C6-C5	6.35	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1178	4AC	C6-C5	6.35	1.49	1.35
27	B1	1067	4AC	C6-C5	6.35	1.49	1.35
1	A1	1181	4AC	C6-C5	6.34	1.49	1.35
1	A1	827	4AC	C6-C5	6.34	1.49	1.35
27	B1	721	4AC	C6-C5	6.34	1.49	1.35
1	A1	231	4AC	C6-C5	6.34	1.49	1.35
27	B1	479	4AC	C6-C5	6.34	1.49	1.35
27	B1	2328	4AC	C6-C5	6.34	1.49	1.35
27	B1	609	4AC	C6-C5	6.34	1.49	1.35
27	B1	940	A2M	O4'-C4'	-6.34	1.30	1.45
1	A1	41	4AC	C6-C5	6.34	1.49	1.35
1	A1	578	4AC	C6-C5	6.34	1.49	1.35
27	B1	2821	4AC	C6-C5	6.33	1.49	1.35
27	B1	48	4AC	C6-C5	6.33	1.49	1.35
27	B1	786	4AC	C6-C5	6.33	1.49	1.35
27	B1	2968	LHH	C2-N3	6.33	1.49	1.36
27	B1	1612	4AC	C6-C5	6.33	1.49	1.35
27	B1	759	4AC	C6-C5	6.33	1.49	1.35
28	B2	120	4AC	C6-C5	6.33	1.49	1.35
27	B1	1107	4AC	C6-C5	6.32	1.49	1.35
27	B1	2020	4AC	C6-C5	6.32	1.49	1.35
27	B1	1442	4AC	C6-C5	6.32	1.49	1.35
27	B1	142	4AC	C6-C5	6.32	1.49	1.35
27	B1	1052	4AC	C6-C5	6.32	1.49	1.35
27	B1	200	4AC	C6-C5	6.32	1.49	1.35
1	A1	1067	4AC	C6-C5	6.32	1.49	1.35
27	B1	715	4AC	C6-C5	6.32	1.49	1.35
27	B1	98	4AC	C6-C5	6.32	1.49	1.35
27	B1	2429	4AC	C6-C5	6.32	1.49	1.35
27	B1	896	4AC	C6-C5	6.32	1.49	1.35
1	A1	816	4AC	C6-C5	6.31	1.49	1.35
27	B1	1743	4AC	C6-C5	6.31	1.49	1.35
1	A1	839	4AC	C6-C5	6.31	1.49	1.35
27	B1	1128	4AC	C6-C5	6.31	1.49	1.35
27	B1	502	LHH	C2-N3	6.31	1.49	1.36
27	B1	1404	4AC	C6-C5	6.31	1.49	1.35
27	B1	580	4AC	C6-C5	6.31	1.49	1.35
1	A1	706	4AC	C6-C5	6.31	1.49	1.35
27	B1	1293	4AC	C6-C5	6.31	1.49	1.35
27	B1	1435	4AC	C6-C5	6.31	1.49	1.35
27	B1	1822	4AC	C6-C5	6.30	1.49	1.35
1	A1	1016	4AC	C6-C5	6.30	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	1254	4AC	C6-C5	6.30	1.49	1.35
1	A1	775	OMU	C6-C5	6.30	1.49	1.35
1	A1	216	4AC	C6-C5	6.30	1.49	1.35
27	B1	741	4AC	C6-C5	6.30	1.49	1.35
27	B1	2526	4AC	C6-C5	6.30	1.49	1.35
1	A1	307	4AC	C6-C5	6.30	1.49	1.35
1	A1	546	4AC	C6-C5	6.30	1.49	1.35
27	B1	19	4AC	C6-C5	6.30	1.49	1.35
1	A1	1288	4AC	C6-C5	6.30	1.49	1.35
27	B1	1546	4AC	C6-C5	6.30	1.49	1.35
1	A1	8	OMU	C6-C5	6.30	1.49	1.35
1	A1	52	OMU	C6-C5	6.30	1.49	1.35
27	B1	2809	4AC	C6-C5	6.30	1.49	1.35
27	B1	1846	4AC	C6-C5	6.30	1.49	1.35
27	B1	2492	4AC	C6-C5	6.30	1.49	1.35
1	A1	1135	4AC	C6-C5	6.30	1.49	1.35
27	B1	1946	LHH	C2-N3	6.30	1.49	1.36
27	B1	2133	4AC	C6-C5	6.29	1.49	1.35
27	B1	1706	4AC	C6-C5	6.29	1.49	1.35
27	B1	2593	OMU	C6-C5	6.29	1.49	1.35
27	B1	688	4AC	C6-C5	6.29	1.49	1.35
27	B1	337	4AC	C6-C5	6.29	1.49	1.35
27	B1	866	4AC	C6-C5	6.29	1.49	1.35
27	B1	1505	4AC	C6-C5	6.29	1.49	1.35
27	B1	807	4AC	C6-C5	6.29	1.49	1.35
27	B1	1478	4AC	C6-C5	6.29	1.49	1.35
27	B1	1703	4AC	C6-C5	6.29	1.49	1.35
27	B1	276	4AC	C6-C5	6.29	1.49	1.35
27	B1	1386	4AC	C6-C5	6.28	1.49	1.35
1	A1	405	4AC	C6-C5	6.28	1.49	1.35
27	B1	2213	4AC	C6-C5	6.28	1.49	1.35
27	B1	1064	4AC	C6-C5	6.28	1.49	1.35
27	B1	1981	OMU	C6-C5	6.28	1.49	1.35
27	B1	2171	4AC	C6-C5	6.28	1.49	1.35
27	B1	2401	OMU	C6-C5	6.28	1.49	1.35
27	B1	130	4AC	C6-C5	6.28	1.49	1.35
27	B1	1488	OMU	C6-C5	6.28	1.49	1.35
27	B1	3006	4AC	C6-C5	6.28	1.49	1.35
1	A1	141	4AC	C6-C5	6.28	1.49	1.35
1	A1	819	A2M	O4'-C4'	-6.28	1.31	1.45
27	B1	813	4AC	C2-N3	6.27	1.49	1.36
27	B1	1264	4AC	C6-C5	6.27	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	540	4AC	C6-C5	6.27	1.49	1.35
27	B1	2876	4AC	C6-C5	6.27	1.49	1.35
27	B1	1757	4AC	C6-C5	6.27	1.49	1.35
1	A1	87	4AC	C6-C5	6.27	1.49	1.35
1	A1	836	4AC	C6-C5	6.27	1.49	1.35
27	B1	1664	4AC	C6-C5	6.27	1.49	1.35
27	B1	599	4AC	C6-C5	6.27	1.49	1.35
27	B1	798	4AC	C6-C5	6.27	1.49	1.35
1	A1	761	4AC	C6-C5	6.27	1.49	1.35
1	A1	499	4AC	C6-C5	6.26	1.49	1.35
27	B1	1911	4AC	C6-C5	6.26	1.49	1.35
27	B1	116	4AC	C6-C5	6.26	1.49	1.35
27	B1	392	4AC	C6-C5	6.26	1.49	1.35
27	B1	3020	4AC	C6-C5	6.26	1.49	1.35
27	B1	227	4AC	C6-C5	6.26	1.49	1.35
1	A1	5	4AC	C6-C5	6.26	1.49	1.35
27	B1	485	4AC	C6-C5	6.26	1.49	1.35
27	B1	1439	4AC	C6-C5	6.26	1.49	1.35
27	B1	1751	4AC	C6-C5	6.26	1.49	1.35
27	B1	80	4AC	C6-C5	6.26	1.49	1.35
27	B1	1551	4AC	C6-C5	6.26	1.49	1.35
27	B1	1769	4AC	C6-C5	6.26	1.49	1.35
27	B1	2668	OMU	C6-C5	6.26	1.49	1.35
28	B2	117	4AC	C6-C5	6.26	1.49	1.35
1	A1	427	4AC	C2-N3	6.26	1.49	1.36
1	A1	1221	4AC	C6-C5	6.25	1.49	1.35
27	B1	2602	4AC	C6-C5	6.25	1.49	1.35
1	A1	1092	4AC	C6-C5	6.25	1.49	1.35
27	B1	2008	4AC	C6-C5	6.25	1.49	1.35
27	B1	2454	4AC	C6-C5	6.25	1.49	1.35
1	A1	382	4AC	C6-C5	6.25	1.49	1.35
27	B1	3023	4AC	C6-C5	6.25	1.49	1.35
27	B1	2792	4AC	C6-C5	6.25	1.49	1.35
1	A1	636	4AC	C6-C5	6.25	1.49	1.35
27	B1	2844	4AC	C6-C5	6.25	1.49	1.35
27	B1	2469	4AC	C6-C5	6.25	1.49	1.35
1	A1	1368	OMU	C6-C5	6.25	1.49	1.35
27	B1	2113	4AC	C6-C5	6.25	1.49	1.35
1	A1	425	OMU	C6-C5	6.25	1.49	1.35
27	B1	142	4AC	C2-N3	6.24	1.49	1.36
1	A1	762	OMU	C6-C5	6.24	1.49	1.35
1	A1	367	4AC	C6-C5	6.24	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B2	90	4AC	C6-C5	6.24	1.49	1.35
27	B1	454	OMU	C6-C5	6.24	1.49	1.35
1	A1	444	4AC	C6-C5	6.24	1.49	1.35
27	B1	271	4AC	C6-C5	6.24	1.49	1.35
1	A1	195	4AC	C2-N3	6.24	1.49	1.36
27	B1	419	4AC	C6-C5	6.24	1.49	1.35
27	B1	1501	4AC	C6-C5	6.24	1.49	1.35
1	A1	810	4AC	C6-C5	6.24	1.49	1.35
1	A1	220	4AC	C6-C5	6.24	1.49	1.35
1	A1	467	4AC	C6-C5	6.24	1.49	1.35
27	B1	434	4AC	C6-C5	6.24	1.49	1.35
1	A1	291	4AC	C6-C5	6.23	1.49	1.35
1	A1	1467	4AC	C6-C5	6.23	1.49	1.35
27	B1	857	A2M	O4'-C4'	-6.23	1.31	1.45
27	B1	1621	4AC	C2-N3	6.23	1.49	1.36
27	B1	1383	4AC	C6-C5	6.23	1.49	1.35
27	B1	2554	OMU	C6-C5	6.22	1.49	1.35
1	A1	1016	4AC	C2-N3	6.22	1.49	1.36
27	B1	979	4AC	C2-N3	6.22	1.49	1.36
27	B1	243	4AC	C6-C5	6.22	1.49	1.35
27	B1	1322	4AC	C6-C5	6.22	1.49	1.35
27	B1	3011	4AC	C6-C5	6.22	1.49	1.35
1	A1	756	4SU	C6-C5	6.22	1.49	1.35
27	B1	1608	4AC	C2-N3	6.21	1.49	1.36
27	B1	3037	4AC	C2-N3	6.21	1.49	1.36
27	B1	23	4AC	C6-C5	6.21	1.49	1.35
27	B1	732	4AC	C6-C5	6.21	1.49	1.35
27	B1	950	4AC	C6-C5	6.21	1.49	1.35
1	A1	614	4AC	C6-C5	6.21	1.49	1.35
27	B1	953	4AC	C6-C5	6.21	1.49	1.35
1	A1	739	4AC	C6-C5	6.20	1.49	1.35
27	B1	3037	4AC	C6-C5	6.20	1.49	1.35
27	B1	1818	4AC	C6-C5	6.20	1.49	1.35
1	A1	467	4AC	C2-N3	6.20	1.48	1.36
27	B1	1374	4AC	C2-N3	6.20	1.48	1.36
27	B1	2749	4AC	C6-C5	6.20	1.49	1.35
1	A1	141	4AC	C2-N3	6.19	1.48	1.36
27	B1	1061	4AC	C6-C5	6.19	1.49	1.35
27	B1	2850	4AC	C6-C5	6.19	1.49	1.35
27	B1	1734	4AC	C6-C5	6.18	1.49	1.35
27	B1	1150	4AC	C2-N3	6.18	1.48	1.36
1	A1	546	4AC	C2-N3	6.18	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	624	4AC	C6-C5	6.18	1.49	1.35
27	B1	2565	4SU	C6-C5	6.18	1.49	1.35
27	B1	3006	4AC	C2-N3	6.18	1.48	1.36
1	A1	1314	4AC	C6-C5	6.17	1.49	1.35
1	A1	405	4AC	C2-N3	6.17	1.48	1.36
1	A1	761	4AC	C2-N3	6.16	1.48	1.36
27	B1	1706	4AC	C2-N3	6.16	1.48	1.36
1	A1	427	4AC	C6-C5	6.16	1.49	1.35
1	A1	624	4AC	C2-N3	6.16	1.48	1.36
1	A1	636	4AC	C2-N3	6.15	1.48	1.36
1	A1	739	4AC	C2-N3	6.15	1.48	1.36
27	B1	1734	4AC	C2-N3	6.15	1.48	1.36
1	A1	1135	4AC	C2-N3	6.15	1.48	1.36
27	B1	732	4AC	C2-N3	6.15	1.48	1.36
1	A1	220	4AC	C2-N3	6.14	1.48	1.36
1	A1	1221	4AC	C2-N3	6.14	1.48	1.36
1	A1	367	4AC	C2-N3	6.14	1.48	1.36
1	A1	1092	4AC	C2-N3	6.14	1.48	1.36
1	A1	1067	4AC	C2-N3	6.14	1.48	1.36
1	A1	691	4AC	C6-C5	6.14	1.49	1.35
1	A1	614	4AC	C2-N3	6.14	1.48	1.36
1	A1	216	4AC	C2-N3	6.13	1.48	1.36
27	B1	80	4AC	C2-N3	6.13	1.48	1.36
27	B1	1762	4AC	C6-C5	6.13	1.49	1.35
27	B1	1061	4AC	C2-N3	6.13	1.48	1.36
27	B1	1612	4AC	C2-N3	6.12	1.48	1.36
1	A1	87	4AC	C2-N3	6.12	1.48	1.36
27	B1	2429	4AC	C2-N3	6.12	1.48	1.36
27	B1	1286	4AC	C2-N3	6.11	1.48	1.36
27	B1	609	4AC	C2-N3	6.11	1.48	1.36
28	B2	120	4AC	C2-N3	6.11	1.48	1.36
27	B1	1150	4AC	C6-C5	6.11	1.49	1.35
1	A1	816	4AC	C2-N3	6.11	1.48	1.36
1	A1	1314	4AC	C2-N3	6.10	1.48	1.36
27	B1	741	4AC	C2-N3	6.10	1.48	1.36
27	B1	1743	4AC	C2-N3	6.10	1.48	1.36
1	A1	5	4AC	C2-N3	6.10	1.48	1.36
1	A1	719	4AC	C2-N3	6.10	1.48	1.36
1	A1	444	4AC	C2-N3	6.10	1.48	1.36
27	B1	1264	4AC	C2-N3	6.10	1.48	1.36
1	A1	1254	4AC	C2-N3	6.10	1.48	1.36
1	A1	540	4AC	C2-N3	6.09	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	1029	4AC	C2-N3	6.09	1.48	1.36
28	B2	90	4AC	C2-N3	6.09	1.48	1.36
27	B1	2821	4AC	C2-N3	6.09	1.48	1.36
1	A1	382	4AC	C2-N3	6.09	1.48	1.36
27	B1	271	4AC	C2-N3	6.09	1.48	1.36
27	B1	896	4AC	C2-N3	6.09	1.48	1.36
27	B1	2454	4AC	C2-N3	6.08	1.48	1.36
1	A1	836	4AC	C2-N3	6.08	1.48	1.36
27	B1	759	4AC	C2-N3	6.08	1.48	1.36
1	A1	691	4AC	C2-N3	6.08	1.48	1.36
27	B1	1751	4AC	C2-N3	6.08	1.48	1.36
1	A1	307	4AC	C2-N3	6.07	1.48	1.36
1	A1	810	4AC	C2-N3	6.07	1.48	1.36
27	B1	1703	4AC	C2-N3	6.07	1.48	1.36
27	B1	227	4AC	C2-N3	6.07	1.48	1.36
27	B1	392	4AC	C2-N3	6.07	1.48	1.36
1	A1	578	4AC	C2-N3	6.07	1.48	1.36
27	B1	1178	4AC	C2-N3	6.06	1.48	1.36
28	B2	117	4AC	C2-N3	6.06	1.48	1.36
27	B1	276	4AC	C2-N3	6.06	1.48	1.36
27	B1	1818	4AC	C2-N3	6.06	1.48	1.36
27	B1	2749	4AC	C2-N3	6.06	1.48	1.36
27	B1	1762	4AC	C2-N3	6.06	1.48	1.36
27	B1	1664	4AC	C2-N3	6.05	1.48	1.36
1	A1	499	4AC	C2-N3	6.05	1.48	1.36
1	A1	534	4AC	C2-N3	6.05	1.48	1.36
27	B1	2876	4AC	C2-N3	6.05	1.48	1.36
27	B1	3020	4AC	C2-N3	6.05	1.48	1.36
27	B1	1439	4AC	C2-N3	6.05	1.48	1.36
27	B1	130	4AC	C2-N3	6.05	1.48	1.36
1	A1	231	4AC	C2-N3	6.05	1.48	1.36
27	B1	1360	4AC	C2-N3	6.04	1.48	1.36
27	B1	243	4AC	C2-N3	6.04	1.48	1.36
27	B1	1322	4AC	C2-N3	6.04	1.48	1.36
27	B1	2602	4AC	C2-N3	6.04	1.48	1.36
27	B1	2432	4AC	C2-N3	6.04	1.48	1.36
1	A1	827	4AC	C2-N3	6.04	1.48	1.36
27	B1	599	4AC	C2-N3	6.04	1.48	1.36
27	B1	1435	4AC	C2-N3	6.04	1.48	1.36
27	B1	2020	4AC	C2-N3	6.04	1.48	1.36
27	B1	3023	4AC	C2-N3	6.04	1.48	1.36
27	B1	721	4AC	C2-N3	6.03	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	41	4AC	C2-N3	6.03	1.48	1.36
27	B1	1293	4AC	C2-N3	6.03	1.48	1.36
27	B1	1374	4AC	C6-C5	6.03	1.49	1.35
27	B1	715	4AC	C2-N3	6.03	1.48	1.36
1	A1	1288	4AC	C2-N3	6.02	1.48	1.36
27	B1	19	4AC	C2-N3	6.02	1.48	1.36
27	B1	360	4AC	C2-N3	6.02	1.48	1.36
27	B1	688	4AC	C2-N3	6.02	1.48	1.36
27	B1	1911	4AC	C2-N3	6.01	1.48	1.36
27	B1	580	4AC	C2-N3	6.01	1.48	1.36
27	B1	23	4AC	C2-N3	6.01	1.48	1.36
27	B1	1383	4AC	C2-N3	6.01	1.48	1.36
27	B1	1621	4AC	C6-C5	6.01	1.49	1.35
27	B1	1386	4AC	C2-N3	6.01	1.48	1.36
27	B1	2328	4AC	C2-N3	6.01	1.48	1.36
27	B1	479	4AC	C2-N3	6.01	1.48	1.36
27	B1	950	4AC	C2-N3	6.01	1.48	1.36
27	B1	866	4AC	C2-N3	6.01	1.48	1.36
27	B1	3011	4AC	C2-N3	6.01	1.48	1.36
1	A1	1467	4AC	C2-N3	6.00	1.48	1.36
27	B1	2850	4AC	C2-N3	6.00	1.48	1.36
27	B1	953	4AC	C2-N3	6.00	1.48	1.36
27	B1	2469	4AC	C2-N3	6.00	1.48	1.36
1	A1	1227	4AC	C2-N3	6.00	1.48	1.36
27	B1	1313	4AC	C2-N3	6.00	1.48	1.36
27	B1	1757	4AC	C2-N3	6.00	1.48	1.36
27	B1	1107	4AC	C2-N3	5.99	1.48	1.36
27	B1	1360	4AC	C6-C5	5.99	1.49	1.35
1	A1	274	4AC	C2-N3	5.99	1.48	1.36
1	A1	1181	4AC	C2-N3	5.99	1.48	1.36
27	B1	1052	4AC	C2-N3	5.99	1.48	1.36
1	A1	839	4AC	C2-N3	5.99	1.48	1.36
1	A1	706	4AC	C2-N3	5.99	1.48	1.36
27	B1	1064	4AC	C2-N3	5.99	1.48	1.36
1	A1	856	4AC	C2-N3	5.99	1.48	1.36
27	B1	1067	4AC	C2-N3	5.99	1.48	1.36
27	B1	1551	4AC	C2-N3	5.98	1.48	1.36
27	B1	813	4AC	C6-C5	5.98	1.49	1.35
27	B1	1649	4AC	C2-N3	5.98	1.48	1.36
27	B1	419	4AC	C2-N3	5.98	1.48	1.36
27	B1	933	4AC	C6-C5	5.97	1.48	1.35
27	B1	979	4AC	C6-C5	5.97	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2792	4AC	C2-N3	5.97	1.48	1.36
27	B1	1404	4AC	C2-N3	5.97	1.48	1.36
27	B1	98	4AC	C2-N3	5.97	1.48	1.36
27	B1	807	4AC	C2-N3	5.97	1.48	1.36
27	B1	1639	4AC	C2-N3	5.96	1.48	1.36
27	B1	1286	4AC	C6-C5	5.96	1.48	1.35
27	B1	2888	4AC	C2-N3	5.96	1.48	1.36
27	B1	1885	4AC	C2-N3	5.95	1.48	1.36
1	A1	291	4AC	C2-N3	5.95	1.48	1.36
27	B1	2492	4AC	C2-N3	5.95	1.48	1.36
27	B1	1478	4AC	C2-N3	5.95	1.48	1.36
27	B1	1769	4AC	C2-N3	5.95	1.48	1.36
27	B1	1442	4AC	C2-N3	5.95	1.48	1.36
27	B1	1290	4AC	C2-N3	5.95	1.48	1.36
27	B1	2213	4AC	C2-N3	5.94	1.48	1.36
27	B1	2844	4AC	C2-N3	5.94	1.48	1.36
27	B1	798	4AC	C2-N3	5.93	1.48	1.36
27	B1	1501	4AC	C2-N3	5.93	1.48	1.36
27	B1	485	4AC	C2-N3	5.93	1.48	1.36
27	B1	1967	4AC	C2-N3	5.93	1.48	1.36
27	B1	2113	4AC	C2-N3	5.93	1.48	1.36
27	B1	1846	4AC	C2-N3	5.93	1.48	1.36
27	B1	337	4AC	C2-N3	5.92	1.48	1.36
27	B1	2171	4AC	C2-N3	5.92	1.48	1.36
27	B1	116	4AC	C2-N3	5.92	1.48	1.36
27	B1	1100	4AC	C2-N3	5.92	1.48	1.36
27	B1	1128	4AC	C2-N3	5.92	1.48	1.36
27	B1	162	4AC	C2-N3	5.92	1.48	1.36
27	B1	1505	4AC	C2-N3	5.91	1.48	1.36
27	B1	933	4AC	C2-N3	5.91	1.48	1.36
27	B1	2008	4AC	C2-N3	5.91	1.48	1.36
27	B1	786	4AC	C2-N3	5.91	1.48	1.36
27	B1	48	4AC	C2-N3	5.90	1.48	1.36
27	B1	2526	4AC	C2-N3	5.90	1.48	1.36
27	B1	1546	4AC	C2-N3	5.89	1.48	1.36
27	B1	1822	4AC	C2-N3	5.89	1.48	1.36
27	B1	1608	4AC	C6-C5	5.89	1.48	1.35
27	B1	652	4AC	C2-N3	5.89	1.48	1.36
27	B1	434	4AC	C2-N3	5.88	1.48	1.36
27	B1	2809	4AC	C2-N3	5.86	1.48	1.36
27	B1	2133	4AC	C2-N3	5.85	1.48	1.36
27	B1	200	4AC	C2-N3	5.84	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	880	A2M	O4'-C4'	-5.83	1.32	1.45
27	B1	2700	UR3	C2-N3	5.82	1.50	1.39
1	A1	481	G7M	C2-N3	5.82	1.47	1.33
1	A1	1362	5MC	C4-N3	5.81	1.44	1.34
1	A1	466	5MC	C4-N3	5.79	1.43	1.34
27	B1	2067	5MC	C4-N3	5.78	1.43	1.34
1	A1	1190	5MC	C4-N3	5.77	1.43	1.34
1	A1	473	5MC	C4-N3	5.77	1.43	1.34
27	B1	2379	4AC	C2-N3	5.76	1.48	1.36
27	B1	1648	5MC	C4-N3	5.76	1.43	1.34
1	A1	826	5MC	C4-N3	5.75	1.43	1.34
1	A1	1015	5MC	C4-N3	5.74	1.43	1.34
27	B1	275	5MC	C4-N3	5.73	1.43	1.34
1	A1	1012	5MC	C4-N3	5.73	1.43	1.34
1	A1	1013	5MC	C4-N3	5.73	1.43	1.34
1	A1	855	5MC	C4-N3	5.72	1.43	1.34
1	A1	681	5MC	C4-N3	5.71	1.43	1.34
27	B1	2453	5MC	C4-N3	5.70	1.43	1.34
1	A1	1348	5MC	C4-N3	5.70	1.43	1.34
1	A1	1486	5MC	C4-N3	5.69	1.43	1.34
27	B1	336	5MC	C4-N3	5.69	1.43	1.34
27	B1	2875	5MC	C4-N3	5.68	1.43	1.34
1	A1	605	5MC	C4-N3	5.67	1.43	1.34
1	A1	523	5MC	C4-N3	5.67	1.43	1.34
27	B1	226	5MC	C4-N3	5.67	1.43	1.34
1	A1	951	5MC	C4-N3	5.67	1.43	1.34
1	A1	230	5MC	C4-N3	5.66	1.43	1.34
1	A1	718	5MC	C4-N3	5.66	1.43	1.34
27	B1	47	5MC	C4-N3	5.66	1.43	1.34
1	A1	17	5MC	C4-N3	5.66	1.43	1.34
1	A1	273	5MC	C4-N3	5.66	1.43	1.34
27	B1	18	5MC	C4-N3	5.65	1.43	1.34
1	A1	623	5MC	C4-N3	5.65	1.43	1.34
27	B1	1966	5MC	C4-N3	5.64	1.43	1.34
1	A1	687	5MC	C4-N3	5.64	1.43	1.34
27	B1	1620	5MC	C4-N3	5.64	1.43	1.34
1	A1	863	5MC	C4-N3	5.64	1.43	1.34
27	B1	2087	5MC	C4-N3	5.63	1.43	1.34
27	B1	97	5MC	C4-N3	5.62	1.43	1.34
27	B1	932	5MC	C4-N3	5.62	1.43	1.34
27	B1	1977	5MC	C4-N3	5.62	1.43	1.34
1	A1	1015	5MC	C2-N3	5.62	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	877	5MC	C4-N3	5.62	1.43	1.34
27	B1	1451	5MC	C4-N3	5.61	1.43	1.34
27	B1	2617	5MC	C4-N3	5.61	1.43	1.34
1	A1	1484	5MC	C4-N3	5.60	1.43	1.34
1	A1	533	5MC	C4-N3	5.59	1.43	1.34
1	A1	681	5MC	C2-N3	5.58	1.47	1.36
1	A1	645	OMG	C2-N3	5.58	1.46	1.33
27	B1	1149	5MC	C4-N3	5.58	1.43	1.34
27	B1	2082	5MC	C4-N3	5.57	1.43	1.34
1	A1	1013	5MC	C2-N3	5.57	1.47	1.36
1	A1	1348	5MC	C2-N3	5.57	1.47	1.36
1	A1	1362	5MC	C2-N3	5.57	1.47	1.36
27	B1	359	5MC	C4-N3	5.57	1.43	1.34
27	B1	1868	5MC	C4-N3	5.56	1.43	1.34
1	A1	863	5MC	C2-N3	5.56	1.47	1.36
27	B1	275	5MC	C2-N3	5.56	1.47	1.36
1	A1	1012	5MC	C2-N3	5.55	1.47	1.36
27	B1	336	5MC	C2-N3	5.55	1.47	1.36
1	A1	1486	5MC	C2-N3	5.55	1.47	1.36
27	B1	18	5MC	C2-N3	5.55	1.47	1.36
1	A1	466	5MC	C2-N3	5.54	1.47	1.36
1	A1	473	5MC	C2-N3	5.54	1.47	1.36
1	A1	951	5MC	C2-N3	5.53	1.47	1.36
27	B1	1983	5MC	C4-N3	5.53	1.43	1.34
1	A1	855	5MC	C2-N3	5.53	1.47	1.36
27	B1	1451	5MC	C2-N3	5.52	1.47	1.36
1	A1	273	5MC	C2-N3	5.52	1.47	1.36
27	B1	226	5MC	C2-N3	5.52	1.47	1.36
27	B1	877	5MC	C2-N3	5.52	1.47	1.36
27	B1	2067	5MC	C2-N3	5.52	1.47	1.36
1	A1	1190	5MC	C2-N3	5.52	1.47	1.36
27	B1	2453	5MC	C2-N3	5.52	1.47	1.36
1	A1	17	5MC	C2-N3	5.52	1.47	1.36
1	A1	523	5MC	C2-N3	5.51	1.47	1.36
27	B1	1648	5MC	C2-N3	5.51	1.47	1.36
1	A1	826	5MC	C2-N3	5.51	1.47	1.36
27	B1	1966	5MC	C2-N3	5.51	1.47	1.36
1	A1	605	5MC	C2-N3	5.50	1.47	1.36
1	A1	230	5MC	C2-N3	5.50	1.47	1.36
1	A1	718	5MC	C2-N3	5.49	1.47	1.36
27	B1	2875	5MC	C2-N3	5.49	1.47	1.36
1	A1	533	5MC	C2-N3	5.49	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	97	5MC	C2-N3	5.49	1.47	1.36
27	B1	359	5MC	C2-N3	5.49	1.47	1.36
1	A1	153	OMG	C2-N3	5.49	1.46	1.33
27	B1	1977	5MC	C2-N3	5.48	1.47	1.36
27	B1	2087	5MC	C2-N3	5.48	1.47	1.36
1	A1	1484	5MC	C2-N3	5.48	1.47	1.36
27	B1	1868	5MC	C2-N3	5.47	1.47	1.36
27	B1	1620	5MC	C2-N3	5.47	1.47	1.36
1	A1	623	5MC	C2-N3	5.45	1.47	1.36
27	B1	932	5MC	C2-N3	5.45	1.47	1.36
27	B1	47	5MC	C2-N3	5.45	1.47	1.36
1	A1	687	5MC	C2-N3	5.44	1.47	1.36
27	B1	1983	5MC	C2-N3	5.44	1.47	1.36
1	A1	833	OMG	C2-N3	5.43	1.46	1.33
27	B1	1149	5MC	C2-N3	5.43	1.47	1.36
1	A1	1003	OMG	C2-N3	5.43	1.46	1.33
27	B1	2617	5MC	C2-N3	5.42	1.47	1.36
1	A1	459	OMG	C2-N3	5.42	1.46	1.33
27	B1	887	OMG	C2-N3	5.41	1.46	1.33
27	B1	920	OMG	C2-N3	5.41	1.46	1.33
27	B1	2082	5MC	C2-N3	5.38	1.47	1.36
27	B1	2365	OMG	C2-N3	5.37	1.46	1.33
27	B1	841	OMG	C2-N3	5.36	1.46	1.33
1	A1	763	OMG	C2-N3	5.35	1.46	1.33
1	A1	455	OMG	C2-N3	5.35	1.46	1.33
1	A1	668	OMG	C2-N3	5.34	1.46	1.33
1	A1	901	OMG	C2-N3	5.34	1.46	1.33
1	A1	1004	2MG	C2-N2	5.34	1.45	1.33
1	A1	329	OMG	C2-N3	5.32	1.46	1.33
27	B1	1557	OMG	C2-N3	5.32	1.46	1.33
27	B1	2540	OMG	C2-N3	5.31	1.46	1.33
27	B1	1965	OMG	C2-N3	5.30	1.46	1.33
27	B1	2740	OMG	C2-N3	5.30	1.46	1.33
27	B1	2428	OMC	C4-N3	5.29	1.45	1.34
1	A1	507	OMG	C2-N3	5.27	1.46	1.33
27	B1	2659	OMG	C2-N3	5.27	1.46	1.33
27	B1	2022	OMG	C2-N3	5.26	1.46	1.33
27	B1	921	OMG	C2-N3	5.26	1.46	1.33
27	B1	1533	OMG	C2-N3	5.26	1.46	1.33
27	B1	2028	OMG	C2-N3	5.25	1.46	1.33
27	B1	2180	OMG	C2-N3	5.25	1.45	1.33
1	A1	426	OMC	C4-N3	5.24	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2684	OMG	C2-N3	5.24	1.45	1.33
1	A1	1252	OMC	C4-N3	5.23	1.45	1.34
27	B1	808	OMG	C2-N3	5.22	1.45	1.33
1	A1	228	OMG	C2-N3	5.21	1.45	1.33
1	A1	861	OMG	C2-N3	5.21	1.45	1.33
27	B1	214	OMG	C2-N3	5.21	1.45	1.33
27	B1	675	OMG	C2-N3	5.20	1.45	1.33
1	A1	1194	OMC	C4-N3	5.20	1.45	1.34
1	A1	117	OMC	C4-N3	5.20	1.45	1.34
27	B1	2984	OMG	C2-N3	5.19	1.45	1.33
27	B1	2562	OMG	C2-N3	5.19	1.45	1.33
27	B1	1601	OMG	C2-N3	5.18	1.45	1.33
27	B1	1832	OMC	C4-N3	5.18	1.44	1.34
1	A1	227	OMG	C2-N3	5.18	1.45	1.33
27	B1	2735	OMC	C4-N3	5.16	1.44	1.34
27	B1	2757	OMG	C2-N3	5.16	1.45	1.33
1	A1	1270	OMC	C4-N3	5.16	1.44	1.34
27	B1	2808	OMC	C4-N3	5.16	1.44	1.34
27	B1	2607	OMC	C4-N3	5.14	1.44	1.34
27	B1	2059	OMC	C4-N3	5.12	1.44	1.34
27	B1	501	OMC	C4-N3	5.12	1.44	1.34
27	B1	1783	OMC	C4-N3	5.11	1.44	1.34
27	B1	2119	OMC	C4-N3	5.11	1.44	1.34
27	B1	1489	OMC	C4-N3	5.09	1.44	1.34
1	A1	834	OMC	C4-N3	5.08	1.44	1.34
27	B1	2557	OMC	C4-N3	5.08	1.44	1.34
27	B1	977	OMC	C4-N3	5.08	1.44	1.34
27	B1	1099	OMC	C4-N3	5.07	1.44	1.34
1	A1	645	OMG	C4-N3	5.07	1.49	1.37
27	B1	2391	OMG	C2-N3	5.04	1.45	1.33
27	B1	1914	OMC	C4-N3	5.00	1.44	1.34
1	A1	153	OMG	C4-N3	5.00	1.49	1.37
1	A1	459	OMG	C4-N3	4.97	1.49	1.37
1	A1	1003	OMG	C4-N3	4.96	1.49	1.37
27	B1	2659	OMG	C4-N3	4.95	1.49	1.37
27	B1	920	OMG	C4-N3	4.95	1.49	1.37
27	B1	1965	OMG	C4-N3	4.94	1.49	1.37
27	B1	841	OMG	C4-N3	4.94	1.49	1.37
1	A1	763	OMG	C4-N3	4.93	1.49	1.37
1	A1	668	OMG	C4-N3	4.93	1.49	1.37
1	A1	833	OMG	C4-N3	4.92	1.49	1.37
27	B1	2022	OMG	C4-N3	4.92	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1557	OMG	C4-N3	4.91	1.49	1.37
27	B1	887	OMG	C4-N3	4.91	1.49	1.37
27	B1	2540	OMG	C4-N3	4.91	1.49	1.37
27	B1	2365	OMG	C4-N3	4.91	1.49	1.37
1	A1	329	OMG	C4-N3	4.91	1.49	1.37
1	A1	901	OMG	C4-N3	4.90	1.49	1.37
27	B1	2028	OMG	C4-N3	4.90	1.49	1.37
1	A1	1004	2MG	C2-N1	4.90	1.44	1.36
1	A1	455	OMG	C4-N3	4.88	1.49	1.37
1	A1	507	OMG	C4-N3	4.87	1.49	1.37
1	A1	1004	2MG	C4-N3	4.87	1.49	1.37
27	B1	813	4AC	C7-N4	4.87	1.46	1.37
27	B1	214	OMG	C4-N3	4.87	1.49	1.37
1	A1	861	OMG	C4-N3	4.86	1.49	1.37
27	B1	2740	OMG	C4-N3	4.86	1.49	1.37
1	A1	427	4AC	C7-N4	4.86	1.46	1.37
27	B1	808	OMG	C4-N3	4.85	1.49	1.37
27	B1	921	OMG	C4-N3	4.85	1.49	1.37
27	B1	1533	OMG	C4-N3	4.85	1.49	1.37
27	B1	2684	OMG	C4-N3	4.83	1.49	1.37
27	B1	1601	OMG	C4-N3	4.82	1.49	1.37
27	B1	2180	OMG	C4-N3	4.82	1.49	1.37
27	B1	2984	OMG	C4-N3	4.82	1.49	1.37
1	A1	1029	4AC	C7-N4	4.82	1.46	1.37
1	A1	228	OMG	C4-N3	4.80	1.49	1.37
27	B1	1064	4AC	C7-N4	4.79	1.46	1.37
1	A1	901	OMG	C2-N2	4.79	1.45	1.34
1	A1	227	OMG	C4-N3	4.79	1.49	1.37
1	A1	459	OMG	C2-N2	4.79	1.45	1.34
27	B1	2757	OMG	C4-N3	4.78	1.49	1.37
27	B1	675	OMG	C4-N3	4.78	1.48	1.37
1	A1	1003	OMG	C2-N2	4.77	1.45	1.34
1	A1	153	OMG	C2-N2	4.77	1.45	1.34
1	A1	481	G7M	C6-N1	4.76	1.45	1.37
1	A1	329	OMG	C2-N2	4.76	1.45	1.34
27	B1	1608	4AC	C7-N4	4.76	1.46	1.37
1	A1	833	OMG	C2-N2	4.76	1.45	1.34
1	A1	624	4AC	C7-N4	4.76	1.46	1.37
1	A1	1366	A1I59	C4-N4	4.76	1.46	1.34
27	B1	920	OMG	C2-N2	4.75	1.45	1.34
1	A1	763	OMG	C2-N2	4.75	1.45	1.34
1	A1	645	OMG	C2-N2	4.75	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	142	4AC	C7-N4	4.75	1.46	1.37
1	A1	455	OMG	C2-N2	4.75	1.45	1.34
27	B1	2562	OMG	C4-N3	4.75	1.48	1.37
1	A1	1364	LHH	C7-N4	4.74	1.46	1.37
27	B1	2740	OMG	C2-N2	4.74	1.45	1.34
27	B1	2391	OMG	C4-N3	4.74	1.48	1.37
1	A1	1221	4AC	C7-N4	4.73	1.46	1.37
1	A1	507	OMG	C2-N2	4.73	1.45	1.34
27	B1	2180	OMG	C2-N2	4.73	1.45	1.34
1	A1	481	G7M	C2-N2	4.72	1.45	1.34
27	B1	1734	4AC	C7-N4	4.72	1.45	1.37
27	B1	979	4AC	C7-N4	4.72	1.45	1.37
27	B1	2540	OMG	C2-N2	4.72	1.45	1.34
27	B1	1965	OMG	C2-N2	4.71	1.45	1.34
1	A1	141	4AC	C7-N4	4.71	1.45	1.37
1	A1	228	OMG	C2-N2	4.71	1.45	1.34
27	B1	2984	OMG	C2-N2	4.71	1.45	1.34
27	B1	887	OMG	C2-N2	4.71	1.45	1.34
27	B1	921	OMG	C2-N2	4.71	1.45	1.34
27	B1	1557	OMG	C2-N2	4.71	1.45	1.34
27	B1	2659	OMG	C2-N2	4.71	1.45	1.34
1	A1	227	OMG	C2-N2	4.71	1.45	1.34
27	B1	841	OMG	C2-N2	4.71	1.45	1.34
27	B1	214	OMG	C2-N2	4.70	1.45	1.34
1	A1	1135	4AC	C7-N4	4.70	1.45	1.37
27	B1	1533	OMG	C2-N2	4.70	1.45	1.34
1	A1	1092	4AC	C7-N4	4.70	1.45	1.37
27	B1	1374	4AC	C7-N4	4.70	1.45	1.37
27	B1	2028	OMG	C2-N2	4.70	1.45	1.34
27	B1	378	4AC	C4-N4	4.70	1.46	1.39
27	B1	2022	OMG	C2-N2	4.69	1.45	1.34
1	A1	668	OMG	C2-N2	4.69	1.45	1.34
1	A1	467	4AC	C7-N4	4.69	1.45	1.37
27	B1	641	LHH	C7-N4	4.69	1.45	1.37
27	B1	1601	OMG	C2-N2	4.69	1.45	1.34
27	B1	904	LHH	C7-N4	4.68	1.45	1.37
27	B1	675	OMG	C2-N2	4.68	1.45	1.34
27	B1	2757	OMG	C2-N2	4.68	1.45	1.34
27	B1	2565	4SU	C5-C4	4.68	1.48	1.42
27	B1	2365	OMG	C2-N2	4.68	1.45	1.34
1	A1	756	4SU	C5-C4	4.68	1.48	1.42
27	B1	378	4AC	C7-N4	4.68	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2684	OMG	C2-N2	4.68	1.45	1.34
1	A1	861	OMG	C2-N2	4.67	1.45	1.34
1	A1	195	4AC	C7-N4	4.67	1.45	1.37
27	B1	1639	4AC	C7-N4	4.66	1.45	1.37
1	A1	810	4AC	C7-N4	4.66	1.45	1.37
27	B1	1061	4AC	C7-N4	4.66	1.45	1.37
27	B1	1621	4AC	C7-N4	4.66	1.45	1.37
1	A1	1016	4AC	C7-N4	4.65	1.45	1.37
27	B1	1612	4AC	C7-N4	4.65	1.45	1.37
27	B1	2562	OMG	C2-N2	4.65	1.45	1.34
28	B2	120	4AC	C7-N4	4.65	1.45	1.37
1	A1	636	4AC	C7-N4	4.65	1.45	1.37
27	B1	3037	4AC	C7-N4	4.65	1.45	1.37
1	A1	546	4AC	C7-N4	4.65	1.45	1.37
27	B1	3006	4AC	C7-N4	4.64	1.45	1.37
27	B1	808	OMG	C2-N2	4.64	1.45	1.34
1	A1	444	4AC	C7-N4	4.64	1.45	1.37
1	A1	761	4AC	C7-N4	4.64	1.45	1.37
27	B1	2454	4AC	C7-N4	4.64	1.45	1.37
27	B1	1150	4AC	C7-N4	4.63	1.45	1.37
27	B1	609	4AC	C7-N4	4.63	1.45	1.37
27	B1	2850	4AC	C7-N4	4.63	1.45	1.37
1	A1	1288	4AC	C7-N4	4.62	1.45	1.37
1	A1	1314	4AC	C7-N4	4.62	1.45	1.37
27	B1	1286	4AC	C7-N4	4.62	1.45	1.37
1	A1	540	4AC	C7-N4	4.62	1.45	1.37
27	B1	243	4AC	C7-N4	4.62	1.45	1.37
1	A1	405	4AC	C7-N4	4.62	1.45	1.37
27	B1	1478	4AC	C7-N4	4.61	1.45	1.37
27	B1	1365	LHH	C7-N4	4.61	1.45	1.37
27	B1	1664	4AC	C7-N4	4.61	1.45	1.37
1	A1	739	4AC	C7-N4	4.61	1.45	1.37
27	B1	759	4AC	C7-N4	4.61	1.45	1.37
1	A1	816	4AC	C7-N4	4.60	1.45	1.37
1	A1	1254	4AC	C7-N4	4.60	1.45	1.37
1	A1	216	4AC	C7-N4	4.60	1.45	1.37
1	A1	836	4AC	C7-N4	4.59	1.45	1.37
27	B1	3020	4AC	C7-N4	4.59	1.45	1.37
27	B1	392	4AC	C7-N4	4.59	1.45	1.37
27	B1	2429	4AC	C7-N4	4.59	1.45	1.37
27	B1	2602	4AC	C7-N4	4.59	1.45	1.37
27	B1	599	4AC	C7-N4	4.59	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1703	4AC	C7-N4	4.59	1.45	1.37
27	B1	741	4AC	C7-N4	4.59	1.45	1.37
1	A1	382	4AC	C7-N4	4.59	1.45	1.37
1	A1	1067	4AC	C7-N4	4.59	1.45	1.37
27	B1	360	4AC	C7-N4	4.58	1.45	1.37
27	B1	2876	4AC	C7-N4	4.58	1.45	1.37
27	B1	271	4AC	C7-N4	4.58	1.45	1.37
27	B1	1743	4AC	C7-N4	4.58	1.45	1.37
1	A1	220	4AC	C7-N4	4.58	1.45	1.37
27	B1	732	4AC	C7-N4	4.58	1.45	1.37
1	A1	614	4AC	C7-N4	4.58	1.45	1.37
27	B1	786	4AC	C7-N4	4.58	1.45	1.37
27	B1	3023	4AC	C7-N4	4.58	1.45	1.37
27	B1	1360	4AC	C7-N4	4.58	1.45	1.37
27	B1	2526	4AC	C7-N4	4.57	1.45	1.37
1	A1	87	4AC	C7-N4	4.57	1.45	1.37
27	B1	1818	4AC	C7-N4	4.57	1.45	1.37
27	B1	2391	OMG	C2-N2	4.57	1.45	1.34
27	B1	23	4AC	C7-N4	4.57	1.45	1.37
1	A1	1181	4AC	C7-N4	4.57	1.45	1.37
1	A1	5	4AC	C7-N4	4.57	1.45	1.37
27	B1	130	4AC	C7-N4	4.56	1.45	1.37
1	A1	367	4AC	C7-N4	4.56	1.45	1.37
27	B1	950	4AC	C7-N4	4.56	1.45	1.37
27	B1	1264	4AC	C7-N4	4.56	1.45	1.37
27	B1	1386	4AC	C7-N4	4.56	1.45	1.37
27	B1	276	4AC	C7-N4	4.56	1.45	1.37
27	B1	1706	4AC	C7-N4	4.56	1.45	1.37
27	B1	1751	4AC	C7-N4	4.56	1.45	1.37
27	B1	2888	4AC	C7-N4	4.55	1.45	1.37
1	A1	827	4AC	C7-N4	4.55	1.45	1.37
27	B1	580	4AC	C7-N4	4.55	1.45	1.37
27	B1	2020	4AC	C7-N4	4.55	1.45	1.37
27	B1	2113	4AC	C7-N4	4.55	1.45	1.37
1	A1	499	4AC	C7-N4	4.55	1.45	1.37
1	A1	856	4AC	C7-N4	4.55	1.45	1.37
1	A1	1467	4AC	C7-N4	4.54	1.45	1.37
27	B1	1439	4AC	C7-N4	4.54	1.45	1.37
28	B2	90	4AC	C7-N4	4.54	1.45	1.37
27	B1	1067	4AC	C7-N4	4.54	1.45	1.37
27	B1	1757	4AC	C7-N4	4.54	1.45	1.37
27	B1	2008	4AC	C7-N4	4.54	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	227	4AC	C7-N4	4.54	1.45	1.37
27	B1	896	4AC	C7-N4	4.54	1.45	1.37
27	B1	1052	4AC	C7-N4	4.54	1.45	1.37
1	A1	291	4AC	C7-N4	4.54	1.45	1.37
27	B1	1501	4AC	C7-N4	4.53	1.45	1.37
27	B1	1762	4AC	C7-N4	4.53	1.45	1.37
1	A1	1227	4AC	C7-N4	4.53	1.45	1.37
27	B1	1546	4AC	C7-N4	4.53	1.45	1.37
27	B1	3011	4AC	C7-N4	4.53	1.45	1.37
27	B1	80	4AC	C7-N4	4.53	1.45	1.37
27	B1	1293	4AC	C7-N4	4.53	1.45	1.37
27	B1	1322	4AC	C7-N4	4.53	1.45	1.37
27	B1	866	4AC	C7-N4	4.52	1.45	1.37
27	B1	1946	LHH	C7-N4	4.52	1.45	1.37
27	B1	688	4AC	C7-N4	4.52	1.45	1.37
1	A1	307	4AC	C7-N4	4.52	1.45	1.37
1	A1	578	4AC	C7-N4	4.52	1.45	1.37
1	A1	719	4AC	C7-N4	4.52	1.45	1.37
1	A1	1029	4AC	C4-N4	4.52	1.46	1.39
28	B2	117	4AC	C7-N4	4.51	1.45	1.37
27	B1	162	4AC	C7-N4	4.51	1.45	1.37
27	B1	652	4AC	C7-N4	4.51	1.45	1.37
27	B1	1178	4AC	C7-N4	4.51	1.45	1.37
1	A1	706	4AC	C7-N4	4.51	1.45	1.37
27	B1	1313	4AC	C7-N4	4.51	1.45	1.37
27	B1	2432	4AC	C7-N4	4.51	1.45	1.37
27	B1	721	4AC	C7-N4	4.51	1.45	1.37
27	B1	807	4AC	C7-N4	4.51	1.45	1.37
27	B1	479	4AC	C7-N4	4.51	1.45	1.37
27	B1	2792	4AC	C7-N4	4.51	1.45	1.37
27	B1	502	LHH	C7-N4	4.51	1.45	1.37
27	B1	798	4AC	C7-N4	4.50	1.45	1.37
27	B1	2821	4AC	C7-N4	4.50	1.45	1.37
27	B1	2469	4AC	C7-N4	4.50	1.45	1.37
27	B1	1911	4AC	C7-N4	4.50	1.45	1.37
27	B1	1435	4AC	C7-N4	4.50	1.45	1.37
27	B1	2328	4AC	C7-N4	4.50	1.45	1.37
1	A1	41	4AC	C7-N4	4.50	1.45	1.37
1	A1	691	4AC	C7-N4	4.50	1.45	1.37
27	B1	2749	4AC	C7-N4	4.49	1.45	1.37
27	B1	715	4AC	C7-N4	4.49	1.45	1.37
27	B1	1383	4AC	C7-N4	4.49	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1846	4AC	C7-N4	4.49	1.45	1.37
27	B1	953	4AC	C7-N4	4.48	1.45	1.37
27	B1	2844	4AC	C7-N4	4.48	1.45	1.37
27	B1	2171	4AC	C7-N4	4.48	1.45	1.37
1	A1	839	4AC	C7-N4	4.47	1.45	1.37
27	B1	2809	4AC	C7-N4	4.47	1.45	1.37
27	B1	1551	4AC	C7-N4	4.47	1.45	1.37
27	B1	1649	4AC	C7-N4	4.47	1.45	1.37
27	B1	200	4AC	C7-N4	4.47	1.45	1.37
1	A1	238	LHH	C7-N4	4.47	1.45	1.37
1	A1	534	4AC	C7-N4	4.46	1.45	1.37
1	A1	274	4AC	C7-N4	4.46	1.45	1.37
27	B1	485	4AC	C7-N4	4.46	1.45	1.37
27	B1	2492	4AC	C7-N4	4.45	1.45	1.37
1	A1	231	4AC	C7-N4	4.45	1.45	1.37
27	B1	2213	4AC	C7-N4	4.45	1.45	1.37
27	B1	419	4AC	C7-N4	4.45	1.45	1.37
27	B1	1442	4AC	C7-N4	4.45	1.45	1.37
27	B1	98	4AC	C7-N4	4.44	1.45	1.37
27	B1	1128	4AC	C7-N4	4.44	1.45	1.37
27	B1	1885	4AC	C7-N4	4.44	1.45	1.37
27	B1	19	4AC	C7-N4	4.44	1.45	1.37
27	B1	2133	4AC	C7-N4	4.43	1.45	1.37
27	B1	116	4AC	C7-N4	4.43	1.45	1.37
27	B1	1404	4AC	C7-N4	4.42	1.45	1.37
27	B1	1822	4AC	C7-N4	4.42	1.45	1.37
1	A1	1362	5MC	C2-N1	4.42	1.49	1.40
27	B1	527	LHH	C7-N4	4.41	1.45	1.37
1	A1	466	5MC	C2-N1	4.41	1.49	1.40
27	B1	1100	4AC	C7-N4	4.41	1.45	1.37
27	B1	434	4AC	C7-N4	4.41	1.45	1.37
27	B1	1290	4AC	C7-N4	4.40	1.45	1.37
1	A1	273	5MC	C2-N1	4.40	1.49	1.40
1	A1	1013	5MC	C2-N1	4.40	1.49	1.40
27	B1	2428	OMC	C2-N1	4.40	1.49	1.40
27	B1	1107	4AC	C7-N4	4.40	1.45	1.37
1	A1	951	5MC	C2-N1	4.40	1.49	1.40
27	B1	1769	4AC	C7-N4	4.40	1.45	1.37
27	B1	1064	4AC	C4-N4	4.39	1.46	1.39
1	A1	426	OMC	C2-N1	4.38	1.49	1.40
27	B1	275	5MC	C2-N1	4.38	1.49	1.40
27	B1	2379	4AC	C7-N4	4.37	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	933	4AC	C7-N4	4.37	1.45	1.37
1	A1	1012	5MC	C2-N1	4.37	1.49	1.40
27	B1	336	5MC	C2-N1	4.37	1.49	1.40
27	B1	1967	4AC	C7-N4	4.37	1.45	1.37
27	B1	2087	5MC	C2-N1	4.37	1.49	1.40
27	B1	1832	OMC	C2-N1	4.37	1.49	1.40
27	B1	1639	4AC	C4-N4	4.37	1.46	1.39
1	A1	1194	OMC	C2-N1	4.36	1.49	1.40
27	B1	2968	LHH	C7-N4	4.36	1.45	1.37
27	B1	337	4AC	C7-N4	4.36	1.45	1.37
1	A1	427	4AC	C4-N4	4.35	1.46	1.39
1	A1	739	4AC	C4-N4	4.35	1.46	1.39
27	B1	2875	5MC	C2-N1	4.34	1.49	1.40
1	A1	1015	5MC	C2-N1	4.34	1.49	1.40
1	A1	1486	5MC	C2-N1	4.34	1.49	1.40
1	A1	1348	5MC	C2-N1	4.34	1.49	1.40
1	A1	1362	5MC	C6-N1	4.34	1.45	1.38
27	B1	1451	5MC	C2-N1	4.34	1.49	1.40
1	A1	1190	5MC	C2-N1	4.33	1.49	1.40
1	A1	17	5MC	C2-N1	4.33	1.49	1.40
27	B1	1505	4AC	C7-N4	4.33	1.45	1.37
27	B1	2617	5MC	C2-N1	4.33	1.49	1.40
1	A1	523	5MC	C2-N1	4.33	1.49	1.40
27	B1	1648	5MC	C2-N1	4.33	1.49	1.40
1	A1	473	5MC	C2-N1	4.33	1.49	1.40
27	B1	275	5MC	C6-N1	4.32	1.45	1.38
1	A1	623	5MC	C2-N1	4.32	1.49	1.40
27	B1	359	5MC	C2-N1	4.32	1.49	1.40
27	B1	2875	5MC	C6-N1	4.32	1.45	1.38
27	B1	1983	5MC	C6-N1	4.32	1.45	1.38
1	A1	605	5MC	C2-N1	4.32	1.49	1.40
1	A1	1254	4AC	C4-N4	4.32	1.46	1.39
1	A1	855	5MC	C2-N1	4.32	1.49	1.40
1	A1	195	4AC	C4-N4	4.31	1.46	1.39
1	A1	467	4AC	C4-N4	4.31	1.46	1.39
27	B1	142	4AC	C4-N4	4.31	1.46	1.39
1	A1	141	4AC	C4-N4	4.31	1.46	1.39
1	A1	1190	5MC	C6-N1	4.31	1.45	1.38
27	B1	97	5MC	C2-N1	4.31	1.49	1.40
27	B1	2067	5MC	C2-N1	4.31	1.49	1.40
27	B1	813	4AC	C4-N4	4.31	1.46	1.39
1	A1	826	5MC	C2-N1	4.31	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	609	4AC	C4-N4	4.31	1.46	1.39
27	B1	18	5MC	C2-N1	4.31	1.49	1.40
27	B1	48	4AC	C7-N4	4.31	1.45	1.37
1	A1	1364	LHH	C4-N3	4.31	1.40	1.32
27	B1	1914	OMC	C2-N1	4.30	1.49	1.40
1	A1	623	5MC	C6-N1	4.30	1.45	1.38
27	B1	2067	5MC	C6-N1	4.30	1.45	1.38
1	A1	473	5MC	C6-N1	4.30	1.45	1.38
1	A1	533	5MC	C6-N1	4.29	1.45	1.38
27	B1	1620	5MC	C2-N1	4.29	1.49	1.40
27	B1	2059	OMC	C2-N1	4.29	1.49	1.40
1	A1	1012	5MC	C6-N1	4.29	1.45	1.38
27	B1	2453	5MC	C6-N1	4.29	1.45	1.38
27	B1	759	4AC	C4-N4	4.29	1.46	1.39
27	B1	1478	4AC	C4-N4	4.29	1.46	1.39
1	A1	1013	5MC	C6-N1	4.29	1.45	1.38
1	A1	718	5MC	C2-N1	4.28	1.49	1.40
27	B1	1743	4AC	C4-N4	4.28	1.46	1.39
1	A1	1252	OMC	C2-N1	4.28	1.49	1.40
27	B1	2087	5MC	C6-N1	4.28	1.45	1.38
1	A1	863	5MC	C6-N1	4.28	1.45	1.38
27	B1	904	LHH	C4-N3	4.28	1.40	1.32
1	A1	687	5MC	C6-N1	4.28	1.45	1.38
27	B1	2808	OMC	C2-N1	4.28	1.49	1.40
1	A1	863	5MC	C2-N1	4.28	1.49	1.40
27	B1	392	4AC	C4-N4	4.28	1.45	1.39
27	B1	1149	5MC	C2-N1	4.28	1.49	1.40
27	B1	47	5MC	C2-N1	4.28	1.49	1.40
27	B1	979	4AC	C4-N4	4.27	1.45	1.39
1	A1	230	5MC	C2-N1	4.27	1.49	1.40
27	B1	1489	OMC	C2-N1	4.27	1.49	1.40
27	B1	1150	4AC	C4-N4	4.27	1.45	1.39
1	A1	533	5MC	C2-N1	4.27	1.49	1.40
27	B1	877	5MC	C2-N1	4.27	1.49	1.40
27	B1	2850	4AC	C4-N4	4.27	1.45	1.39
1	A1	1015	5MC	C6-N1	4.27	1.45	1.38
1	A1	1348	5MC	C6-N1	4.27	1.45	1.38
1	A1	546	4AC	C4-N4	4.27	1.45	1.39
1	A1	827	4AC	C4-N4	4.27	1.45	1.39
1	A1	466	5MC	C6-N1	4.27	1.45	1.38
28	B2	120	4AC	C4-N4	4.27	1.45	1.39
1	A1	718	5MC	C6-N1	4.26	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1706	4AC	C4-N4	4.26	1.45	1.39
1	A1	291	4AC	C4-N4	4.26	1.45	1.39
1	A1	405	4AC	C4-N4	4.26	1.45	1.39
27	B1	2020	4AC	C4-N4	4.26	1.45	1.39
1	A1	681	5MC	C2-N1	4.26	1.49	1.40
1	A1	17	5MC	C6-N1	4.26	1.45	1.38
27	B1	1868	5MC	C6-N1	4.26	1.45	1.38
27	B1	3006	4AC	C4-N4	4.26	1.45	1.39
1	A1	826	5MC	C6-N1	4.26	1.45	1.38
1	A1	534	4AC	C4-N4	4.26	1.45	1.39
1	A1	761	4AC	C4-N4	4.26	1.45	1.39
27	B1	1734	4AC	C4-N4	4.26	1.45	1.39
1	A1	1486	5MC	C6-N1	4.26	1.45	1.38
27	B1	3037	4AC	C4-N4	4.25	1.45	1.39
27	B1	1648	5MC	C6-N1	4.25	1.45	1.38
1	A1	1270	OMC	C2-N1	4.25	1.49	1.40
1	A1	1067	4AC	C4-N4	4.25	1.45	1.39
27	B1	1608	4AC	C4-N4	4.25	1.45	1.39
27	B1	1620	5MC	C6-N1	4.25	1.45	1.38
1	A1	1016	4AC	C4-N4	4.25	1.45	1.39
27	B1	1783	OMC	C2-N1	4.25	1.49	1.40
27	B1	2607	OMC	C2-N1	4.25	1.49	1.40
1	A1	523	5MC	C6-N1	4.25	1.45	1.38
1	A1	636	4AC	C4-N4	4.25	1.45	1.39
27	B1	932	5MC	C2-N1	4.25	1.49	1.40
27	B1	1977	5MC	C6-N1	4.25	1.45	1.38
1	A1	1221	4AC	C4-N4	4.25	1.45	1.39
27	B1	1612	4AC	C4-N4	4.25	1.45	1.39
1	A1	1135	4AC	C4-N4	4.24	1.45	1.39
27	B1	1966	5MC	C2-N1	4.24	1.49	1.40
27	B1	2792	4AC	C4-N4	4.24	1.45	1.39
1	A1	687	5MC	C2-N1	4.24	1.49	1.40
27	B1	3037	4AC	C2-N1	4.24	1.49	1.40
1	A1	1227	4AC	C4-N4	4.24	1.45	1.39
27	B1	359	5MC	C6-N1	4.24	1.45	1.38
27	B1	2379	4AC	C4-N4	4.24	1.45	1.39
1	A1	540	4AC	C4-N4	4.24	1.45	1.39
27	B1	688	4AC	C4-N4	4.24	1.45	1.39
27	B1	1313	4AC	C4-N4	4.24	1.45	1.39
1	A1	230	5MC	C6-N1	4.24	1.45	1.38
1	A1	951	5MC	C6-N1	4.24	1.45	1.38
27	B1	1546	4AC	C4-N4	4.24	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2453	5MC	C2-N1	4.24	1.49	1.40
1	A1	856	4AC	C4-N4	4.24	1.45	1.39
1	A1	141	4AC	C2-N1	4.24	1.49	1.40
27	B1	226	5MC	C2-N1	4.23	1.49	1.40
27	B1	1703	4AC	C4-N4	4.23	1.45	1.39
1	A1	681	5MC	C6-N1	4.23	1.45	1.38
1	A1	41	4AC	C4-N4	4.23	1.45	1.39
1	A1	810	4AC	C4-N4	4.23	1.45	1.39
1	A1	382	4AC	C4-N4	4.23	1.45	1.39
27	B1	130	4AC	C4-N4	4.23	1.45	1.39
27	B1	580	4AC	C4-N4	4.23	1.45	1.39
1	A1	444	4AC	C4-N4	4.23	1.45	1.39
27	B1	2821	4AC	C4-N4	4.23	1.45	1.39
1	A1	706	4AC	C4-N4	4.23	1.45	1.39
27	B1	1365	LHH	C4-N3	4.23	1.40	1.32
1	A1	1484	5MC	C2-N1	4.23	1.49	1.40
27	B1	2454	4AC	C4-N4	4.23	1.45	1.39
27	B1	2617	5MC	C6-N1	4.23	1.45	1.38
27	B1	641	LHH	C4-N3	4.23	1.40	1.32
1	A1	220	4AC	C4-N4	4.23	1.45	1.39
27	B1	2082	5MC	C2-N1	4.23	1.49	1.40
1	A1	624	4AC	C4-N4	4.22	1.45	1.39
1	A1	1092	4AC	C4-N4	4.22	1.45	1.39
27	B1	2432	4AC	C4-N4	4.22	1.45	1.39
1	A1	195	4AC	C2-N1	4.22	1.49	1.40
1	A1	614	4AC	C4-N4	4.22	1.45	1.39
27	B1	2565	4SU	C4-S4	-4.22	1.60	1.68
1	A1	855	5MC	C6-N1	4.22	1.45	1.38
27	B1	97	5MC	C6-N1	4.22	1.45	1.38
27	B1	1868	5MC	C2-N1	4.22	1.49	1.40
27	B1	2082	5MC	C6-N1	4.22	1.45	1.38
27	B1	715	4AC	C4-N4	4.22	1.45	1.39
1	A1	427	4AC	C2-N1	4.22	1.49	1.40
1	A1	273	5MC	C6-N1	4.22	1.45	1.38
27	B1	1264	4AC	C4-N4	4.22	1.45	1.39
27	B1	2113	4AC	C4-N4	4.22	1.45	1.39
27	B1	337	4AC	C5-C4	4.21	1.49	1.40
27	B1	866	4AC	C4-N4	4.21	1.45	1.39
27	B1	1846	4AC	C4-N4	4.21	1.45	1.39
27	B1	1099	OMC	C2-N1	4.21	1.49	1.40
1	A1	238	LHH	C4-N3	4.21	1.40	1.32
1	A1	605	5MC	C6-N1	4.21	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1818	4AC	C4-N4	4.21	1.45	1.39
1	A1	87	4AC	C4-N4	4.21	1.45	1.39
1	A1	1288	4AC	C4-N4	4.21	1.45	1.39
27	B1	1067	4AC	C4-N4	4.21	1.45	1.39
27	B1	1061	4AC	C4-N4	4.20	1.45	1.39
27	B1	1293	4AC	C4-N4	4.20	1.45	1.39
27	B1	1374	4AC	C4-N4	4.20	1.45	1.39
1	A1	816	4AC	C4-N4	4.20	1.45	1.39
27	B1	2557	OMC	C2-N1	4.20	1.49	1.40
27	B1	243	4AC	C4-N4	4.20	1.45	1.39
1	A1	367	4AC	C4-N4	4.20	1.45	1.39
27	B1	271	4AC	C4-N4	4.20	1.45	1.39
27	B1	2429	4AC	C4-N4	4.20	1.45	1.39
1	A1	834	OMC	C2-N1	4.20	1.49	1.40
27	B1	1639	4AC	C5-C4	4.20	1.49	1.40
1	A1	274	4AC	C4-N4	4.20	1.45	1.39
27	B1	1977	5MC	C2-N1	4.20	1.49	1.40
27	B1	652	4AC	C4-N4	4.20	1.45	1.39
27	B1	2328	4AC	C4-N4	4.20	1.45	1.39
27	B1	1885	4AC	C4-N4	4.20	1.45	1.39
1	A1	756	4SU	C4-S4	-4.20	1.60	1.68
27	B1	1966	5MC	C6-N1	4.20	1.45	1.38
27	B1	276	4AC	C4-N4	4.20	1.45	1.39
1	A1	1467	4AC	C4-N4	4.19	1.45	1.39
27	B1	1664	4AC	C4-N4	4.19	1.45	1.39
27	B1	2171	4AC	C4-N4	4.19	1.45	1.39
1	A1	307	4AC	C4-N4	4.19	1.45	1.39
27	B1	18	5MC	C6-N1	4.19	1.45	1.38
1	A1	839	4AC	C4-N4	4.19	1.45	1.39
27	B1	2008	4AC	C4-N4	4.19	1.45	1.39
27	B1	1100	4AC	C4-N4	4.19	1.45	1.39
27	B1	1439	4AC	C4-N4	4.19	1.45	1.39
1	A1	1181	4AC	C4-N4	4.19	1.45	1.39
27	B1	227	4AC	C4-N4	4.19	1.45	1.39
27	B1	1551	4AC	C4-N4	4.19	1.45	1.39
27	B1	3020	4AC	C4-N4	4.19	1.45	1.39
27	B1	1703	4AC	C2-N1	4.19	1.49	1.40
1	A1	1314	4AC	C4-N4	4.19	1.45	1.39
27	B1	2133	4AC	C4-N4	4.19	1.45	1.39
27	B1	360	4AC	C4-N4	4.18	1.45	1.39
27	B1	896	4AC	C4-N4	4.18	1.45	1.39
27	B1	1751	4AC	C4-N4	4.18	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	117	OMC	C2-N1	4.18	1.49	1.40
27	B1	741	4AC	C4-N4	4.18	1.45	1.39
27	B1	200	4AC	C4-N4	4.18	1.45	1.39
27	B1	599	4AC	C4-N4	4.18	1.45	1.39
1	A1	5	4AC	C4-N4	4.18	1.45	1.39
27	B1	1178	4AC	C4-N4	4.18	1.45	1.39
27	B1	1621	4AC	C4-N4	4.18	1.45	1.39
1	A1	231	4AC	C4-N4	4.18	1.45	1.39
27	B1	2526	4AC	C4-N4	4.18	1.45	1.39
27	B1	732	4AC	C4-N4	4.18	1.45	1.39
27	B1	1608	4AC	C2-N1	4.18	1.49	1.40
27	B1	1639	4AC	C2-N1	4.18	1.49	1.40
1	A1	624	4AC	C2-N1	4.18	1.49	1.40
27	B1	226	5MC	C6-N1	4.18	1.45	1.38
27	B1	1451	5MC	C6-N1	4.18	1.45	1.38
27	B1	162	4AC	C4-N4	4.17	1.45	1.39
27	B1	2888	4AC	C4-N4	4.17	1.45	1.39
27	B1	47	5MC	C6-N1	4.17	1.45	1.38
1	A1	1029	4AC	C5-C4	4.17	1.49	1.40
27	B1	2876	4AC	C4-N4	4.17	1.45	1.39
27	B1	1052	4AC	C4-N4	4.17	1.45	1.39
1	A1	216	4AC	C4-N4	4.17	1.45	1.39
27	B1	1757	4AC	C4-N4	4.17	1.45	1.39
27	B1	2119	OMC	C2-N1	4.17	1.49	1.40
1	A1	499	4AC	C4-N4	4.16	1.45	1.39
28	B2	120	4AC	C5-C4	4.16	1.49	1.40
1	A1	578	4AC	C4-N4	4.16	1.45	1.39
27	B1	1822	4AC	C4-N4	4.16	1.45	1.39
1	A1	467	4AC	C2-N1	4.16	1.49	1.40
27	B1	786	4AC	C4-N4	4.16	1.45	1.39
27	B1	2492	4AC	C4-N4	4.16	1.45	1.39
1	A1	1484	5MC	C6-N1	4.16	1.45	1.38
27	B1	953	4AC	C4-N4	4.16	1.45	1.39
27	B1	1649	4AC	C4-N4	4.16	1.45	1.39
27	B1	813	4AC	C2-N1	4.16	1.49	1.40
28	B2	117	4AC	C4-N4	4.16	1.45	1.39
27	B1	877	5MC	C6-N1	4.16	1.45	1.38
27	B1	2602	4AC	C4-N4	4.16	1.45	1.39
27	B1	641	LHH	C4-N4	4.16	1.45	1.39
1	A1	1135	4AC	C2-N1	4.15	1.49	1.40
1	A1	195	4AC	C5-C4	4.15	1.49	1.40
1	A1	836	4AC	C4-N4	4.15	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	1092	4AC	C2-N1	4.15	1.49	1.40
27	B1	977	OMC	C2-N1	4.15	1.49	1.40
1	A1	52	OMU	C4-N3	4.15	1.46	1.38
27	B1	23	4AC	C4-N4	4.15	1.45	1.39
27	B1	798	4AC	C4-N4	4.15	1.45	1.39
27	B1	3011	4AC	C4-N4	4.15	1.45	1.39
27	B1	3023	4AC	C4-N4	4.15	1.45	1.39
27	B1	2735	OMC	C2-N1	4.15	1.49	1.40
1	A1	141	4AC	C5-C4	4.15	1.49	1.40
1	A1	481	G7M	C4-N3	4.15	1.47	1.37
27	B1	80	4AC	C4-N4	4.14	1.45	1.39
27	B1	721	4AC	C4-N4	4.14	1.45	1.39
27	B1	2469	4AC	C4-N4	4.14	1.45	1.39
27	B1	950	4AC	C4-N4	4.14	1.45	1.39
1	A1	739	4AC	C2-N1	4.14	1.49	1.40
1	A1	405	4AC	C5-C4	4.14	1.49	1.40
28	B2	90	4AC	C4-N4	4.14	1.45	1.39
27	B1	1435	4AC	C4-N4	4.13	1.45	1.39
27	B1	904	LHH	C4-N4	4.13	1.45	1.39
27	B1	807	4AC	C2-N1	4.13	1.49	1.40
27	B1	116	4AC	C4-N4	4.13	1.45	1.39
27	B1	1612	4AC	C2-N1	4.13	1.48	1.40
27	B1	2213	4AC	C4-N4	4.13	1.45	1.39
1	A1	719	4AC	C4-N4	4.13	1.45	1.39
27	B1	609	4AC	C2-N1	4.13	1.48	1.40
27	B1	1313	4AC	C5-C4	4.13	1.49	1.40
27	B1	2749	4AC	C4-N4	4.13	1.45	1.39
27	B1	142	4AC	C2-N1	4.13	1.48	1.40
27	B1	19	4AC	C4-N4	4.13	1.45	1.39
27	B1	1505	4AC	C4-N4	4.13	1.45	1.39
27	B1	501	OMC	C2-N1	4.13	1.48	1.40
1	A1	706	4AC	C5-C4	4.12	1.49	1.40
27	B1	1290	4AC	C4-N4	4.12	1.45	1.39
1	A1	1067	4AC	C5-C4	4.12	1.49	1.40
27	B1	479	4AC	C5-C4	4.12	1.49	1.40
27	B1	1983	5MC	C2-N1	4.12	1.48	1.40
1	A1	231	4AC	C5-C4	4.12	1.49	1.40
1	A1	216	4AC	C2-N1	4.12	1.48	1.40
1	A1	1227	4AC	C5-C4	4.12	1.49	1.40
27	B1	1734	4AC	C2-N1	4.12	1.48	1.40
1	A1	856	4AC	C5-C4	4.12	1.49	1.40
27	B1	1178	4AC	C5-C4	4.12	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1612	4AC	C5-C4	4.12	1.49	1.40
27	B1	932	5MC	C6-N1	4.12	1.45	1.38
27	B1	98	4AC	C4-N4	4.12	1.45	1.39
1	A1	1221	4AC	C2-N1	4.11	1.48	1.40
27	B1	419	4AC	C4-N4	4.11	1.45	1.39
1	A1	1221	4AC	C5-C4	4.11	1.49	1.40
1	A1	624	4AC	C5-C4	4.11	1.49	1.40
27	B1	3006	4AC	C2-N1	4.11	1.48	1.40
1	A1	636	4AC	C2-N1	4.11	1.48	1.40
27	B1	527	LHH	C4-N3	4.11	1.40	1.32
27	B1	1383	4AC	C4-N4	4.11	1.45	1.39
27	B1	1981	OMU	C4-N3	4.11	1.45	1.38
27	B1	2008	4AC	C5-C4	4.10	1.49	1.40
27	B1	360	4AC	C5-C4	4.10	1.49	1.40
27	B1	2821	4AC	C5-C4	4.10	1.49	1.40
27	B1	2379	4AC	C5-C4	4.10	1.49	1.40
27	B1	479	4AC	C4-N4	4.10	1.45	1.39
1	A1	816	4AC	C5-C4	4.10	1.49	1.40
27	B1	1621	4AC	C2-N1	4.10	1.48	1.40
27	B1	2526	4AC	C5-C4	4.10	1.49	1.40
27	B1	2809	4AC	C4-N4	4.10	1.45	1.39
1	A1	1181	4AC	C5-C4	4.10	1.49	1.40
27	B1	1706	4AC	C5-C4	4.10	1.49	1.40
27	B1	741	4AC	C2-N1	4.10	1.48	1.40
1	A1	41	4AC	C5-C4	4.10	1.49	1.40
27	B1	1386	4AC	C4-N4	4.10	1.45	1.39
1	A1	1092	4AC	C5-C4	4.10	1.49	1.40
27	B1	1064	4AC	C5-C4	4.10	1.49	1.40
27	B1	502	LHH	C4-N3	4.09	1.39	1.32
27	B1	271	4AC	C2-N1	4.09	1.48	1.40
27	B1	2020	4AC	C5-C4	4.09	1.49	1.40
27	B1	2328	4AC	C5-C4	4.09	1.49	1.40
27	B1	1762	4AC	C4-N4	4.09	1.45	1.39
1	A1	499	4AC	C5-C4	4.09	1.49	1.40
27	B1	1911	4AC	C2-N1	4.09	1.48	1.40
1	A1	836	4AC	C5-C4	4.09	1.49	1.40
27	B1	1501	4AC	C4-N4	4.09	1.45	1.39
1	A1	367	4AC	C5-C4	4.09	1.49	1.40
27	B1	2429	4AC	C5-C4	4.08	1.49	1.40
1	A1	1135	4AC	C5-C4	4.08	1.49	1.40
27	B1	741	4AC	C5-C4	4.08	1.49	1.40
27	B1	1150	4AC	C2-N1	4.08	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	1364	LHH	C4-N4	4.08	1.45	1.39
27	B1	1743	4AC	C5-C4	4.08	1.49	1.40
27	B1	1365	LHH	C4-N4	4.08	1.45	1.39
27	B1	609	4AC	C5-C4	4.08	1.49	1.40
27	B1	434	4AC	C4-N4	4.08	1.45	1.39
27	B1	392	4AC	C2-N1	4.08	1.48	1.40
27	B1	1374	4AC	C2-N1	4.08	1.48	1.40
27	B1	227	4AC	C5-C4	4.08	1.49	1.40
27	B1	1911	4AC	C4-N4	4.08	1.45	1.39
1	A1	827	4AC	C5-C4	4.08	1.49	1.40
1	A1	1368	OMU	C4-N3	4.08	1.45	1.38
27	B1	1404	4AC	C4-N4	4.08	1.45	1.39
1	A1	467	4AC	C5-C4	4.08	1.49	1.40
27	B1	227	4AC	C2-N1	4.08	1.48	1.40
27	B1	715	4AC	C2-N1	4.08	1.48	1.40
1	A1	719	4AC	C5-C4	4.07	1.49	1.40
27	B1	759	4AC	C2-N1	4.07	1.48	1.40
27	B1	1293	4AC	C5-C4	4.07	1.49	1.40
1	A1	5	4AC	C5-C4	4.07	1.49	1.40
27	B1	2821	4AC	C2-N1	4.07	1.48	1.40
1	A1	367	4AC	C2-N1	4.07	1.48	1.40
27	B1	1322	4AC	C4-N4	4.07	1.45	1.39
1	A1	1467	4AC	C5-C4	4.07	1.49	1.40
27	B1	715	4AC	C5-C4	4.07	1.49	1.40
1	A1	1067	4AC	C2-N1	4.07	1.48	1.40
1	A1	546	4AC	C5-C4	4.07	1.49	1.40
27	B1	1743	4AC	C2-N1	4.07	1.48	1.40
27	B1	142	4AC	C5-C4	4.07	1.49	1.40
1	A1	87	4AC	C2-N1	4.07	1.48	1.40
27	B1	1100	4AC	C5-C4	4.07	1.49	1.40
28	B2	120	4AC	C2-N1	4.07	1.48	1.40
1	A1	827	4AC	C2-N1	4.07	1.48	1.40
1	A1	1288	4AC	C5-C4	4.07	1.49	1.40
27	B1	798	4AC	C5-C4	4.06	1.49	1.40
27	B1	2809	4AC	C5-C4	4.06	1.49	1.40
27	B1	1107	4AC	C4-N4	4.06	1.45	1.39
27	B1	2454	4AC	C5-C4	4.06	1.49	1.40
27	B1	1946	LHH	C4-N3	4.06	1.39	1.32
1	A1	578	4AC	C5-C4	4.06	1.49	1.40
1	A1	1016	4AC	C2-N1	4.06	1.48	1.40
27	B1	2968	LHH	C4-N3	4.06	1.39	1.32
1	A1	216	4AC	C5-C4	4.06	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	652	4AC	C5-C4	4.06	1.49	1.40
1	A1	762	OMU	C4-N3	4.06	1.45	1.38
1	A1	444	4AC	C2-N1	4.06	1.48	1.40
27	B1	2593	OMU	C4-N3	4.06	1.45	1.38
1	A1	739	4AC	C5-C4	4.06	1.49	1.40
27	B1	721	4AC	C5-C4	4.06	1.49	1.40
27	B1	1649	4AC	C5-C4	4.06	1.49	1.40
1	A1	41	4AC	C2-N1	4.06	1.48	1.40
1	A1	810	4AC	C2-N1	4.06	1.48	1.40
27	B1	1128	4AC	C4-N4	4.06	1.45	1.39
27	B1	1442	4AC	C4-N4	4.06	1.45	1.39
1	A1	274	4AC	C5-C4	4.06	1.49	1.40
1	A1	382	4AC	C2-N1	4.06	1.48	1.40
27	B1	732	4AC	C2-N1	4.06	1.48	1.40
27	B1	2668	OMU	C4-N3	4.06	1.45	1.38
1	A1	761	4AC	C2-N1	4.06	1.48	1.40
27	B1	1822	4AC	C5-C4	4.06	1.49	1.40
27	B1	1967	4AC	C5-C4	4.06	1.49	1.40
27	B1	2429	4AC	C2-N1	4.06	1.48	1.40
27	B1	807	4AC	C5-C4	4.06	1.49	1.40
27	B1	896	4AC	C5-C4	4.06	1.49	1.40
1	A1	220	4AC	C2-N1	4.06	1.48	1.40
1	A1	810	4AC	C5-C4	4.05	1.49	1.40
27	B1	1313	4AC	C2-N1	4.05	1.48	1.40
1	A1	534	4AC	C5-C4	4.05	1.49	1.40
27	B1	2432	4AC	C5-C4	4.05	1.49	1.40
27	B1	580	4AC	C5-C4	4.05	1.49	1.40
27	B1	2792	4AC	C5-C4	4.05	1.49	1.40
1	A1	546	4AC	C2-N1	4.05	1.48	1.40
1	A1	444	4AC	C5-C4	4.05	1.49	1.40
1	A1	1016	4AC	C5-C4	4.05	1.49	1.40
27	B1	2876	4AC	C2-N1	4.05	1.48	1.40
27	B1	1360	4AC	C4-N4	4.05	1.45	1.39
27	B1	19	4AC	C5-C4	4.05	1.49	1.40
27	B1	2133	4AC	C5-C4	4.05	1.49	1.40
1	A1	405	4AC	C2-N1	4.05	1.48	1.40
1	A1	540	4AC	C5-C4	4.05	1.49	1.40
27	B1	98	4AC	C5-C4	4.05	1.49	1.40
1	A1	1254	4AC	C2-N1	4.05	1.48	1.40
27	B1	392	4AC	C5-C4	4.05	1.49	1.40
27	B1	276	4AC	C5-C4	4.05	1.49	1.40
27	B1	1290	4AC	C5-C4	4.05	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	5	4AC	C2-N1	4.05	1.48	1.40
27	B1	1757	4AC	C5-C4	4.05	1.49	1.40
27	B1	2328	4AC	C2-N1	4.04	1.48	1.40
27	B1	1264	4AC	C2-N1	4.04	1.48	1.40
1	A1	839	4AC	C5-C4	4.04	1.49	1.40
27	B1	1052	4AC	C2-N1	4.04	1.48	1.40
27	B1	3006	4AC	C5-C4	4.04	1.49	1.40
27	B1	2554	OMU	C4-N3	4.04	1.45	1.38
27	B1	1061	4AC	C2-N1	4.04	1.48	1.40
1	A1	220	4AC	C5-C4	4.04	1.49	1.40
27	B1	1478	4AC	C5-C4	4.04	1.49	1.40
27	B1	2876	4AC	C5-C4	4.04	1.49	1.40
27	B1	1100	4AC	C2-N1	4.04	1.48	1.40
1	A1	691	4AC	C4-N4	4.04	1.45	1.39
27	B1	2844	4AC	C4-N4	4.04	1.45	1.39
1	A1	578	4AC	C2-N1	4.04	1.48	1.40
1	A1	8	OMU	C4-N3	4.04	1.45	1.38
27	B1	1885	4AC	C5-C4	4.04	1.49	1.40
1	A1	775	OMU	C4-N3	4.04	1.45	1.38
27	B1	866	4AC	C5-C4	4.04	1.49	1.40
27	B1	1505	4AC	C5-C4	4.04	1.49	1.40
1	A1	836	4AC	C2-N1	4.04	1.48	1.40
1	A1	1181	4AC	C2-N1	4.04	1.48	1.40
27	B1	1551	4AC	C5-C4	4.04	1.49	1.40
1	A1	1288	4AC	C2-N1	4.04	1.48	1.40
27	B1	2401	OMU	C4-N3	4.04	1.45	1.38
27	B1	1067	4AC	C5-C4	4.04	1.49	1.40
27	B1	276	4AC	C2-N1	4.03	1.48	1.40
27	B1	2432	4AC	C2-N1	4.03	1.48	1.40
27	B1	1546	4AC	C5-C4	4.03	1.49	1.40
27	B1	19	4AC	C2-N1	4.03	1.48	1.40
1	A1	636	4AC	C5-C4	4.03	1.49	1.40
27	B1	1178	4AC	C2-N1	4.03	1.48	1.40
28	B2	117	4AC	C2-N1	4.03	1.48	1.40
27	B1	48	4AC	C4-N4	4.03	1.45	1.39
1	A1	499	4AC	C2-N1	4.03	1.48	1.40
27	B1	1439	4AC	C5-C4	4.03	1.49	1.40
27	B1	759	4AC	C5-C4	4.03	1.49	1.40
27	B1	130	4AC	C2-N1	4.03	1.48	1.40
27	B1	502	LHH	C4-N4	4.03	1.45	1.39
1	A1	1314	4AC	C2-N1	4.03	1.48	1.40
27	B1	1757	4AC	C2-N1	4.03	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	807	4AC	C4-N4	4.03	1.45	1.39
27	B1	1435	4AC	C5-C4	4.03	1.49	1.40
27	B1	2888	4AC	C5-C4	4.03	1.49	1.40
1	A1	274	4AC	C2-N1	4.03	1.48	1.40
27	B1	1293	4AC	C2-N1	4.02	1.48	1.40
27	B1	454	OMU	C4-N3	4.02	1.45	1.38
27	B1	485	4AC	C5-C4	4.02	1.49	1.40
27	B1	1052	4AC	C5-C4	4.02	1.49	1.40
27	B1	1383	4AC	C5-C4	4.02	1.49	1.40
28	B2	90	4AC	C2-N1	4.02	1.48	1.40
27	B1	162	4AC	C5-C4	4.02	1.49	1.40
27	B1	1967	4AC	C4-N4	4.02	1.45	1.39
1	A1	691	4AC	C2-N1	4.02	1.48	1.40
27	B1	48	4AC	C5-C4	4.02	1.49	1.40
27	B1	1264	4AC	C5-C4	4.02	1.49	1.40
27	B1	721	4AC	C2-N1	4.02	1.48	1.40
27	B1	2602	4AC	C5-C4	4.02	1.49	1.40
27	B1	3020	4AC	C5-C4	4.02	1.49	1.40
28	B2	117	4AC	C5-C4	4.02	1.49	1.40
1	A1	1227	4AC	C2-N1	4.02	1.48	1.40
1	A1	425	OMU	C4-N3	4.02	1.45	1.38
27	B1	485	4AC	C4-N4	4.02	1.45	1.39
27	B1	337	4AC	C2-N1	4.01	1.48	1.40
27	B1	1751	4AC	C2-N1	4.01	1.48	1.40
1	A1	427	4AC	C5-C4	4.01	1.49	1.40
27	B1	2020	4AC	C2-N1	4.01	1.48	1.40
1	A1	534	4AC	C2-N1	4.01	1.48	1.40
27	B1	580	4AC	C2-N1	4.01	1.48	1.40
28	B2	90	4AC	C5-C4	4.01	1.49	1.40
27	B1	98	4AC	C2-N1	4.01	1.48	1.40
27	B1	1149	5MC	C6-N1	4.01	1.44	1.38
27	B1	130	4AC	C5-C4	4.01	1.49	1.40
1	A1	1314	4AC	C5-C4	4.01	1.49	1.40
27	B1	979	4AC	C2-N1	4.01	1.48	1.40
27	B1	1322	4AC	C2-N1	4.01	1.48	1.40
27	B1	786	4AC	C5-C4	4.01	1.49	1.40
27	B1	1846	4AC	C2-N1	4.01	1.48	1.40
27	B1	2454	4AC	C2-N1	4.01	1.48	1.40
1	A1	291	4AC	C5-C4	4.01	1.49	1.40
27	B1	1649	4AC	C2-N1	4.01	1.48	1.40
27	B1	271	4AC	C5-C4	4.01	1.49	1.40
27	B1	1703	4AC	C5-C4	4.01	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2213	4AC	C5-C4	4.01	1.49	1.40
27	B1	1286	4AC	C2-N1	4.01	1.48	1.40
27	B1	1439	4AC	C2-N1	4.01	1.48	1.40
1	A1	1467	4AC	C2-N1	4.00	1.48	1.40
27	B1	896	4AC	C2-N1	4.00	1.48	1.40
27	B1	1751	4AC	C5-C4	4.00	1.49	1.40
1	A1	761	4AC	C5-C4	4.00	1.49	1.40
1	A1	816	4AC	C2-N1	4.00	1.48	1.40
27	B1	732	4AC	C5-C4	4.00	1.49	1.40
1	A1	307	4AC	C5-C4	4.00	1.49	1.40
27	B1	1442	4AC	C5-C4	4.00	1.49	1.40
27	B1	1946	LHH	C4-N4	4.00	1.45	1.39
27	B1	1769	4AC	C5-C4	3.99	1.49	1.40
27	B1	200	4AC	C5-C4	3.99	1.49	1.40
27	B1	3023	4AC	C2-N1	3.99	1.48	1.40
27	B1	599	4AC	C5-C4	3.99	1.49	1.40
27	B1	688	4AC	C5-C4	3.99	1.49	1.40
27	B1	2526	4AC	C2-N1	3.99	1.48	1.40
1	A1	691	4AC	C5-C4	3.99	1.49	1.40
27	B1	162	4AC	C2-N1	3.99	1.48	1.40
27	B1	652	4AC	C2-N1	3.99	1.48	1.40
27	B1	1846	4AC	C5-C4	3.99	1.49	1.40
27	B1	1128	4AC	C5-C4	3.99	1.49	1.40
1	A1	706	4AC	C2-N1	3.99	1.48	1.40
27	B1	2844	4AC	C5-C4	3.99	1.49	1.40
27	B1	80	4AC	C5-C4	3.98	1.49	1.40
27	B1	1911	4AC	C5-C4	3.98	1.49	1.40
1	A1	1254	4AC	C5-C4	3.98	1.49	1.40
27	B1	1107	4AC	C5-C4	3.98	1.49	1.40
27	B1	2850	4AC	C2-N1	3.98	1.48	1.40
27	B1	1664	4AC	C2-N1	3.98	1.48	1.40
1	A1	87	4AC	C5-C4	3.98	1.49	1.40
27	B1	2492	4AC	C5-C4	3.98	1.49	1.40
27	B1	2171	4AC	C5-C4	3.98	1.49	1.40
27	B1	243	4AC	C5-C4	3.98	1.49	1.40
1	A1	719	4AC	C2-N1	3.98	1.48	1.40
27	B1	3037	4AC	C5-C4	3.98	1.49	1.40
27	B1	1386	4AC	C5-C4	3.98	1.49	1.40
27	B1	1818	4AC	C2-N1	3.98	1.48	1.40
27	B1	337	4AC	C4-N4	3.98	1.45	1.39
27	B1	1322	4AC	C5-C4	3.98	1.49	1.40
27	B1	3020	4AC	C2-N1	3.97	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	116	4AC	C5-C4	3.97	1.49	1.40
27	B1	2809	4AC	C2-N1	3.97	1.48	1.40
27	B1	2749	4AC	C5-C4	3.97	1.49	1.40
27	B1	1505	4AC	C2-N1	3.97	1.48	1.40
27	B1	3023	4AC	C5-C4	3.97	1.49	1.40
27	B1	599	4AC	C2-N1	3.97	1.48	1.40
27	B1	1734	4AC	C5-C4	3.97	1.49	1.40
27	B1	2008	4AC	C2-N1	3.97	1.48	1.40
1	A1	382	4AC	C5-C4	3.97	1.49	1.40
27	B1	23	4AC	C5-C4	3.97	1.49	1.40
27	B1	1290	4AC	C2-N1	3.97	1.48	1.40
27	B1	1762	4AC	C2-N1	3.96	1.48	1.40
27	B1	1360	4AC	C2-N1	3.96	1.48	1.40
27	B1	378	4AC	C5-C4	3.96	1.49	1.40
27	B1	786	4AC	C2-N1	3.96	1.48	1.40
27	B1	1107	4AC	C2-N1	3.96	1.48	1.40
1	A1	614	4AC	C2-N1	3.96	1.48	1.40
1	A1	839	4AC	C2-N1	3.96	1.48	1.40
27	B1	1286	4AC	C4-N4	3.96	1.45	1.39
27	B1	798	4AC	C2-N1	3.96	1.48	1.40
27	B1	479	4AC	C2-N1	3.96	1.48	1.40
27	B1	419	4AC	C2-N1	3.96	1.48	1.40
27	B1	1383	4AC	C2-N1	3.96	1.48	1.40
27	B1	1150	4AC	C5-C4	3.96	1.49	1.40
27	B1	1442	4AC	C2-N1	3.96	1.48	1.40
27	B1	1488	OMU	C4-N3	3.96	1.45	1.38
27	B1	1067	4AC	C2-N1	3.96	1.48	1.40
27	B1	2792	4AC	C2-N1	3.95	1.48	1.40
27	B1	1501	4AC	C5-C4	3.95	1.49	1.40
27	B1	1967	4AC	C2-N1	3.95	1.48	1.40
27	B1	360	4AC	C2-N1	3.95	1.48	1.40
27	B1	378	4AC	C2-N1	3.95	1.48	1.40
27	B1	3011	4AC	C5-C4	3.95	1.49	1.40
27	B1	243	4AC	C2-N1	3.95	1.48	1.40
27	B1	1769	4AC	C4-N4	3.95	1.45	1.39
27	B1	953	4AC	C2-N1	3.95	1.48	1.40
27	B1	933	4AC	C2-N1	3.95	1.48	1.40
27	B1	1818	4AC	C5-C4	3.94	1.49	1.40
1	A1	291	4AC	C2-N1	3.94	1.48	1.40
1	A1	238	LHH	C4-N4	3.94	1.45	1.39
27	B1	2469	4AC	C5-C4	3.94	1.49	1.40
1	A1	540	4AC	C2-N1	3.94	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	1270	OMC	C4-N4	3.94	1.43	1.33
27	B1	1551	4AC	C2-N1	3.94	1.48	1.40
27	B1	2428	OMC	C4-N4	3.94	1.43	1.33
27	B1	2968	LHH	C4-N4	3.94	1.45	1.39
27	B1	23	4AC	C2-N1	3.94	1.48	1.40
27	B1	1061	4AC	C5-C4	3.93	1.49	1.40
27	B1	434	4AC	C5-C4	3.93	1.49	1.40
27	B1	1360	4AC	C5-C4	3.93	1.49	1.40
27	B1	688	4AC	C2-N1	3.93	1.48	1.40
27	B1	116	4AC	C2-N1	3.93	1.48	1.40
27	B1	1128	4AC	C2-N1	3.93	1.48	1.40
27	B1	2602	4AC	C2-N1	3.93	1.48	1.40
27	B1	2844	4AC	C2-N1	3.93	1.48	1.40
27	B1	1706	4AC	C2-N1	3.93	1.48	1.40
27	B1	2171	4AC	C2-N1	3.92	1.48	1.40
1	A1	231	4AC	C2-N1	3.92	1.48	1.40
27	B1	2850	4AC	C5-C4	3.92	1.49	1.40
27	B1	1435	4AC	C2-N1	3.92	1.48	1.40
27	B1	2469	4AC	C2-N1	3.92	1.48	1.40
27	B1	953	4AC	C5-C4	3.92	1.49	1.40
27	B1	1374	4AC	C5-C4	3.92	1.49	1.40
27	B1	1608	4AC	C5-C4	3.92	1.49	1.40
27	B1	1885	4AC	C2-N1	3.92	1.48	1.40
27	B1	1621	4AC	C5-C4	3.92	1.49	1.40
27	B1	950	4AC	C5-C4	3.92	1.49	1.40
27	B1	1769	4AC	C2-N1	3.91	1.48	1.40
27	B1	1546	4AC	C2-N1	3.91	1.48	1.40
27	B1	419	4AC	C5-C4	3.91	1.49	1.40
27	B1	1664	4AC	C5-C4	3.91	1.49	1.40
1	A1	856	4AC	C2-N1	3.91	1.48	1.40
27	B1	1478	4AC	C2-N1	3.91	1.48	1.40
27	B1	336	5MC	C6-N1	3.91	1.44	1.38
27	B1	813	4AC	C5-C4	3.91	1.49	1.40
27	B1	866	4AC	C2-N1	3.91	1.48	1.40
27	B1	1501	4AC	C2-N1	3.91	1.48	1.40
27	B1	1286	4AC	C5-C4	3.91	1.49	1.40
27	B1	1404	4AC	C5-C4	3.90	1.49	1.40
1	A1	1029	4AC	C2-N1	3.90	1.48	1.40
27	B1	1386	4AC	C2-N1	3.90	1.48	1.40
27	B1	1822	4AC	C2-N1	3.90	1.48	1.40
27	B1	2749	4AC	C2-N1	3.90	1.48	1.40
27	B1	1064	4AC	C2-N1	3.90	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	307	4AC	C2-N1	3.90	1.48	1.40
27	B1	950	4AC	C2-N1	3.90	1.48	1.40
1	A1	426	OMC	C4-N4	3.90	1.43	1.33
27	B1	80	4AC	C2-N1	3.90	1.48	1.40
27	B1	2492	4AC	C2-N1	3.90	1.48	1.40
1	A1	614	4AC	C5-C4	3.89	1.49	1.40
27	B1	48	4AC	C2-N1	3.89	1.48	1.40
27	B1	2213	4AC	C2-N1	3.89	1.48	1.40
1	A1	901	OMG	C6-N1	3.89	1.43	1.37
27	B1	1783	OMC	C4-N4	3.89	1.43	1.33
27	B1	3011	4AC	C2-N1	3.89	1.48	1.40
1	A1	1252	OMC	C4-N4	3.89	1.43	1.33
27	B1	200	4AC	C2-N1	3.88	1.48	1.40
27	B1	2607	OMC	C4-N4	3.88	1.43	1.33
1	A1	1194	OMC	C4-N4	3.88	1.43	1.33
27	B1	2735	OMC	C4-N4	3.88	1.43	1.33
27	B1	1404	4AC	C2-N1	3.87	1.48	1.40
27	B1	2888	4AC	C2-N1	3.87	1.48	1.40
27	B1	2059	OMC	C4-N4	3.86	1.43	1.33
27	B1	1762	4AC	C5-C4	3.86	1.49	1.40
27	B1	2133	4AC	C2-N1	3.86	1.48	1.40
1	A1	117	OMC	C4-N4	3.86	1.43	1.33
27	B1	485	4AC	C2-N1	3.86	1.48	1.40
27	B1	933	4AC	C5-C4	3.86	1.49	1.40
1	A1	834	OMC	C4-N4	3.85	1.43	1.33
27	B1	1099	OMC	C4-N4	3.85	1.43	1.33
27	B1	1832	OMC	C4-N4	3.84	1.43	1.33
27	B1	1489	OMC	C4-N4	3.84	1.43	1.33
27	B1	434	4AC	C2-N1	3.84	1.48	1.40
1	A1	507	OMG	C6-N1	3.83	1.43	1.37
1	A1	1004	2MG	C6-N1	3.83	1.43	1.37
27	B1	501	OMC	C4-N4	3.83	1.42	1.33
27	B1	2113	4AC	C5-C4	3.82	1.49	1.40
1	A1	329	OMG	C6-N1	3.82	1.43	1.37
27	B1	1601	OMG	C6-N1	3.82	1.43	1.37
27	B1	2119	OMC	C4-N4	3.82	1.42	1.33
27	B1	977	OMC	C4-N4	3.82	1.42	1.33
27	B1	2808	OMC	C4-N4	3.81	1.42	1.33
27	B1	933	4AC	C4-N4	3.81	1.45	1.39
27	B1	2984	OMG	C6-N1	3.81	1.43	1.37
27	B1	1914	OMC	C4-N4	3.81	1.42	1.33
27	B1	2557	OMC	C4-N4	3.80	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2757	OMG	C6-N1	3.80	1.43	1.37
27	B1	527	LHH	C4-N4	3.80	1.45	1.39
1	A1	227	OMG	C6-N1	3.79	1.43	1.37
27	B1	2113	4AC	C2-N1	3.78	1.48	1.40
1	A1	481	G7M	C2-N1	3.78	1.47	1.37
1	A1	1003	OMG	C6-N1	3.78	1.43	1.37
27	B1	675	OMG	C6-N1	3.77	1.43	1.37
27	B1	2740	OMG	C6-N1	3.76	1.43	1.37
27	B1	979	4AC	C5-C4	3.76	1.48	1.40
1	A1	455	OMG	C6-N1	3.75	1.43	1.37
27	B1	1557	OMG	C6-N1	3.75	1.43	1.37
1	A1	228	OMG	C6-N1	3.75	1.43	1.37
27	B1	214	OMG	C6-N1	3.75	1.43	1.37
1	A1	153	OMG	C6-N1	3.74	1.43	1.37
27	B1	2684	OMG	C6-N1	3.74	1.43	1.37
27	B1	2379	4AC	C2-N1	3.73	1.48	1.40
27	B1	2562	OMG	C6-N1	3.72	1.43	1.37
1	A1	861	OMG	C6-N1	3.70	1.43	1.37
27	B1	887	OMG	C6-N1	3.70	1.43	1.37
1	A1	763	OMG	C6-N1	3.70	1.43	1.37
27	B1	2180	OMG	C6-N1	3.69	1.43	1.37
27	B1	1965	OMG	C6-N1	3.68	1.43	1.37
27	B1	2659	OMG	C6-N1	3.66	1.43	1.37
27	B1	2365	OMG	C6-N1	3.65	1.43	1.37
1	A1	833	OMG	C6-N1	3.63	1.43	1.37
27	B1	808	OMG	C6-N1	3.61	1.43	1.37
27	B1	2391	OMG	C6-N1	3.61	1.43	1.37
27	B1	2540	OMG	C6-N1	3.60	1.43	1.37
1	A1	668	OMG	C6-N1	3.60	1.43	1.37
27	B1	920	OMG	C6-N1	3.58	1.43	1.37
27	B1	2028	OMG	C6-N1	3.56	1.43	1.37
27	B1	841	OMG	C6-N1	3.56	1.43	1.37
1	A1	1366	A1I59	C6-C5	3.56	1.40	1.34
1	A1	459	OMG	C6-N1	3.56	1.43	1.37
1	A1	645	OMG	C6-N1	3.52	1.43	1.37
27	B1	2022	OMG	C6-N1	3.52	1.43	1.37
27	B1	921	OMG	C6-N1	3.49	1.43	1.37
27	B1	378	4AC	C6-N1	3.48	1.46	1.38
27	B1	2428	OMC	C6-N1	3.46	1.46	1.38
1	A1	1194	OMC	C6-N1	3.43	1.46	1.38
27	B1	1832	OMC	C6-N1	3.42	1.46	1.38
27	B1	1533	OMG	C6-N1	3.42	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1914	OMC	C6-N1	3.41	1.46	1.38
27	B1	1489	OMC	C6-N1	3.41	1.46	1.38
1	A1	1366	A1I59	C2-N1	-3.39	1.32	1.40
1	A1	426	OMC	C6-N1	3.39	1.46	1.38
27	B1	2059	OMC	C6-N1	3.39	1.46	1.38
27	B1	2119	OMC	C6-N1	3.39	1.46	1.38
27	B1	1099	OMC	C6-N1	3.39	1.46	1.38
27	B1	2557	OMC	C6-N1	3.39	1.46	1.38
1	A1	1252	OMC	C6-N1	3.37	1.46	1.38
1	A1	1270	OMC	C6-N1	3.36	1.46	1.38
27	B1	2808	OMC	C6-N1	3.36	1.46	1.38
27	B1	2607	OMC	C6-N1	3.36	1.46	1.38
1	A1	834	OMC	C6-N1	3.35	1.46	1.38
1	A1	117	OMC	C6-N1	3.34	1.46	1.38
27	B1	2735	OMC	C6-N1	3.34	1.46	1.38
27	B1	501	OMC	C6-N1	3.33	1.46	1.38
27	B1	977	OMC	C6-N1	3.33	1.46	1.38
27	B1	1783	OMC	C6-N1	3.31	1.46	1.38
1	A1	1314	4AC	C6-N1	3.25	1.45	1.38
27	B1	162	4AC	C6-N1	3.24	1.45	1.38
27	B1	2328	4AC	C6-N1	3.22	1.45	1.38
27	B1	2008	4AC	C6-N1	3.22	1.45	1.38
27	B1	1649	4AC	C6-N1	3.22	1.45	1.38
27	B1	2700	UR3	O4-C4	-3.21	1.16	1.23
27	B1	1290	4AC	C6-N1	3.21	1.45	1.38
27	B1	1612	4AC	C6-N1	3.21	1.45	1.38
27	B1	896	4AC	C6-N1	3.21	1.45	1.38
1	A1	195	4AC	C6-N1	3.21	1.45	1.38
27	B1	2020	4AC	C6-N1	3.21	1.45	1.38
27	B1	2492	4AC	C6-N1	3.20	1.45	1.38
27	B1	2749	4AC	C6-N1	3.20	1.45	1.38
27	B1	2171	4AC	C6-N1	3.20	1.45	1.38
27	B1	48	4AC	C6-N1	3.20	1.45	1.38
1	A1	1067	4AC	C6-N1	3.20	1.45	1.38
1	A1	274	4AC	C6-N1	3.20	1.45	1.38
27	B1	2526	4AC	C6-N1	3.19	1.45	1.38
1	A1	1181	4AC	C6-N1	3.19	1.45	1.38
27	B1	1067	4AC	C6-N1	3.19	1.45	1.38
1	A1	231	4AC	C6-N1	3.19	1.45	1.38
1	A1	1135	4AC	C6-N1	3.19	1.45	1.38
27	B1	609	4AC	C6-N1	3.18	1.45	1.38
27	B1	1442	4AC	C6-N1	3.18	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	98	4AC	C6-N1	3.18	1.45	1.38
27	B1	2888	4AC	C6-N1	3.18	1.45	1.38
27	B1	688	4AC	C6-N1	3.18	1.45	1.38
27	B1	1706	4AC	C6-N1	3.18	1.45	1.38
27	B1	1100	4AC	C6-N1	3.18	1.45	1.38
27	B1	1967	4AC	C6-N1	3.18	1.45	1.38
1	A1	1029	4AC	C6-N1	3.18	1.45	1.38
27	B1	1264	4AC	C6-N1	3.18	1.45	1.38
1	A1	719	4AC	C6-N1	3.18	1.45	1.38
1	A1	1227	4AC	C6-N1	3.18	1.45	1.38
27	B1	1107	4AC	C6-N1	3.18	1.45	1.38
1	A1	706	4AC	C6-N1	3.17	1.45	1.38
1	A1	839	4AC	C6-N1	3.17	1.45	1.38
27	B1	759	4AC	C6-N1	3.17	1.45	1.38
27	B1	1052	4AC	C6-N1	3.17	1.45	1.38
27	B1	2432	4AC	C6-N1	3.17	1.45	1.38
27	B1	1846	4AC	C6-N1	3.17	1.45	1.38
28	B2	117	4AC	C6-N1	3.17	1.45	1.38
1	A1	1092	4AC	C6-N1	3.17	1.45	1.38
27	B1	130	4AC	C6-N1	3.17	1.45	1.38
27	B1	1822	4AC	C6-N1	3.17	1.45	1.38
27	B1	2821	4AC	C6-N1	3.17	1.45	1.38
27	B1	1885	4AC	C6-N1	3.17	1.45	1.38
27	B1	786	4AC	C6-N1	3.16	1.45	1.38
27	B1	1751	4AC	C6-N1	3.16	1.45	1.38
27	B1	142	4AC	C6-N1	3.16	1.45	1.38
27	B1	1664	4AC	C6-N1	3.16	1.45	1.38
27	B1	1546	4AC	C6-N1	3.16	1.45	1.38
27	B1	741	4AC	C6-N1	3.16	1.45	1.38
27	B1	732	4AC	C6-N1	3.16	1.45	1.38
1	A1	546	4AC	C6-N1	3.16	1.45	1.38
1	A1	856	4AC	C6-N1	3.16	1.45	1.38
1	A1	216	4AC	C6-N1	3.16	1.45	1.38
1	A1	1288	4AC	C6-N1	3.16	1.45	1.38
1	A1	578	4AC	C6-N1	3.16	1.45	1.38
27	B1	3023	4AC	C6-N1	3.15	1.45	1.38
27	B1	721	4AC	C6-N1	3.15	1.45	1.38
27	B1	360	4AC	C6-N1	3.15	1.45	1.38
27	B1	1703	4AC	C6-N1	3.15	1.45	1.38
27	B1	1501	4AC	C6-N1	3.15	1.45	1.38
1	A1	405	4AC	C6-N1	3.15	1.45	1.38
27	B1	3006	4AC	C6-N1	3.15	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	41	4AC	C6-N1	3.15	1.45	1.38
27	B1	940	A2M	C6-N6	3.15	1.45	1.34
27	B1	1734	4AC	C6-N1	3.15	1.45	1.38
27	B1	2454	4AC	C6-N1	3.15	1.45	1.38
27	B1	580	4AC	C6-N1	3.15	1.45	1.38
1	A1	816	4AC	C6-N1	3.14	1.45	1.38
27	B1	116	4AC	C6-N1	3.14	1.45	1.38
27	B1	276	4AC	C6-N1	3.14	1.45	1.38
27	B1	1061	4AC	C6-N1	3.14	1.45	1.38
27	B1	2379	4AC	C6-N1	3.14	1.45	1.38
27	B1	652	4AC	C6-N1	3.14	1.45	1.38
1	A1	361	A2M	C6-N6	3.14	1.45	1.34
27	B1	1743	4AC	C6-N1	3.14	1.45	1.38
27	B1	19	4AC	C6-N1	3.14	1.45	1.38
1	A1	827	4AC	C6-N1	3.14	1.45	1.38
27	B1	2133	4AC	C6-N1	3.14	1.45	1.38
1	A1	291	4AC	C6-N1	3.14	1.45	1.38
27	B1	485	4AC	C6-N1	3.14	1.45	1.38
1	A1	819	A2M	C6-N6	3.14	1.45	1.34
1	A1	810	4AC	C6-N1	3.14	1.45	1.38
27	B1	2429	4AC	C6-N1	3.14	1.45	1.38
27	B1	807	4AC	C6-N1	3.14	1.45	1.38
27	B1	200	4AC	C6-N1	3.14	1.45	1.38
27	B1	271	4AC	C6-N1	3.14	1.45	1.38
27	B1	392	4AC	C6-N1	3.14	1.45	1.38
27	B1	243	4AC	C6-N1	3.14	1.45	1.38
27	B1	866	4AC	C6-N1	3.14	1.45	1.38
27	B1	1404	4AC	C6-N1	3.14	1.45	1.38
1	A1	499	4AC	C6-N1	3.14	1.45	1.38
27	B1	479	4AC	C6-N1	3.14	1.45	1.38
1	A1	534	4AC	C6-N1	3.14	1.45	1.38
1	A1	739	4AC	C6-N1	3.14	1.45	1.38
27	B1	2602	4AC	C6-N1	3.13	1.45	1.38
27	B1	2876	4AC	C6-N1	3.13	1.45	1.38
27	B1	2792	4AC	C6-N1	3.13	1.45	1.38
27	B1	1178	4AC	C6-N1	3.13	1.45	1.38
27	B1	1293	4AC	C6-N1	3.13	1.45	1.38
27	B1	506	A2M	C6-N6	3.13	1.45	1.34
27	B1	1505	4AC	C6-N1	3.13	1.45	1.38
27	B1	1313	4AC	C6-N1	3.13	1.45	1.38
27	B1	880	A2M	C6-N6	3.13	1.45	1.34
1	A1	467	4AC	C6-N1	3.13	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	367	4AC	C6-N1	3.13	1.45	1.38
27	B1	1911	4AC	C6-N1	3.13	1.45	1.38
28	B2	120	4AC	C6-N1	3.13	1.45	1.38
27	B1	2809	4AC	C6-N1	3.13	1.45	1.38
1	A1	1467	4AC	C6-N1	3.13	1.45	1.38
27	B1	1478	4AC	C6-N1	3.13	1.45	1.38
1	A1	1004	2MG	C5-C6	3.12	1.53	1.47
1	A1	636	4AC	C6-N1	3.12	1.45	1.38
27	B1	1386	4AC	C6-N1	3.12	1.45	1.38
1	A1	87	4AC	C6-N1	3.12	1.45	1.38
27	B1	1128	4AC	C6-N1	3.12	1.45	1.38
1	A1	1221	4AC	C6-N1	3.12	1.45	1.38
1	A1	220	4AC	C6-N1	3.12	1.45	1.38
1	A1	141	4AC	C6-N1	3.12	1.45	1.38
1	A1	836	4AC	C6-N1	3.12	1.45	1.38
27	B1	2844	4AC	C6-N1	3.12	1.45	1.38
27	B1	857	A2M	C6-N6	3.12	1.45	1.34
27	B1	1322	4AC	C6-N1	3.12	1.45	1.38
28	B2	90	4AC	C6-N1	3.12	1.45	1.38
1	A1	5	4AC	C6-N1	3.11	1.45	1.38
27	B1	1383	4AC	C6-N1	3.11	1.45	1.38
27	B1	1551	4AC	C6-N1	3.11	1.45	1.38
27	B1	1435	4AC	C6-N1	3.11	1.45	1.38
27	B1	3020	4AC	C6-N1	3.11	1.45	1.38
27	B1	715	4AC	C6-N1	3.11	1.45	1.38
1	A1	1016	4AC	C6-N1	3.10	1.45	1.38
1	A1	1254	4AC	C6-N1	3.10	1.45	1.38
27	B1	1639	4AC	C6-N1	3.10	1.45	1.38
1	A1	444	4AC	C6-N1	3.10	1.45	1.38
27	B1	2469	4AC	C6-N1	3.10	1.45	1.38
27	B1	23	4AC	C6-N1	3.10	1.45	1.38
27	B1	2213	4AC	C6-N1	3.10	1.45	1.38
27	B1	2850	4AC	C6-N1	3.10	1.45	1.38
27	B1	1818	4AC	C6-N1	3.09	1.45	1.38
1	A1	382	4AC	C6-N1	3.09	1.45	1.38
27	B1	3011	4AC	C6-N1	3.09	1.45	1.38
27	B1	2057	A2M	C6-N6	3.09	1.45	1.34
1	A1	761	4AC	C6-N1	3.09	1.45	1.38
1	A1	329	OMG	C5-C6	3.09	1.53	1.47
27	B1	798	4AC	C6-N1	3.09	1.45	1.38
27	B1	434	4AC	C6-N1	3.09	1.45	1.38
27	B1	419	4AC	C6-N1	3.09	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1769	4AC	C6-N1	3.09	1.45	1.38
27	B1	599	4AC	C6-N1	3.09	1.45	1.38
27	B1	3037	4AC	C6-N1	3.08	1.45	1.38
27	B1	950	4AC	C6-N1	3.08	1.45	1.38
27	B1	2506	A2M	C6-N6	3.08	1.45	1.34
1	A1	307	4AC	C6-N1	3.07	1.45	1.38
27	B1	337	4AC	C6-N1	3.07	1.45	1.38
1	A1	763	OMG	C5-C6	3.07	1.53	1.47
1	A1	624	4AC	C6-N1	3.07	1.45	1.38
27	B1	2057	A2M	O3'-C3'	-3.07	1.35	1.43
1	A1	455	OMG	C5-C6	3.06	1.53	1.47
27	B1	1064	4AC	C6-N1	3.06	1.45	1.38
27	B1	2757	OMG	C5-C6	3.06	1.53	1.47
1	A1	540	4AC	C6-N1	3.06	1.45	1.38
27	B1	1757	4AC	C6-N1	3.06	1.45	1.38
27	B1	953	4AC	C6-N1	3.06	1.45	1.38
27	B1	227	4AC	C6-N1	3.06	1.45	1.38
27	B1	1439	4AC	C6-N1	3.06	1.45	1.38
1	A1	1003	OMG	C5-C6	3.05	1.53	1.47
1	A1	691	4AC	C6-N1	3.05	1.45	1.38
1	A1	427	4AC	C6-N1	3.04	1.45	1.38
1	A1	507	OMG	C5-C6	3.04	1.53	1.47
27	B1	1557	OMG	C5-C6	3.03	1.53	1.47
27	B1	2684	OMG	C5-C6	3.03	1.53	1.47
27	B1	80	4AC	C6-N1	3.03	1.45	1.38
27	B1	940	A2M	O3'-C3'	-3.02	1.35	1.43
1	A1	227	OMG	C5-C6	3.02	1.53	1.47
1	A1	668	OMG	C5-C6	3.02	1.53	1.47
1	A1	153	OMG	C5-C6	3.01	1.53	1.47
27	B1	880	A2M	O3'-C3'	-3.01	1.35	1.43
27	B1	920	OMG	C5-C6	3.01	1.53	1.47
27	B1	2506	A2M	O3'-C3'	-3.00	1.35	1.43
27	B1	2562	OMG	C5-C6	3.00	1.53	1.47
27	B1	1601	OMG	C5-C6	3.00	1.53	1.47
27	B1	1621	4AC	C6-N1	3.00	1.45	1.38
27	B1	2113	4AC	C6-N1	2.99	1.45	1.38
1	A1	833	OMG	C5-C6	2.99	1.53	1.47
27	B1	1762	4AC	C6-N1	2.99	1.45	1.38
1	A1	901	OMG	C5-C6	2.99	1.53	1.47
1	A1	228	OMG	C5-C6	2.98	1.53	1.47
1	A1	775	OMU	C6-N1	2.98	1.45	1.38
27	B1	2740	OMG	C5-C6	2.97	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	214	OMG	C5-C6	2.97	1.53	1.47
27	B1	2984	OMG	C5-C6	2.97	1.53	1.47
1	A1	459	OMG	C5-C6	2.97	1.53	1.47
27	B1	2180	OMG	C5-C6	2.97	1.53	1.47
27	B1	979	4AC	C6-N1	2.96	1.45	1.38
27	B1	1360	4AC	C6-N1	2.96	1.45	1.38
27	B1	2540	OMG	C5-C6	2.96	1.53	1.47
1	A1	819	A2M	O3'-C3'	-2.96	1.36	1.43
27	B1	808	OMG	C5-C6	2.95	1.53	1.47
1	A1	861	OMG	C5-C6	2.95	1.53	1.47
27	B1	841	OMG	C5-C6	2.95	1.53	1.47
27	B1	933	4AC	C6-N1	2.95	1.45	1.38
27	B1	1965	OMG	C5-C6	2.95	1.53	1.47
27	B1	1286	4AC	C6-N1	2.94	1.45	1.38
1	A1	8	OMU	C6-N1	2.94	1.45	1.38
27	B1	857	A2M	O3'-C3'	-2.93	1.36	1.43
27	B1	675	OMG	C5-C6	2.93	1.53	1.47
1	A1	645	OMG	C5-C6	2.93	1.53	1.47
27	B1	1608	4AC	C6-N1	2.93	1.45	1.38
27	B1	2659	OMG	C5-C6	2.92	1.53	1.47
27	B1	2401	OMU	C6-N1	2.92	1.45	1.38
27	B1	2391	OMG	C5-C6	2.92	1.53	1.47
27	B1	1374	4AC	C6-N1	2.92	1.45	1.38
27	B1	2022	OMG	C5-C6	2.91	1.53	1.47
1	A1	52	OMU	C6-N1	2.91	1.45	1.38
27	B1	2365	OMG	C5-C6	2.91	1.53	1.47
27	B1	506	A2M	O3'-C3'	-2.91	1.36	1.43
27	B1	1488	OMU	C6-N1	2.91	1.45	1.38
1	A1	826	5MC	CM5-C5	2.90	1.57	1.50
1	A1	533	5MC	CM5-C5	2.90	1.57	1.50
1	A1	1348	5MC	CM5-C5	2.90	1.57	1.50
1	A1	951	5MC	CM5-C5	2.90	1.57	1.50
1	A1	614	4AC	C6-N1	2.90	1.45	1.38
1	A1	762	OMU	C6-N1	2.89	1.45	1.38
1	A1	863	5MC	CM5-C5	2.89	1.57	1.50
1	A1	361	A2M	O2'-C2'	2.89	1.50	1.42
27	B1	97	5MC	CM5-C5	2.89	1.57	1.50
27	B1	1983	5MC	CM5-C5	2.89	1.57	1.50
1	A1	1013	5MC	CM5-C5	2.89	1.57	1.50
1	A1	425	OMU	O4-C4	-2.89	1.18	1.24
27	B1	275	5MC	CM5-C5	2.88	1.57	1.50
27	B1	454	OMU	O4-C4	-2.88	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1620	5MC	CM5-C5	2.88	1.57	1.50
1	A1	1012	5MC	CM5-C5	2.88	1.57	1.50
1	A1	466	5MC	CM5-C5	2.88	1.57	1.50
1	A1	1015	5MC	CM5-C5	2.88	1.57	1.50
1	A1	1190	5MC	CM5-C5	2.88	1.57	1.50
27	B1	813	4AC	C6-N1	2.88	1.44	1.38
27	B1	2593	OMU	C6-N1	2.88	1.44	1.38
27	B1	18	5MC	CM5-C5	2.88	1.57	1.50
1	A1	1362	5MC	CM5-C5	2.88	1.57	1.50
27	B1	1149	5MC	CM5-C5	2.88	1.57	1.50
27	B1	2875	5MC	CM5-C5	2.88	1.57	1.50
27	B1	2554	OMU	C6-N1	2.88	1.44	1.38
27	B1	454	OMU	C6-N1	2.87	1.44	1.38
1	A1	605	5MC	CM5-C5	2.87	1.57	1.50
27	B1	921	OMG	C5-C6	2.87	1.53	1.47
27	B1	887	OMG	C5-C6	2.87	1.53	1.47
27	B1	2554	OMU	O4-C4	-2.87	1.18	1.24
1	A1	473	5MC	CM5-C5	2.87	1.57	1.50
1	A1	855	5MC	CM5-C5	2.87	1.57	1.50
1	A1	687	5MC	CM5-C5	2.87	1.57	1.50
27	B1	359	5MC	CM5-C5	2.87	1.57	1.50
1	A1	1486	5MC	CM5-C5	2.87	1.57	1.50
27	B1	2453	5MC	CM5-C5	2.87	1.57	1.50
27	B1	2087	5MC	CM5-C5	2.87	1.57	1.50
1	A1	1368	OMU	C6-N1	2.87	1.44	1.38
27	B1	2668	OMU	C6-N1	2.86	1.44	1.38
27	B1	2593	OMU	O4-C4	-2.86	1.18	1.24
1	A1	718	5MC	CM5-C5	2.86	1.57	1.50
27	B1	1981	OMU	C6-N1	2.86	1.44	1.38
27	B1	226	5MC	CM5-C5	2.86	1.57	1.50
1	A1	17	5MC	CM5-C5	2.86	1.57	1.50
27	B1	1100	4AC	O2-C2	-2.86	1.18	1.23
27	B1	877	5MC	CM5-C5	2.86	1.57	1.50
1	A1	523	5MC	CM5-C5	2.86	1.57	1.50
27	B1	2028	OMG	C5-C6	2.86	1.53	1.47
27	B1	932	5MC	CM5-C5	2.86	1.57	1.50
1	A1	1484	5MC	CM5-C5	2.86	1.57	1.50
27	B1	2668	OMU	O4-C4	-2.85	1.19	1.24
27	B1	1868	5MC	CM5-C5	2.85	1.57	1.50
1	A1	8	OMU	O4-C4	-2.85	1.19	1.24
1	A1	762	OMU	O4-C4	-2.85	1.19	1.24
1	A1	775	OMU	O4-C4	-2.85	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	681	5MC	CM5-C5	2.85	1.57	1.50
27	B1	2757	OMG	C5-C4	-2.85	1.35	1.43
27	B1	1981	OMU	O4-C4	-2.84	1.19	1.24
1	A1	756	4SU	C6-N1	2.84	1.44	1.38
27	B1	1648	5MC	CM5-C5	2.84	1.57	1.50
27	B1	1533	OMG	C5-C6	2.84	1.53	1.47
27	B1	1977	5MC	CM5-C5	2.84	1.57	1.50
27	B1	1769	4AC	O2-C2	-2.84	1.18	1.23
1	A1	623	5MC	CM5-C5	2.84	1.57	1.50
27	B1	1488	OMU	O4-C4	-2.84	1.19	1.24
27	B1	1150	4AC	C6-N1	2.83	1.44	1.38
27	B1	1966	5MC	CM5-C5	2.82	1.57	1.50
1	A1	819	A2M	O2'-C2'	2.82	1.49	1.42
1	A1	425	OMU	C6-N1	2.82	1.44	1.38
27	B1	2401	OMU	O4-C4	-2.82	1.19	1.24
1	A1	273	5MC	CM5-C5	2.82	1.57	1.50
1	A1	230	5MC	CM5-C5	2.82	1.57	1.50
27	B1	2067	5MC	CM5-C5	2.81	1.57	1.50
27	B1	485	4AC	O2-C2	-2.81	1.18	1.23
1	A1	1366	A1I59	C1-C3	2.81	1.54	1.51
27	B1	2082	5MC	CM5-C5	2.81	1.57	1.50
1	A1	52	OMU	O4-C4	-2.81	1.19	1.24
1	A1	1368	OMU	O4-C4	-2.81	1.19	1.24
27	B1	2984	OMG	C5-C4	-2.80	1.35	1.43
27	B1	2057	A2M	O2'-C2'	2.80	1.49	1.42
27	B1	2391	OMG	C5-C4	-2.80	1.35	1.43
1	A1	361	A2M	O3'-C3'	-2.79	1.36	1.43
27	B1	1981	OMU	C5-C4	2.79	1.49	1.43
27	B1	857	A2M	O2'-C2'	2.79	1.49	1.42
1	A1	329	OMG	C5-C4	-2.79	1.36	1.43
27	B1	2735	OMC	O2-C2	-2.78	1.18	1.23
27	B1	675	OMG	C5-C4	-2.78	1.36	1.43
27	B1	2617	5MC	CM5-C5	2.78	1.57	1.50
27	B1	2659	OMG	C5-C4	-2.78	1.36	1.43
1	A1	775	OMU	C5-C4	2.78	1.49	1.43
27	B1	1489	OMC	O2-C2	-2.78	1.18	1.23
27	B1	940	A2M	O2'-C2'	2.78	1.49	1.42
27	B1	336	5MC	CM5-C5	2.77	1.57	1.50
1	A1	117	OMC	O2-C2	-2.77	1.18	1.23
27	B1	1439	4AC	O2-C2	-2.77	1.18	1.23
27	B1	1639	4AC	O2-C2	-2.77	1.18	1.23
27	B1	880	A2M	O2'-C2'	2.76	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	3020	4AC	O2-C2	-2.76	1.18	1.23
27	B1	921	OMG	C5-C4	-2.76	1.36	1.43
27	B1	2022	OMG	C5-C4	-2.76	1.36	1.43
1	A1	228	OMG	C5-C4	-2.76	1.36	1.43
27	B1	2668	OMU	C5-C4	2.76	1.49	1.43
27	B1	2565	4SU	C6-N1	2.76	1.44	1.38
27	B1	580	4AC	O2-C2	-2.76	1.18	1.23
1	A1	228	OMG	C2-N1	2.76	1.44	1.37
27	B1	2984	OMG	C2-N1	2.76	1.44	1.37
27	B1	1822	4AC	O2-C2	-2.75	1.18	1.23
27	B1	1533	OMG	C5-C4	-2.75	1.36	1.43
27	B1	1360	4AC	O2-C2	-2.75	1.18	1.23
27	B1	214	OMG	C5-C4	-2.75	1.36	1.43
1	A1	8	OMU	C5-C4	2.75	1.49	1.43
1	A1	861	OMG	C5-C4	-2.75	1.36	1.43
27	B1	1967	4AC	O2-C2	-2.75	1.18	1.23
1	A1	507	OMG	C2-N1	2.75	1.44	1.37
27	B1	200	4AC	O2-C2	-2.75	1.18	1.23
27	B1	1052	4AC	O2-C2	-2.74	1.18	1.23
27	B1	2809	4AC	O2-C2	-2.74	1.18	1.23
1	A1	1003	OMG	C2-N1	2.74	1.44	1.37
27	B1	1762	4AC	O2-C2	-2.74	1.18	1.23
1	A1	1368	OMU	C5-C4	2.74	1.49	1.43
27	B1	2391	OMG	C2-N1	2.74	1.44	1.37
27	B1	1404	4AC	O2-C2	-2.74	1.18	1.23
1	A1	455	OMG	C2-N1	2.74	1.44	1.37
27	B1	841	OMG	C5-C4	-2.74	1.36	1.43
27	B1	2740	OMG	C5-C4	-2.74	1.36	1.43
27	B1	1551	4AC	O2-C2	-2.74	1.18	1.23
27	B1	2506	A2M	O2'-C2'	2.74	1.49	1.42
27	B1	2844	4AC	O2-C2	-2.74	1.18	1.23
1	A1	719	4AC	O2-C2	-2.74	1.18	1.23
27	B1	2740	OMG	C2-N1	2.74	1.44	1.37
27	B1	2180	OMG	C5-C4	-2.74	1.36	1.43
27	B1	2562	OMG	C5-C4	-2.74	1.36	1.43
27	B1	47	5MC	CM5-C5	2.73	1.57	1.50
27	B1	813	4AC	O2-C2	-2.73	1.18	1.23
27	B1	1832	OMC	O2-C2	-2.73	1.18	1.23
27	B1	501	OMC	O2-C2	-2.73	1.18	1.23
27	B1	506	A2M	C5-C4	-2.73	1.33	1.40
27	B1	2659	OMG	C2-N1	2.73	1.44	1.37
1	A1	901	OMG	C2-N1	2.73	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2401	OMU	C5-C4	2.73	1.49	1.43
1	A1	1288	4AC	O2-C2	-2.73	1.18	1.23
27	B1	808	OMG	C5-C4	-2.73	1.36	1.43
27	B1	950	4AC	O2-C2	-2.73	1.18	1.23
27	B1	1374	4AC	O2-C2	-2.73	1.18	1.23
27	B1	2379	4AC	O2-C2	-2.73	1.18	1.23
27	B1	2028	OMG	C2-N1	2.73	1.44	1.37
27	B1	2850	4AC	O2-C2	-2.72	1.18	1.23
27	B1	721	4AC	O2-C2	-2.72	1.18	1.23
27	B1	1286	4AC	O2-C2	-2.72	1.18	1.23
27	B1	857	A2M	C5-C4	-2.72	1.33	1.40
27	B1	506	A2M	O2'-C2'	2.72	1.49	1.42
27	B1	1601	OMG	C5-C4	-2.72	1.36	1.43
27	B1	1451	5MC	CM5-C5	2.72	1.57	1.50
27	B1	2028	OMG	C5-C4	-2.72	1.36	1.43
27	B1	1914	OMC	O2-C2	-2.72	1.18	1.23
1	A1	227	OMG	C2-N1	2.72	1.44	1.37
27	B1	2506	A2M	C5-C4	-2.72	1.33	1.40
1	A1	1475	MA6	C5-C4	-2.72	1.33	1.40
1	A1	425	OMU	C5-C4	2.72	1.49	1.43
27	B1	2602	4AC	O2-C2	-2.72	1.18	1.23
27	B1	2593	OMU	C5-C4	2.72	1.49	1.43
27	B1	2171	4AC	O2-C2	-2.72	1.18	1.23
27	B1	940	A2M	C5-C4	-2.71	1.33	1.40
1	A1	540	4AC	O2-C2	-2.71	1.18	1.23
1	A1	856	4AC	O2-C2	-2.71	1.18	1.23
27	B1	1264	4AC	O2-C2	-2.71	1.18	1.23
27	B1	2113	4AC	O2-C2	-2.71	1.18	1.23
27	B1	1601	OMG	C2-N1	2.71	1.44	1.37
1	A1	507	OMG	C5-C4	-2.71	1.36	1.43
27	B1	1557	OMG	C2-N1	2.71	1.44	1.37
1	A1	153	OMG	C2-N1	2.71	1.44	1.37
27	B1	2684	OMG	C2-N1	2.71	1.44	1.37
1	A1	227	OMG	C5-C4	-2.71	1.36	1.43
1	A1	861	OMG	C2-N1	2.71	1.44	1.37
27	B1	434	4AC	O2-C2	-2.71	1.18	1.23
27	B1	741	4AC	O2-C2	-2.71	1.18	1.23
27	B1	1150	4AC	O2-C2	-2.71	1.18	1.23
27	B1	2133	4AC	O2-C2	-2.71	1.18	1.23
27	B1	977	OMC	O2-C2	-2.71	1.18	1.23
27	B1	2469	4AC	O2-C2	-2.71	1.18	1.23
27	B1	1293	4AC	O2-C2	-2.71	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1612	4AC	O2-C2	-2.71	1.18	1.23
27	B1	2213	4AC	O2-C2	-2.71	1.18	1.23
1	A1	1476	MA6	C5-C4	-2.70	1.33	1.40
27	B1	880	A2M	C5-C4	-2.70	1.33	1.40
27	B1	652	4AC	O2-C2	-2.70	1.18	1.23
27	B1	933	4AC	O2-C2	-2.70	1.18	1.23
1	A1	614	4AC	O2-C2	-2.70	1.18	1.23
27	B1	1386	4AC	O2-C2	-2.70	1.18	1.23
1	A1	1457	MA6	C5-C4	-2.70	1.33	1.40
27	B1	2684	OMG	C5-C4	-2.70	1.36	1.43
1	A1	52	OMU	C5-C4	2.70	1.49	1.43
27	B1	1067	4AC	O2-C2	-2.70	1.18	1.23
27	B1	1107	4AC	O2-C2	-2.70	1.18	1.23
27	B1	1783	OMC	O2-C2	-2.70	1.18	1.23
1	A1	762	OMU	C5-C4	2.70	1.49	1.43
27	B1	1435	4AC	O2-C2	-2.70	1.18	1.23
27	B1	2888	4AC	O2-C2	-2.70	1.18	1.23
27	B1	2700	UR3	C6-N1	2.70	1.44	1.38
27	B1	214	OMG	C2-N1	2.70	1.44	1.37
1	A1	834	OMC	O2-C2	-2.70	1.18	1.23
1	A1	578	4AC	O2-C2	-2.70	1.18	1.23
1	A1	307	4AC	O2-C2	-2.70	1.18	1.23
27	B1	130	4AC	O2-C2	-2.69	1.18	1.23
27	B1	2180	OMG	C2-N1	2.69	1.44	1.37
1	A1	836	4AC	O2-C2	-2.69	1.18	1.23
27	B1	2492	4AC	O2-C2	-2.69	1.18	1.23
27	B1	1965	OMG	C5-C4	-2.69	1.36	1.43
27	B1	2876	4AC	O2-C2	-2.69	1.18	1.23
1	A1	5	4AC	O2-C2	-2.69	1.18	1.23
1	A1	291	4AC	O2-C2	-2.69	1.18	1.23
1	A1	231	4AC	O2-C2	-2.69	1.18	1.23
27	B1	1451	5MC	C4-N4	2.69	1.41	1.34
27	B1	2554	OMU	C5-C4	2.69	1.49	1.43
1	A1	361	A2M	C5-C4	-2.69	1.33	1.40
27	B1	1099	OMC	O2-C2	-2.69	1.18	1.23
1	A1	810	4AC	O2-C2	-2.69	1.18	1.23
27	B1	1442	4AC	O2-C2	-2.69	1.18	1.23
27	B1	2757	OMG	C2-N1	2.69	1.44	1.37
27	B1	953	4AC	O2-C2	-2.69	1.18	1.23
27	B1	1322	4AC	O2-C2	-2.69	1.18	1.23
27	B1	1557	OMG	C5-C4	-2.69	1.36	1.43
27	B1	2821	4AC	O2-C2	-2.69	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	833	OMG	C2-N1	2.69	1.44	1.37
27	B1	675	OMG	C2-N1	2.69	1.44	1.37
27	B1	454	OMU	C5-C4	2.69	1.49	1.43
27	B1	116	4AC	O2-C2	-2.68	1.18	1.23
27	B1	360	4AC	O2-C2	-2.68	1.18	1.23
27	B1	378	4AC	O2-C2	-2.68	1.18	1.23
1	A1	87	4AC	O2-C2	-2.68	1.18	1.23
27	B1	1911	4AC	O2-C2	-2.68	1.18	1.23
27	B1	2557	OMC	O2-C2	-2.68	1.18	1.23
1	A1	901	OMG	C5-C4	-2.68	1.36	1.43
27	B1	276	4AC	O2-C2	-2.68	1.18	1.23
27	B1	1885	4AC	O2-C2	-2.68	1.18	1.23
1	A1	274	4AC	O2-C2	-2.68	1.18	1.23
27	B1	2020	4AC	O2-C2	-2.68	1.18	1.23
27	B1	2540	OMG	C5-C4	-2.68	1.36	1.43
27	B1	1313	4AC	O2-C2	-2.68	1.18	1.23
27	B1	2749	4AC	O2-C2	-2.68	1.18	1.23
1	A1	819	A2M	C5-C4	-2.68	1.33	1.40
27	B1	2057	A2M	C5-C4	-2.68	1.33	1.40
27	B1	2365	OMG	C5-C4	-2.68	1.36	1.43
27	B1	1061	4AC	O2-C2	-2.68	1.18	1.23
27	B1	2119	OMC	O2-C2	-2.68	1.18	1.23
27	B1	19	4AC	O2-C2	-2.68	1.18	1.23
27	B1	1757	4AC	O2-C2	-2.68	1.18	1.23
27	B1	1533	OMG	C2-N1	2.68	1.44	1.37
27	B1	80	4AC	O2-C2	-2.68	1.18	1.23
27	B1	1064	4AC	O2-C2	-2.68	1.18	1.23
27	B1	23	4AC	O2-C2	-2.68	1.18	1.23
27	B1	1649	4AC	O2-C2	-2.67	1.18	1.23
27	B1	48	4AC	O2-C2	-2.67	1.18	1.23
27	B1	920	OMG	C2-N1	2.67	1.44	1.37
1	A1	220	4AC	O2-C2	-2.67	1.18	1.23
27	B1	337	4AC	O2-C2	-2.67	1.18	1.23
1	A1	455	OMG	C5-C4	-2.67	1.36	1.43
1	A1	1314	4AC	O2-C2	-2.67	1.18	1.23
27	B1	1734	4AC	O2-C2	-2.67	1.18	1.23
27	B1	1488	OMU	C5-C4	2.67	1.49	1.43
1	A1	1221	4AC	O2-C2	-2.67	1.18	1.23
27	B1	2607	OMC	O2-C2	-2.67	1.18	1.23
27	B1	2059	OMC	O2-C2	-2.67	1.18	1.23
1	A1	763	OMG	C5-C4	-2.67	1.36	1.43
27	B1	142	4AC	O2-C2	-2.67	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	827	4AC	O2-C2	-2.67	1.18	1.23
1	A1	1029	4AC	O2-C2	-2.67	1.18	1.23
27	B1	896	4AC	O2-C2	-2.67	1.18	1.23
1	A1	1067	4AC	O2-C2	-2.67	1.18	1.23
27	B1	98	4AC	O2-C2	-2.67	1.18	1.23
27	B1	227	4AC	O2-C2	-2.67	1.18	1.23
1	A1	855	5MC	C4-N4	2.67	1.41	1.34
1	A1	1003	OMG	C5-C4	-2.67	1.36	1.43
1	A1	833	OMG	C5-C4	-2.67	1.36	1.43
27	B1	732	4AC	O2-C2	-2.66	1.18	1.23
1	A1	216	4AC	O2-C2	-2.66	1.18	1.23
1	A1	1015	5MC	C4-N4	2.66	1.41	1.34
1	A1	1348	5MC	C4-N4	2.66	1.41	1.34
27	B1	887	OMG	C5-C4	-2.66	1.36	1.43
27	B1	866	4AC	O2-C2	-2.66	1.18	1.23
1	A1	1004	2MG	C5-C4	-2.66	1.36	1.43
1	A1	706	4AC	O2-C2	-2.66	1.18	1.23
27	B1	798	4AC	O2-C2	-2.66	1.18	1.23
27	B1	2365	OMG	C2-N1	2.66	1.44	1.37
27	B1	1965	OMG	C2-N1	2.66	1.44	1.37
27	B1	1383	4AC	O2-C2	-2.66	1.18	1.23
28	B2	117	4AC	O2-C2	-2.66	1.18	1.23
27	B1	921	OMG	C2-N1	2.66	1.44	1.37
1	A1	763	OMG	C2-N1	2.66	1.44	1.37
1	A1	624	4AC	O2-C2	-2.66	1.18	1.23
27	B1	688	4AC	O2-C2	-2.66	1.18	1.23
27	B1	887	OMG	C2-N1	2.66	1.44	1.37
1	A1	499	4AC	O2-C2	-2.66	1.18	1.23
27	B1	2562	OMG	C2-N1	2.66	1.44	1.37
27	B1	2429	4AC	O2-C2	-2.66	1.18	1.23
27	B1	243	4AC	O2-C2	-2.66	1.18	1.23
27	B1	1706	4AC	O2-C2	-2.66	1.18	1.23
1	A1	329	OMG	C2-N1	2.66	1.44	1.37
1	A1	41	4AC	O2-C2	-2.66	1.18	1.23
27	B1	786	4AC	O2-C2	-2.66	1.18	1.23
27	B1	979	4AC	O2-C2	-2.66	1.18	1.23
1	A1	1013	5MC	C4-N4	2.65	1.41	1.34
27	B1	2453	5MC	C4-N4	2.65	1.41	1.34
1	A1	1270	OMC	O2-C2	-2.65	1.18	1.23
28	B2	90	4AC	O2-C2	-2.65	1.18	1.23
27	B1	271	4AC	O2-C2	-2.65	1.18	1.23
1	A1	1194	OMC	O2-C2	-2.65	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	715	4AC	O2-C2	-2.65	1.18	1.23
1	A1	691	4AC	O2-C2	-2.65	1.18	1.23
27	B1	807	4AC	O2-C2	-2.65	1.18	1.23
1	A1	1016	4AC	O2-C2	-2.65	1.18	1.23
1	A1	427	4AC	O2-C2	-2.65	1.18	1.23
27	B1	920	OMG	C5-C4	-2.65	1.36	1.43
27	B1	2432	4AC	O2-C2	-2.65	1.18	1.23
27	B1	3037	4AC	O2-C2	-2.65	1.18	1.23
1	A1	668	OMG	C5-C4	-2.65	1.36	1.43
27	B1	392	4AC	O2-C2	-2.65	1.18	1.23
1	A1	605	5MC	C4-N4	2.65	1.41	1.34
1	A1	1227	4AC	O2-C2	-2.65	1.18	1.23
27	B1	1846	4AC	O2-C2	-2.65	1.18	1.23
1	A1	839	4AC	O2-C2	-2.65	1.18	1.23
27	B1	419	4AC	O2-C2	-2.65	1.18	1.23
1	A1	466	5MC	C4-N4	2.65	1.41	1.34
1	A1	459	OMG	C2-N1	2.65	1.44	1.37
27	B1	808	OMG	C2-N1	2.65	1.44	1.37
27	B1	1290	4AC	O2-C2	-2.65	1.18	1.23
1	A1	668	OMG	C2-N1	2.65	1.44	1.37
27	B1	2808	OMC	O2-C2	-2.65	1.18	1.23
27	B1	1178	4AC	O2-C2	-2.65	1.18	1.23
27	B1	1546	4AC	O2-C2	-2.65	1.18	1.23
1	A1	1252	OMC	O2-C2	-2.64	1.18	1.23
27	B1	2792	4AC	O2-C2	-2.64	1.18	1.23
27	B1	599	4AC	O2-C2	-2.64	1.18	1.23
1	A1	473	5MC	C4-N4	2.64	1.41	1.34
27	B1	1608	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1818	4AC	O2-C2	-2.64	1.18	1.23
1	A1	1362	5MC	C4-N4	2.64	1.41	1.34
27	B1	1743	4AC	O2-C2	-2.64	1.18	1.23
1	A1	761	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1478	4AC	O2-C2	-2.64	1.18	1.23
1	A1	623	5MC	C4-N4	2.64	1.40	1.34
1	A1	1190	5MC	C4-N4	2.64	1.40	1.34
27	B1	877	5MC	C4-N4	2.64	1.40	1.34
1	A1	459	OMG	C5-C4	-2.64	1.36	1.43
27	B1	2540	OMG	C2-N1	2.64	1.44	1.37
1	A1	382	4AC	O2-C2	-2.64	1.18	1.23
27	B1	162	4AC	O2-C2	-2.63	1.18	1.23
1	A1	739	4AC	O2-C2	-2.63	1.18	1.23
1	A1	523	5MC	C4-N4	2.63	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	18	5MC	C4-N4	2.63	1.40	1.34
1	A1	367	4AC	O2-C2	-2.63	1.18	1.23
27	B1	1664	4AC	O2-C2	-2.63	1.18	1.23
1	A1	273	5MC	C4-N4	2.63	1.40	1.34
1	A1	1254	4AC	O2-C2	-2.63	1.18	1.23
27	B1	275	5MC	C4-N4	2.63	1.40	1.34
27	B1	97	5MC	C4-N4	2.63	1.40	1.34
27	B1	2328	4AC	O2-C2	-2.63	1.18	1.23
27	B1	3011	4AC	O2-C2	-2.63	1.18	1.23
27	B1	932	5MC	C4-N4	2.63	1.40	1.34
1	A1	230	5MC	C4-N4	2.63	1.40	1.34
1	A1	405	4AC	O2-C2	-2.63	1.18	1.23
27	B1	1703	4AC	O2-C2	-2.63	1.18	1.23
27	B1	609	4AC	O2-C2	-2.63	1.18	1.23
1	A1	687	5MC	C4-N4	2.62	1.40	1.34
1	A1	1486	5MC	C4-N4	2.62	1.40	1.34
27	B1	1501	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1621	4AC	O2-C2	-2.62	1.18	1.23
27	B1	2526	4AC	O2-C2	-2.62	1.18	1.23
27	B1	3006	4AC	O2-C2	-2.62	1.18	1.23
1	A1	481	G7M	C5-C6	2.62	1.52	1.45
1	A1	426	OMC	O2-C2	-2.62	1.18	1.23
1	A1	195	4AC	O2-C2	-2.62	1.18	1.23
1	A1	826	5MC	C4-N4	2.62	1.40	1.34
27	B1	2087	5MC	C4-N4	2.62	1.40	1.34
27	B1	1977	5MC	C4-N4	2.62	1.40	1.34
27	B1	3023	4AC	O2-C2	-2.62	1.18	1.23
27	B1	2008	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1620	5MC	C4-N4	2.62	1.40	1.34
1	A1	636	4AC	O2-C2	-2.62	1.18	1.23
1	A1	1467	4AC	O2-C2	-2.62	1.18	1.23
1	A1	1181	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1505	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1128	4AC	O2-C2	-2.62	1.18	1.23
27	B1	2875	5MC	C4-N4	2.62	1.40	1.34
1	A1	534	4AC	O2-C2	-2.62	1.18	1.23
27	B1	2454	4AC	O2-C2	-2.62	1.18	1.23
1	A1	681	5MC	C4-N4	2.61	1.40	1.34
27	B1	2617	5MC	C4-N4	2.61	1.40	1.34
27	B1	2022	OMG	C2-N1	2.61	1.44	1.37
1	A1	718	5MC	C4-N4	2.61	1.40	1.34
28	B2	120	4AC	O2-C2	-2.61	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	1012	5MC	C4-N4	2.61	1.40	1.34
1	A1	546	4AC	O2-C2	-2.61	1.18	1.23
27	B1	336	5MC	C4-N4	2.61	1.40	1.34
1	A1	1484	5MC	C4-N4	2.61	1.40	1.34
27	B1	1149	5MC	C4-N4	2.61	1.40	1.34
1	A1	533	5MC	C4-N4	2.61	1.40	1.34
27	B1	1751	4AC	O2-C2	-2.60	1.18	1.23
27	B1	47	5MC	C4-N4	2.60	1.40	1.34
1	A1	153	OMG	C5-C4	-2.60	1.36	1.43
1	A1	816	4AC	O2-C2	-2.60	1.18	1.23
27	B1	479	4AC	O2-C2	-2.60	1.18	1.23
27	B1	1648	5MC	C4-N4	2.60	1.40	1.34
27	B1	2067	5MC	C4-N4	2.60	1.40	1.34
1	A1	1135	4AC	O2-C2	-2.60	1.18	1.23
1	A1	863	5MC	C4-N4	2.60	1.40	1.34
1	A1	467	4AC	O2-C2	-2.60	1.18	1.23
1	A1	645	OMG	C2-N1	2.59	1.44	1.37
27	B1	2700	UR3	C5-C4	2.59	1.50	1.43
1	A1	17	5MC	C4-N4	2.59	1.40	1.34
27	B1	2428	OMC	O2-C2	-2.59	1.18	1.23
27	B1	359	5MC	C4-N4	2.59	1.40	1.34
1	A1	141	4AC	O2-C2	-2.59	1.18	1.23
27	B1	2428	OMC	C5-C4	2.59	1.48	1.42
27	B1	759	4AC	O2-C2	-2.58	1.18	1.23
27	B1	841	OMG	C2-N1	2.58	1.44	1.37
27	B1	1868	5MC	C4-N4	2.57	1.40	1.34
27	B1	2082	5MC	C4-N4	2.57	1.40	1.34
1	A1	951	5MC	C4-N4	2.57	1.40	1.34
1	A1	426	OMC	C5-C4	2.57	1.48	1.42
1	A1	444	4AC	O2-C2	-2.57	1.18	1.23
27	B1	226	5MC	C4-N4	2.57	1.40	1.34
1	A1	1194	OMC	C5-C4	2.57	1.48	1.42
27	B1	1983	5MC	C4-N4	2.57	1.40	1.34
1	A1	645	OMG	C5-C4	-2.56	1.36	1.43
27	B1	2607	OMC	C5-C4	2.56	1.48	1.42
1	A1	1252	OMC	C5-C4	2.55	1.48	1.42
1	A1	1092	4AC	O2-C2	-2.55	1.19	1.23
27	B1	2059	OMC	C5-C4	2.53	1.48	1.42
27	B1	1966	5MC	C4-N4	2.53	1.40	1.34
1	A1	1366	A1I59	C6-N1	-2.53	1.33	1.38
27	B1	2557	OMC	C5-C4	2.51	1.48	1.42
27	B1	2735	OMC	C5-C4	2.50	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2119	OMC	C5-C4	2.50	1.48	1.42
27	B1	2700	UR3	O2-C2	-2.49	1.18	1.22
1	A1	834	OMC	C5-C4	2.49	1.48	1.42
1	A1	117	OMC	C5-C4	2.47	1.48	1.42
27	B1	1489	OMC	C5-C4	2.46	1.48	1.42
27	B1	1832	OMC	C5-C4	2.46	1.48	1.42
27	B1	2808	OMC	C5-C4	2.46	1.48	1.42
27	B1	1783	OMC	C5-C4	2.45	1.48	1.42
1	A1	1270	OMC	C5-C4	2.45	1.48	1.42
27	B1	1914	OMC	C5-C4	2.45	1.48	1.42
27	B1	1099	OMC	C5-C4	2.43	1.48	1.42
27	B1	501	OMC	C5-C4	2.43	1.48	1.42
27	B1	977	OMC	C5-C4	2.41	1.48	1.42
1	A1	329	OMG	O6-C6	-2.35	1.18	1.23
27	B1	2740	OMG	O6-C6	-2.34	1.18	1.23
27	B1	921	OMG	O6-C6	-2.34	1.18	1.23
27	B1	2540	OMG	O6-C6	-2.34	1.18	1.23
27	B1	2562	OMG	O6-C6	-2.33	1.18	1.23
1	A1	861	OMG	O6-C6	-2.33	1.18	1.23
27	B1	2684	OMG	O6-C6	-2.33	1.18	1.23
27	B1	214	OMG	O6-C6	-2.32	1.18	1.23
27	B1	808	OMG	O6-C6	-2.32	1.18	1.23
27	B1	887	OMG	O6-C6	-2.31	1.18	1.23
27	B1	2365	OMG	O6-C6	-2.31	1.18	1.23
27	B1	2757	OMG	O6-C6	-2.31	1.18	1.23
27	B1	1533	OMG	O6-C6	-2.31	1.18	1.23
27	B1	675	OMG	O6-C6	-2.31	1.18	1.23
27	B1	2659	OMG	O6-C6	-2.31	1.18	1.23
1	A1	833	OMG	O6-C6	-2.30	1.18	1.23
27	B1	2028	OMG	O6-C6	-2.30	1.18	1.23
27	B1	1965	OMG	O6-C6	-2.30	1.18	1.23
27	B1	337	4AC	O7-C7	-2.30	1.18	1.23
1	A1	455	OMG	O6-C6	-2.29	1.18	1.23
27	B1	2565	4SU	O2-C2	-2.29	1.18	1.23
27	B1	1557	OMG	O6-C6	-2.29	1.18	1.23
1	A1	756	4SU	O2-C2	-2.29	1.18	1.23
27	B1	2984	OMG	O6-C6	-2.29	1.18	1.23
1	A1	481	G7M	C5-C4	2.29	1.43	1.39
27	B1	920	OMG	O6-C6	-2.29	1.18	1.23
27	B1	2022	OMG	O6-C6	-2.28	1.18	1.23
1	A1	901	OMG	O6-C6	-2.28	1.18	1.23
27	B1	2180	OMG	O6-C6	-2.28	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	645	OMG	O6-C6	-2.28	1.18	1.23
1	A1	227	OMG	O6-C6	-2.27	1.18	1.23
1	A1	763	OMG	O6-C6	-2.26	1.18	1.23
27	B1	2391	OMG	O6-C6	-2.26	1.18	1.23
27	B1	1601	OMG	O6-C6	-2.26	1.18	1.23
1	A1	507	OMG	O6-C6	-2.26	1.18	1.23
1	A1	668	OMG	O6-C6	-2.25	1.18	1.23
1	A1	481	G7M	O6-C6	-2.24	1.18	1.23
27	B1	841	OMG	O6-C6	-2.24	1.18	1.23
1	A1	153	OMG	O6-C6	-2.24	1.18	1.23
1	A1	459	OMG	O6-C6	-2.24	1.18	1.23
1	A1	228	OMG	O6-C6	-2.24	1.18	1.23
1	A1	1003	OMG	O6-C6	-2.22	1.18	1.23
1	A1	1004	2MG	O6-C6	-2.20	1.18	1.23
1	A1	819	A2M	C2-N3	2.18	1.35	1.32
1	A1	361	A2M	C2-N3	2.18	1.35	1.32
27	B1	485	4AC	O7-C7	-2.17	1.18	1.23
27	B1	378	4AC	O7-C7	-2.15	1.18	1.23
27	B1	2844	4AC	O7-C7	-2.15	1.18	1.23
27	B1	1478	4AC	O7-C7	-2.14	1.18	1.23
27	B1	1150	4AC	O7-C7	-2.13	1.18	1.23
27	B1	1818	4AC	O7-C7	-2.13	1.18	1.23
27	B1	866	4AC	O7-C7	-2.13	1.18	1.23
1	A1	706	4AC	O7-C7	-2.13	1.18	1.23
27	B1	1505	4AC	O7-C7	-2.13	1.18	1.23
27	B1	200	4AC	O7-C7	-2.12	1.18	1.23
27	B1	419	4AC	O7-C7	-2.12	1.18	1.23
27	B1	688	4AC	O7-C7	-2.12	1.18	1.23
27	B1	1435	4AC	O7-C7	-2.12	1.18	1.23
27	B1	2213	4AC	O7-C7	-2.12	1.18	1.23
27	B1	19	4AC	O7-C7	-2.12	1.18	1.23
27	B1	1107	4AC	O7-C7	-2.12	1.18	1.23
27	B1	2454	4AC	O7-C7	-2.12	1.18	1.23
27	B1	1822	4AC	O7-C7	-2.11	1.18	1.23
27	B1	1551	4AC	O7-C7	-2.11	1.18	1.23
27	B1	48	4AC	O7-C7	-2.11	1.18	1.23
27	B1	1100	4AC	O7-C7	-2.11	1.18	1.23
27	B1	2850	4AC	O7-C7	-2.11	1.18	1.23
27	B1	953	4AC	O7-C7	-2.11	1.18	1.23
27	B1	857	A2M	C2-N3	2.11	1.35	1.32
27	B1	2469	4AC	O7-C7	-2.10	1.18	1.23
27	B1	1967	4AC	O7-C7	-2.10	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1290	4AC	O7-C7	-2.10	1.18	1.23
1	A1	839	4AC	O7-C7	-2.10	1.18	1.23
27	B1	1128	4AC	O7-C7	-2.10	1.18	1.23
27	B1	580	4AC	O7-C7	-2.10	1.18	1.23
27	B1	1762	4AC	O7-C7	-2.10	1.18	1.23
1	A1	827	4AC	O7-C7	-2.09	1.18	1.23
27	B1	2171	4AC	O7-C7	-2.09	1.18	1.23
27	B1	3037	4AC	O7-C7	-2.09	1.18	1.23
27	B1	1404	4AC	O7-C7	-2.09	1.18	1.23
27	B1	2888	4AC	O7-C7	-2.09	1.18	1.23
1	A1	231	4AC	O7-C7	-2.09	1.18	1.23
27	B1	271	4AC	O7-C7	-2.09	1.18	1.23
27	B1	243	4AC	O7-C7	-2.09	1.18	1.23
27	B1	1501	4AC	O7-C7	-2.09	1.18	1.23
27	B1	979	4AC	O7-C7	-2.09	1.18	1.23
27	B1	2526	4AC	O7-C7	-2.09	1.18	1.23
28	B2	117	4AC	O7-C7	-2.09	1.18	1.23
27	B1	2113	4AC	O7-C7	-2.09	1.18	1.23
27	B1	262	A2M	C8-N7	-2.08	1.31	1.34
1	A1	614	4AC	O7-C7	-2.08	1.18	1.23
27	B1	2328	4AC	O7-C7	-2.08	1.18	1.23
27	B1	2876	4AC	O7-C7	-2.08	1.18	1.23
1	A1	382	4AC	O7-C7	-2.08	1.18	1.23
27	B1	1264	4AC	O7-C7	-2.08	1.18	1.23
27	B1	2809	4AC	O7-C7	-2.08	1.18	1.23
27	B1	434	4AC	O7-C7	-2.08	1.18	1.23
27	B1	1546	4AC	O7-C7	-2.08	1.18	1.23
27	B1	227	4AC	O7-C7	-2.08	1.18	1.23
1	A1	5	4AC	O7-C7	-2.07	1.18	1.23
1	A1	367	4AC	O7-C7	-2.07	1.18	1.23
1	A1	1181	4AC	O7-C7	-2.07	1.18	1.23
27	B1	479	4AC	O7-C7	-2.07	1.18	1.23
27	B1	896	4AC	O7-C7	-2.07	1.18	1.23
27	B1	1442	4AC	O7-C7	-2.07	1.18	1.23
27	B1	1911	4AC	O7-C7	-2.07	1.18	1.23
27	B1	2602	4AC	O7-C7	-2.07	1.18	1.23
27	B1	1360	4AC	O7-C7	-2.07	1.18	1.23
27	B1	2792	4AC	O7-C7	-2.07	1.18	1.23
27	B1	1649	4AC	O7-C7	-2.07	1.18	1.23
27	B1	786	4AC	O7-C7	-2.07	1.18	1.23
27	B1	950	4AC	O7-C7	-2.07	1.18	1.23
1	A1	41	4AC	O7-C7	-2.07	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	116	4AC	O7-C7	-2.07	1.18	1.23
1	A1	1467	4AC	O7-C7	-2.07	1.18	1.23
27	B1	80	4AC	O7-C7	-2.07	1.18	1.23
27	B1	502	LHH	O7-C7	-2.07	1.18	1.23
27	B1	3023	4AC	O7-C7	-2.07	1.18	1.23
27	B1	807	4AC	O7-C7	-2.07	1.18	1.23
27	B1	1178	4AC	O7-C7	-2.07	1.18	1.23
27	B1	1061	4AC	O7-C7	-2.06	1.18	1.23
27	B1	1383	4AC	O7-C7	-2.06	1.18	1.23
27	B1	721	4AC	O7-C7	-2.06	1.18	1.23
27	B1	741	4AC	O7-C7	-2.06	1.18	1.23
28	B2	90	4AC	O7-C7	-2.06	1.18	1.23
27	B1	1757	4AC	O7-C7	-2.06	1.18	1.23
27	B1	1846	4AC	O7-C7	-2.06	1.18	1.23
27	B1	162	4AC	O7-C7	-2.06	1.18	1.23
27	B1	1322	4AC	O7-C7	-2.06	1.18	1.23
1	A1	291	4AC	O7-C7	-2.06	1.18	1.23
1	A1	467	4AC	O7-C7	-2.06	1.18	1.23
27	B1	360	4AC	O7-C7	-2.06	1.18	1.23
1	A1	307	4AC	O7-C7	-2.06	1.18	1.23
1	A1	739	4AC	O7-C7	-2.06	1.18	1.23
1	A1	1288	4AC	O7-C7	-2.06	1.18	1.23
27	B1	940	A2M	C2-N3	2.06	1.35	1.32
27	B1	2379	4AC	O7-C7	-2.06	1.18	1.23
1	A1	534	4AC	O7-C7	-2.06	1.18	1.23
27	B1	1885	4AC	O7-C7	-2.06	1.18	1.23
27	B1	652	4AC	O7-C7	-2.06	1.18	1.23
27	B1	130	4AC	O7-C7	-2.06	1.18	1.23
27	B1	933	4AC	O7-C7	-2.06	1.18	1.23
1	A1	540	4AC	O7-C7	-2.06	1.18	1.23
27	B1	641	LHH	O7-C7	-2.06	1.18	1.23
1	A1	1135	4AC	O7-C7	-2.05	1.18	1.23
27	B1	1769	4AC	O7-C7	-2.05	1.18	1.23
27	B1	2492	4AC	O7-C7	-2.05	1.18	1.23
27	B1	1439	4AC	O7-C7	-2.05	1.18	1.23
1	A1	1016	4AC	O7-C7	-2.05	1.18	1.23
27	B1	1293	4AC	O7-C7	-2.05	1.18	1.23
1	A1	816	4AC	O7-C7	-2.05	1.18	1.23
1	A1	444	4AC	O7-C7	-2.05	1.18	1.23
27	B1	715	4AC	O7-C7	-2.05	1.18	1.23
1	A1	87	4AC	O7-C7	-2.05	1.18	1.23
27	B1	2432	4AC	O7-C7	-2.05	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	274	4AC	O7-C7	-2.05	1.18	1.23
27	B1	2749	4AC	O7-C7	-2.05	1.18	1.23
27	B1	1608	4AC	O7-C7	-2.04	1.18	1.23
27	B1	3011	4AC	O7-C7	-2.04	1.18	1.23
1	A1	546	4AC	O7-C7	-2.04	1.18	1.23
27	B1	1703	4AC	O7-C7	-2.04	1.18	1.23
1	A1	195	4AC	O7-C7	-2.04	1.18	1.23
27	B1	1374	4AC	O7-C7	-2.04	1.18	1.23
27	B1	506	A2M	C2-N3	2.04	1.35	1.32
27	B1	798	4AC	O7-C7	-2.04	1.18	1.23
27	B1	1743	4AC	O7-C7	-2.04	1.18	1.23
27	B1	3020	4AC	O7-C7	-2.04	1.18	1.23
1	A1	216	4AC	O7-C7	-2.04	1.18	1.23
27	B1	1313	4AC	O7-C7	-2.04	1.18	1.23
27	B1	759	4AC	O7-C7	-2.03	1.18	1.23
27	B1	1067	4AC	O7-C7	-2.03	1.18	1.23
1	A1	220	4AC	O7-C7	-2.03	1.18	1.23
1	A1	636	4AC	O7-C7	-2.03	1.18	1.23
27	B1	142	4AC	O7-C7	-2.03	1.18	1.23
27	B1	276	4AC	O7-C7	-2.03	1.18	1.23
27	B1	1286	4AC	O7-C7	-2.03	1.18	1.23
1	A1	578	4AC	O7-C7	-2.03	1.18	1.23
27	B1	1365	LHH	O7-C7	-2.03	1.18	1.23
1	A1	1227	4AC	O7-C7	-2.03	1.18	1.23
1	A1	624	4AC	O7-C7	-2.03	1.18	1.23
27	B1	2429	4AC	O7-C7	-2.03	1.18	1.23
1	A1	810	4AC	O7-C7	-2.03	1.18	1.23
1	A1	836	4AC	O7-C7	-2.03	1.18	1.23
27	B1	98	4AC	O7-C7	-2.03	1.18	1.23
1	A1	719	4AC	O7-C7	-2.03	1.18	1.23
27	B1	1664	4AC	O7-C7	-2.02	1.18	1.23
1	A1	856	4AC	O7-C7	-2.02	1.18	1.23
1	A1	1221	4AC	O7-C7	-2.02	1.18	1.23
27	B1	1052	4AC	O7-C7	-2.02	1.18	1.23
27	B1	1386	4AC	O7-C7	-2.02	1.18	1.23
1	A1	238	LHH	O7-C7	-2.02	1.18	1.23
1	A1	1092	4AC	O7-C7	-2.02	1.18	1.23
27	B1	813	4AC	O7-C7	-2.02	1.18	1.23
1	A1	1254	4AC	O7-C7	-2.02	1.18	1.23
27	B1	904	LHH	O7-C7	-2.02	1.18	1.23
27	B1	732	4AC	O7-C7	-2.02	1.18	1.23
27	B1	1946	LHH	O7-C7	-2.02	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1621	4AC	O7-C7	-2.02	1.18	1.23
27	B1	2008	4AC	O7-C7	-2.02	1.18	1.23
1	A1	1067	4AC	O7-C7	-2.02	1.18	1.23
27	B1	1706	4AC	O7-C7	-2.02	1.18	1.23
27	B1	2057	A2M	O5'-C5'	-2.02	1.39	1.44
1	A1	761	4AC	O7-C7	-2.02	1.18	1.23
1	A1	691	4AC	O7-C7	-2.01	1.18	1.23
28	B2	120	4AC	O7-C7	-2.01	1.18	1.23
27	B1	1064	4AC	O7-C7	-2.01	1.18	1.23
27	B1	527	LHH	O7-C7	-2.01	1.18	1.23
27	B1	1751	4AC	O7-C7	-2.01	1.18	1.23
27	B1	1612	4AC	O7-C7	-2.01	1.18	1.23
1	A1	1314	4AC	O7-C7	-2.01	1.18	1.23
27	B1	3006	4AC	O7-C7	-2.01	1.18	1.23
27	B1	599	4AC	O7-C7	-2.01	1.18	1.23
27	B1	392	4AC	O7-C7	-2.00	1.18	1.23
27	B1	2133	4AC	O7-C7	-2.00	1.18	1.23
27	B1	2057	A2M	C2-N3	2.00	1.35	1.32
27	B1	23	4AC	O7-C7	-2.00	1.18	1.23
1	A1	405	4AC	O7-C7	-2.00	1.18	1.23

All (1109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1457	MA6	N1-C6-N6	-13.75	102.58	117.06
1	A1	1476	MA6	N1-C6-N6	-13.50	102.85	117.06
1	A1	1475	MA6	N1-C6-N6	-13.39	102.97	117.06
1	A1	1475	MA6	C1'-N9-C4	12.84	149.20	126.64
1	A1	1457	MA6	C1'-N9-C4	12.37	148.38	126.64
1	A1	1476	MA6	C1'-N9-C4	11.94	147.63	126.64
27	B1	2565	4SU	C4-N3-C2	-7.82	119.75	127.34
1	A1	756	4SU	C4-N3-C2	-7.71	119.85	127.34
27	B1	527	LHH	C4-N3-C2	-5.83	112.18	120.12
27	B1	880	A2M	C1'-N9-C4	5.74	136.73	126.64
1	A1	1364	LHH	C4-N3-C2	-5.70	112.36	120.12
1	A1	361	A2M	C1'-N9-C4	5.63	136.53	126.64
1	A1	238	LHH	C4-N3-C2	-5.59	112.50	120.12
27	B1	2968	LHH	C4-N3-C2	-5.59	112.51	120.12
27	B1	940	A2M	C1'-N9-C4	5.54	136.37	126.64
27	B1	880	A2M	N3-C2-N1	-5.53	120.03	128.68
1	A1	1475	MA6	N3-C2-N1	-5.52	120.06	128.68
27	B1	1365	LHH	C4-N3-C2	-5.47	112.67	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	819	A2M	C1'-N9-C4	5.46	136.23	126.64
27	B1	857	A2M	N3-C2-N1	-5.45	120.16	128.68
1	A1	1457	MA6	N3-C2-N1	-5.44	120.17	128.68
27	B1	904	LHH	C4-N3-C2	-5.42	112.73	120.12
27	B1	502	LHH	C4-N3-C2	-5.42	112.74	120.12
27	B1	2057	A2M	C1'-N9-C4	5.42	136.16	126.64
1	A1	1476	MA6	N3-C2-N1	-5.41	120.22	128.68
1	A1	819	A2M	N3-C2-N1	-5.41	120.22	128.68
27	B1	2057	A2M	N3-C2-N1	-5.40	120.23	128.68
27	B1	940	A2M	N3-C2-N1	-5.39	120.25	128.68
27	B1	2506	A2M	N3-C2-N1	-5.38	120.28	128.68
27	B1	857	A2M	C1'-N9-C4	5.37	136.07	126.64
27	B1	506	A2M	N3-C2-N1	-5.35	120.32	128.68
1	A1	8	OMU	C4-N3-C2	-5.33	119.55	126.58
27	B1	2565	4SU	C5-C4-N3	5.33	119.63	114.69
27	B1	506	A2M	C1'-N9-C4	5.32	135.99	126.64
27	B1	1946	LHH	C4-N3-C2	-5.31	112.88	120.12
27	B1	2668	OMU	C4-N3-C2	-5.30	119.58	126.58
1	A1	775	OMU	C4-N3-C2	-5.29	119.60	126.58
1	A1	361	A2M	N3-C2-N1	-5.29	120.41	128.68
27	B1	2506	A2M	C1'-N9-C4	5.28	135.92	126.64
1	A1	756	4SU	C5-C4-N3	5.26	119.56	114.69
27	B1	2554	OMU	C4-N3-C2	-5.26	119.65	126.58
27	B1	641	LHH	C4-N3-C2	-5.25	112.96	120.12
1	A1	425	OMU	C4-N3-C2	-5.25	119.66	126.58
27	B1	1981	OMU	C4-N3-C2	-5.23	119.68	126.58
1	A1	1029	4AC	CM7-C7-N4	5.22	124.33	115.29
27	B1	1488	OMU	C4-N3-C2	-5.20	119.72	126.58
1	A1	1368	OMU	C4-N3-C2	-5.20	119.73	126.58
1	A1	762	OMU	C4-N3-C2	-5.18	119.75	126.58
1	A1	52	OMU	C4-N3-C2	-5.18	119.75	126.58
27	B1	2401	OMU	C4-N3-C2	-5.14	119.80	126.58
27	B1	1064	4AC	CM7-C7-N4	5.12	124.16	115.29
27	B1	454	OMU	C4-N3-C2	-5.11	119.83	126.58
27	B1	2593	OMU	C4-N3-C2	-5.06	119.90	126.58
27	B1	2700	UR3	C4-N3-C2	-4.74	120.10	124.56
1	A1	819	A2M	C5-C6-N6	-4.17	114.02	120.35
1	A1	762	OMU	O3'-C3'-C2'	4.04	122.64	111.17
27	B1	940	A2M	C5-C6-N6	-4.03	114.23	120.35
27	B1	880	A2M	C5-C6-N6	-4.03	114.23	120.35
27	B1	1488	OMU	N3-C2-N1	4.03	120.23	114.89
1	A1	775	OMU	N3-C2-N1	4.00	120.21	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	1965	OMG	O3'-C3'-C2'	3.98	122.47	111.17
1	A1	361	A2M	C5-C6-N6	-3.98	114.30	120.35
27	B1	2506	A2M	C5-C6-N6	-3.95	114.35	120.35
27	B1	841	OMG	O3'-C3'-C2'	3.92	122.30	111.17
27	B1	1914	OMC	O3'-C3'-C2'	3.92	122.30	111.17
27	B1	2057	A2M	C5-C6-N6	-3.91	114.41	120.35
1	A1	216	4AC	O3'-C3'-C4'	3.90	122.33	111.05
1	A1	756	4SU	N3-C2-N1	3.89	120.05	114.89
27	B1	857	A2M	C5-C6-N6	-3.89	114.45	120.35
1	A1	1368	OMU	N3-C2-N1	3.87	120.03	114.89
27	B1	506	A2M	C5-C6-N6	-3.87	114.47	120.35
27	B1	2565	4SU	N3-C2-N1	3.86	120.02	114.89
1	A1	8	OMU	N3-C2-N1	3.84	119.99	114.89
27	B1	2749	4AC	O4'-C1'-N1	3.82	117.10	108.36
27	B1	933	4AC	O3'-C3'-C4'	3.81	122.07	111.05
1	A1	425	OMU	N3-C2-N1	3.81	119.95	114.89
27	B1	454	OMU	N3-C2-N1	3.81	119.94	114.89
27	B1	2668	OMU	N3-C2-N1	3.80	119.93	114.89
1	A1	1348	5MC	O3'-C3'-C4'	3.79	122.01	111.05
1	A1	1314	4AC	O4'-C1'-N1	3.77	116.97	108.36
27	B1	2401	OMU	N3-C2-N1	3.76	119.89	114.89
1	A1	762	OMU	N3-C2-N1	3.73	119.84	114.89
27	B1	1981	OMU	N3-C2-N1	3.71	119.82	114.89
27	B1	2554	OMU	N3-C2-N1	3.71	119.82	114.89
1	A1	1467	4AC	O3'-C3'-C4'	3.71	121.79	111.05
1	A1	52	OMU	N3-C2-N1	3.71	119.81	114.89
27	B1	2492	4AC	O3'-C3'-C4'	3.69	121.73	111.05
27	B1	841	OMG	O3'-C3'-C4'	3.68	121.68	111.05
27	B1	130	4AC	O3'-C3'-C4'	3.66	121.64	111.05
27	B1	2593	OMU	N3-C2-N1	3.66	119.75	114.89
27	B1	979	4AC	O4'-C1'-N1	3.65	116.71	108.36
27	B1	1914	OMC	O3'-C3'-C4'	3.60	121.46	111.05
27	B1	1818	4AC	O3'-C3'-C4'	3.59	121.43	111.05
27	B1	2067	5MC	O3'-C3'-C4'	3.54	121.28	111.05
1	A1	329	OMG	C5-C6-N1	3.53	120.18	113.95
27	B1	1965	OMG	O3'-C3'-C4'	3.52	121.23	111.05
27	B1	880	A2M	N6-C6-N1	3.52	125.88	118.57
1	A1	762	OMU	O3'-C3'-C4'	3.50	121.17	111.05
27	B1	808	OMG	C5-C6-N1	3.49	120.12	113.95
27	B1	2562	OMG	C5-C6-N1	3.49	120.11	113.95
27	B1	3037	4AC	O3'-C3'-C4'	3.49	121.13	111.05
1	A1	819	A2M	N6-C6-N1	3.48	125.81	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	920	OMG	C5-C6-N1	3.48	120.09	113.95
27	B1	2740	OMG	C5-C6-N1	3.48	120.09	113.95
1	A1	216	4AC	O3'-C3'-C2'	3.48	123.06	111.82
1	A1	763	OMG	C5-C6-N1	3.47	120.08	113.95
27	B1	2659	OMG	C5-C6-N1	3.47	120.08	113.95
27	B1	887	OMG	C5-C6-N1	3.47	120.07	113.95
27	B1	214	OMG	C5-C6-N1	3.46	120.07	113.95
27	B1	813	4AC	N4-C4-N3	3.46	119.66	113.85
27	B1	1965	OMG	C5-C6-N1	3.46	120.06	113.95
27	B1	921	OMG	C5-C6-N1	3.46	120.06	113.95
1	A1	153	OMG	C5-C6-N1	3.44	120.03	113.95
27	B1	2365	OMG	C5-C6-N1	3.44	120.03	113.95
1	A1	459	OMG	C5-C6-N1	3.44	120.03	113.95
27	B1	2984	OMG	C5-C6-N1	3.44	120.03	113.95
1	A1	1003	OMG	C5-C6-N1	3.44	120.02	113.95
1	A1	901	OMG	C5-C6-N1	3.43	120.00	113.95
1	A1	1004	2MG	C5-C6-N1	3.42	119.99	113.95
1	A1	645	OMG	C5-C6-N1	3.42	119.99	113.95
27	B1	2565	4SU	C5-C4-S4	-3.42	120.06	124.47
27	B1	2757	OMG	C5-C6-N1	3.42	119.98	113.95
27	B1	1818	4AC	O3'-C3'-C2'	3.41	122.87	111.82
1	A1	227	OMG	C5-C6-N1	3.41	119.98	113.95
27	B1	1557	OMG	C5-C6-N1	3.41	119.98	113.95
27	B1	1601	OMG	C5-C6-N1	3.41	119.98	113.95
1	A1	668	OMG	C5-C6-N1	3.41	119.98	113.95
27	B1	2028	OMG	C5-C6-N1	3.41	119.98	113.95
27	B1	2540	OMG	C5-C6-N1	3.41	119.97	113.95
1	A1	361	A2M	N6-C6-N1	3.40	125.64	118.57
27	B1	1608	4AC	N4-C4-N3	3.40	119.56	113.85
1	A1	507	OMG	C5-C6-N1	3.39	119.94	113.95
1	A1	833	OMG	C5-C6-N1	3.39	119.94	113.95
1	A1	228	OMG	C5-C6-N1	3.39	119.94	113.95
27	B1	2180	OMG	C5-C6-N1	3.38	119.93	113.95
1	A1	861	OMG	C5-C6-N1	3.38	119.92	113.95
1	A1	455	OMG	C5-C6-N1	3.38	119.92	113.95
1	A1	8	OMU	C5-C4-N3	3.37	119.88	114.84
27	B1	933	4AC	O3'-C3'-C2'	3.37	122.72	111.82
1	A1	1348	5MC	O3'-C3'-C2'	3.37	122.72	111.82
1	A1	756	4SU	C5-C4-S4	-3.37	120.13	124.47
27	B1	2492	4AC	O3'-C3'-C2'	3.36	122.70	111.82
1	A1	1366	A1I59	C5-C6-N1	-3.36	119.05	123.38
27	B1	2554	OMU	C5-C4-N3	3.36	119.86	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	940	A2M	N6-C6-N1	3.36	125.54	118.57
27	B1	675	OMG	C5-C6-N1	3.35	119.87	113.95
27	B1	841	OMG	C5-C6-N1	3.35	119.86	113.95
27	B1	2391	OMG	C5-C6-N1	3.35	119.86	113.95
27	B1	2684	OMG	C5-C6-N1	3.35	119.86	113.95
27	B1	2668	OMU	C5-C4-N3	3.34	119.83	114.84
27	B1	130	4AC	O3'-C3'-C2'	3.34	122.61	111.82
27	B1	2617	5MC	C5-C6-N1	-3.34	119.91	123.34
27	B1	506	A2M	N6-C6-N1	3.33	125.49	118.57
27	B1	1981	OMU	C5-C4-N3	3.32	119.81	114.84
27	B1	47	5MC	C5-C6-N1	-3.32	119.92	123.34
1	A1	623	5MC	C5-C6-N1	-3.32	119.93	123.34
27	B1	275	5MC	C5-C6-N1	-3.31	119.93	123.34
27	B1	979	4AC	N4-C4-N3	3.30	119.40	113.85
27	B1	2057	A2M	N6-C6-N1	3.30	125.43	118.57
27	B1	1533	OMG	C5-C6-N1	3.30	119.78	113.95
1	A1	273	5MC	C5-C6-N1	-3.30	119.94	123.34
1	A1	230	5MC	C5-C6-N1	-3.29	119.95	123.34
1	A1	52	OMU	C5-C4-N3	3.29	119.76	114.84
1	A1	1364	LHH	C5-C4-N4	-3.29	117.21	122.92
1	A1	687	5MC	C5-C6-N1	-3.28	119.96	123.34
27	B1	2401	OMU	C5-C4-N3	3.28	119.75	114.84
1	A1	718	5MC	C5-C6-N1	-3.28	119.96	123.34
1	A1	762	OMU	C5-C4-N3	3.27	119.74	114.84
27	B1	2506	A2M	N6-C6-N1	3.27	125.37	118.57
1	A1	775	OMU	C5-C4-N3	3.27	119.73	114.84
27	B1	877	5MC	C5-C6-N1	-3.27	119.98	123.34
27	B1	857	A2M	N6-C6-N1	3.26	125.35	118.57
27	B1	2022	OMG	C5-C6-N1	3.25	119.70	113.95
27	B1	2082	5MC	C5-C6-N1	-3.25	120.00	123.34
27	B1	2067	5MC	O3'-C3'-C2'	3.25	122.33	111.82
1	A1	425	OMU	C5-C4-N3	3.25	119.70	114.84
1	A1	1348	5MC	C5-C6-N1	-3.23	120.01	123.34
1	A1	1467	4AC	O3'-C3'-C2'	3.23	122.27	111.82
27	B1	454	OMU	C5-C4-N3	3.23	119.67	114.84
27	B1	359	5MC	C5-C6-N1	-3.21	120.03	123.34
1	A1	1368	OMU	C5-C4-N3	3.21	119.64	114.84
27	B1	2593	OMU	C5-C4-N3	3.21	119.64	114.84
1	A1	466	5MC	C5-C6-N1	-3.21	120.04	123.34
27	B1	1488	OMU	C5-C4-N3	3.19	119.62	114.84
1	A1	863	5MC	C5-C6-N1	-3.19	120.05	123.34
27	B1	1451	5MC	C5-C6-N1	-3.19	120.06	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	1374	4AC	N4-C4-N3	3.18	119.18	113.85
1	A1	473	5MC	C5-C6-N1	-3.17	120.08	123.34
27	B1	2453	5MC	C5-C6-N1	-3.17	120.08	123.34
1	A1	951	5MC	C5-C6-N1	-3.16	120.09	123.34
27	B1	18	5MC	C5-C6-N1	-3.14	120.10	123.34
27	B1	1150	4AC	N4-C4-N3	3.14	119.12	113.85
27	B1	3037	4AC	O3'-C3'-C2'	3.14	121.97	111.82
27	B1	97	5MC	C5-C6-N1	-3.14	120.11	123.34
1	A1	826	5MC	C5-C6-N1	-3.13	120.12	123.34
27	B1	2875	5MC	C5-C6-N1	-3.13	120.12	123.34
1	A1	523	5MC	C5-C6-N1	-3.12	120.13	123.34
1	A1	1362	5MC	C5-C6-N1	-3.12	120.13	123.34
1	A1	533	5MC	C5-C6-N1	-3.12	120.13	123.34
1	A1	605	5MC	C5-C6-N1	-3.11	120.14	123.34
1	A1	1013	5MC	C5-C6-N1	-3.11	120.14	123.34
1	A1	427	4AC	N4-C4-N3	3.10	119.06	113.85
27	B1	1977	5MC	C5-C6-N1	-3.10	120.15	123.34
27	B1	1621	4AC	N4-C4-N3	3.09	119.04	113.85
1	A1	681	5MC	C5-C6-N1	-3.09	120.16	123.34
27	B1	1149	5MC	C5-C6-N1	-3.08	120.17	123.34
27	B1	1966	5MC	C5-C6-N1	-3.07	120.17	123.34
1	A1	1012	5MC	C5-C6-N1	-3.05	120.20	123.34
1	A1	645	OMG	C2-N1-C6	-3.05	119.48	125.10
27	B1	920	OMG	C2-N1-C6	-3.05	119.48	125.10
27	B1	2067	5MC	C5-C6-N1	-3.04	120.21	123.34
27	B1	1620	5MC	C5-C6-N1	-3.04	120.21	123.34
27	B1	378	4AC	C6-C5-C4	3.03	120.67	116.96
27	B1	378	4AC	N4-C4-N3	3.03	118.94	113.85
1	A1	1015	5MC	C5-C6-N1	-3.03	120.23	123.34
27	B1	1868	5MC	C5-C6-N1	-3.03	120.23	123.34
27	B1	2087	5MC	C5-C6-N1	-3.02	120.23	123.34
1	A1	668	OMG	C2-N1-C6	-3.02	119.53	125.10
1	A1	833	OMG	C2-N1-C6	-3.01	119.55	125.10
27	B1	226	5MC	C5-C6-N1	-3.00	120.26	123.34
1	A1	1486	5MC	C5-C6-N1	-3.00	120.26	123.34
27	B1	336	5MC	C5-C6-N1	-3.00	120.26	123.34
27	B1	979	4AC	C2'-C1'-N1	2.99	121.69	113.22
1	A1	763	OMG	C2-N1-C6	-2.99	119.59	125.10
27	B1	2562	OMG	C2-N1-C6	-2.99	119.60	125.10
1	A1	1190	5MC	C5-C6-N1	-2.99	120.27	123.34
1	A1	153	OMG	C2-N1-C6	-2.98	119.61	125.10
27	B1	2659	OMG	C2-N1-C6	-2.98	119.62	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	228	OMG	C2-N1-C6	-2.97	119.62	125.10
27	B1	1965	OMG	C2-N1-C6	-2.97	119.62	125.10
27	B1	1286	4AC	N4-C4-N3	2.97	118.84	113.85
27	B1	808	OMG	C2-N1-C6	-2.96	119.64	125.10
1	A1	1003	OMG	C2-N1-C6	-2.96	119.65	125.10
27	B1	2365	OMG	C2-N1-C6	-2.95	119.66	125.10
1	A1	901	OMG	C2-N1-C6	-2.95	119.66	125.10
27	B1	1557	OMG	C2-N1-C6	-2.95	119.66	125.10
1	A1	459	OMG	C2-N1-C6	-2.95	119.66	125.10
27	B1	2984	OMG	C2-N1-C6	-2.95	119.67	125.10
1	A1	855	5MC	C5-C6-N1	-2.94	120.31	123.34
27	B1	887	OMG	C2-N1-C6	-2.94	119.68	125.10
27	B1	2540	OMG	C2-N1-C6	-2.94	119.68	125.10
1	A1	455	OMG	C2-N1-C6	-2.94	119.69	125.10
27	B1	214	OMG	C2-N1-C6	-2.94	119.69	125.10
27	B1	2740	OMG	C2-N1-C6	-2.94	119.69	125.10
27	B1	1822	4AC	O4'-C4'-C5'	2.93	119.00	109.37
27	B1	813	4AC	C6-C5-C4	2.92	120.53	116.96
1	A1	227	OMG	C2-N1-C6	-2.91	119.73	125.10
27	B1	841	OMG	C8-N7-C5	2.91	108.54	102.99
1	A1	507	OMG	C2-N1-C6	-2.91	119.74	125.10
27	B1	1601	OMG	C2-N1-C6	-2.91	119.74	125.10
1	A1	17	5MC	C5-C6-N1	-2.91	120.35	123.34
27	B1	2554	OMU	O4-C4-C5	-2.91	120.05	125.16
27	B1	1981	OMU	O4-C4-C5	-2.91	120.05	125.16
27	B1	841	OMG	C2-N1-C6	-2.90	119.76	125.10
1	A1	762	OMU	O4-C4-C5	-2.89	120.07	125.16
27	B1	2684	OMG	C2-N1-C6	-2.89	119.78	125.10
27	B1	1360	4AC	N4-C4-N3	2.89	118.70	113.85
1	A1	329	OMG	C2-N1-C6	-2.88	119.79	125.10
27	B1	2757	OMG	C2-N1-C6	-2.88	119.80	125.10
27	B1	1150	4AC	C6-C5-C4	2.87	120.47	116.96
27	B1	2757	OMG	C8-N7-C5	2.87	108.45	102.99
27	B1	921	OMG	C2-N1-C6	-2.87	119.82	125.10
1	A1	329	OMG	C8-N7-C5	2.87	108.45	102.99
1	A1	833	OMG	C8-N7-C5	2.86	108.45	102.99
27	B1	2659	OMG	C8-N7-C5	2.86	108.43	102.99
27	B1	675	OMG	C2-N1-C6	-2.85	119.84	125.10
27	B1	2028	OMG	C2-N1-C6	-2.85	119.84	125.10
1	A1	624	4AC	N4-C4-N3	2.85	118.64	113.85
1	A1	52	OMU	O4-C4-C5	-2.85	120.14	125.16
27	B1	2180	OMG	C2-N1-C6	-2.85	119.86	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	454	OMU	O4-C4-C5	-2.84	120.16	125.16
1	A1	861	OMG	C2-N1-C6	-2.83	119.88	125.10
27	B1	2391	OMG	C2-N1-C6	-2.83	119.89	125.10
1	A1	1004	2MG	C8-N7-C5	2.83	108.38	102.99
1	A1	1368	OMU	O4-C4-C5	-2.83	120.19	125.16
1	A1	481	G7M	C2-N1-C6	-2.82	119.90	125.10
1	A1	228	OMG	C8-N7-C5	2.82	108.37	102.99
27	B1	813	4AC	CM7-C7-N4	2.82	120.17	115.29
1	A1	1003	OMG	C8-N7-C5	2.82	108.36	102.99
27	B1	932	5MC	C5-C6-N1	-2.81	120.45	123.34
27	B1	2984	OMG	C8-N7-C5	2.81	108.34	102.99
27	B1	1965	OMG	C8-N7-C5	2.80	108.32	102.99
1	A1	425	OMU	O4-C4-C5	-2.79	120.25	125.16
27	B1	2668	OMU	O4-C4-C5	-2.79	120.25	125.16
27	B1	1488	OMU	O4-C4-C5	-2.79	120.25	125.16
1	A1	455	OMG	C8-N7-C5	2.79	108.30	102.99
27	B1	2180	OMG	C8-N7-C5	2.79	108.30	102.99
1	A1	227	OMG	C8-N7-C5	2.78	108.29	102.99
27	B1	2401	OMU	O4-C4-C5	-2.78	120.27	125.16
1	A1	763	OMG	C8-N7-C5	2.78	108.29	102.99
27	B1	214	OMG	C8-N7-C5	2.78	108.28	102.99
27	B1	808	OMG	C8-N7-C5	2.77	108.27	102.99
27	B1	1150	4AC	CM7-C7-N4	2.77	120.09	115.29
27	B1	2365	OMG	C8-N7-C5	2.77	108.27	102.99
27	B1	2540	OMG	C8-N7-C5	2.77	108.27	102.99
1	A1	645	OMG	C8-N7-C5	2.77	108.27	102.99
27	B1	1533	OMG	C2-N1-C6	-2.77	120.00	125.10
1	A1	624	4AC	C6-C5-C4	2.77	120.35	116.96
1	A1	8	OMU	O4-C4-C5	-2.77	120.30	125.16
1	A1	467	4AC	N4-C4-N3	2.76	118.49	113.85
27	B1	920	OMG	C8-N7-C5	2.76	108.25	102.99
1	A1	775	OMU	O4-C4-C5	-2.76	120.31	125.16
1	A1	668	OMG	C8-N7-C5	2.76	108.25	102.99
27	B1	675	OMG	C8-N7-C5	2.76	108.24	102.99
27	B1	2593	OMU	O4-C4-C5	-2.76	120.31	125.16
27	B1	2684	OMG	C8-N7-C5	2.76	108.24	102.99
27	B1	1734	4AC	N4-C4-N3	2.76	118.48	113.85
27	B1	2028	OMG	C8-N7-C5	2.75	108.24	102.99
1	A1	153	OMG	C8-N7-C5	2.75	108.23	102.99
1	A1	507	OMG	C8-N7-C5	2.75	108.23	102.99
27	B1	1557	OMG	C8-N7-C5	2.75	108.23	102.99
27	B1	3037	4AC	N4-C4-N3	2.75	118.47	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	337	4AC	C6-C5-C4	2.75	120.33	116.96
27	B1	887	OMG	C8-N7-C5	2.75	108.22	102.99
1	A1	459	OMG	C8-N7-C5	2.75	108.22	102.99
1	A1	901	OMG	C8-N7-C5	2.74	108.21	102.99
27	B1	2740	OMG	C8-N7-C5	2.74	108.21	102.99
1	A1	238	LHH	C5-C4-N4	-2.73	118.18	122.92
27	B1	2391	OMG	C8-N7-C5	2.73	108.19	102.99
27	B1	3037	4AC	C2'-C3'-C4'	2.72	107.93	102.64
27	B1	1404	4AC	O4'-C4'-C5'	2.72	118.33	109.37
1	A1	861	OMG	C8-N7-C5	2.72	108.17	102.99
27	B1	2968	LHH	C5-C4-N4	-2.72	118.19	122.92
27	B1	1533	OMG	C8-N7-C5	2.72	108.17	102.99
27	B1	921	OMG	C8-N7-C5	2.71	108.16	102.99
27	B1	337	4AC	CM7-C7-N4	2.71	119.97	115.29
27	B1	1061	4AC	O4'-C4'-C5'	2.70	118.27	109.37
1	A1	1254	4AC	N4-C4-N3	2.70	118.38	113.85
1	A1	1364	LHH	CM7-C7-N4	2.70	119.96	115.29
27	B1	1648	5MC	C5-C6-N1	-2.69	120.57	123.34
27	B1	2562	OMG	C8-N7-C5	2.69	108.12	102.99
1	A1	195	4AC	C6-C5-C4	2.69	120.25	116.96
27	B1	1064	4AC	C6-C5-C4	2.69	120.25	116.96
27	B1	2428	OMC	O4'-C4'-C5'	2.69	118.23	109.37
1	A1	1314	4AC	N4-C4-N3	2.69	118.37	113.85
27	B1	527	LHH	C5-C4-N4	-2.69	118.25	122.92
27	B1	1601	OMG	C8-N7-C5	2.69	108.11	102.99
27	B1	1762	4AC	N4-C4-N3	2.68	118.36	113.85
27	B1	360	4AC	O4'-C4'-C5'	2.68	118.21	109.37
27	B1	2022	OMG	C8-N7-C5	2.68	108.10	102.99
27	B1	142	4AC	N4-C4-N3	2.68	118.35	113.85
1	A1	141	4AC	C6-C5-C4	2.68	120.24	116.96
1	A1	141	4AC	N4-C4-N3	2.67	118.34	113.85
1	A1	739	4AC	N4-C4-N3	2.67	118.33	113.85
1	A1	691	4AC	N4-C4-N3	2.67	118.33	113.85
1	A1	444	4AC	N4-C4-N3	2.66	118.33	113.85
1	A1	427	4AC	C6-C5-C4	2.66	120.22	116.96
27	B1	336	5MC	CM5-C5-C6	-2.66	119.29	122.85
1	A1	367	4AC	C6-C5-C4	2.66	120.21	116.96
1	A1	614	4AC	N4-C4-N3	2.66	118.31	113.85
27	B1	3006	4AC	N4-C4-N3	2.66	118.31	113.85
27	B1	741	4AC	C6-C5-C4	2.65	120.21	116.96
1	A1	1029	4AC	C6-C5-C4	2.65	120.21	116.96
1	A1	761	4AC	N4-C4-N3	2.65	118.30	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	243	4AC	N4-C4-N3	2.65	118.30	113.85
27	B1	1706	4AC	C6-C5-C4	2.65	120.20	116.96
1	A1	1484	5MC	C5-C6-N1	-2.64	120.62	123.34
27	B1	1983	5MC	C5-C6-N1	-2.64	120.63	123.34
1	A1	739	4AC	C6-C5-C4	2.63	120.18	116.96
1	A1	1092	4AC	N4-C4-N3	2.63	118.27	113.85
27	B1	1608	4AC	C6-C5-C4	2.63	120.18	116.96
27	B1	142	4AC	C6-C5-C4	2.63	120.18	116.96
27	B1	1052	4AC	C6-C5-C4	2.63	120.17	116.96
27	B1	2022	OMG	C2-N1-C6	-2.62	120.27	125.10
27	B1	1061	4AC	N4-C4-N3	2.62	118.25	113.85
1	A1	810	4AC	N4-C4-N3	2.62	118.25	113.85
1	A1	816	4AC	C6-C5-C4	2.62	120.17	116.96
1	A1	1067	4AC	C6-C5-C4	2.62	120.17	116.96
1	A1	1221	4AC	N4-C4-N3	2.62	118.24	113.85
1	A1	216	4AC	C6-C5-C4	2.61	120.16	116.96
27	B1	807	4AC	C6-C5-C4	2.61	120.16	116.96
27	B1	243	4AC	C6-C5-C4	2.61	120.16	116.96
27	B1	2850	4AC	N4-C4-N3	2.61	118.23	113.85
1	A1	636	4AC	C6-C5-C4	2.61	120.15	116.96
1	A1	546	4AC	C6-C5-C4	2.61	120.15	116.96
27	B1	1178	4AC	C6-C5-C4	2.60	120.15	116.96
28	B2	120	4AC	C6-C5-C4	2.60	120.15	116.96
1	A1	540	4AC	C6-C5-C4	2.60	120.15	116.96
27	B1	732	4AC	N4-C4-N3	2.60	118.22	113.85
27	B1	1383	4AC	C6-C5-C4	2.60	120.14	116.96
27	B1	1374	4AC	C6-C5-C4	2.59	120.14	116.96
27	B1	1439	4AC	C6-C5-C4	2.59	120.14	116.96
27	B1	1649	4AC	C6-C5-C4	2.59	120.13	116.96
1	A1	1092	4AC	C6-C5-C4	2.59	120.13	116.96
1	A1	1288	4AC	C6-C5-C4	2.59	120.13	116.96
27	B1	1757	4AC	C6-C5-C4	2.59	120.13	116.96
27	B1	2876	4AC	C6-C5-C4	2.59	120.13	116.96
27	B1	130	4AC	C6-C5-C4	2.59	120.13	116.96
1	A1	719	4AC	C6-C5-C4	2.59	120.13	116.96
27	B1	609	4AC	C6-C5-C4	2.59	120.12	116.96
27	B1	1100	4AC	C6-C5-C4	2.59	120.12	116.96
28	B2	90	4AC	N4-C4-N3	2.58	118.19	113.85
1	A1	636	4AC	N4-C4-N3	2.58	118.19	113.85
27	B1	3037	4AC	C6-C5-C4	2.58	120.12	116.96
27	B1	1734	4AC	C6-C5-C4	2.58	120.12	116.96
1	A1	238	LHH	CM7-C7-N4	2.58	119.75	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	741	4AC	N4-C4-N3	2.58	118.18	113.85
1	A1	274	4AC	C6-C5-C4	2.58	120.11	116.96
1	A1	1254	4AC	C6-C5-C4	2.57	120.11	116.96
27	B1	1612	4AC	C6-C5-C4	2.57	120.11	116.96
1	A1	534	4AC	C6-C5-C4	2.57	120.11	116.96
27	B1	2113	4AC	N4-C4-N3	2.57	118.17	113.85
27	B1	1435	4AC	C6-C5-C4	2.57	120.10	116.96
27	B1	1703	4AC	N4-C4-N3	2.57	118.16	113.85
27	B1	1061	4AC	C5'-C4'-C3'	2.57	124.80	115.18
27	B1	1621	4AC	C6-C5-C4	2.57	120.10	116.96
1	A1	578	4AC	C6-C5-C4	2.57	120.10	116.96
27	B1	1313	4AC	C6-C5-C4	2.57	120.10	116.96
27	B1	2379	4AC	C6-C5-C4	2.57	120.10	116.96
27	B1	360	4AC	C6-C5-C4	2.56	120.10	116.96
27	B1	715	4AC	C6-C5-C4	2.56	120.10	116.96
1	A1	1221	4AC	C6-C5-C4	2.56	120.10	116.96
27	B1	1064	4AC	C5-C4-N3	-2.56	118.47	122.59
27	B1	599	4AC	N4-C4-N3	2.56	118.15	113.85
27	B1	2700	UR3	C1'-N1-C2	2.56	121.31	116.99
1	A1	1016	4AC	N4-C4-N3	2.56	118.15	113.85
27	B1	798	4AC	C6-C5-C4	2.56	120.09	116.96
27	B1	1322	4AC	N4-C4-N3	2.56	118.15	113.85
1	A1	467	4AC	C6-C5-C4	2.56	120.09	116.96
27	B1	1286	4AC	C6-C5-C4	2.56	120.09	116.96
27	B1	271	4AC	C6-C5-C4	2.55	120.09	116.96
27	B1	276	4AC	C6-C5-C4	2.55	120.09	116.96
27	B1	2821	4AC	C6-C5-C4	2.55	120.09	116.96
27	B1	392	4AC	C6-C5-C4	2.55	120.09	116.96
27	B1	721	4AC	C6-C5-C4	2.55	120.09	116.96
27	B1	1743	4AC	C6-C5-C4	2.55	120.09	116.96
1	A1	1016	4AC	C6-C5-C4	2.55	120.08	116.96
27	B1	479	4AC	C6-C5-C4	2.55	120.08	116.96
27	B1	80	4AC	N4-C4-N3	2.55	118.13	113.85
27	B1	527	LHH	CM7-C7-N4	2.55	119.70	115.29
27	B1	688	4AC	C6-C5-C4	2.55	120.08	116.96
27	B1	1703	4AC	C6-C5-C4	2.55	120.08	116.96
1	A1	291	4AC	O2'-C2'-C3'	2.55	120.07	111.82
27	B1	950	4AC	N4-C4-N3	2.55	118.13	113.85
1	A1	839	4AC	C6-C5-C4	2.55	120.08	116.96
1	A1	41	4AC	C6-C5-C4	2.54	120.07	116.96
27	B1	227	4AC	C6-C5-C4	2.54	120.07	116.96
27	B1	1822	4AC	C5'-C4'-C3'	2.54	124.71	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	499	4AC	C6-C5-C4	2.54	120.07	116.96
27	B1	1818	4AC	C6-C5-C4	2.54	120.07	116.96
1	A1	231	4AC	C6-C5-C4	2.54	120.07	116.96
1	A1	856	4AC	C6-C5-C4	2.54	120.07	116.96
1	A1	87	4AC	N4-C4-N3	2.54	118.11	113.85
1	A1	827	4AC	C6-C5-C4	2.54	120.07	116.96
1	A1	1181	4AC	C6-C5-C4	2.54	120.07	116.96
27	B1	1769	4AC	C6-C5-C4	2.54	120.07	116.96
27	B1	1360	4AC	C6-C5-C4	2.54	120.07	116.96
1	A1	220	4AC	N4-C4-N3	2.54	118.11	113.85
27	B1	880	A2M	C3'-C2'-C1'	-2.54	98.12	102.89
1	A1	1029	4AC	C5-C4-N3	-2.54	118.51	122.59
27	B1	2429	4AC	N4-C4-N3	2.54	118.11	113.85
1	A1	761	4AC	C6-C5-C4	2.53	120.06	116.96
27	B1	2454	4AC	C6-C5-C4	2.53	120.06	116.96
27	B1	1743	4AC	N4-C4-N3	2.53	118.11	113.85
27	B1	3020	4AC	C6-C5-C4	2.53	120.06	116.96
1	A1	87	4AC	C6-C5-C4	2.53	120.06	116.96
1	A1	367	4AC	N4-C4-N3	2.53	118.10	113.85
27	B1	2749	4AC	N4-C4-N3	2.53	118.10	113.85
27	B1	2602	4AC	C6-C5-C4	2.53	120.06	116.96
1	A1	836	4AC	C6-C5-C4	2.53	120.06	116.96
27	B1	1967	4AC	C6-C5-C4	2.53	120.06	116.96
1	A1	1467	4AC	C6-C5-C4	2.53	120.06	116.96
27	B1	1911	4AC	C6-C5-C4	2.53	120.05	116.96
1	A1	1135	4AC	N4-C4-N3	2.53	118.09	113.85
27	B1	2429	4AC	C6-C5-C4	2.53	120.05	116.96
27	B1	2428	OMC	C5'-C4'-C3'	2.53	124.64	115.18
1	A1	220	4AC	C6-C5-C4	2.52	120.05	116.96
27	B1	1067	4AC	C6-C5-C4	2.52	120.05	116.96
1	A1	810	4AC	C6-C5-C4	2.52	120.04	116.96
27	B1	1751	4AC	C6-C5-C4	2.52	120.04	116.96
27	B1	2792	4AC	C6-C5-C4	2.52	120.04	116.96
1	A1	444	4AC	C6-C5-C4	2.52	120.04	116.96
27	B1	732	4AC	C6-C5-C4	2.52	120.04	116.96
27	B1	1505	4AC	C6-C5-C4	2.52	120.04	116.96
1	A1	405	4AC	C6-C5-C4	2.52	120.04	116.96
27	B1	1061	4AC	C6-C5-C4	2.51	120.04	116.96
27	B1	953	4AC	C6-C5-C4	2.51	120.04	116.96
27	B1	1374	4AC	CM7-C7-N4	2.51	119.64	115.29
27	B1	392	4AC	N4-C4-N3	2.51	118.07	113.85
27	B1	1128	4AC	C6-C5-C4	2.51	120.03	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	382	4AC	N4-C4-N3	2.51	118.07	113.85
1	A1	1135	4AC	C6-C5-C4	2.51	120.03	116.96
27	B1	1822	4AC	C6-C5-C4	2.51	120.03	116.96
27	B1	759	4AC	C6-C5-C4	2.51	120.03	116.96
27	B1	271	4AC	N4-C4-N3	2.51	118.06	113.85
27	B1	652	4AC	C6-C5-C4	2.51	120.03	116.96
27	B1	1290	4AC	C6-C5-C4	2.51	120.03	116.96
27	B1	2113	4AC	O2'-C2'-C3'	2.50	119.92	111.82
27	B1	1404	4AC	C5'-C4'-C3'	2.50	124.56	115.18
27	B1	485	4AC	C6-C5-C4	2.50	120.02	116.96
1	A1	5	4AC	C6-C5-C4	2.50	120.02	116.96
1	A1	1067	4AC	N4-C4-N3	2.50	118.05	113.85
27	B1	360	4AC	C5'-C4'-C3'	2.50	124.54	115.18
27	B1	1064	4AC	O7-C7-N4	-2.50	117.78	121.82
27	B1	1293	4AC	C6-C5-C4	2.50	120.02	116.96
1	A1	195	4AC	N4-C4-N3	2.50	118.04	113.85
27	B1	1818	4AC	N4-C4-N3	2.50	118.04	113.85
1	A1	1227	4AC	C6-C5-C4	2.50	120.01	116.96
1	A1	1314	4AC	C2'-C1'-N1	2.49	120.28	113.22
27	B1	130	4AC	N4-C4-N3	2.49	118.04	113.85
27	B1	2850	4AC	C6-C5-C4	2.49	120.01	116.96
28	B2	90	4AC	C6-C5-C4	2.49	120.01	116.96
27	B1	609	4AC	N4-C4-N3	2.49	118.04	113.85
1	A1	291	4AC	C6-C5-C4	2.49	120.01	116.96
27	B1	2020	4AC	C6-C5-C4	2.49	120.01	116.96
1	A1	706	4AC	C6-C5-C4	2.49	120.01	116.96
1	A1	1029	4AC	O7-C7-N4	-2.49	117.79	121.82
1	A1	405	4AC	N4-C4-N3	2.49	118.03	113.85
27	B1	715	4AC	N4-C4-N3	2.49	118.03	113.85
27	B1	1612	4AC	N4-C4-N3	2.49	118.03	113.85
1	A1	307	4AC	C6-C5-C4	2.49	120.00	116.96
27	B1	2454	4AC	N4-C4-N3	2.49	118.02	113.85
27	B1	19	4AC	C6-C5-C4	2.48	120.00	116.96
27	B1	2008	4AC	C6-C5-C4	2.48	120.00	116.96
27	B1	2432	4AC	C6-C5-C4	2.48	120.00	116.96
27	B1	378	4AC	C5-C4-N3	-2.48	118.60	122.59
27	B1	2469	4AC	C6-C5-C4	2.48	120.00	116.96
27	B1	98	4AC	C6-C5-C4	2.48	119.99	116.96
27	B1	580	4AC	C6-C5-C4	2.48	119.99	116.96
27	B1	896	4AC	C6-C5-C4	2.48	119.99	116.96
27	B1	3006	4AC	C6-C5-C4	2.48	119.99	116.96
27	B1	227	4AC	N4-C4-N3	2.48	118.01	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	1365	LHH	CM7-C7-N4	2.48	119.58	115.29
27	B1	162	4AC	C6-C5-C4	2.48	119.99	116.96
27	B1	580	4AC	N4-C4-N3	2.48	118.01	113.85
1	A1	691	4AC	C6-C5-C4	2.47	119.99	116.96
27	B1	2526	4AC	C6-C5-C4	2.47	119.99	116.96
1	A1	5	4AC	N4-C4-N3	2.47	118.00	113.85
27	B1	933	4AC	N4-C4-N3	2.47	118.00	113.85
27	B1	23	4AC	C6-C5-C4	2.47	119.99	116.96
27	B1	1442	4AC	C6-C5-C4	2.47	119.99	116.96
1	A1	1314	4AC	C6-C5-C4	2.47	119.99	116.96
27	B1	2888	4AC	C6-C5-C4	2.47	119.98	116.96
28	B2	117	4AC	N4-C4-N3	2.47	118.00	113.85
27	B1	378	4AC	CM7-C7-N4	2.47	119.56	115.29
27	B1	1478	4AC	C6-C5-C4	2.47	119.98	116.96
1	A1	546	4AC	N4-C4-N3	2.46	117.99	113.85
27	B1	3020	4AC	N4-C4-N3	2.46	117.98	113.85
27	B1	23	4AC	N4-C4-N3	2.46	117.98	113.85
27	B1	1386	4AC	C6-C5-C4	2.46	119.97	116.96
27	B1	1264	4AC	C6-C5-C4	2.46	119.97	116.96
27	B1	2328	4AC	C6-C5-C4	2.46	119.97	116.96
1	A1	624	4AC	CM7-C7-N4	2.46	119.54	115.29
27	B1	1664	4AC	N4-C4-N3	2.46	117.98	113.85
27	B1	1551	4AC	C6-C5-C4	2.46	119.97	116.96
27	B1	2876	4AC	N4-C4-N3	2.45	117.97	113.85
27	B1	866	4AC	C6-C5-C4	2.45	119.96	116.96
28	B2	117	4AC	C6-C5-C4	2.45	119.96	116.96
27	B1	2469	4AC	N4-C4-N3	2.45	117.96	113.85
1	A1	836	4AC	N4-C4-N3	2.45	117.96	113.85
27	B1	759	4AC	N4-C4-N3	2.45	117.96	113.85
27	B1	3023	4AC	N4-C4-N3	2.45	117.96	113.85
27	B1	116	4AC	C6-C5-C4	2.45	119.95	116.96
27	B1	2809	4AC	C6-C5-C4	2.45	119.95	116.96
27	B1	1435	4AC	N4-C4-N3	2.45	117.96	113.85
27	B1	953	4AC	N4-C4-N3	2.45	117.96	113.85
27	B1	1608	4AC	CM7-C7-N4	2.44	119.52	115.29
27	B1	979	4AC	C6-C5-C4	2.44	119.95	116.96
27	B1	1846	4AC	C6-C5-C4	2.44	119.95	116.96
27	B1	1365	LHH	C5-C4-N4	-2.44	118.68	122.92
1	A1	534	4AC	N4-C4-N3	2.43	117.94	113.85
27	B1	1639	4AC	C6-C5-C4	2.43	119.94	116.96
1	A1	706	4AC	CM7-C7-N4	2.43	119.50	115.29
27	B1	2213	4AC	C6-C5-C4	2.43	119.93	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	291	4AC	N4-C4-N3	2.43	117.93	113.85
1	A1	499	4AC	N4-C4-N3	2.43	117.93	113.85
27	B1	599	4AC	C6-C5-C4	2.43	119.93	116.96
27	B1	2844	4AC	C6-C5-C4	2.43	119.93	116.96
1	A1	540	4AC	N4-C4-N3	2.43	117.92	113.85
27	B1	2113	4AC	C6-C5-C4	2.42	119.92	116.96
27	B1	419	4AC	C6-C5-C4	2.42	119.92	116.96
27	B1	434	4AC	C6-C5-C4	2.42	119.92	116.96
27	B1	950	4AC	C6-C5-C4	2.42	119.92	116.96
27	B1	1546	4AC	C6-C5-C4	2.42	119.92	116.96
1	A1	1467	4AC	N4-C4-N3	2.42	117.91	113.85
27	B1	786	4AC	C6-C5-C4	2.41	119.92	116.96
27	B1	2171	4AC	C6-C5-C4	2.41	119.92	116.96
27	B1	3023	4AC	C6-C5-C4	2.41	119.91	116.96
27	B1	721	4AC	N4-C4-N3	2.41	117.90	113.85
1	A1	216	4AC	N4-C4-N3	2.41	117.90	113.85
1	A1	382	4AC	C6-C5-C4	2.41	119.91	116.96
1	A1	307	4AC	N4-C4-N3	2.41	117.90	113.85
27	B1	688	4AC	N4-C4-N3	2.41	117.90	113.85
27	B1	1664	4AC	C6-C5-C4	2.41	119.91	116.96
1	A1	1288	4AC	N4-C4-N3	2.41	117.90	113.85
27	B1	1762	4AC	C6-C5-C4	2.41	119.91	116.96
27	B1	1757	4AC	N4-C4-N3	2.41	117.89	113.85
1	A1	614	4AC	C6-C5-C4	2.41	119.90	116.96
27	B1	1322	4AC	C6-C5-C4	2.40	119.90	116.96
27	B1	1885	4AC	C6-C5-C4	2.40	119.90	116.96
27	B1	2133	4AC	C6-C5-C4	2.40	119.90	116.96
27	B1	1439	4AC	N4-C4-N3	2.40	117.88	113.85
27	B1	887	OMG	O6-C6-C5	-2.40	119.69	124.37
27	B1	1178	4AC	N4-C4-N3	2.40	117.88	113.85
27	B1	1383	4AC	N4-C4-N3	2.40	117.87	113.85
27	B1	1107	4AC	C6-C5-C4	2.39	119.89	116.96
1	A1	427	4AC	CM7-C7-N4	2.39	119.43	115.29
27	B1	1264	4AC	N4-C4-N3	2.38	117.86	113.85
27	B1	3011	4AC	N4-C4-N3	2.38	117.85	113.85
1	A1	816	4AC	N4-C4-N3	2.38	117.85	113.85
27	B1	276	4AC	N4-C4-N3	2.38	117.85	113.85
27	B1	80	4AC	C6-C5-C4	2.38	119.88	116.96
27	B1	1546	4AC	N4-C4-N3	2.38	117.85	113.85
1	A1	827	4AC	N4-C4-N3	2.38	117.84	113.85
27	B1	813	4AC	O7-C7-CM7	-2.37	117.65	122.06
27	B1	1404	4AC	C6-C5-C4	2.37	119.86	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	1706	4AC	N4-C4-N3	2.37	117.83	113.85
27	B1	1478	4AC	CM7-C7-N4	2.37	119.39	115.29
27	B1	798	4AC	N4-C4-N3	2.36	117.82	113.85
27	B1	1501	4AC	N4-C4-N3	2.36	117.82	113.85
27	B1	2749	4AC	C6-C5-C4	2.36	119.85	116.96
27	B1	688	4AC	C5-C4-N3	-2.36	118.80	122.59
27	B1	813	4AC	C5-C4-N3	-2.36	118.80	122.59
27	B1	485	4AC	N4-C4-N3	2.35	117.80	113.85
27	B1	48	4AC	C6-C5-C4	2.35	119.84	116.96
1	A1	1364	LHH	N4-C4-N3	2.35	117.80	113.85
1	A1	578	4AC	N4-C4-N3	2.35	117.80	113.85
28	B2	120	4AC	N4-C4-N3	2.35	117.79	113.85
27	B1	979	4AC	CM7-C7-N4	2.35	119.35	115.29
27	B1	200	4AC	C6-C5-C4	2.35	119.83	116.96
27	B1	1451	5MC	CM5-C5-C6	-2.35	119.72	122.85
27	B1	1911	4AC	N4-C4-N3	2.34	117.78	113.85
27	B1	2602	4AC	N4-C4-N3	2.34	117.78	113.85
27	B1	933	4AC	C6-C5-C4	2.33	119.82	116.96
27	B1	419	4AC	N4-C4-N3	2.33	117.77	113.85
27	B1	1386	4AC	N4-C4-N3	2.33	117.77	113.85
27	B1	2792	4AC	N4-C4-N3	2.33	117.77	113.85
27	B1	19	4AC	N4-C4-N3	2.33	117.76	113.85
27	B1	2391	OMG	O6-C6-C5	-2.33	119.82	124.37
27	B1	1478	4AC	N4-C4-N3	2.33	117.76	113.85
27	B1	2740	OMG	O6-C6-C5	-2.33	119.83	124.37
27	B1	2565	4SU	O2-C2-N1	-2.33	119.69	122.79
27	B1	2492	4AC	C6-C5-C4	2.33	119.81	116.96
27	B1	1846	4AC	N4-C4-N3	2.32	117.75	113.85
1	A1	839	4AC	N4-C4-N3	2.32	117.75	113.85
27	B1	3011	4AC	C6-C5-C4	2.32	119.79	116.96
27	B1	1150	4AC	O7-C7-CM7	-2.32	117.76	122.06
27	B1	2844	4AC	N4-C4-N3	2.31	117.74	113.85
27	B1	2700	UR3	C6-N1-C2	-2.31	119.72	121.79
1	A1	614	4AC	C5-C4-N3	-2.31	118.87	122.59
27	B1	2659	OMG	O6-C6-C5	-2.31	119.86	124.37
27	B1	360	4AC	N4-C4-N3	2.31	117.73	113.85
27	B1	1501	4AC	C6-C5-C4	2.31	119.78	116.96
27	B1	1966	5MC	CM5-C5-C6	-2.31	119.77	122.85
27	B1	1621	4AC	CM7-C7-N4	2.31	119.28	115.29
27	B1	1360	4AC	CM7-C7-N4	2.31	119.28	115.29
27	B1	641	LHH	CM7-C7-N4	2.30	119.28	115.29
1	A1	1227	4AC	CM7-C7-N4	2.30	119.28	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	2984	OMG	O6-C6-C5	-2.30	119.89	124.37
1	A1	1254	4AC	C5-C4-N3	-2.30	118.90	122.59
1	A1	459	OMG	O6-C6-C5	-2.29	119.89	124.37
27	B1	741	4AC	CM7-C7-N4	2.29	119.26	115.29
27	B1	2432	4AC	N4-C4-N3	2.29	117.70	113.85
1	A1	1467	4AC	CM7-C7-N4	2.29	119.26	115.29
27	B1	2850	4AC	CM7-C7-N4	2.29	119.26	115.29
27	B1	896	4AC	N4-C4-N3	2.29	117.70	113.85
27	B1	2968	LHH	CM7-C7-N4	2.29	119.25	115.29
27	B1	2113	4AC	C5-C4-N3	-2.29	118.91	122.59
27	B1	2171	4AC	N4-C4-N3	2.29	117.69	113.85
1	A1	307	4AC	C5-C4-N3	-2.29	118.91	122.59
27	B1	2365	OMG	O6-C6-C5	-2.29	119.91	124.37
1	A1	195	4AC	C5-C4-N3	-2.28	118.92	122.59
27	B1	243	4AC	C5-C4-N3	-2.28	118.92	122.59
27	B1	1965	OMG	O6-C6-C5	-2.28	119.92	124.37
1	A1	614	4AC	CM7-C7-N4	2.28	119.24	115.29
1	A1	228	OMG	O6-C6-C5	-2.28	119.92	124.37
27	B1	2379	4AC	C5-C4-N3	-2.28	118.93	122.59
27	B1	419	4AC	C5-C4-N3	-2.28	118.93	122.59
27	B1	1313	4AC	N4-C4-N3	2.27	117.67	113.85
1	A1	291	4AC	O2'-C2'-C1'	2.27	117.62	110.02
27	B1	1557	OMG	O6-C6-C5	-2.27	119.94	124.37
27	B1	1404	4AC	C5-C4-N3	-2.27	118.94	122.59
27	B1	807	4AC	N4-C4-N3	2.27	117.66	113.85
1	A1	1003	OMG	O6-C6-C5	-2.27	119.94	124.37
1	A1	901	OMG	O6-C6-C5	-2.27	119.94	124.37
27	B1	1107	4AC	C5-C4-N3	-2.27	118.94	122.59
27	B1	2469	4AC	CM7-C7-N4	2.27	119.22	115.29
27	B1	1150	4AC	C5-C4-N3	-2.27	118.95	122.59
27	B1	688	4AC	CM7-C7-N4	2.27	119.21	115.29
1	A1	861	OMG	O6-C6-C5	-2.26	119.95	124.37
1	A1	87	4AC	C5-C4-N3	-2.26	118.95	122.59
27	B1	1751	4AC	N4-C4-N3	2.26	117.65	113.85
27	B1	866	4AC	N4-C4-N3	2.26	117.65	113.85
27	B1	214	OMG	O6-C6-C5	-2.26	119.95	124.37
27	B1	921	OMG	O6-C6-C5	-2.26	119.96	124.37
1	A1	507	OMG	O6-C6-C5	-2.26	119.96	124.37
1	A1	1254	4AC	CM7-C7-N4	2.26	119.20	115.29
27	B1	2328	4AC	CM7-C7-N4	2.26	119.20	115.29
27	B1	866	4AC	CM7-C7-N4	2.26	119.20	115.29
27	B1	1601	OMG	O6-C6-C5	-2.26	119.97	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	2171	4AC	C5-C4-N3	-2.26	118.96	122.59
1	A1	1181	4AC	N4-C4-N3	2.26	117.64	113.85
1	A1	1227	4AC	N4-C4-N3	2.26	117.64	113.85
27	B1	1293	4AC	N4-C4-N3	2.25	117.64	113.85
27	B1	2821	4AC	N4-C4-N3	2.25	117.64	113.85
27	B1	1442	4AC	C5-C4-N3	-2.25	118.97	122.59
27	B1	2391	OMG	N2-C2-N1	2.25	121.51	116.71
27	B1	2888	4AC	CM7-C7-N4	2.25	119.19	115.29
1	A1	307	4AC	CM7-C7-N4	2.25	119.19	115.29
27	B1	2113	4AC	O2'-C2'-C1'	2.25	117.55	110.02
27	B1	3037	4AC	CM7-C7-N4	2.25	119.18	115.29
1	A1	231	4AC	N4-C4-N3	2.25	117.63	113.85
27	B1	2113	4AC	CM7-C7-N4	2.25	119.18	115.29
27	B1	732	4AC	C5-C4-N3	-2.25	118.98	122.59
27	B1	877	5MC	CM5-C5-C6	-2.25	119.85	122.85
1	A1	1029	4AC	O7-C7-CM7	-2.25	117.89	122.06
27	B1	1442	4AC	N4-C4-N3	2.24	117.62	113.85
1	A1	1067	4AC	C5-C4-N3	-2.24	118.98	122.59
27	B1	1061	4AC	C5-C4-N3	-2.24	118.98	122.59
1	A1	761	4AC	CM7-C7-N4	2.24	119.17	115.29
1	A1	763	OMG	O6-C6-C5	-2.24	119.99	124.37
27	B1	1639	4AC	N4-C4-N3	2.24	117.62	113.85
27	B1	262	A2M	C5-C6-N6	2.24	123.76	120.35
27	B1	1435	4AC	C5-C4-N3	-2.24	118.99	122.59
1	A1	645	OMG	O6-C6-C5	-2.24	120.00	124.37
1	A1	833	OMG	O6-C6-C5	-2.24	120.00	124.37
27	B1	741	4AC	C5-C4-N3	-2.24	118.99	122.59
27	B1	759	4AC	C5-C4-N3	-2.24	118.99	122.59
27	B1	1706	4AC	CM7-C7-N4	2.24	119.17	115.29
27	B1	485	4AC	CM7-C7-N4	2.24	119.17	115.29
27	B1	2429	4AC	CM7-C7-N4	2.24	119.16	115.29
1	A1	681	5MC	CM5-C5-C6	-2.24	119.86	122.85
1	A1	455	OMG	O6-C6-C5	-2.24	120.00	124.37
27	B1	1743	4AC	CM7-C7-N4	2.24	119.16	115.29
27	B1	116	4AC	C5-C4-N3	-2.23	119.00	122.59
27	B1	3006	4AC	C5-C4-N3	-2.23	119.00	122.59
27	B1	1052	4AC	N4-C4-N3	2.23	117.60	113.85
27	B1	271	4AC	CM7-C7-N4	2.23	119.16	115.29
1	A1	153	OMG	O6-C6-C5	-2.23	120.02	124.37
27	B1	80	4AC	CM7-C7-N4	2.23	119.15	115.29
1	A1	668	OMG	O6-C6-C5	-2.23	120.02	124.37
27	B1	130	4AC	CM7-C7-N4	2.23	119.15	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	2850	4AC	C5-C4-N3	-2.23	119.01	122.59
27	B1	3037	4AC	C5-C4-N3	-2.23	119.01	122.59
27	B1	2469	4AC	C5-C4-N3	-2.22	119.01	122.59
27	B1	2180	OMG	O6-C6-C5	-2.22	120.03	124.37
27	B1	2213	4AC	N4-C4-N3	2.22	117.58	113.85
27	B1	721	4AC	C5-C4-N3	-2.22	119.02	122.59
27	B1	98	4AC	N4-C4-N3	2.22	117.58	113.85
27	B1	1383	4AC	CM7-C7-N4	2.22	119.14	115.29
27	B1	2028	OMG	O6-C6-C5	-2.22	120.03	124.37
27	B1	2684	OMG	O6-C6-C5	-2.22	120.03	124.37
1	A1	775	OMU	O2'-C2'-C1'	2.22	113.41	109.08
1	A1	1004	2MG	O6-C6-C5	-2.22	120.03	124.37
27	B1	434	4AC	N4-C4-N3	2.22	117.58	113.85
27	B1	786	4AC	N4-C4-N3	2.22	117.58	113.85
27	B1	1488	OMU	O2'-C2'-C1'	2.22	113.41	109.08
1	A1	141	4AC	CM7-C7-N4	2.22	119.13	115.29
27	B1	732	4AC	CM7-C7-N4	2.22	119.13	115.29
1	A1	444	4AC	CM7-C7-N4	2.22	119.13	115.29
1	A1	1221	4AC	CM7-C7-N4	2.22	119.13	115.29
27	B1	434	4AC	C5-C4-N3	-2.22	119.03	122.59
27	B1	920	OMG	O6-C6-C5	-2.22	120.05	124.37
1	A1	719	4AC	N4-C4-N3	2.22	117.57	113.85
27	B1	1052	4AC	CM7-C7-N4	2.21	119.12	115.29
1	A1	816	4AC	C5-C4-N3	-2.21	119.03	122.59
1	A1	856	4AC	N4-C4-N3	2.21	117.57	113.85
27	B1	1822	4AC	N4-C4-N3	2.21	117.57	113.85
1	A1	534	4AC	C5-C4-N3	-2.21	119.03	122.59
27	B1	979	4AC	C5-C4-N3	-2.21	119.03	122.59
27	B1	116	4AC	N4-C4-N3	2.21	117.57	113.85
27	B1	1067	4AC	N4-C4-N3	2.21	117.57	113.85
27	B1	1734	4AC	C5-C4-N3	-2.21	119.03	122.59
1	A1	329	OMG	O6-C6-C5	-2.21	120.05	124.37
27	B1	80	4AC	C5-C4-N3	-2.21	119.03	122.59
1	A1	739	4AC	CM7-C7-N4	2.21	119.12	115.29
27	B1	502	LHH	CM7-C7-N4	2.21	119.12	115.29
1	A1	1227	4AC	C5-C4-N3	-2.21	119.04	122.59
1	A1	540	4AC	CM7-C7-N4	2.21	119.11	115.29
27	B1	1290	4AC	C5-C4-N3	-2.21	119.04	122.59
27	B1	2876	4AC	CM7-C7-N4	2.21	119.11	115.29
1	A1	839	4AC	CM7-C7-N4	2.21	119.11	115.29
27	B1	609	4AC	CM7-C7-N4	2.20	119.11	115.29
1	A1	274	4AC	C5-C4-N3	-2.20	119.05	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	142	4AC	CM7-C7-N4	2.20	119.10	115.29
27	B1	1107	4AC	N4-C4-N3	2.20	117.55	113.85
27	B1	2526	4AC	N4-C4-N3	2.20	117.55	113.85
27	B1	2540	OMG	O6-C6-C5	-2.20	120.07	124.37
27	B1	1639	4AC	C5-C4-N3	-2.20	119.05	122.59
27	B1	130	4AC	C5-C4-N3	-2.20	119.05	122.59
27	B1	1612	4AC	C5-C4-N3	-2.20	119.06	122.59
27	B1	1608	4AC	O7-C7-CM7	-2.20	117.97	122.06
27	B1	2526	4AC	CM7-C7-N4	2.20	119.10	115.29
1	A1	382	4AC	C5-C4-N3	-2.20	119.06	122.59
1	A1	810	4AC	C5-C4-N3	-2.20	119.06	122.59
27	B1	675	OMG	O6-C6-C5	-2.20	120.08	124.37
27	B1	23	4AC	C5-C4-N3	-2.20	119.06	122.59
27	B1	3011	4AC	C5-C4-N3	-2.20	119.06	122.59
1	A1	856	4AC	CM7-C7-N4	2.20	119.09	115.29
1	A1	719	4AC	C5-C4-N3	-2.19	119.06	122.59
1	A1	227	OMG	O6-C6-C5	-2.19	120.09	124.37
27	B1	2888	4AC	C5-C4-N3	-2.19	119.06	122.59
27	B1	759	4AC	CM7-C7-N4	2.19	119.09	115.29
27	B1	1374	4AC	C5-C4-N3	-2.19	119.06	122.59
27	B1	1734	4AC	CM7-C7-N4	2.19	119.09	115.29
1	A1	951	5MC	CM5-C5-C6	-2.19	119.92	122.85
1	A1	1092	4AC	CM7-C7-N4	2.19	119.08	115.29
27	B1	2213	4AC	C5-C4-N3	-2.19	119.07	122.59
27	B1	580	4AC	CM7-C7-N4	2.19	119.08	115.29
27	B1	1264	4AC	C5-C4-N3	-2.19	119.07	122.59
1	A1	706	4AC	N4-C4-N3	2.19	117.53	113.85
27	B1	2067	5MC	C2'-C3'-C4'	2.19	106.89	102.64
1	A1	367	4AC	CM7-C7-N4	2.19	119.08	115.29
27	B1	2888	4AC	N4-C4-N3	2.19	117.52	113.85
1	A1	220	4AC	CM7-C7-N4	2.19	119.08	115.29
27	B1	715	4AC	CM7-C7-N4	2.19	119.08	115.29
27	B1	2020	4AC	N4-C4-N3	2.19	117.52	113.85
1	A1	816	4AC	CM7-C7-N4	2.19	119.07	115.29
1	A1	1016	4AC	CM7-C7-N4	2.19	119.07	115.29
27	B1	1293	4AC	C5-C4-N3	-2.18	119.08	122.59
27	B1	1885	4AC	C5-C4-N3	-2.18	119.08	122.59
27	B1	1100	4AC	C5-C4-N3	-2.18	119.08	122.59
27	B1	1612	4AC	CM7-C7-N4	2.18	119.07	115.29
27	B1	1946	LHH	CM7-C7-N4	2.18	119.07	115.29
27	B1	2562	OMG	O6-C6-C5	-2.18	120.11	124.37
1	A1	839	4AC	C5-C4-N3	-2.18	119.08	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	17	5MC	CM5-C5-C6	-2.18	119.93	122.85
27	B1	226	5MC	CM5-C5-C6	-2.18	119.93	122.85
27	B1	1818	4AC	CM7-C7-N4	2.18	119.07	115.29
27	B1	950	4AC	C5-C4-N3	-2.18	119.08	122.59
1	A1	1015	5MC	CM5-C5-C6	-2.18	119.94	122.85
27	B1	359	5MC	CM5-C5-C6	-2.18	119.94	122.85
1	A1	706	4AC	C5-C4-N3	-2.18	119.09	122.59
27	B1	200	4AC	N4-C4-N3	2.18	117.51	113.85
27	B1	1706	4AC	C5-C4-N3	-2.18	119.09	122.59
27	B1	2792	4AC	C5-C4-N3	-2.18	119.09	122.59
27	B1	1061	4AC	CM7-C7-N4	2.18	119.06	115.29
27	B1	419	4AC	CM7-C7-N4	2.18	119.06	115.29
27	B1	2757	OMG	O6-C6-C5	-2.18	120.12	124.37
1	A1	605	5MC	CM5-C5-C6	-2.18	119.94	122.85
27	B1	1551	4AC	N4-C4-N3	2.18	117.50	113.85
27	B1	609	4AC	C5-C4-N3	-2.17	119.09	122.59
27	B1	1264	4AC	CM7-C7-N4	2.17	119.05	115.29
1	A1	1181	4AC	C5-C4-N3	-2.17	119.10	122.59
1	A1	427	4AC	C5-C4-N3	-2.17	119.10	122.59
27	B1	1439	4AC	CM7-C7-N4	2.17	119.05	115.29
27	B1	2432	4AC	C5-C4-N3	-2.17	119.10	122.59
28	B2	90	4AC	C5-C4-N3	-2.17	119.10	122.59
1	A1	624	4AC	C5-C4-N3	-2.17	119.10	122.59
1	A1	1221	4AC	C5-C4-N3	-2.17	119.10	122.59
1	A1	578	4AC	C5-C4-N3	-2.17	119.10	122.59
27	B1	3020	4AC	CM7-C7-N4	2.17	119.05	115.29
27	B1	599	4AC	C5-C4-N3	-2.17	119.10	122.59
27	B1	1505	4AC	CM7-C7-N4	2.17	119.05	115.29
27	B1	2379	4AC	CM7-C7-N4	2.17	119.05	115.29
27	B1	2876	4AC	C5-C4-N3	-2.17	119.10	122.59
27	B1	1762	4AC	C5-C4-N3	-2.17	119.11	122.59
27	B1	786	4AC	CM7-C7-N4	2.17	119.04	115.29
27	B1	1546	4AC	CM7-C7-N4	2.17	119.04	115.29
27	B1	243	4AC	CM7-C7-N4	2.17	119.04	115.29
27	B1	580	4AC	C5-C4-N3	-2.17	119.11	122.59
27	B1	1822	4AC	C5-C4-N3	-2.17	119.11	122.59
27	B1	23	4AC	CM7-C7-N4	2.17	119.04	115.29
27	B1	2171	4AC	CM7-C7-N4	2.17	119.04	115.29
27	B1	2602	4AC	C5-C4-N3	-2.17	119.11	122.59
27	B1	97	5MC	CM5-C5-C6	-2.16	119.96	122.85
27	B1	1743	4AC	C5-C4-N3	-2.16	119.11	122.59
1	A1	540	4AC	C5-C4-N3	-2.16	119.11	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	1322	4AC	CM7-C7-N4	2.16	119.03	115.29
1	A1	1467	4AC	C5-C4-N3	-2.16	119.12	122.59
1	A1	1092	4AC	C5-C4-N3	-2.16	119.12	122.59
27	B1	227	4AC	CM7-C7-N4	2.16	119.03	115.29
1	A1	41	4AC	N4-C4-N3	2.16	117.47	113.85
1	A1	719	4AC	CM7-C7-N4	2.16	119.03	115.29
27	B1	2213	4AC	CM7-C7-N4	2.16	119.03	115.29
1	A1	291	4AC	CM7-C7-N4	2.16	119.03	115.29
27	B1	2328	4AC	N4-C4-N3	2.16	117.47	113.85
1	A1	231	4AC	CM7-C7-N4	2.16	119.02	115.29
27	B1	162	4AC	N4-C4-N3	2.15	117.47	113.85
27	B1	2454	4AC	CM7-C7-N4	2.15	119.02	115.29
27	B1	1649	4AC	C5-C4-N3	-2.15	119.13	122.59
1	A1	1067	4AC	CM7-C7-N4	2.15	119.02	115.29
27	B1	271	4AC	C5-C4-N3	-2.15	119.13	122.59
27	B1	715	4AC	C5-C4-N3	-2.15	119.13	122.59
27	B1	1067	4AC	C5-C4-N3	-2.15	119.13	122.59
27	B1	2454	4AC	C5-C4-N3	-2.15	119.13	122.59
27	B1	1374	4AC	O7-C7-CM7	-2.15	118.06	122.06
27	B1	1128	4AC	N4-C4-N3	2.15	117.46	113.85
1	A1	425	OMU	O2-C2-N1	-2.15	119.93	122.79
27	B1	652	4AC	N4-C4-N3	2.15	117.46	113.85
27	B1	1290	4AC	N4-C4-N3	2.15	117.46	113.85
27	B1	652	4AC	C5-C4-N3	-2.15	119.14	122.59
27	B1	1064	4AC	O7-C7-CM7	-2.15	118.07	122.06
27	B1	1818	4AC	C5-C4-N3	-2.15	119.14	122.59
27	B1	1128	4AC	C5-C4-N3	-2.15	119.14	122.59
27	B1	2429	4AC	C5-C4-N3	-2.15	119.14	122.59
27	B1	200	4AC	CM7-C7-N4	2.15	119.00	115.29
27	B1	1404	4AC	N4-C4-N3	2.15	117.45	113.85
27	B1	360	4AC	C5-C4-N3	-2.15	119.14	122.59
1	A1	761	4AC	C5-C4-N3	-2.14	119.14	122.59
1	A1	499	4AC	C5-C4-N3	-2.14	119.14	122.59
27	B1	162	4AC	C5-C4-N3	-2.14	119.14	122.59
27	B1	1505	4AC	C5-C4-N3	-2.14	119.14	122.59
27	B1	1442	4AC	CM7-C7-N4	2.14	119.00	115.29
27	B1	3006	4AC	CM7-C7-N4	2.14	119.00	115.29
1	A1	1314	4AC	C5-C4-N3	-2.14	119.14	122.59
27	B1	1608	4AC	C5-C4-N3	-2.14	119.14	122.59
27	B1	200	4AC	C5-C4-N3	-2.14	119.14	122.59
1	A1	1368	OMU	O2-C2-N1	-2.14	119.94	122.79
1	A1	405	4AC	C5-C4-N3	-2.14	119.15	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	1621	4AC	C5-C4-N3	-2.14	119.15	122.59
27	B1	1769	4AC	C5-C4-N3	-2.14	119.15	122.59
1	A1	274	4AC	CM7-C7-N4	2.14	119.00	115.29
1	A1	578	4AC	CM7-C7-N4	2.14	119.00	115.29
27	B1	841	OMG	O6-C6-C5	-2.14	120.19	124.37
1	A1	367	4AC	C5-C4-N3	-2.14	119.15	122.59
27	B1	1501	4AC	CM7-C7-N4	2.14	119.00	115.29
1	A1	117	OMC	O3'-C3'-C2'	2.14	117.25	111.17
27	B1	1286	4AC	CM7-C7-N4	2.14	119.00	115.29
28	B2	117	4AC	CM7-C7-N4	2.14	119.00	115.29
27	B1	1052	4AC	C5-C4-N3	-2.14	119.15	122.59
1	A1	534	4AC	CM7-C7-N4	2.14	118.99	115.29
1	A1	231	4AC	C5-C4-N3	-2.14	119.15	122.59
1	A1	467	4AC	C5-C4-N3	-2.14	119.15	122.59
1	A1	810	4AC	CM7-C7-N4	2.14	118.99	115.29
27	B1	434	4AC	CM7-C7-N4	2.14	118.99	115.29
1	A1	1135	4AC	C5-C4-N3	-2.14	119.15	122.59
27	B1	2749	4AC	C5-C4-N3	-2.14	119.15	122.59
1	A1	41	4AC	C5-C4-N3	-2.14	119.15	122.59
1	A1	826	5MC	CM5-C5-C6	-2.14	119.99	122.85
27	B1	953	4AC	C5-C4-N3	-2.14	119.16	122.59
1	A1	1362	5MC	CM5-C5-C6	-2.14	120.00	122.85
27	B1	1478	4AC	C5-C4-N3	-2.13	119.16	122.59
27	B1	2133	4AC	C5-C4-N3	-2.13	119.16	122.59
1	A1	827	4AC	CM7-C7-N4	2.13	118.99	115.29
27	B1	2008	4AC	N4-C4-N3	2.13	117.44	113.85
27	B1	1322	4AC	C5-C4-N3	-2.13	119.16	122.59
27	B1	1178	4AC	CM7-C7-N4	2.13	118.98	115.29
27	B1	1664	4AC	CM7-C7-N4	2.13	118.98	115.29
27	B1	2067	5MC	CM5-C5-C6	-2.13	120.00	122.85
27	B1	1751	4AC	CM7-C7-N4	2.13	118.98	115.29
1	A1	636	4AC	CM7-C7-N4	2.13	118.98	115.29
27	B1	1546	4AC	C5-C4-N3	-2.13	119.16	122.59
27	B1	1313	4AC	CM7-C7-N4	2.13	118.98	115.29
27	B1	2526	4AC	C5-C4-N3	-2.13	119.16	122.59
1	A1	141	4AC	C5-C4-N3	-2.13	119.17	122.59
1	A1	466	5MC	CM5-C5-C6	-2.13	120.00	122.85
1	A1	1012	5MC	CM5-C5-C6	-2.13	120.00	122.85
27	B1	1769	4AC	N4-C4-N3	2.13	117.43	113.85
1	A1	827	4AC	C5-C4-N3	-2.13	119.17	122.59
27	B1	3023	4AC	C5-C4-N3	-2.13	119.17	122.59
27	B1	142	4AC	C5-C4-N3	-2.13	119.17	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	2792	4AC	CM7-C7-N4	2.13	118.97	115.29
27	B1	1846	4AC	C5-C4-N3	-2.13	119.17	122.59
27	B1	479	4AC	N4-C4-N3	2.13	117.42	113.85
27	B1	2602	4AC	CM7-C7-N4	2.13	118.97	115.29
1	A1	216	4AC	CM7-C7-N4	2.13	118.97	115.29
1	A1	855	5MC	CM5-C5-C6	-2.13	120.01	122.85
28	B2	117	4AC	C5-C4-N3	-2.13	119.17	122.59
27	B1	1435	4AC	CM7-C7-N4	2.13	118.97	115.29
28	B2	90	4AC	CM7-C7-N4	2.13	118.97	115.29
1	A1	291	4AC	C5-C4-N3	-2.12	119.17	122.59
1	A1	499	4AC	CM7-C7-N4	2.12	118.97	115.29
1	A1	636	4AC	C5-C4-N3	-2.12	119.18	122.59
27	B1	1846	4AC	CM7-C7-N4	2.12	118.97	115.29
27	B1	1757	4AC	C5-C4-N3	-2.12	119.18	122.59
27	B1	2492	4AC	C5-C4-N3	-2.12	119.18	122.59
27	B1	360	4AC	CM7-C7-N4	2.12	118.96	115.29
27	B1	896	4AC	C5-C4-N3	-2.12	119.18	122.59
1	A1	41	4AC	CM7-C7-N4	2.12	118.96	115.29
27	B1	1501	4AC	C5-C4-N3	-2.12	119.18	122.59
27	B1	392	4AC	C5-C4-N3	-2.12	119.18	122.59
27	B1	1664	4AC	C5-C4-N3	-2.12	119.18	122.59
27	B1	1967	4AC	C5-C4-N3	-2.12	119.19	122.59
27	B1	1293	4AC	CM7-C7-N4	2.12	118.96	115.29
27	B1	798	4AC	C5-C4-N3	-2.12	119.19	122.59
27	B1	1178	4AC	C5-C4-N3	-2.12	119.19	122.59
27	B1	3020	4AC	C5-C4-N3	-2.12	119.19	122.59
1	A1	1314	4AC	CM7-C7-N4	2.12	118.96	115.29
1	A1	216	4AC	C5-C4-N3	-2.12	119.19	122.59
27	B1	1649	4AC	CM7-C7-N4	2.12	118.95	115.29
27	B1	652	4AC	CM7-C7-N4	2.11	118.95	115.29
27	B1	950	4AC	CM7-C7-N4	2.11	118.95	115.29
27	B1	1439	4AC	C5-C4-N3	-2.11	119.19	122.59
27	B1	1703	4AC	C5-C4-N3	-2.11	119.19	122.59
27	B1	2328	4AC	C5-C4-N3	-2.11	119.19	122.59
1	A1	195	4AC	CM7-C7-N4	2.11	118.95	115.29
1	A1	227	OMG	N2-C2-N1	2.11	121.21	116.71
1	A1	1348	5MC	CM5-C5-C6	-2.11	120.03	122.85
27	B1	2492	4AC	CM7-C7-N4	2.11	118.95	115.29
1	A1	220	4AC	C5-C4-N3	-2.11	119.19	122.59
27	B1	485	4AC	C5-C4-N3	-2.11	119.19	122.59
27	B1	798	4AC	CM7-C7-N4	2.11	118.95	115.29
1	A1	756	4SU	O2-C2-N1	-2.11	119.98	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	1100	4AC	CM7-C7-N4	2.11	118.94	115.29
1	A1	467	4AC	CM7-C7-N4	2.11	118.94	115.29
27	B1	1290	4AC	CM7-C7-N4	2.11	118.94	115.29
27	B1	18	5MC	CM5-C5-C6	-2.11	120.03	122.85
27	B1	1703	4AC	CM7-C7-N4	2.11	118.94	115.29
1	A1	775	OMU	O2-C2-N1	-2.11	119.98	122.79
27	B1	1404	4AC	CM7-C7-N4	2.11	118.94	115.29
27	B1	808	OMG	O6-C6-C5	-2.11	120.25	124.37
27	B1	2984	OMG	N2-C2-N1	2.11	121.20	116.71
1	A1	1181	4AC	CM7-C7-N4	2.11	118.94	115.29
1	A1	1016	4AC	C5-C4-N3	-2.11	119.20	122.59
1	A1	87	4AC	CM7-C7-N4	2.10	118.93	115.29
27	B1	786	4AC	C5-C4-N3	-2.10	119.21	122.59
27	B1	1386	4AC	C5-C4-N3	-2.10	119.21	122.59
27	B1	1533	OMG	O6-C6-C5	-2.10	120.26	124.37
27	B1	2022	OMG	O6-C6-C5	-2.10	120.27	124.37
27	B1	1649	4AC	N4-C4-N3	2.10	117.38	113.85
27	B1	2492	4AC	N4-C4-N3	2.10	117.38	113.85
1	A1	1288	4AC	CM7-C7-N4	2.10	118.93	115.29
1	A1	405	4AC	CM7-C7-N4	2.10	118.93	115.29
1	A1	1486	5MC	CM5-C5-C6	-2.10	120.04	122.85
1	A1	546	4AC	CM7-C7-N4	2.10	118.92	115.29
27	B1	1885	4AC	CM7-C7-N4	2.10	118.92	115.29
1	A1	382	4AC	CM7-C7-N4	2.10	118.92	115.29
28	B2	120	4AC	CM7-C7-N4	2.10	118.92	115.29
1	A1	444	4AC	C5-C4-N3	-2.10	119.22	122.59
27	B1	2020	4AC	C5-C4-N3	-2.10	119.22	122.59
1	A1	856	4AC	C5-C4-N3	-2.09	119.22	122.59
27	B1	2617	5MC	CM5-C5-C6	-2.09	120.05	122.85
27	B1	98	4AC	C5-C4-N3	-2.09	119.22	122.59
1	A1	1013	5MC	CM5-C5-C6	-2.09	120.05	122.85
27	B1	1977	5MC	CM5-C5-C6	-2.09	120.05	122.85
1	A1	739	4AC	C5-C4-N3	-2.09	119.22	122.59
27	B1	2133	4AC	CM7-C7-N4	2.09	118.91	115.29
27	B1	2757	OMG	N2-C2-N1	2.09	121.17	116.71
27	B1	904	LHH	CM7-C7-N4	2.09	118.91	115.29
27	B1	887	OMG	CM2-O2'-C2'	2.09	120.01	114.52
1	A1	523	5MC	CM5-C5-C6	-2.09	120.06	122.85
27	B1	2809	4AC	N4-C4-N3	2.09	117.36	113.85
27	B1	1757	4AC	CM7-C7-N4	2.09	118.91	115.29
27	B1	1488	OMU	O2-C2-N1	-2.09	120.01	122.79
1	A1	5	4AC	C5-C4-N3	-2.09	119.23	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	227	4AC	C5-C4-N3	-2.09	119.23	122.59
1	A1	546	4AC	C5-C4-N3	-2.09	119.23	122.59
27	B1	1751	4AC	C5-C4-N3	-2.09	119.23	122.59
27	B1	276	4AC	CM7-C7-N4	2.09	118.91	115.29
27	B1	1822	4AC	CM7-C7-N4	2.09	118.91	115.29
27	B1	2008	4AC	C5-C4-N3	-2.09	119.23	122.59
1	A1	836	4AC	CM7-C7-N4	2.09	118.90	115.29
27	B1	1639	4AC	CM7-C7-N4	2.09	118.90	115.29
27	B1	1149	5MC	CM5-C5-C6	-2.09	120.06	122.85
27	B1	276	4AC	C5-C4-N3	-2.09	119.24	122.59
27	B1	1505	4AC	N4-C4-N3	2.09	117.35	113.85
27	B1	98	4AC	CM7-C7-N4	2.08	118.90	115.29
27	B1	866	4AC	C5-C4-N3	-2.08	119.24	122.59
1	A1	473	5MC	CM5-C5-C6	-2.08	120.07	122.85
27	B1	1551	4AC	C5-C4-N3	-2.08	119.24	122.59
27	B1	2875	5MC	CM5-C5-C6	-2.08	120.07	122.85
27	B1	721	4AC	CM7-C7-N4	2.08	118.89	115.29
27	B1	1383	4AC	C5-C4-N3	-2.08	119.25	122.59
27	B1	2432	4AC	CM7-C7-N4	2.08	118.89	115.29
27	B1	1648	5MC	CM5-C5-C6	-2.08	120.07	122.85
27	B1	2844	4AC	C5-C4-N3	-2.08	119.25	122.59
27	B1	675	OMG	N2-C2-N1	2.08	121.13	116.71
27	B1	599	4AC	CM7-C7-N4	2.08	118.88	115.29
27	B1	896	4AC	CM7-C7-N4	2.07	118.88	115.29
27	B1	1313	4AC	C5-C4-N3	-2.07	119.26	122.59
27	B1	2749	4AC	CM7-C7-N4	2.07	118.88	115.29
27	B1	116	4AC	CM7-C7-N4	2.07	118.88	115.29
27	B1	392	4AC	CM7-C7-N4	2.07	118.88	115.29
1	A1	1288	4AC	C5-C4-N3	-2.07	119.27	122.59
27	B1	1946	LHH	C5-C4-N4	-2.06	119.33	122.92
27	B1	932	5MC	CM5-C5-C6	-2.06	120.09	122.85
1	A1	1135	4AC	CM7-C7-N4	2.06	118.86	115.29
27	B1	3023	4AC	CM7-C7-N4	2.06	118.86	115.29
27	B1	1107	4AC	CM7-C7-N4	2.06	118.86	115.29
27	B1	3011	4AC	CM7-C7-N4	2.06	118.86	115.29
27	B1	2008	4AC	CM7-C7-N4	2.06	118.86	115.29
27	B1	953	4AC	CM7-C7-N4	2.06	118.85	115.29
1	A1	5	4AC	CM7-C7-N4	2.06	118.85	115.29
27	B1	1981	OMU	O2-C2-N1	-2.06	120.05	122.79
27	B1	1762	4AC	CM7-C7-N4	2.05	118.84	115.29
27	B1	1621	4AC	O7-C7-CM7	-2.05	118.25	122.06
27	B1	2844	4AC	CM7-C7-N4	2.05	118.84	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	19	4AC	CM7-C7-N4	2.05	118.84	115.29
1	A1	863	5MC	CM5-C5-C6	-2.05	120.11	122.85
27	B1	47	5MC	CM5-C5-C6	-2.05	120.11	122.85
27	B1	2087	5MC	CM5-C5-C6	-2.05	120.11	122.85
27	B1	1100	4AC	N4-C4-N3	2.05	117.29	113.85
27	B1	19	4AC	C5-C4-N3	-2.05	119.30	122.59
27	B1	1128	4AC	CM7-C7-N4	2.05	118.83	115.29
1	A1	1366	A1I59	O2-C2-N3	-2.04	119.01	122.33
27	B1	2554	OMU	O2-C2-N1	-2.04	120.07	122.79
1	A1	1190	5MC	CM5-C5-C6	-2.04	120.12	122.85
27	B1	2668	OMU	O2-C2-N1	-2.04	120.07	122.79
27	B1	1885	4AC	N4-C4-N3	2.04	117.28	113.85
27	B1	48	4AC	C5-C4-N3	-2.04	119.31	122.59
1	A1	274	4AC	N4-C4-N3	2.04	117.27	113.85
27	B1	479	4AC	C5-C4-N3	-2.04	119.32	122.59
27	B1	1067	4AC	CM7-C7-N4	2.04	118.81	115.29
27	B1	2821	4AC	CM7-C7-N4	2.04	118.81	115.29
1	A1	533	5MC	CM5-C5-C6	-2.03	120.13	122.85
27	B1	1286	4AC	O7-C7-CM7	-2.03	118.28	122.06
27	B1	275	5MC	CM5-C5-C6	-2.03	120.13	122.85
1	A1	230	5MC	CM5-C5-C6	-2.03	120.14	122.85
1	A1	762	OMU	O2-C2-N1	-2.03	120.09	122.79
27	B1	1488	OMU	CM2-O2'-C2'	2.03	119.85	114.52
27	B1	2020	4AC	CM7-C7-N4	2.03	118.81	115.29
27	B1	1551	4AC	CM7-C7-N4	2.03	118.80	115.29
27	B1	502	LHH	C5-C4-N4	-2.02	119.40	122.92
27	B1	2133	4AC	N4-C4-N3	2.02	117.25	113.85
27	B1	454	OMU	O2-C2-N1	-2.02	120.10	122.79
1	A1	691	4AC	CM7-C7-N4	2.02	118.79	115.29
28	B2	120	4AC	C5-C4-N3	-2.02	119.35	122.59
27	B1	2453	5MC	CM5-C5-C6	-2.01	120.16	122.85
27	B1	2809	4AC	C5-C4-N3	-2.01	119.35	122.59
27	B1	2809	4AC	CM7-C7-N4	2.01	118.78	115.29
27	B1	2821	4AC	C5-C4-N3	-2.01	119.35	122.59
1	A1	52	OMU	O2-C2-N1	-2.01	120.11	122.79
27	B1	2401	OMU	C1'-N1-C2	2.01	121.21	117.57
27	B1	2562	OMG	N2-C2-N1	2.01	120.99	116.71
1	A1	691	4AC	C5-C4-N3	-2.00	119.37	122.59
27	B1	2749	4AC	C2'-C1'-N1	2.00	118.89	113.22
1	A1	8	OMU	O2-C2-N1	-2.00	120.12	122.79
27	B1	1911	4AC	C5-C4-N3	-2.00	119.37	122.59

There are no chirality outliers.

All (209) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A1	8	OMU	C3'-C4'-C5'-O5'
1	A1	238	LHH	C5-C4-N4-C7
1	A1	238	LHH	N3-C4-N4-C7
1	A1	466	5MC	C3'-C4'-C5'-O5'
1	A1	481	G7M	O4'-C4'-C5'-O5'
1	A1	481	G7M	C3'-C4'-C5'-O5'
1	A1	775	OMU	C1'-C2'-O2'-CM2
1	A1	861	OMG	O4'-C4'-C5'-O5'
1	A1	926	5MU	O4'-C4'-C5'-O5'
1	A1	951	5MC	C3'-C4'-C5'-O5'
1	A1	1012	5MC	O4'-C4'-C5'-O5'
1	A1	1012	5MC	C3'-C4'-C5'-O5'
1	A1	1270	OMC	C3'-C4'-C5'-O5'
1	A1	1270	OMC	O4'-C4'-C5'-O5'
1	A1	1364	LHH	C5-C4-N4-C7
1	A1	1364	LHH	N3-C4-N4-C7
1	A1	1364	LHH	C3'-C4'-C5'-O5'
1	A1	1364	LHH	O4'-C4'-C5'-O5'
1	A1	1366	A1I59	CM5-C1-C3-O1
1	A1	1366	A1I59	CM5-C1-C3-O4
1	A1	1366	A1I59	C3-C1-CM5-N5
1	A1	1457	MA6	C5-C6-N6-C9
1	A1	1457	MA6	C5-C6-N6-C10
1	A1	1092	4AC	O4'-C4'-C5'-O5'
27	B1	47	5MC	C4'-C5'-O5'-P
27	B1	392	4AC	O4'-C4'-C5'-O5'
27	B1	392	4AC	C3'-C4'-C5'-O5'
27	B1	502	LHH	C5-C4-N4-C7
27	B1	502	LHH	N3-C4-N4-C7
27	B1	527	LHH	C5-C4-N4-C7
27	B1	527	LHH	N3-C4-N4-C7
27	B1	641	LHH	C3'-C4'-C5'-O5'
27	B1	641	LHH	O4'-C4'-C5'-O5'
27	B1	813	4AC	O4'-C4'-C5'-O5'
27	B1	813	4AC	C3'-C4'-C5'-O5'
27	B1	887	OMG	C1'-C2'-O2'-CM2
27	B1	904	LHH	C3'-C4'-C5'-O5'
27	B1	904	LHH	O4'-C4'-C5'-O5'
27	B1	1365	LHH	C5-C4-N4-C7
27	B1	1365	LHH	N3-C4-N4-C7
27	B1	1451	5MC	C3'-C4'-C5'-O5'
27	B1	1488	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
27	B1	1601	OMG	C1'-C2'-O2'-CM2
27	B1	1639	4AC	O4'-C4'-C5'-O5'
27	B1	1703	4AC	C3'-C4'-C5'-O5'
27	B1	1818	4AC	C3'-C4'-C5'-O5'
27	B1	1946	LHH	C5-C4-N4-C7
27	B1	1946	LHH	N3-C4-N4-C7
27	B1	1965	OMG	O4'-C4'-C5'-O5'
27	B1	1965	OMG	C3'-C4'-C5'-O5'
27	B1	1966	5MC	C3'-C4'-C5'-O5'
27	B1	2057	A2M	O4'-C4'-C5'-O5'
27	B1	2057	A2M	C3'-C4'-C5'-O5'
27	B1	2365	OMG	O4'-C4'-C5'-O5'
27	B1	2401	OMU	O4'-C1'-N1-C2
27	B1	2401	OMU	O4'-C1'-N1-C6
27	B1	2401	OMU	C3'-C4'-C5'-O5'
27	B1	2700	UR3	O4'-C1'-N1-C6
27	B1	2700	UR3	O4'-C1'-N1-C2
27	B1	2850	4AC	C3'-C4'-C5'-O5'
27	B1	2902	4AC	O7-C7-N4-C4
27	B1	2902	4AC	CM7-C7-N4-C4
27	B1	2968	LHH	C5-C4-N4-C7
27	B1	2968	LHH	N3-C4-N4-C7
27	B1	3037	4AC	C4'-C5'-O5'-P
28	B2	117	4AC	O4'-C4'-C5'-O5'
28	B2	117	4AC	C3'-C4'-C5'-O5'
1	A1	17	5MC	O4'-C4'-C5'-O5'
1	A1	533	5MC	O4'-C4'-C5'-O5'
1	A1	861	OMG	C3'-C4'-C5'-O5'
1	A1	926	5MU	C3'-C4'-C5'-O5'
1	A1	951	5MC	O4'-C4'-C5'-O5'
1	A1	1366	A1I59	C3'-C4'-C5'-O5'
1	A1	1366	A1I59	O4'-C4'-C5'-O5'
27	B1	275	5MC	O4'-C4'-C5'-O5'
27	B1	276	4AC	O4'-C4'-C5'-O5'
27	B1	276	4AC	C3'-C4'-C5'-O5'
27	B1	715	4AC	O4'-C4'-C5'-O5'
27	B1	933	4AC	O4'-C4'-C5'-O5'
27	B1	1178	4AC	C3'-C4'-C5'-O5'
27	B1	1383	4AC	O4'-C4'-C5'-O5'
27	B1	1383	4AC	C3'-C4'-C5'-O5'
27	B1	1489	OMC	O4'-C4'-C5'-O5'
27	B1	1533	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
27	B1	1612	4AC	C3'-C4'-C5'-O5'
27	B1	1639	4AC	C3'-C4'-C5'-O5'
27	B1	1703	4AC	O4'-C4'-C5'-O5'
27	B1	1818	4AC	O4'-C4'-C5'-O5'
27	B1	1966	5MC	O4'-C4'-C5'-O5'
27	B1	2180	OMG	O4'-C4'-C5'-O5'
27	B1	2365	OMG	C3'-C4'-C5'-O5'
27	B1	2850	4AC	O4'-C4'-C5'-O5'
27	B1	2902	4AC	O4'-C4'-C5'-O5'
27	B1	2902	4AC	C3'-C4'-C5'-O5'
27	B1	2391	OMG	C4'-C5'-O5'-P
1	A1	17	5MC	C3'-C4'-C5'-O5'
1	A1	455	OMG	O4'-C4'-C5'-O5'
1	A1	466	5MC	O4'-C4'-C5'-O5'
1	A1	1190	5MC	O4'-C4'-C5'-O5'
1	A1	1348	5MC	O4'-C4'-C5'-O5'
1	A1	5	4AC	O4'-C4'-C5'-O5'
1	A1	467	4AC	O4'-C4'-C5'-O5'
1	A1	706	4AC	O4'-C4'-C5'-O5'
1	A1	1016	4AC	O4'-C4'-C5'-O5'
1	A1	1016	4AC	C3'-C4'-C5'-O5'
1	A1	1092	4AC	C3'-C4'-C5'-O5'
27	B1	275	5MC	C3'-C4'-C5'-O5'
27	B1	675	OMG	O4'-C4'-C5'-O5'
27	B1	688	4AC	O4'-C4'-C5'-O5'
27	B1	933	4AC	C3'-C4'-C5'-O5'
27	B1	1178	4AC	O4'-C4'-C5'-O5'
27	B1	1451	5MC	O4'-C4'-C5'-O5'
27	B1	1533	OMG	O4'-C4'-C5'-O5'
27	B1	1612	4AC	O4'-C4'-C5'-O5'
27	B1	1914	OMC	O4'-C4'-C5'-O5'
27	B1	2401	OMU	O4'-C4'-C5'-O5'
1	A1	1457	MA6	N1-C6-N6-C9
27	B1	887	OMG	C3'-C2'-O2'-CM2
1	A1	775	OMU	C2'-C1'-N1-C6
1	A1	533	5MC	C3'-C4'-C5'-O5'
27	B1	715	4AC	C3'-C4'-C5'-O5'
27	B1	1648	5MC	C3'-C4'-C5'-O5'
27	B1	2180	OMG	C3'-C4'-C5'-O5'
1	A1	8	OMU	O4'-C4'-C5'-O5'
1	A1	1190	5MC	C3'-C4'-C5'-O5'
1	A1	5	4AC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A1	467	4AC	C3'-C4'-C5'-O5'
1	A1	1467	4AC	O4'-C4'-C5'-O5'
27	B1	688	4AC	C3'-C4'-C5'-O5'
27	B1	1648	5MC	O4'-C4'-C5'-O5'
27	B1	1846	4AC	O4'-C4'-C5'-O5'
27	B1	732	4AC	O4'-C4'-C5'-O5'
27	B1	741	4AC	C3'-C4'-C5'-O5'
27	B1	979	4AC	O4'-C4'-C5'-O5'
27	B1	1365	LHH	O4'-C4'-C5'-O5'
1	A1	87	4AC	O4'-C4'-C5'-O5'
27	B1	798	4AC	O4'-C4'-C5'-O5'
27	B1	1743	4AC	O4'-C4'-C5'-O5'
27	B1	2379	4AC	O4'-C4'-C5'-O5'
27	B1	2469	4AC	O4'-C4'-C5'-O5'
1	A1	1029	4AC	O7-C7-N4-C4
1	A1	1029	4AC	CM7-C7-N4-C4
27	B1	1064	4AC	O7-C7-N4-C4
27	B1	1064	4AC	CM7-C7-N4-C4
1	A1	775	OMU	O4'-C1'-N1-C6
1	A1	775	OMU	C2'-C1'-N1-C2
27	B1	857	A2M	C4'-C5'-O5'-P
1	A1	763	OMG	C3'-C4'-C5'-O5'
1	A1	1476	MA6	C3'-C4'-C5'-O5'
1	A1	706	4AC	C3'-C4'-C5'-O5'
1	A1	1486	5MC	O4'-C1'-N1-C6
1	A1	228	OMG	C3'-C4'-C5'-O5'
1	A1	455	OMG	C3'-C4'-C5'-O5'
1	A1	1348	5MC	C3'-C4'-C5'-O5'
27	B1	2391	OMG	C3'-C4'-C5'-O5'
1	A1	1362	5MC	O4'-C4'-C5'-O5'
1	A1	839	4AC	O4'-C4'-C5'-O5'
27	B1	97	5MC	O4'-C4'-C5'-O5'
1	A1	775	OMU	O4'-C1'-N1-C2
1	A1	329	OMG	C4'-C5'-O5'-P
27	B1	2557	OMC	C4'-C5'-O5'-P
1	A1	718	5MC	O4'-C4'-C5'-O5'
1	A1	499	4AC	O4'-C4'-C5'-O5'
27	B1	675	OMG	C3'-C4'-C5'-O5'
27	B1	2876	4AC	C3'-C4'-C5'-O5'
1	A1	826	5MC	C4'-C5'-O5'-P
27	B1	1914	OMC	C3'-C4'-C5'-O5'
27	B1	979	4AC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
27	B1	979	4AC	C2'-C1'-N1-C6
27	B1	1914	OMC	C2'-C1'-N1-C6
1	A1	1486	5MC	O4'-C1'-N1-C2
1	A1	763	OMG	C3'-C2'-O2'-CM2
27	B1	1639	4AC	C4'-C5'-O5'-P
27	B1	741	4AC	O4'-C4'-C5'-O5'
27	B1	2757	OMG	O4'-C4'-C5'-O5'
27	B1	1743	4AC	C2'-C1'-N1-C2
1	A1	763	OMG	O4'-C4'-C5'-O5'
1	A1	1467	4AC	C3'-C4'-C5'-O5'
27	B1	979	4AC	C3'-C4'-C5'-O5'
27	B1	1365	LHH	C3'-C4'-C5'-O5'
27	B1	1846	4AC	C3'-C4'-C5'-O5'
1	A1	8	OMU	C3'-C2'-O2'-CM2
1	A1	87	4AC	C2'-C1'-N1-C2
1	A1	87	4AC	C3'-C4'-C5'-O5'
27	B1	732	4AC	C3'-C4'-C5'-O5'
27	B1	920	OMG	C3'-C4'-C5'-O5'
1	A1	1486	5MC	C2'-C1'-N1-C2
27	B1	688	4AC	C2'-C1'-N1-C2
27	B1	1734	4AC	C2'-C1'-N1-C2
27	B1	1914	OMC	C2'-C1'-N1-C2
27	B1	1734	4AC	C4'-C5'-O5'-P
1	A1	459	OMG	O4'-C4'-C5'-O5'
1	A1	1362	5MC	C3'-C4'-C5'-O5'
27	B1	652	4AC	O4'-C4'-C5'-O5'
27	B1	798	4AC	C3'-C4'-C5'-O5'
27	B1	921	OMG	C3'-C4'-C5'-O5'
27	B1	1743	4AC	C3'-C4'-C5'-O5'
27	B1	2469	4AC	C3'-C4'-C5'-O5'
27	B1	1451	5MC	C2'-C1'-N1-C2
27	B1	1612	4AC	C2'-C1'-N1-C2
27	B1	1648	5MC	C2'-C1'-N1-C2
27	B1	3037	4AC	C2'-C1'-N1-C2
1	A1	605	5MC	O4'-C4'-C5'-O5'
1	A1	1486	5MC	O4'-C4'-C5'-O5'
1	A1	216	4AC	O4'-C4'-C5'-O5'
27	B1	2379	4AC	C3'-C4'-C5'-O5'
1	A1	425	OMU	C2'-C1'-N1-C2
1	A1	951	5MC	C2'-C1'-N1-C2
27	B1	1489	OMC	C4'-C5'-O5'-P

There are no ring outliers.

208 monomers are involved in 320 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A1	273	5MC	2	0
27	B1	1313	4AC	4	0
27	B1	2020	4AC	1	0
1	A1	195	4AC	1	0
27	B1	1451	5MC	1	0
27	B1	1706	4AC	3	0
27	B1	2809	4AC	2	0
27	B1	933	4AC	6	0
27	B1	80	4AC	2	0
27	B1	1751	4AC	1	0
27	B1	1149	5MC	4	0
1	A1	231	4AC	1	0
27	B1	3037	4AC	4	0
27	B1	1293	4AC	1	0
27	B1	877	5MC	1	0
27	B1	1649	4AC	1	0
27	B1	378	4AC	1	0
27	B1	813	4AC	3	0
27	B1	1762	4AC	2	0
27	B1	2082	5MC	1	0
27	B1	479	4AC	2	0
27	B1	1383	4AC	1	0
27	B1	2171	4AC	1	0
27	B1	1290	4AC	1	0
1	A1	1067	4AC	1	0
1	A1	827	4AC	1	0
27	B1	1150	4AC	5	0
27	B1	896	4AC	2	0
27	B1	392	4AC	1	0
27	B1	2133	4AC	2	0
1	A1	1314	4AC	2	0
27	B1	2469	4AC	1	0
27	B1	715	4AC	1	0
28	B2	117	4AC	1	0
1	A1	636	4AC	1	0
27	B1	1612	4AC	1	0
27	B1	1374	4AC	6	0
1	A1	1476	MA6	2	0
27	B1	599	4AC	2	0
27	B1	1783	OMC	2	0
1	A1	1194	OMC	1	0
27	B1	48	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A1	329	OMG	1	0
27	B1	1107	4AC	2	0
27	B1	786	4AC	1	0
1	A1	87	4AC	2	0
1	A1	1227	4AC	4	0
27	B1	1435	4AC	1	0
1	A1	624	4AC	4	0
1	A1	691	4AC	5	0
28	B2	90	4AC	2	0
27	B1	1601	OMG	3	0
27	B1	3020	4AC	1	0
1	A1	836	4AC	1	0
27	B1	1639	4AC	4	0
27	B1	866	4AC	1	0
1	A1	1181	4AC	1	0
27	B1	2888	4AC	2	0
27	B1	142	4AC	1	0
27	B1	921	OMG	2	0
27	B1	1981	OMU	1	0
27	B1	1551	4AC	2	0
27	B1	950	4AC	1	0
1	A1	719	4AC	1	0
27	B1	1404	4AC	2	0
1	A1	1364	LHH	1	0
1	A1	1016	4AC	2	0
1	A1	220	4AC	1	0
1	A1	1029	4AC	4	0
27	B1	2087	5MC	1	0
1	A1	1012	5MC	1	0
27	B1	1977	5MC	1	0
1	A1	367	4AC	1	0
27	B1	1100	4AC	1	0
27	B1	2844	4AC	1	0
27	B1	1439	4AC	2	0
27	B1	2492	4AC	3	0
27	B1	337	4AC	1	0
1	A1	1254	4AC	2	0
27	B1	1734	4AC	1	0
27	B1	271	4AC	1	0
27	B1	2454	4AC	1	0
1	A1	405	4AC	1	0
27	B1	2526	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	262	A2M	2	0
27	B1	2850	4AC	2	0
27	B1	1911	4AC	1	0
27	B1	1769	4AC	3	0
27	B1	116	4AC	1	0
27	B1	1064	4AC	4	0
27	B1	2379	4AC	1	0
1	A1	274	4AC	1	0
27	B1	1501	4AC	1	0
27	B1	1608	4AC	6	0
27	B1	1822	4AC	1	0
27	B1	360	4AC	1	0
1	A1	361	A2M	1	0
27	B1	276	4AC	1	0
27	B1	2876	4AC	1	0
27	B1	1386	4AC	1	0
1	A1	425	OMU	1	0
1	A1	578	4AC	1	0
1	A1	427	4AC	4	0
1	A1	706	4AC	2	0
27	B1	3011	4AC	1	0
27	B1	721	4AC	1	0
1	A1	534	4AC	1	0
27	B1	759	4AC	1	0
27	B1	454	OMU	1	0
1	A1	1368	OMU	1	0
1	A1	540	4AC	1	0
27	B1	741	4AC	1	0
1	A1	739	4AC	1	0
1	A1	1135	4AC	1	0
27	B1	1546	4AC	1	0
27	B1	2659	OMG	1	0
27	B1	23	4AC	1	0
27	B1	130	4AC	1	0
27	B1	2328	4AC	1	0
27	B1	2617	5MC	1	0
27	B1	1743	4AC	1	0
1	A1	291	4AC	1	0
27	B1	2749	4AC	3	0
27	B1	1967	4AC	1	0
27	B1	485	4AC	4	0
27	B1	243	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	200	4AC	1	0
27	B1	2213	4AC	2	0
27	B1	2792	4AC	2	0
1	A1	307	4AC	2	0
1	A1	499	4AC	1	0
27	B1	1505	4AC	1	0
27	B1	1286	4AC	4	0
1	A1	645	OMG	2	0
27	B1	953	4AC	1	0
27	B1	1178	4AC	1	0
1	A1	467	4AC	1	0
27	B1	2429	4AC	1	0
27	B1	2432	4AC	2	0
27	B1	1868	5MC	1	0
1	A1	41	4AC	1	0
27	B1	580	4AC	1	0
27	B1	1128	4AC	1	0
27	B1	2428	OMC	3	0
1	A1	668	OMG	1	0
27	B1	920	OMG	2	0
27	B1	2067	5MC	1	0
27	B1	1703	4AC	1	0
27	B1	1264	4AC	1	0
1	A1	839	4AC	1	0
27	B1	1067	4AC	1	0
27	B1	2113	4AC	2	0
1	A1	141	4AC	1	0
27	B1	98	4AC	1	0
27	B1	798	4AC	1	0
27	B1	1052	4AC	2	0
27	B1	1360	4AC	6	0
1	A1	1467	4AC	1	0
27	B1	162	4AC	1	0
27	B1	527	LHH	1	0
1	A1	546	4AC	1	0
1	A1	1221	4AC	1	0
27	B1	732	4AC	1	0
27	B1	19	4AC	1	0
1	A1	1475	MA6	2	0
27	B1	979	4AC	5	0
27	B1	1818	4AC	1	0
1	A1	216	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A1	1092	4AC	1	0
1	A1	1366	A1I59	1	0
1	A1	1288	4AC	3	0
27	B1	227	4AC	1	0
27	B1	47	5MC	1	0
27	B1	688	4AC	1	0
27	B1	3023	4AC	1	0
27	B1	652	4AC	1	0
27	B1	419	4AC	2	0
27	B1	1885	4AC	3	0
27	B1	1757	4AC	1	0
27	B1	2008	4AC	1	0
1	A1	687	5MC	1	0
27	B1	1488	OMU	1	0
27	B1	3006	4AC	2	0
27	B1	434	4AC	1	0
27	B1	1061	4AC	1	0
1	A1	5	4AC	1	0
27	B1	1478	4AC	4	0
27	B1	336	5MC	3	0
27	B1	1442	4AC	1	0
27	B1	2602	4AC	1	0
1	A1	382	4AC	2	0
1	A1	810	4AC	1	0
1	A1	816	4AC	1	0
27	B1	807	4AC	1	0
27	B1	1322	4AC	2	0
27	B1	2607	OMC	2	0
27	B1	609	4AC	1	0
1	A1	614	4AC	2	0
27	B1	1846	4AC	1	0
27	B1	1621	4AC	6	0
1	A1	819	A2M	1	0
28	B2	120	4AC	1	0
1	A1	856	4AC	1	0
27	B1	1664	4AC	2	0
27	B1	2821	4AC	2	0
27	B1	214	OMG	1	0
1	A1	444	4AC	3	0
1	A1	761	4AC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 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](#)

There are no chain breaks in this entry.

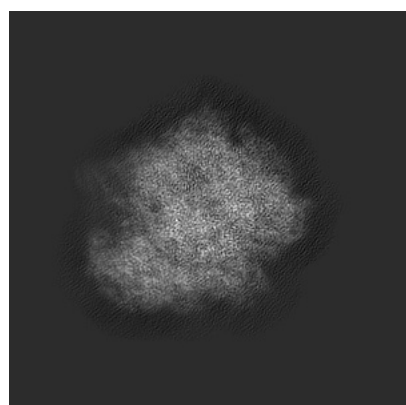
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53099. These allow visual inspection of the internal detail of the map and identification of artifacts.

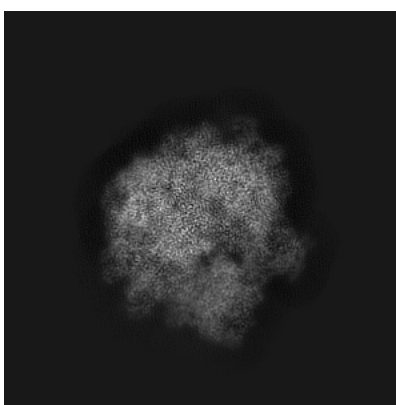
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

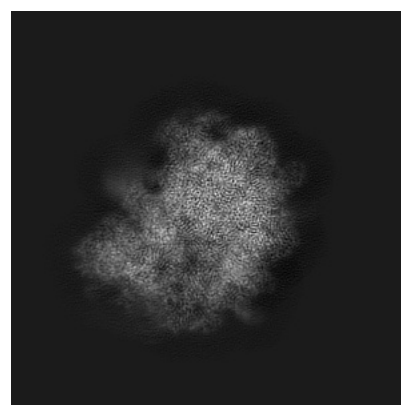
6.1.1 Primary map



X



Y

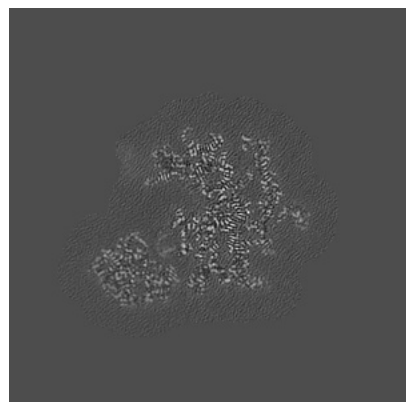


Z

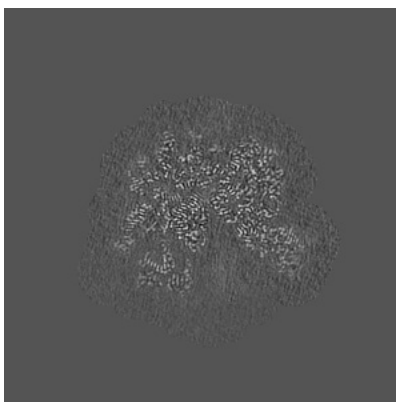
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

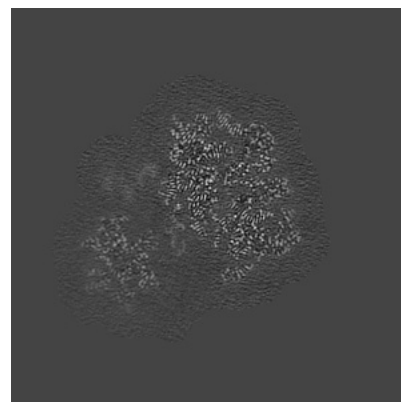
6.2.1 Primary map



X Index: 224



Y Index: 224

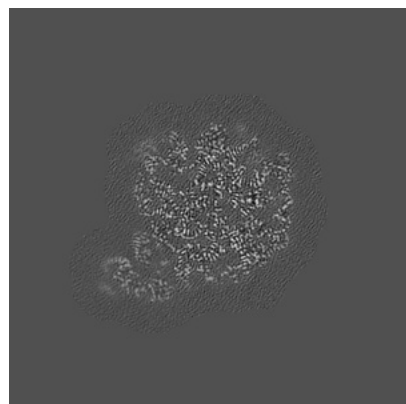


Z Index: 224

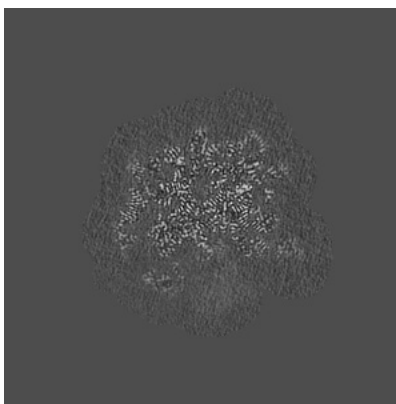
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

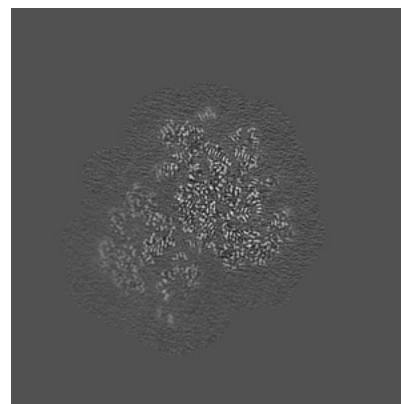
6.3.1 Primary map



X Index: 257



Y Index: 243

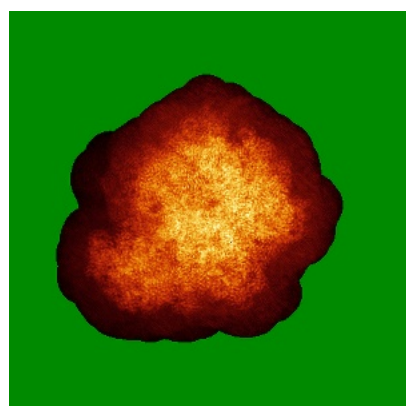


Z Index: 202

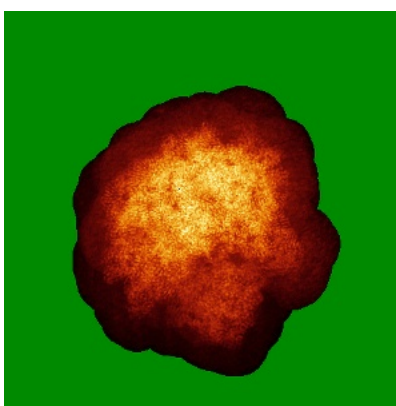
The images above show the largest variance slices of the map in three orthogonal directions.

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

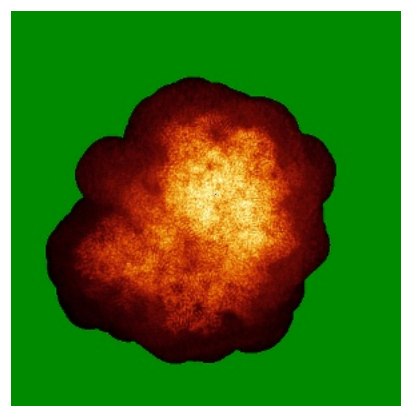
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

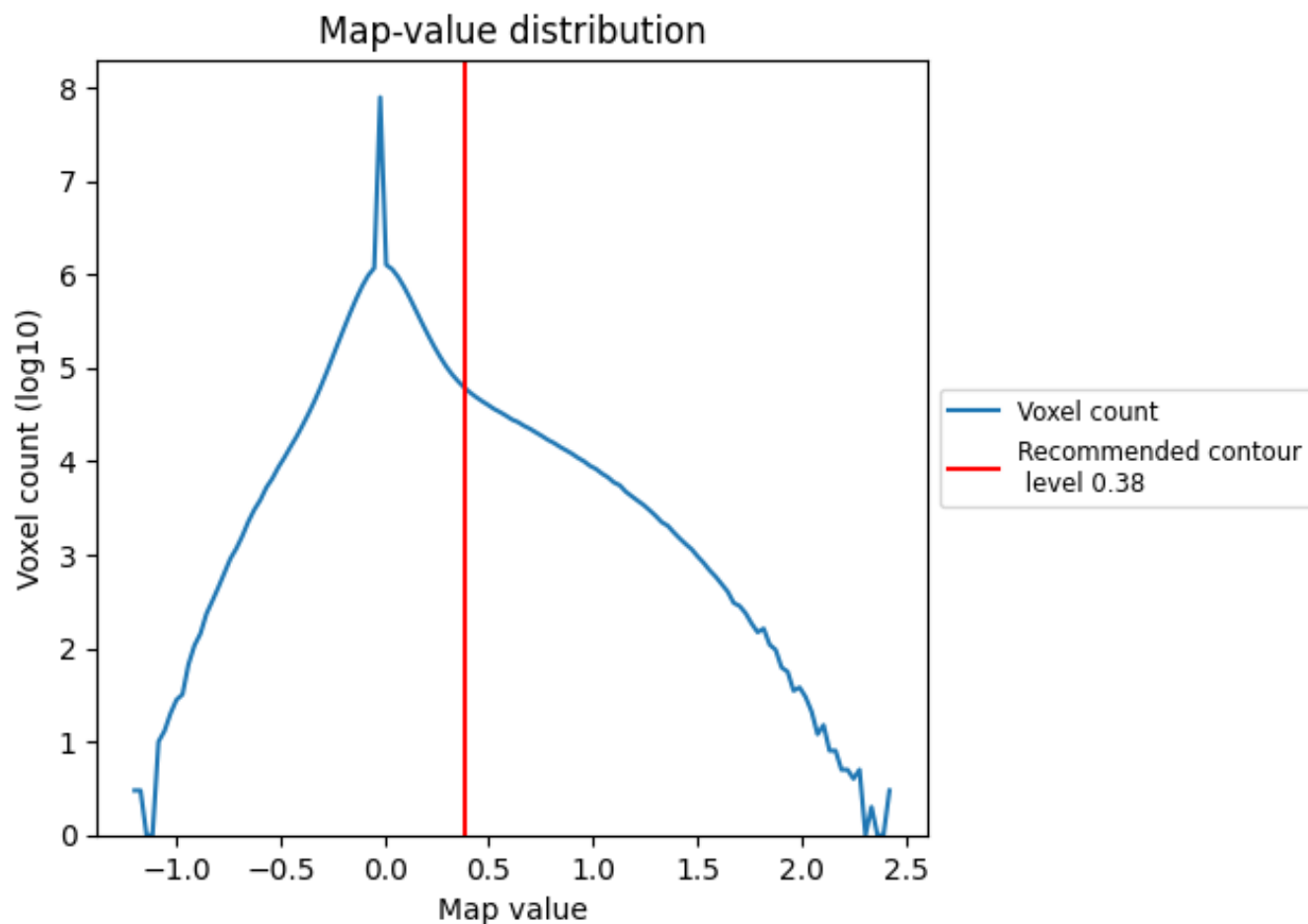
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

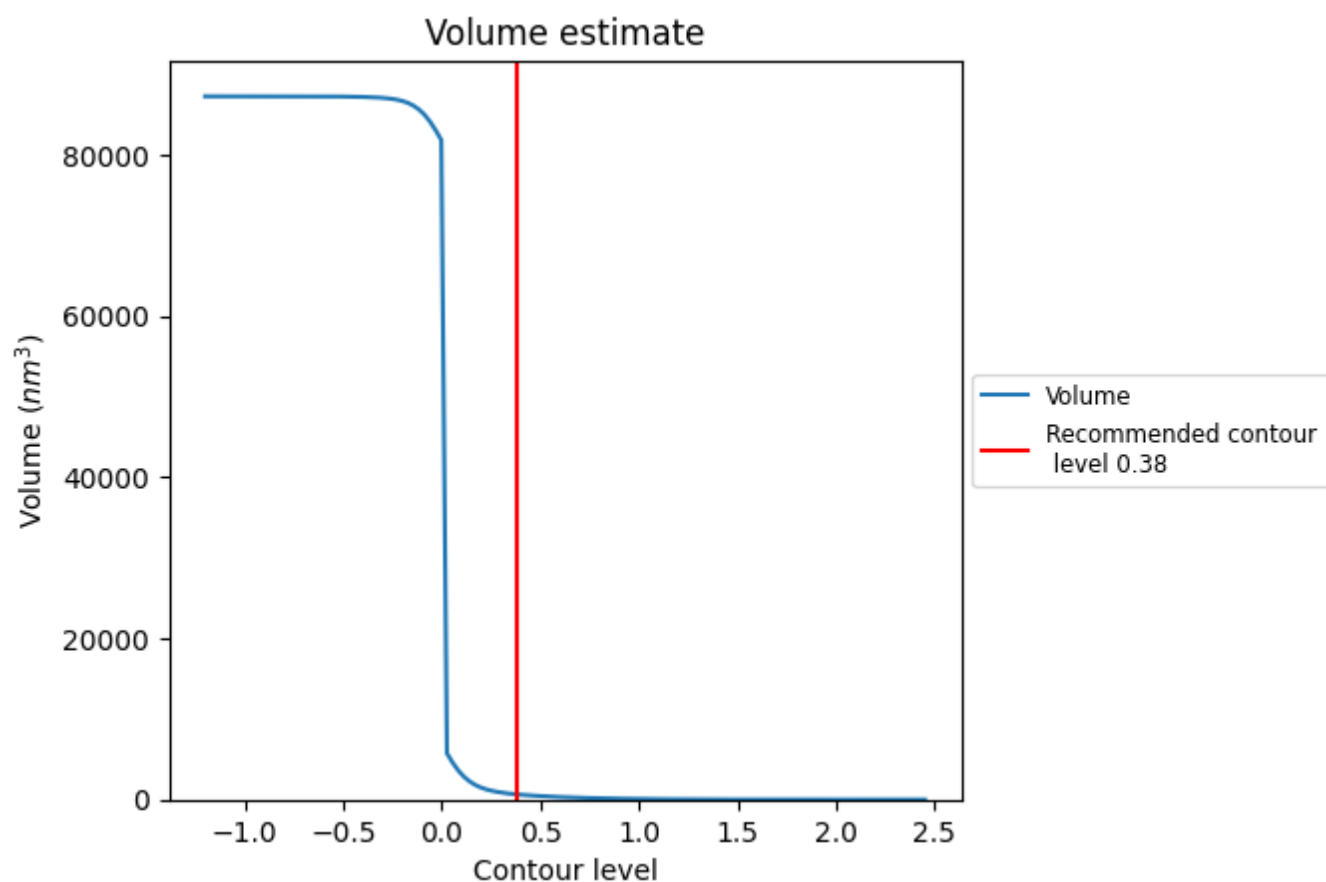
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

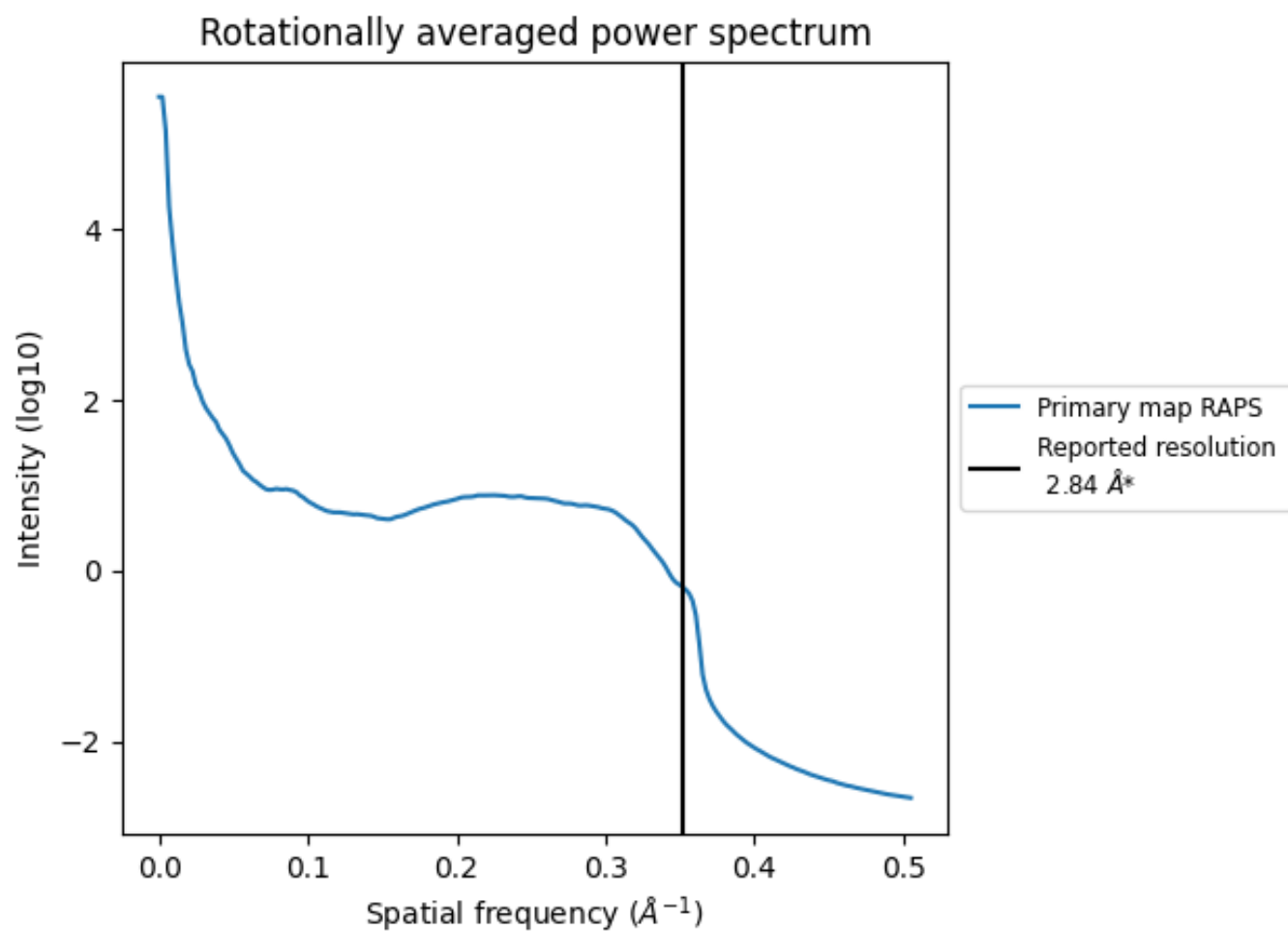
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 646 nm^3 ; this corresponds to an approximate mass of 583 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 0.352 Å⁻¹

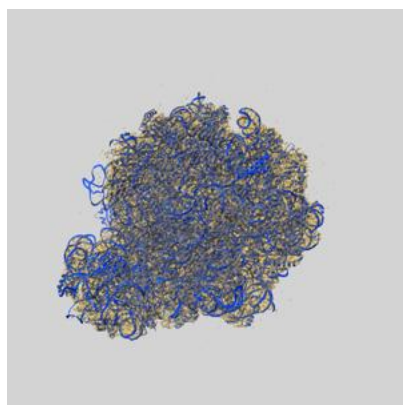
8 Fourier-Shell correlation ⓘ

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

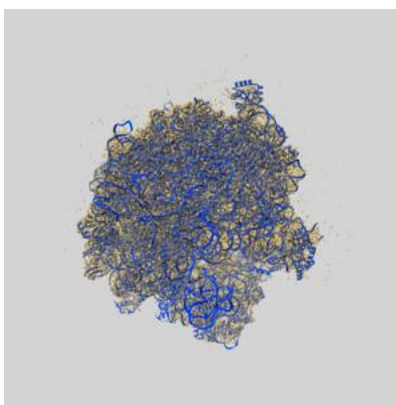
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53099 and PDB model 9QF5. Per-residue inclusion information can be found in section [3](#) on page [19](#).

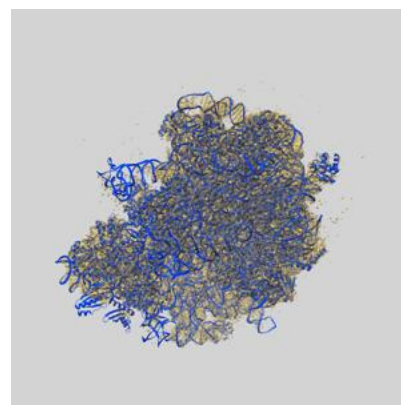
9.1 Map-model overlay [i](#)



X



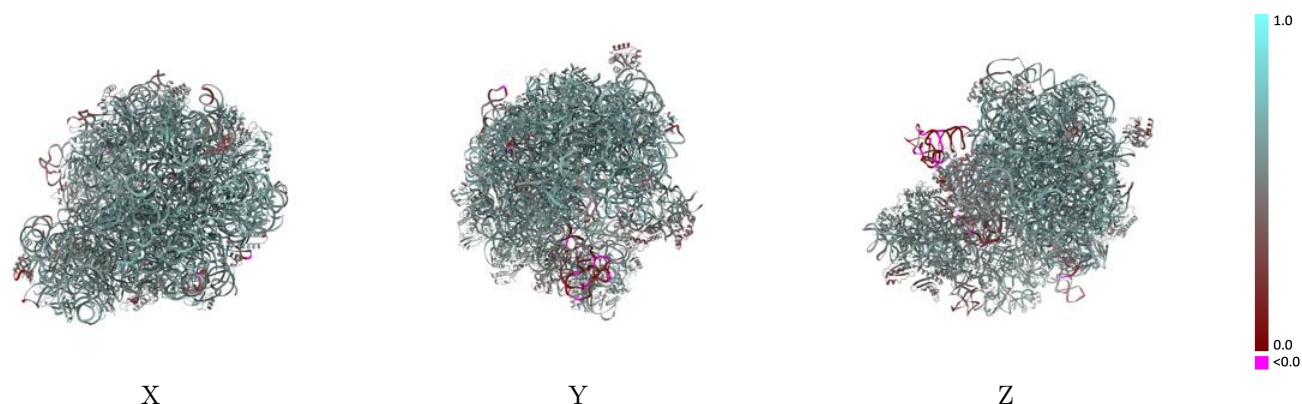
Y



Z

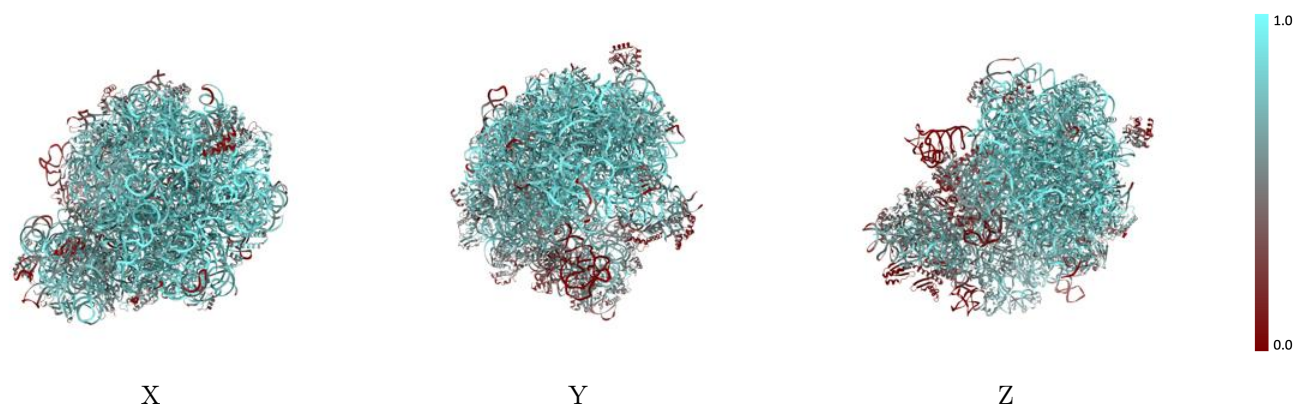
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



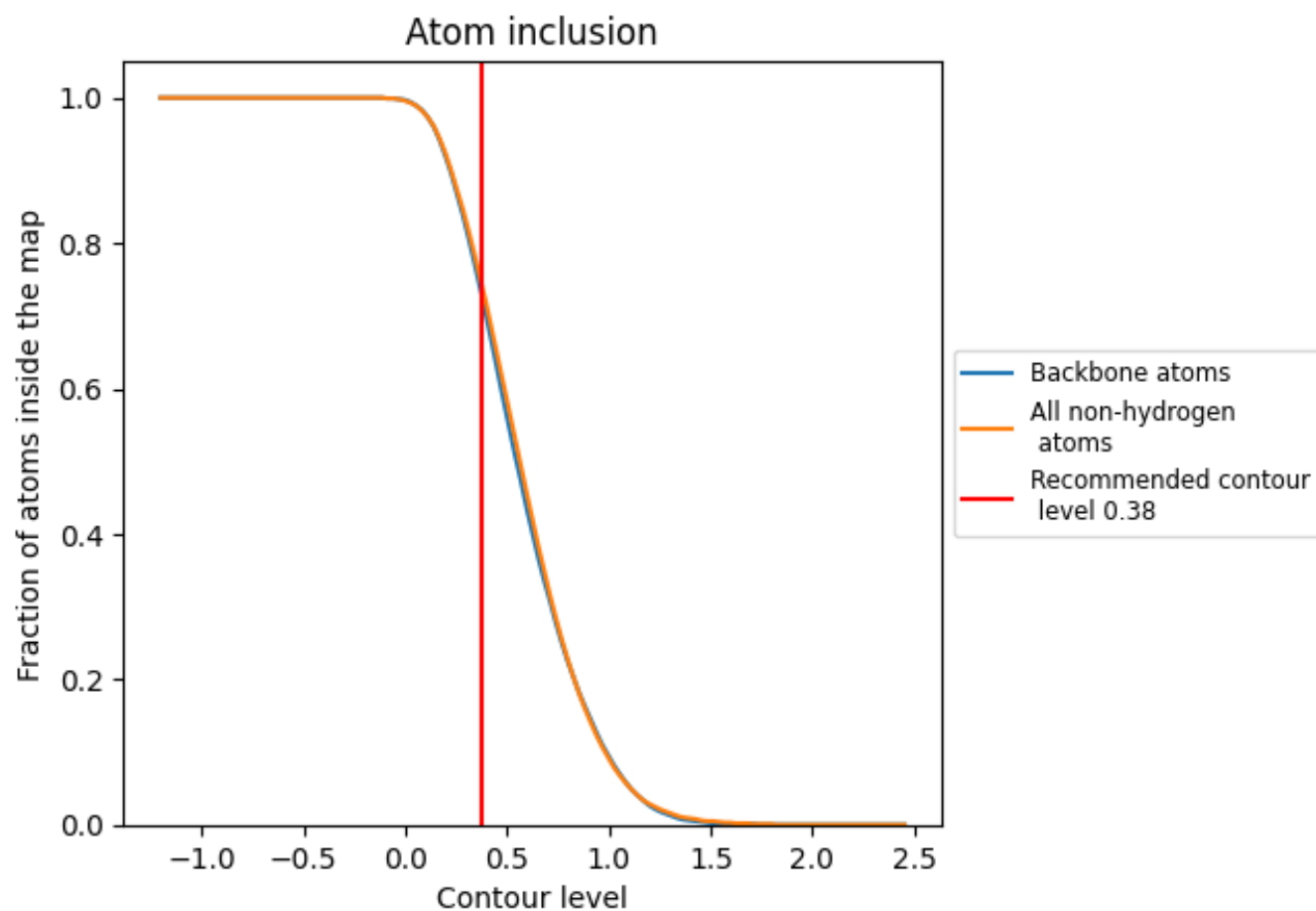
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.38).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 74% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.5690
A1	 0.7140	 0.5590
Aa	 0.4590	 0.5340
Ab	 0.2300	 0.4740
Ac	 0.5110	 0.5470
Ad	 0.6540	 0.5750
Ae	 0.6820	 0.5790
Af	 0.6220	 0.5660
Ag	 0.3420	 0.5060
Ah	 0.4780	 0.5210
Ai	 0.6960	 0.5910
Aj	 0.6300	 0.5690
Ak	 0.5180	 0.5470
Al	 0.2630	 0.4380
Am	 0.4870	 0.5200
An	 0.5890	 0.5720
Ao	 0.5540	 0.5490
Ap	 0.5040	 0.5390
Aq	 0.6180	 0.5590
Ar	 0.6780	 0.5880
As	 0.0310	 0.4100
At	 0.5460	 0.5440
Au	 0.5770	 0.5630
Av	 0.5630	 0.5490
Aw	 0.5390	 0.5530
Ax	 0.3070	 0.4810
Ay	 0.5480	 0.5570
B1	 0.8510	 0.5820
B2	 0.7310	 0.5440
BA	 0.8650	 0.6210
BB	 0.7960	 0.6040
BC	 0.8090	 0.6050
BD	 0.2950	 0.4130
BE	 0.6810	 0.5670
BF	 0.6210	 0.5480



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Chain	Atom inclusion	Q-score
BG	 0.2570	 0.4080
BH	 0.7990	 0.5980
BI	 0.8190	 0.6070
BJ	 0.8200	 0.6160
BK	 0.5700	 0.5410
BL	 0.6200	 0.5530
BM	 0.6070	 0.5220
BN	 0.8970	 0.6300
BO	 0.5130	 0.4990
BP	 0.7820	 0.5920
BQ	 0.7830	 0.5860
BR	 0.8290	 0.6140
BS	 0.8590	 0.6150
BT	 0.7750	 0.5850
BU	 0.7930	 0.5950
BV	 0.7900	 0.6090
BW	 0.6760	 0.5350
BX	 0.8020	 0.6010
BY	 0.6140	 0.5520
BZ	 0.7410	 0.5810
Ba	 0.8350	 0.6050
Bb	 0.8260	 0.5940
Bc	 0.8150	 0.6050
Bd	 0.9170	 0.6290
Be	 0.8200	 0.6020
Bf	 0.8740	 0.6170
Bg	 0.6600	 0.5690
Bh	 0.6980	 0.5900
Bi	 0.7930	 0.5970
Bj	 0.6060	 0.5380
Bk	 0.7930	 0.5950