



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 04:39 am BST

PDB ID : 6SKG / pdb_00006skg
EMDB ID : EMD-10224
Title : Cryo-EM Structure of T. kodakarensis 70S ribosome in TkNat10 deleted strain
Authors : Matzov, D.; Sas-Chen, A.; Thomas, J.M.; Santangelo, T.; Meier, J.L.; Schwartz, S.; Shalev-Benami, M.
Deposited on : 2019-08-15
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

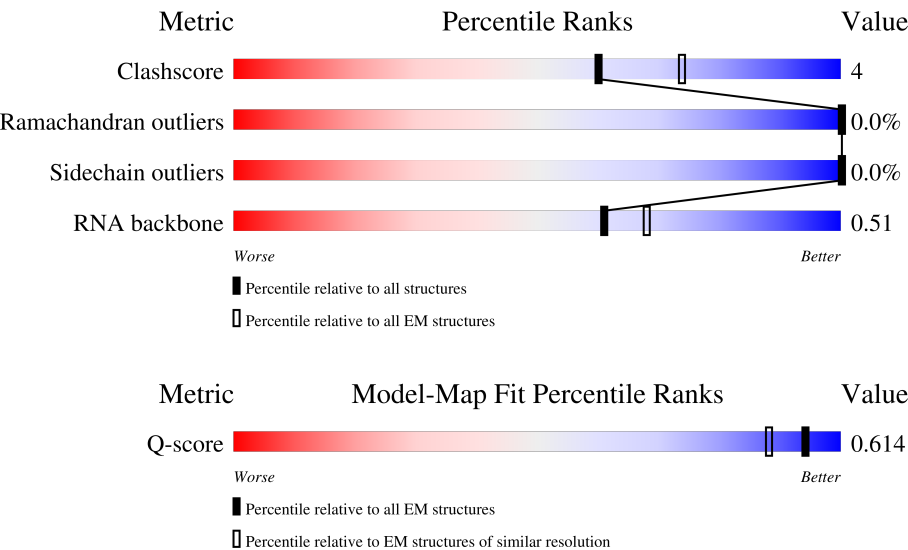
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9050 (2.15 - 3.15)

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	Aa	1498	8% 68% 22% 7% ••
2	Ab	201	20% 90% 7% •
3	Ac	209	71% 86% 8% 7%

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Mol	Chain	Length	Quality of chain
4	Ad	200	
5	Ae	180	
6	Af	243	
7	Ag	235	
8	Ah	125	
9	Ai	215	
10	Aj	130	
11	Ak	130	
12	Al	135	
13	Am	102	
14	An	140	
15	Ao	147	
16	Ap	149	
17	Aq	151	
18	Ar	56	
19	As	114	
20	At	67	
20	Bm	67	
21	Au	133	
22	Av	150	
23	Aw	98	
23	Bn	98	
24	Ax	65	
25	Ay	70	
26	Az	62	

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Mol	Chain	Length	Quality of chain
27	BA	3037	
28	BB	126	
29	BC	239	
30	BD	346	
31	BE	255	
32	BF	183	
33	BG	184	
34	BH	123	
34	BI	123	
35	BJ	182	
36	BK	142	
37	BL	141	
38	BM	83	
38	BN	83	
39	BO	148	
40	BP	194	
41	BQ	201	
42	BR	121	
43	BS	150	
44	BT	77	
45	BU	98	
46	BV	156	
47	BW	86	
48	BX	121	
49	BY	67	

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Mol	Chain	Length	Quality of chain
50	BZ	66	
51	Ba	155	
52	Bb	102	
53	Bc	90	
54	Bd	125	
55	Be	90	
56	Bf	101	
57	Bg	86	
58	Bh	63	
59	Bi	51	
60	Bj	51	
61	Bk	37	
62	Bl	94	
63	Bo	47	
64	Bp	236	
65	Bq	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	5MC	Aa	1007	-	-	X	-

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 167400 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	1463	Total	C	N	O	P	0	0
			31531	14063	5836	10169	1463		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	196	Total	C	N	O	S	0	0
			1580	1021	272	284	3		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ac	195	Total	C	N	O	S	0	0
			1536	979	283	271	3		

- Molecule 4 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ad	190	Total	C	N	O	S	0	0
			1550	997	277	273	3		

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ae	174	Total	C	N	O	S	0	0
			1454	912	287	253	2		

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Af	242	Total	C	N	O	S	0	0
			1952	1261	349	337	5		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ag	223	Total	C	N	O	S	0	0
			1753	1107	327	312	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ah	123	Total	C	N	O	S	0	0
			952	599	179	172	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ai	214	Total	C	N	O	S	0	0
			1715	1087	317	303	8		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Aj	129	Total	C	N	O	S	0	0
			1020	662	176	180	2		

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ak	125	Total	C	N	O		0	0
			982	615	198	169			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Al	133	Total	C	N	O	S	0	0
			1054	656	205	188	5		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Am	100	Total	C	N	O	S	0	0
			803	498	154	148	3		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	An	127	Total	C	N	O	S	0	0
			953	587	190	173	3		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ao	143	Total	C	N	O	S	0	0
			1122	712	216	192	2		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ap	135	Total	C	N	O	S	0	0
			1090	691	214	181	4		

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Aq	149	Total	C	N	O	S	0	0
			1217	776	233	206	2		

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ar	54	Total	C	N	O	S	0	0
			447	284	92	65	6		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	As	108	Total	C	N	O	S	0	0
			879	560	164	152	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	At	64	Total	C	N	O	S	0	0
			538	338	103	95	2		
20	Bm	63	Total	C	N	O	S	0	0
			534	336	102	94	2		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Au	116	Total	C	N	O	S	0	0
			952	608	175	163	6		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Av	149	Total	C	N	O	S	0	0
			1216	788	215	213			

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Aw	95	Total	C	N	O	S	0	0
			777	497	131	146	3		
23	Bn	92	Total	C	N	O	S	0	0
			752	481	126	142	3		

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ax	61	Total	C	N	O	S	0	0
			461	294	83	79	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ax	64	GLU	LEU	conflict	UNP Q5JE50

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ay	64	Total	C	N	O	S	0	0
			499	307	99	93			

- Molecule 26 is a protein called Predicted zinc-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Az	55	Total	C	N	O	S	0	0
			426	269	74	75	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
27	BA	2934	Total	C	N	O	P	S	0	0
			63209	28168	11754	20351	2934	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BB	125	Total	C	N	O	P	0	0
			2678	1191	492	870	125		

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BC	237	Total	C	N	O	S	0	0
			1820	1150	356	311	3		

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BD	344	Total	C	N	O	S	0	0
			2746	1765	505	469	7		

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BE	255	Total	C	N	O	S	0	0
			2026	1286	389	347	4		

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BF	166	Total	C	N	O	S	0	0
			1338	839	258	234	7		

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BG	183	Total	C	N	O	S	0	0
			1463	942	253	266	2		

- Molecule 34 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BH	121	Total	C	N	O	S	0	0
			928	591	154	180	3		
34	BI	121	Total	C	N	O	S	0	0
			928	591	154	180	3		

- Molecule 35 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BJ	171	Total	C	N	O	S	0	0
			1399	891	261	240	7		

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	142	Total	C	N	O	S	0	0
			1146	731	213	198	4		

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	140	Total	C	N	O	S	0	0
			1055	658	214	180	3		

- Molecule 38 is a protein called 50S ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	81	Total	C	N	O	S	0	0
			610	382	119	108	1		
38	BN	81	Total	C	N	O	S	0	0
			610	382	119	108	1		

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BO	148	Total	C	N	O	S	0	0
			1166	743	222	198	3		

- Molecule 40 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BP	193	Total	C	N	O	S	0	0
			1582	1010	316	250	6		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BQ	164	Total	C	N	O	S	0	0
			1314	841	243	228	2		

- Molecule 42 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BR	120	Total	C	N	O	S	0	0
			959	601	187	169	2		

- Molecule 43 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BS	146	Total	C	N	O	S	0	0
			1200	753	246	194	7		

- Molecule 44 is a protein called 50S ribosomal protein L18Ae.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	BT	74	Total	C	N	O	0	0
			624	399	113	112		

- Molecule 45 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BU	96	Total	C	N	O	S	0	0
			784	502	158	123	1		

- Molecule 46 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	154	Total	C	N	O	S	0	0
			1234	777	242	211	4		

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	85	Total	C	N	O	S	0	0
			683	438	119	123	3		

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BX	120	Total	C	N	O	S	0	0
			991	628	188	170	5		

- Molecule 49 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	62	Total	C	N	O	S	0	0
			524	334	99	85	6		

- Molecule 50 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BZ	60	Total	C	N	O	S	0	0
			506	314	98	90	4		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ba	154	Total	C	N	O	S	0	0
			1242	788	235	214	5		

- Molecule 52 is a protein called 50S ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bb	96	Total	C	N	O	S	0	0
			730	473	123	133	1		

- Molecule 53 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Bc	89	Total	C	N	O	0	0
			721	463	140	118		

- Molecule 54 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bd	124	Total	C	N	O	S	0	0
			1022	650	208	162	2		

- Molecule 55 is a protein called 50S ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Be	89	Total	C	N	O	S	0	0
			728	454	155	110	9		

- Molecule 56 is a protein called Ribosomal protein eL35A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bf	86	Total	C	N	O	S	0	0
			669	424	133	112			

- Molecule 57 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Bg	84	Total	C	N	O	S	0	0
			630	392	132	101	5		

- Molecule 58 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bh	62	Total	C	N	O	S	0	0
			512	314	118	75	5		

- Molecule 59 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bi	50	Total	C	N	O	S	0	0
			432	276	97	59			

- Molecule 60 is a protein called 50S ribosomal protein L40e.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bj	47	Total	C	N	O	S	0	0
			373	233	79	56	5		

- Molecule 61 is a protein called LSU ribosomal protein L41E.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bk	36	Total	C	N	O	S	0	0
			345	218	86	39	2		

- Molecule 62 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bl	93	Total	C	N	O	S	0	0
			778	494	160	119	5		

- Molecule 63 is a protein called Nucleic acid-binding protein, containing C2H2 zinc-finger.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bo	43	Total	C	N	O	S	0	0
			349	222	69	55	3		

- Molecule 64 is a protein called Predicted exosome subunit, UPF0023 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bp	232	Total	C	N	O	S	0	0
			1861	1193	323	341	4		

- Molecule 65 is a protein called Unknown ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	Bq	34	Total	C	N	O	0	0
			170	102	34	34		

- Molecule 66 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
66	Ag	1	Total	Zn	0
			1	1	
66	Ar	1	Total	Zn	0
			1	1	
66	As	1	Total	Zn	0
			1	1	
66	Ax	1	Total	Zn	0
			1	1	
66	Az	2	Total	Zn	0
			2	2	
66	BY	1	Total	Zn	0
			1	1	
66	Be	2	Total	Zn	0
			2	2	
66	Bg	1	Total	Zn	0
			1	1	
66	Bh	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
66	Bj	1	Total 1	Zn 1	0
66	Bl	1	Total 1	Zn 1	0
66	Bo	1	Total 1	Zn 1	0

- Molecule 67 is water.

Mol	Chain	Residues	Atoms		AltConf
67	Aa	266	Total 266	O 266	0
67	Ad	1	Total 1	O 1	0
67	Af	4	Total 4	O 4	0
67	Ag	1	Total 1	O 1	0
67	Ai	1	Total 1	O 1	0
67	Aj	2	Total 2	O 2	0
67	Ak	6	Total 6	O 6	0
67	Al	2	Total 2	O 2	0
67	Am	2	Total 2	O 2	0
67	An	2	Total 2	O 2	0
67	Ao	1	Total 1	O 1	0
67	Ap	3	Total 3	O 3	0
67	Aq	5	Total 5	O 5	0
67	As	2	Total 2	O 2	0
67	Au	1	Total 1	O 1	0
67	Av	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
67	Az	1	Total 1	O 1	0
67	BA	2715	Total 2715	O 2715	0
67	BB	23	Total 23	O 23	0
67	BC	51	Total 51	O 51	0
67	BD	59	Total 59	O 59	0
67	BE	41	Total 41	O 41	0
67	BF	2	Total 2	O 2	0
67	BG	1	Total 1	O 1	0
67	BH	1	Total 1	O 1	0
67	BJ	13	Total 13	O 13	0
67	BK	18	Total 18	O 18	0
67	BL	15	Total 15	O 15	0
67	BM	3	Total 3	O 3	0
67	BN	3	Total 3	O 3	0
67	BO	30	Total 30	O 30	0
67	BP	36	Total 36	O 36	0
67	BQ	6	Total 6	O 6	0
67	BR	14	Total 14	O 14	0
67	BS	17	Total 17	O 17	0
67	BT	2	Total 2	O 2	0
67	BU	13	Total 13	O 13	0

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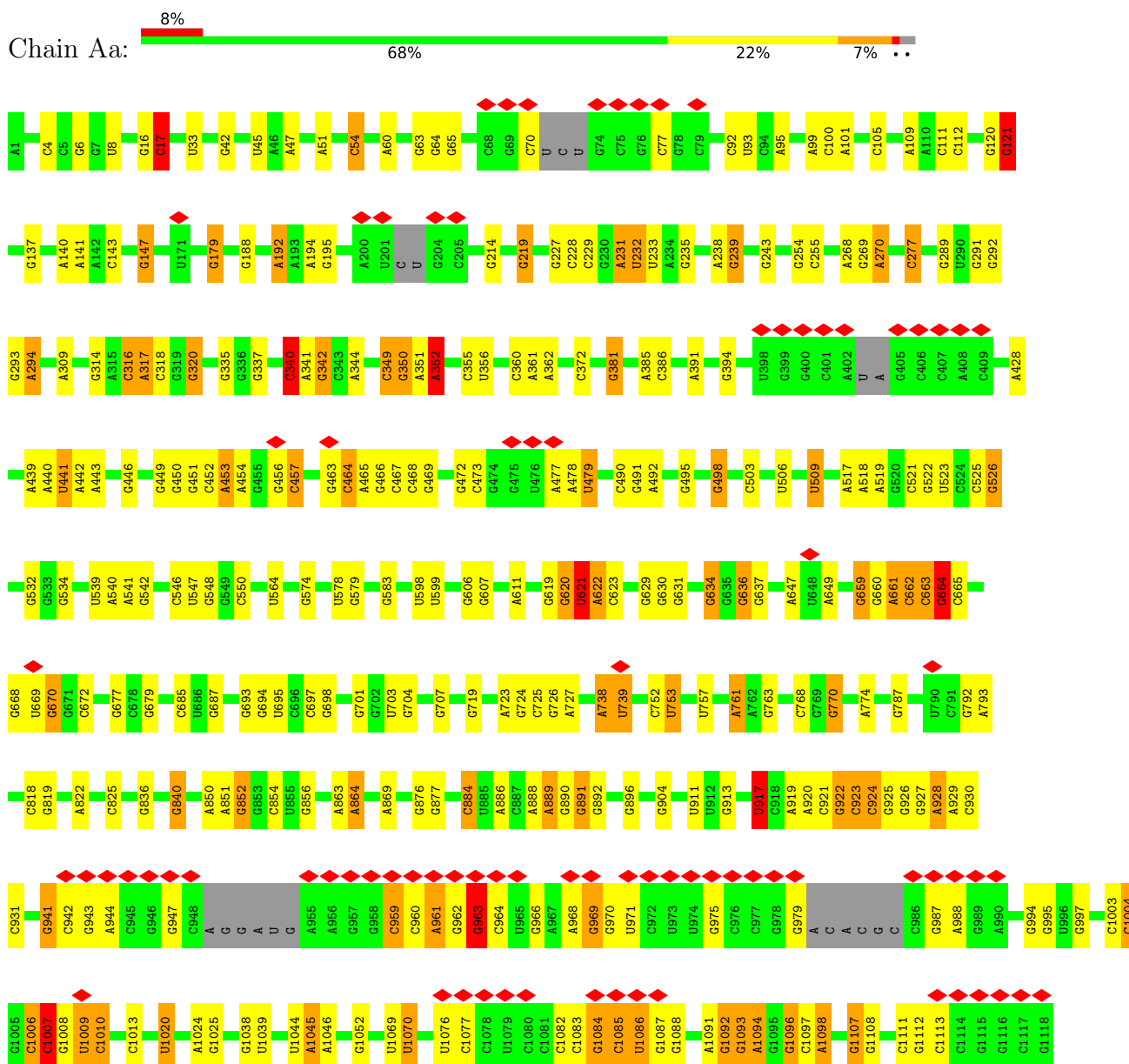
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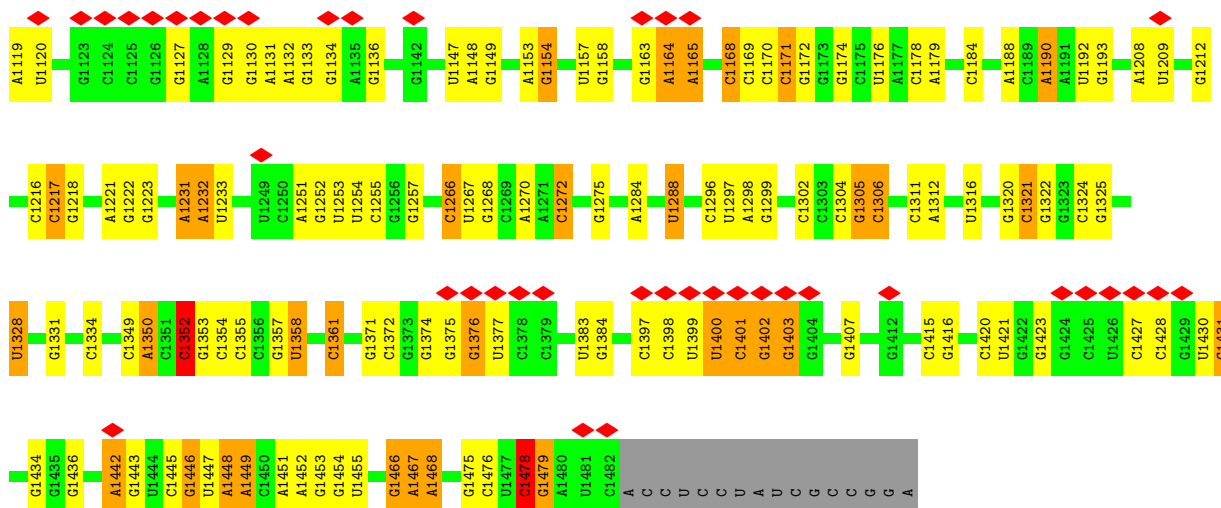
Mol	Chain	Residues	Atoms		AltConf
67	BV	22	Total 22	O 22	0
67	BW	3	Total 3	O 3	0
67	BX	10	Total 10	O 10	0
67	BY	12	Total 12	O 12	0
67	BZ	7	Total 7	O 7	0
67	Ba	14	Total 14	O 14	0
67	Bb	8	Total 8	O 8	0
67	Bc	10	Total 10	O 10	0
67	Bd	23	Total 23	O 23	0
67	Be	8	Total 8	O 8	0
67	Bf	7	Total 7	O 7	0
67	Bg	15	Total 15	O 15	0
67	Bh	23	Total 23	O 23	0
67	Bi	10	Total 10	O 10	0
67	Bj	3	Total 3	O 3	0
67	Bk	3	Total 3	O 3	0
67	Bl	8	Total 8	O 8	0
67	Bm	1	Total 1	O 1	0
67	Bn	1	Total 1	O 1	0
67	Bo	4	Total 4	O 4	0

3 Residue-property plots [i](#)

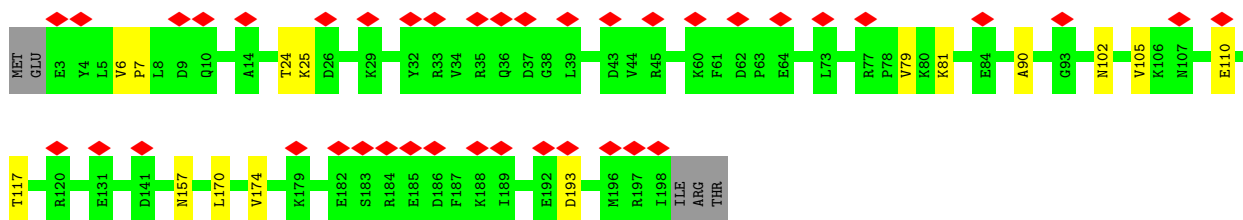
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

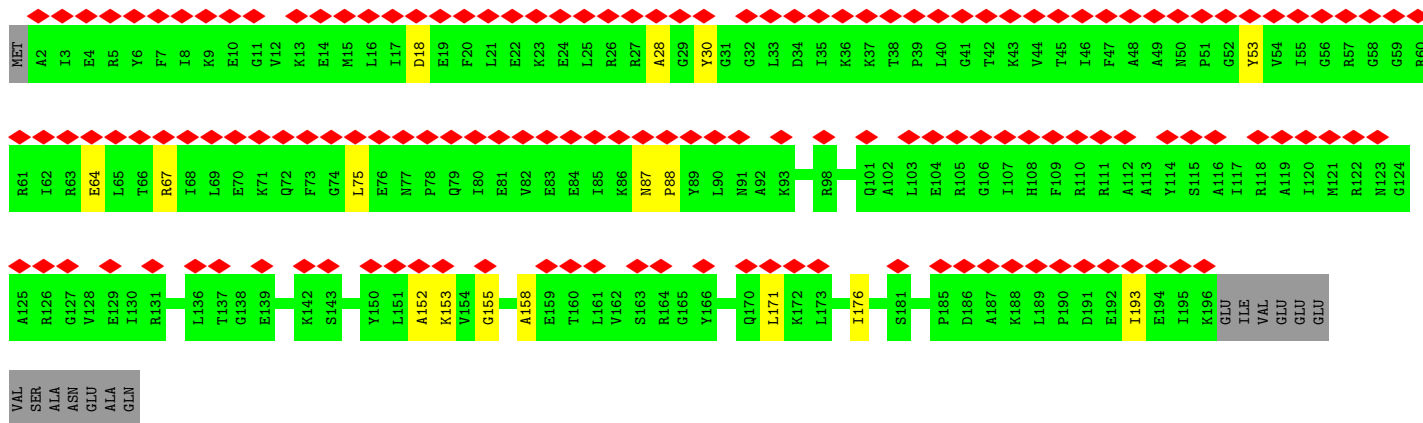
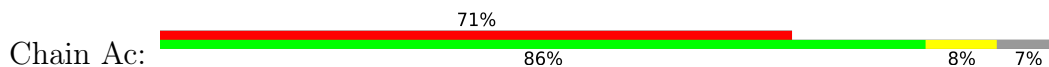




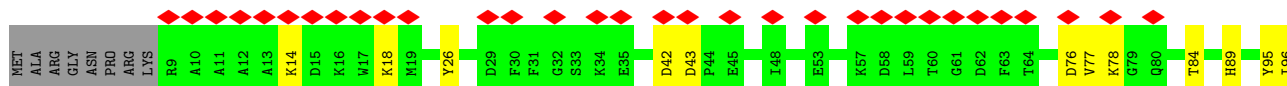
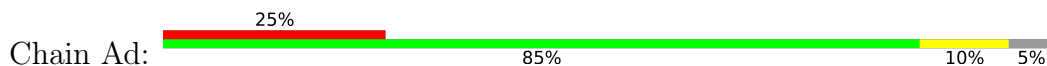
• Molecule 2: 30S ribosomal protein S2

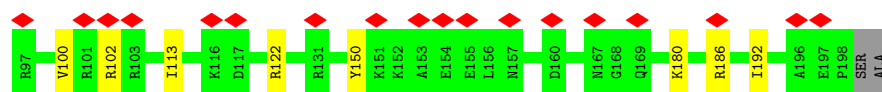


• Molecule 3: 30S ribosomal protein S3

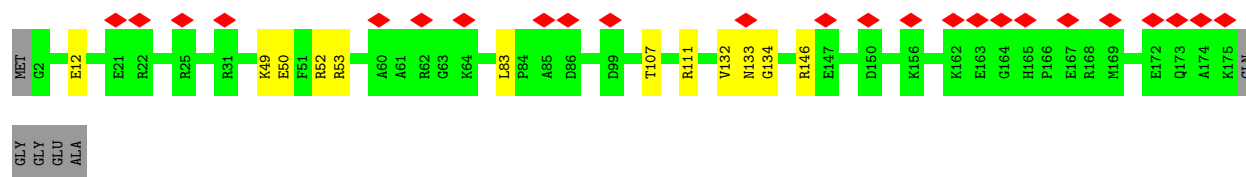


• Molecule 4: 30S ribosomal protein S3Ae

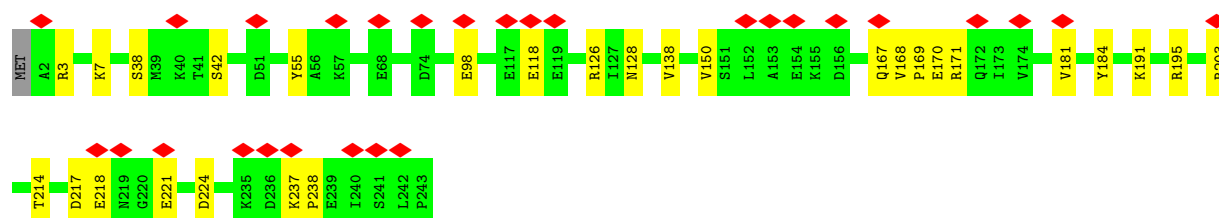
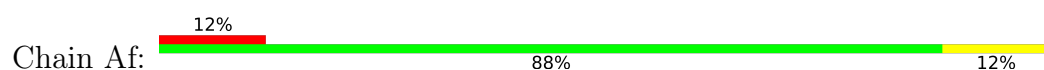




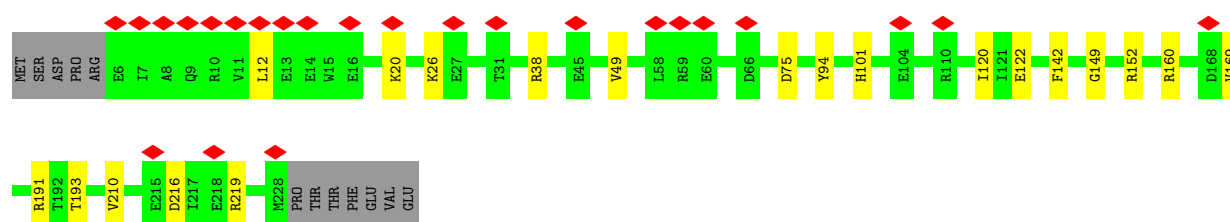
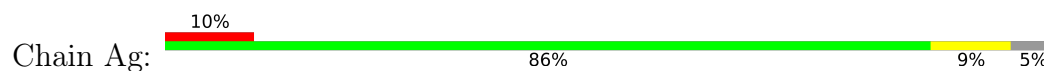
- Molecule 5: 30S ribosomal protein S4



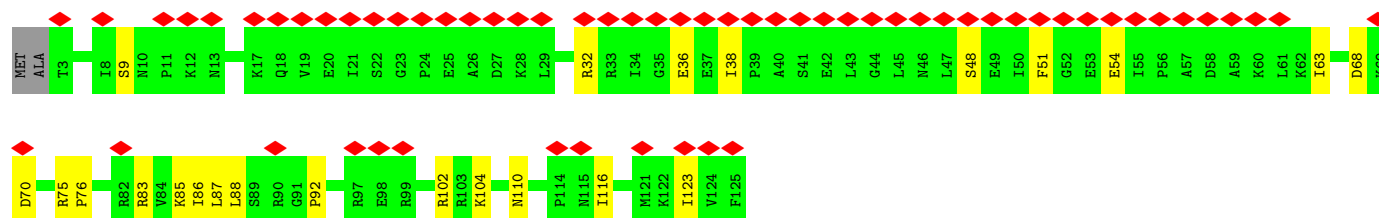
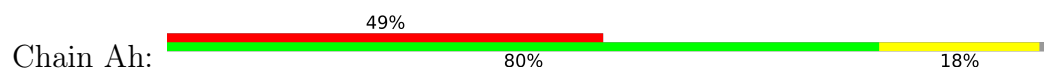
- Molecule 6: 30S ribosomal protein S4e



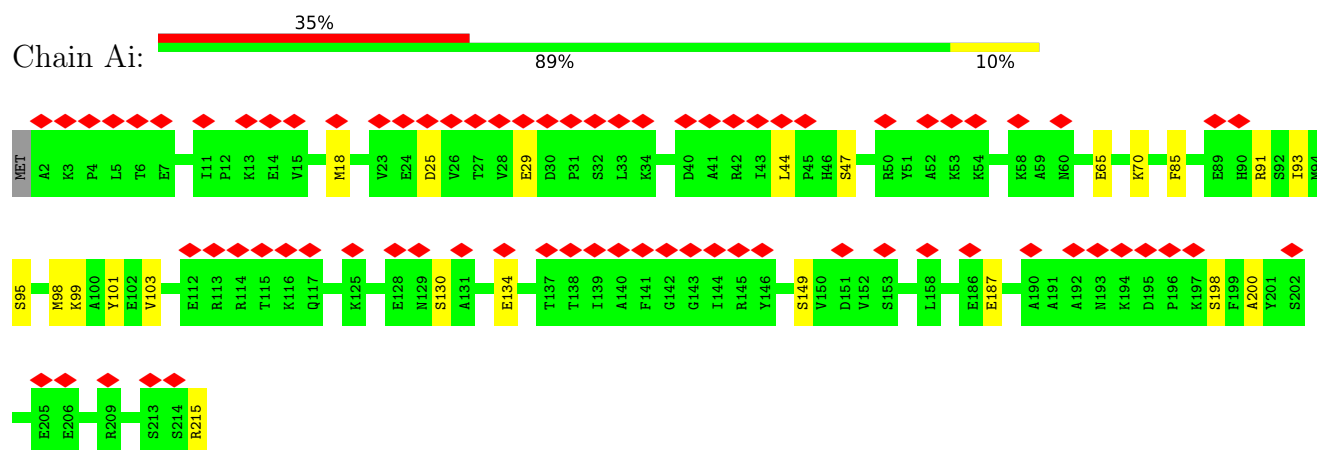
- Molecule 7: 30S ribosomal protein S5



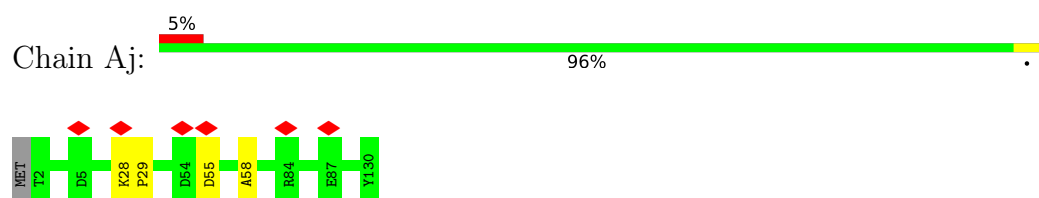
- Molecule 8: 30S ribosomal protein S6e



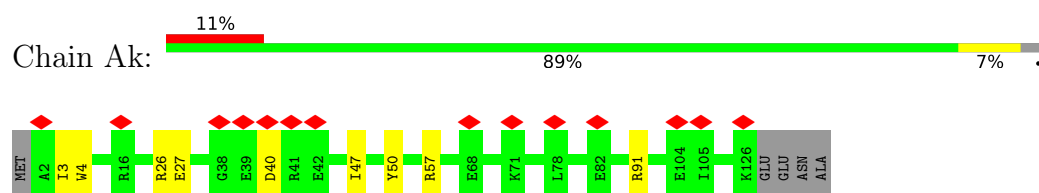
- Molecule 9: 30S ribosomal protein S7



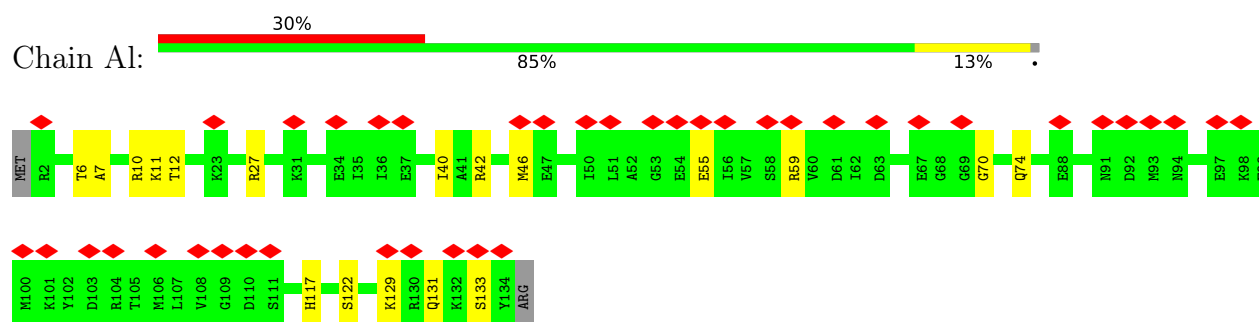
- Molecule 10: 30S ribosomal protein S8



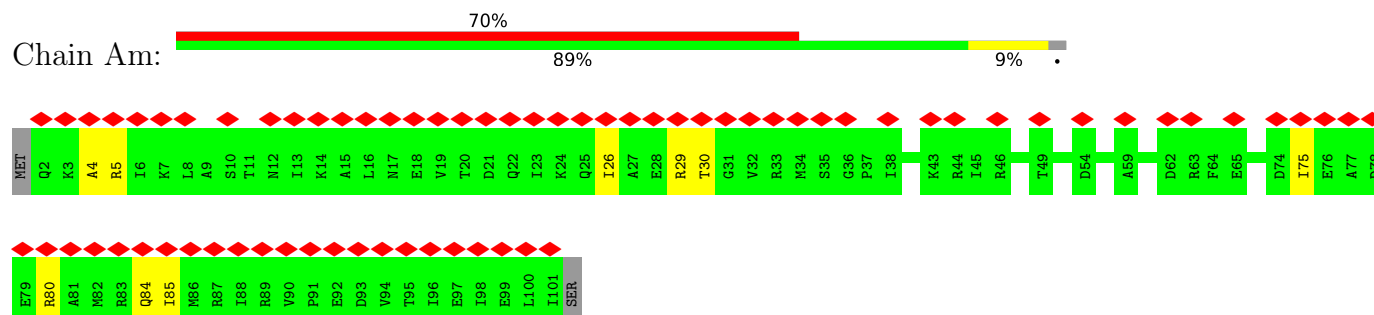
- Molecule 11: 30S ribosomal protein S8e



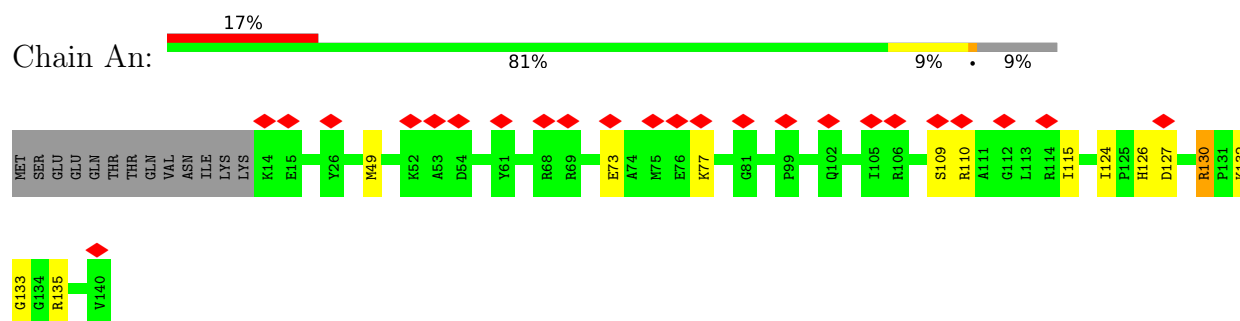
- Molecule 12: 30S ribosomal protein S9



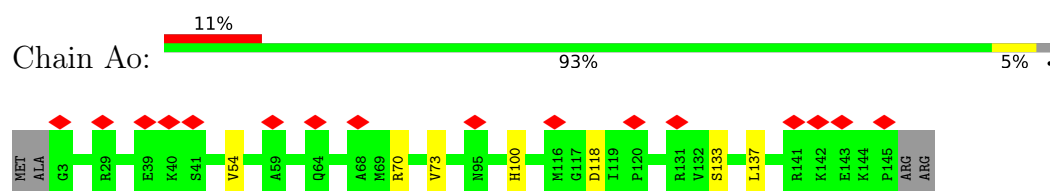
- Molecule 13: 30S ribosomal protein S10



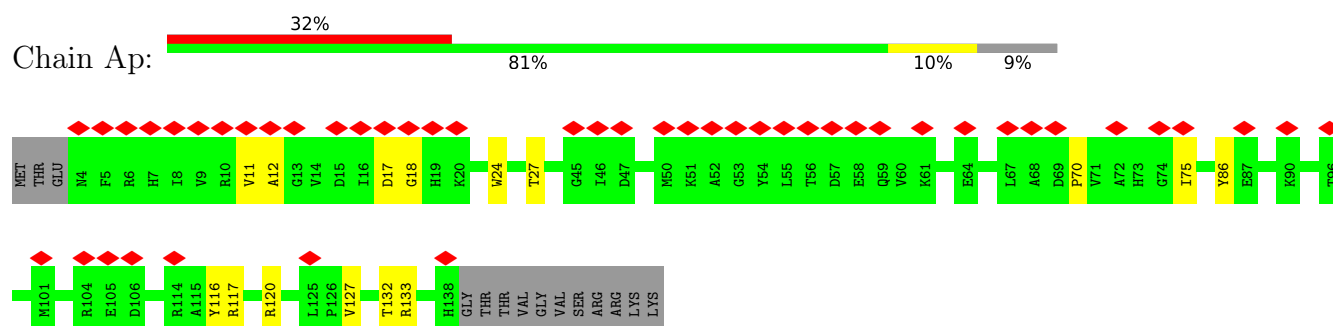
- Molecule 14: 30S ribosomal protein S11



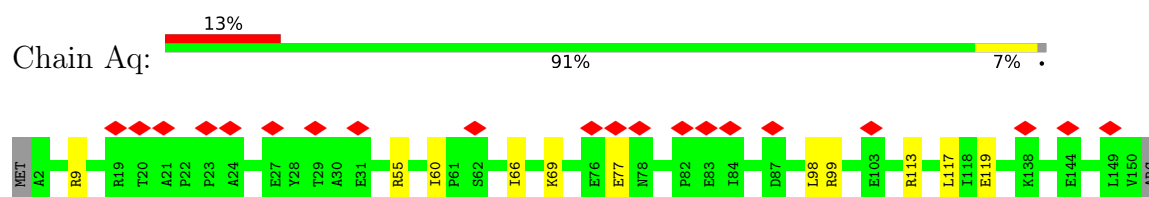
- Molecule 15: 30S ribosomal protein S12



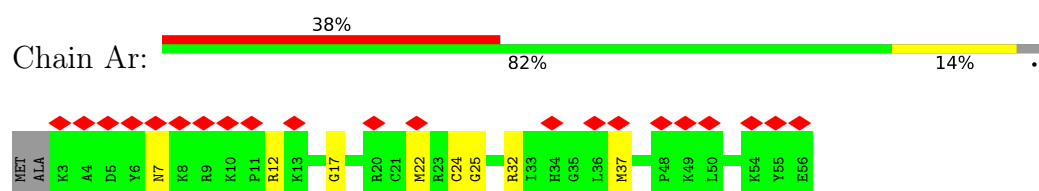
- Molecule 16: 30S ribosomal protein S13



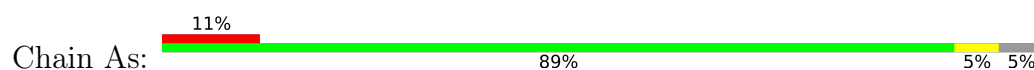
- Molecule 17: 30S ribosomal protein S15

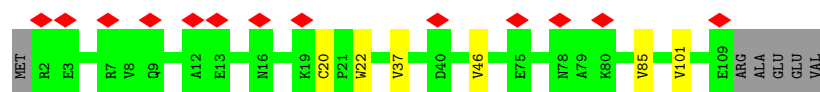


- Molecule 18: 30S ribosomal protein S14 type Z

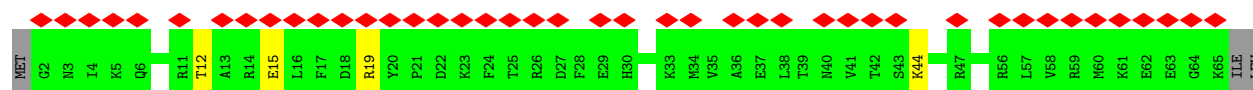
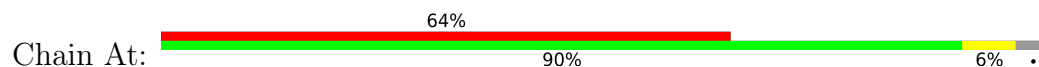


- Molecule 19: 30S ribosomal protein S17

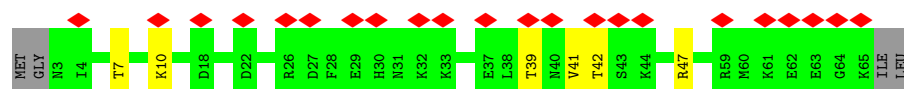
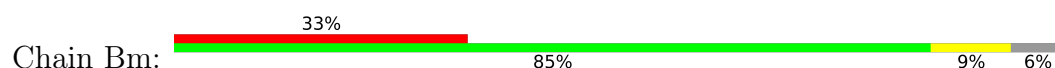




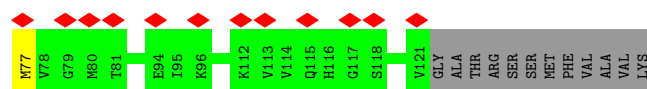
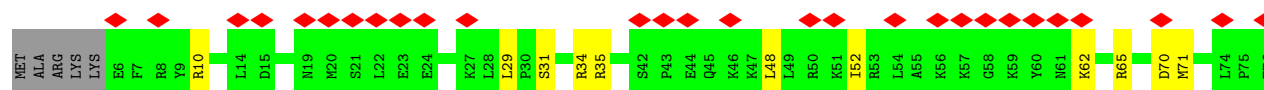
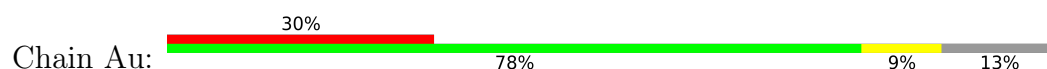
- Molecule 20: 30S ribosomal protein S17e



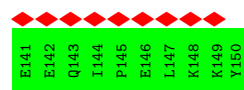
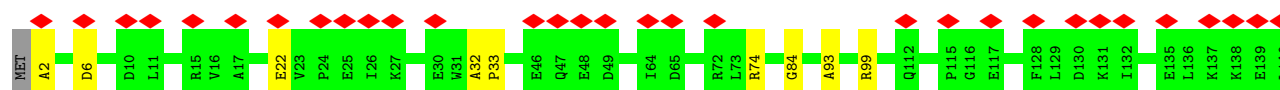
- Molecule 20: 30S ribosomal protein S17e



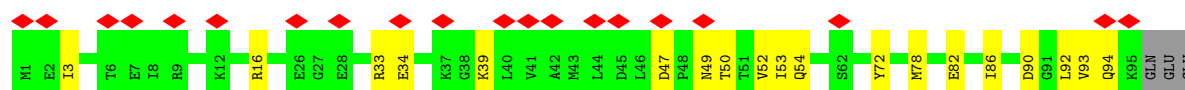
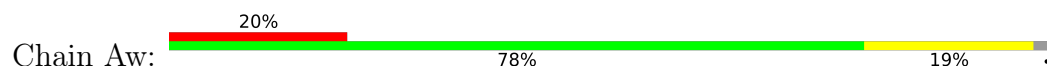
- Molecule 21: 30S ribosomal protein S19



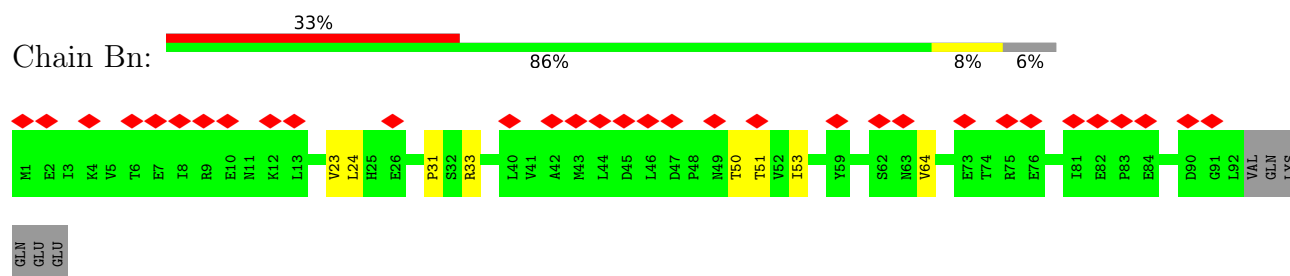
- Molecule 22: 30S ribosomal protein S19e



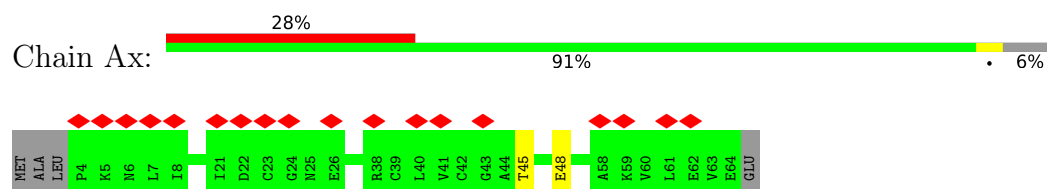
- Molecule 23: 30S ribosomal protein S24e



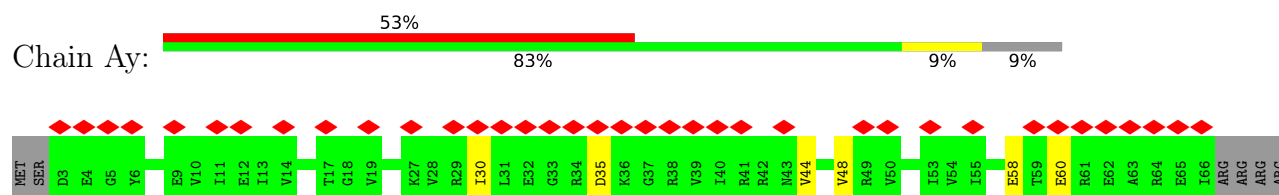
- Molecule 23: 30S ribosomal protein S24e



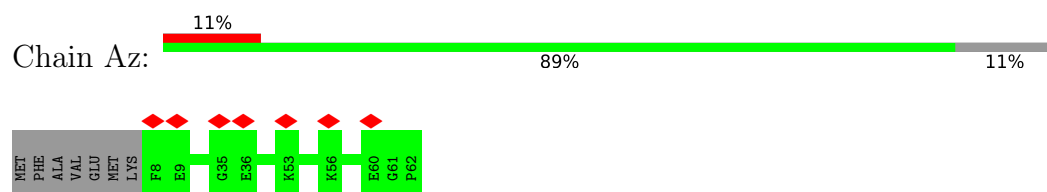
- Molecule 24: 30S ribosomal protein S27e



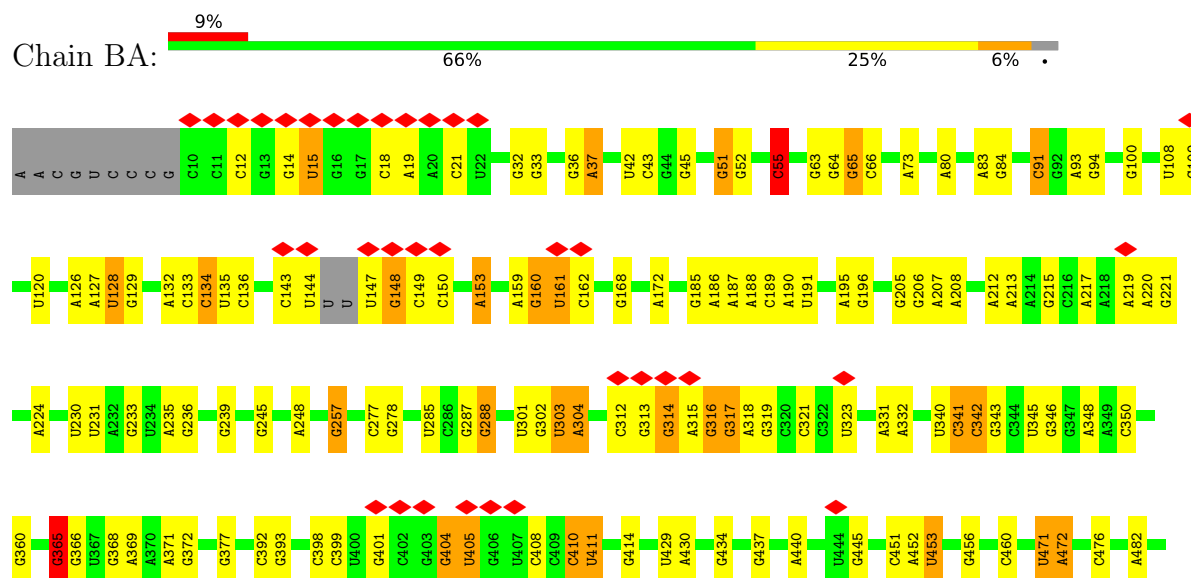
- Molecule 25: 30S ribosomal protein S28e

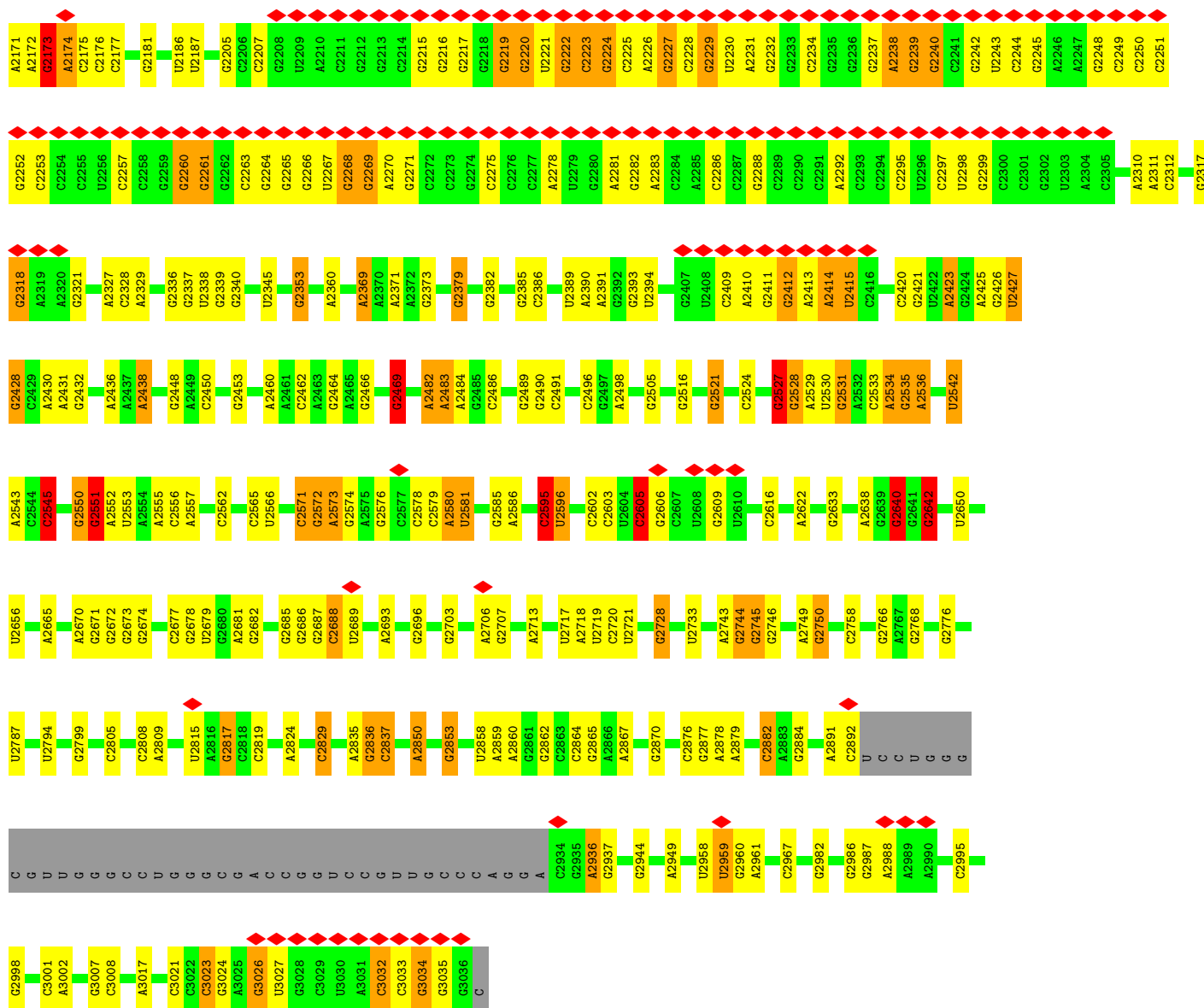


- Molecule 26: Predicted zinc-ribbon RNA-binding protein involved in translation



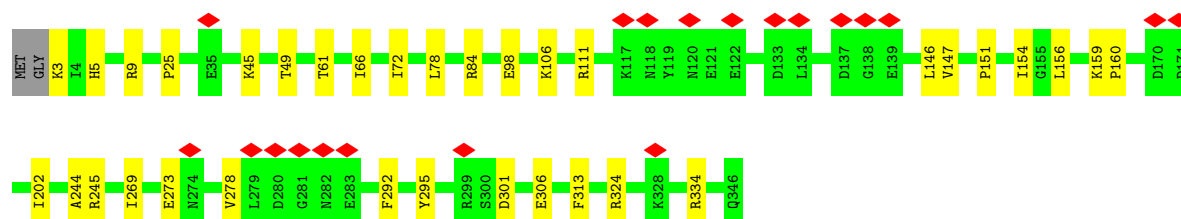
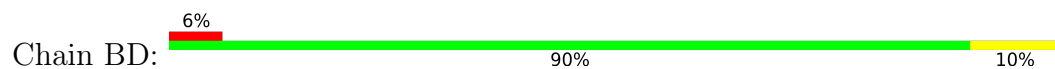
- Molecule 27: 23S ribosomal RNA



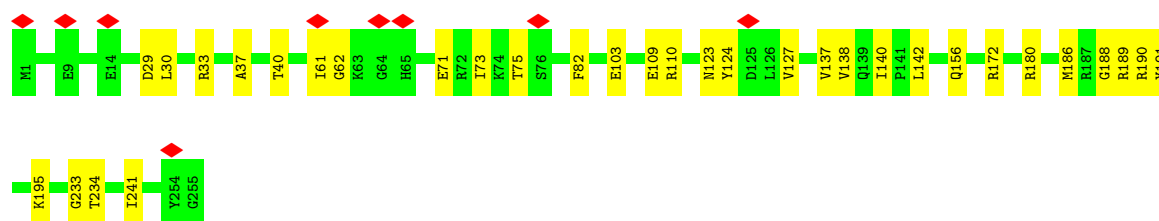




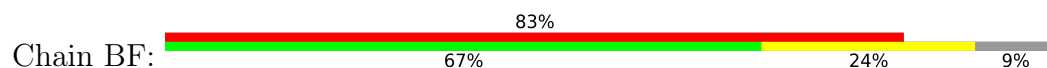
- Molecule 30: 50S ribosomal protein L3



- Molecule 31: 50S ribosomal protein L4



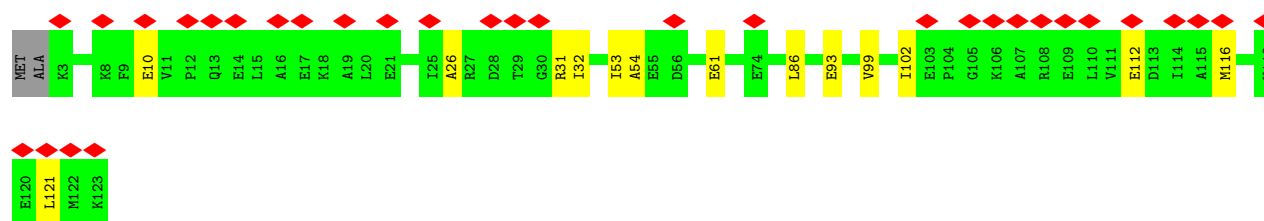
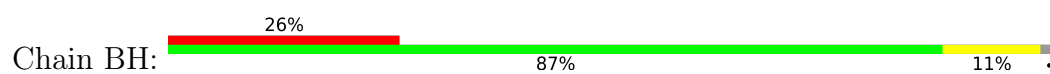
- Molecule 32: 50S ribosomal protein L5



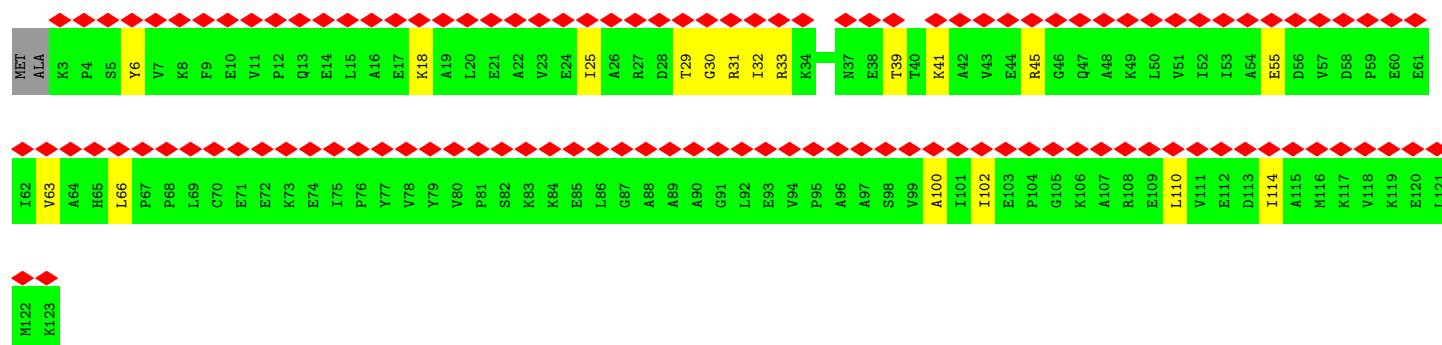
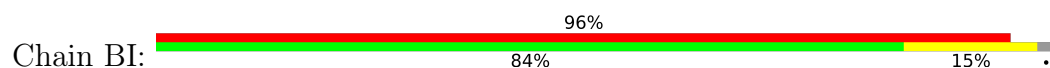
- Molecule 33: 50S ribosomal protein L6



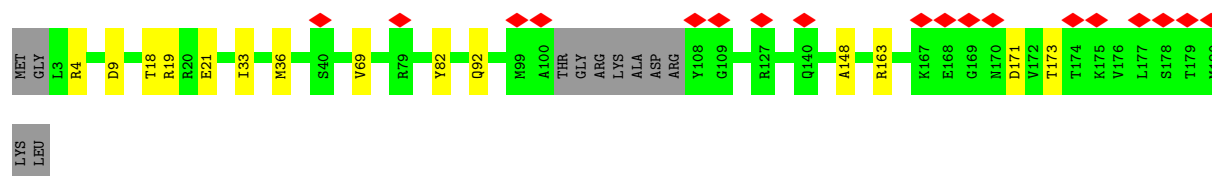
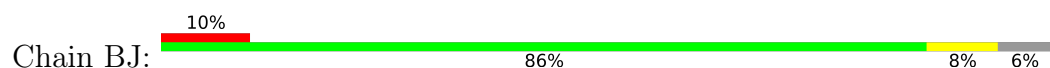
- Molecule 34: 50S ribosomal protein L7Ae



- Molecule 34: 50S ribosomal protein L7Ae



- Molecule 35: 50S ribosomal protein L10e



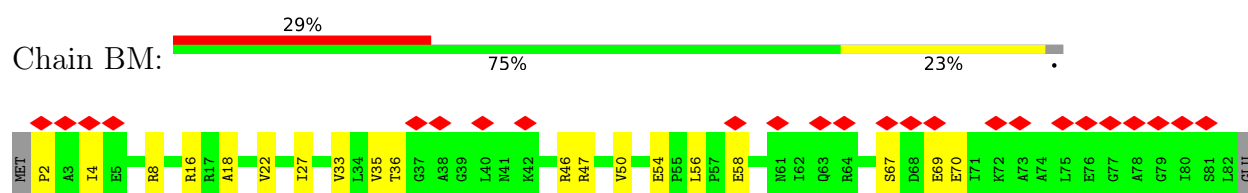
- Molecule 36: 50S ribosomal protein L13



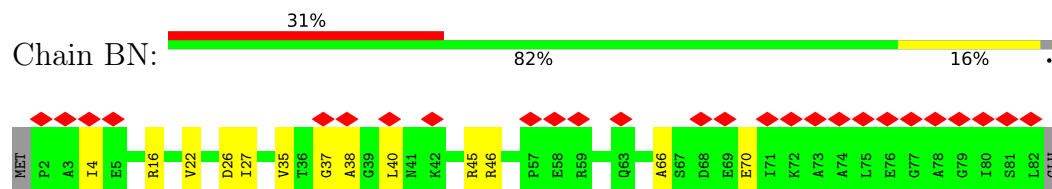
- Molecule 37: 50S ribosomal protein L14



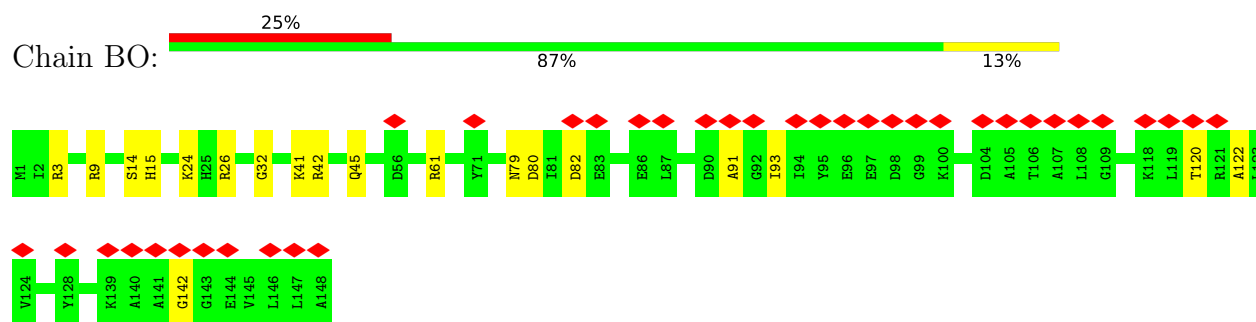
- Molecule 38: 50S ribosomal protein L14e



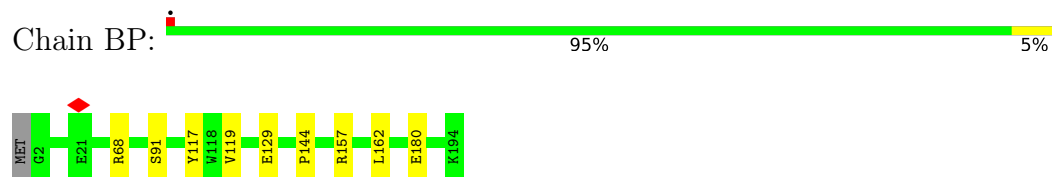
- Molecule 38: 50S ribosomal protein L14e



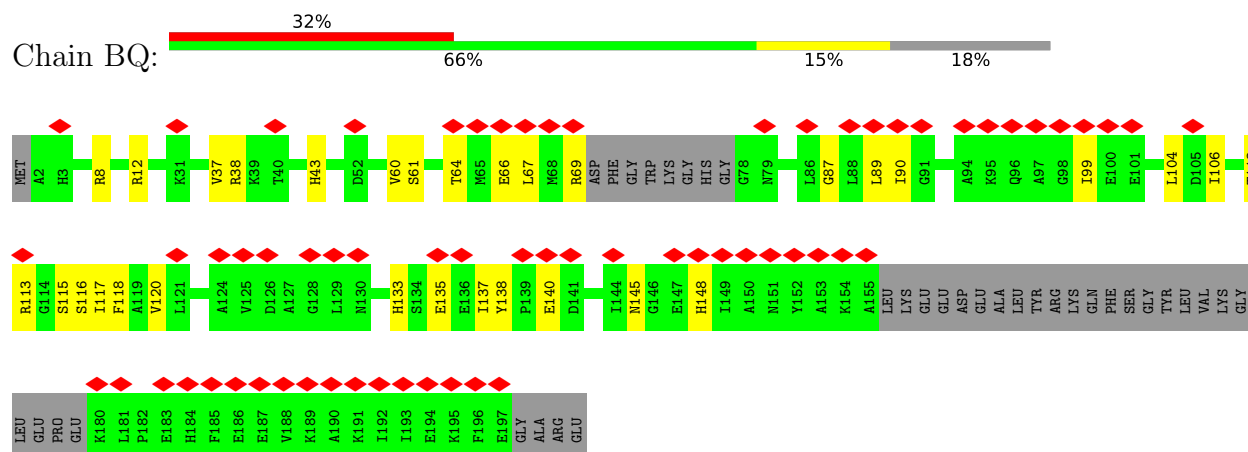
- Molecule 39: 50S ribosomal protein L15



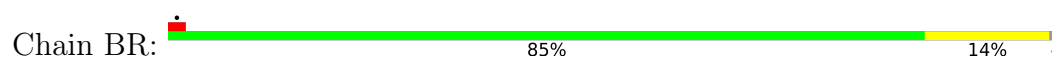
- Molecule 40: 50S ribosomal protein L15e

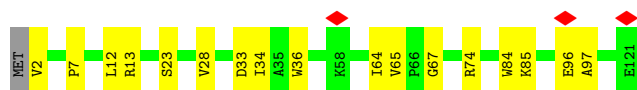


- Molecule 41: 50S ribosomal protein L18

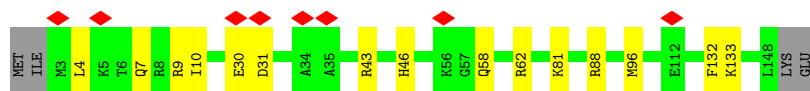
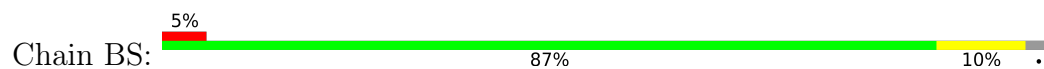


- Molecule 42: 50S ribosomal protein L18e





- Molecule 43: 50S ribosomal protein L19e



- Molecule 44: 50S ribosomal protein L18Ae



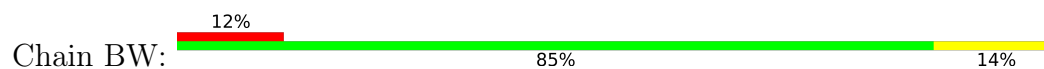
- Molecule 45: 50S ribosomal protein L21e



- Molecule 46: 50S ribosomal protein L22



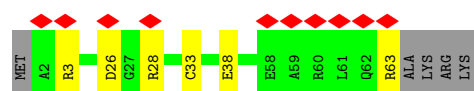
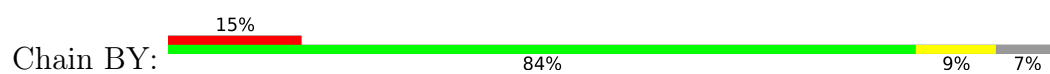
- Molecule 47: 50S ribosomal protein L23



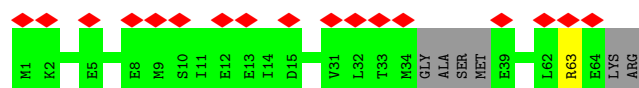
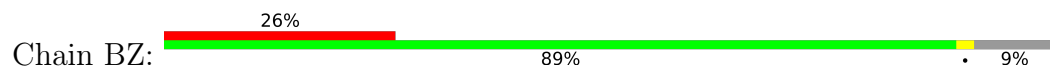
- Molecule 48: 50S ribosomal protein L24



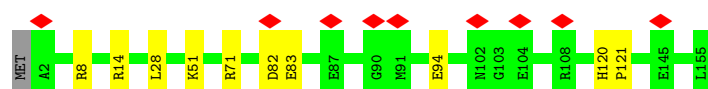
- Molecule 49: 50S ribosomal protein L24e



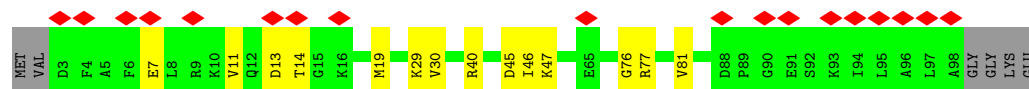
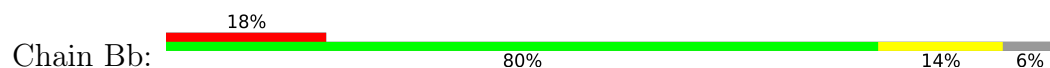
- Molecule 50: 50S ribosomal protein L29



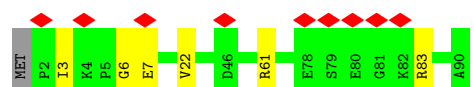
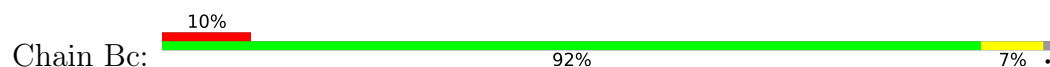
- Molecule 51: 50S ribosomal protein L30



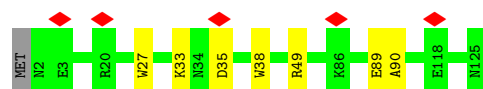
- Molecule 52: 50S ribosomal protein L30e



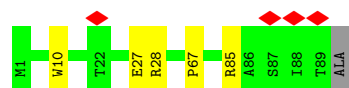
- Molecule 53: 50S ribosomal protein L31e



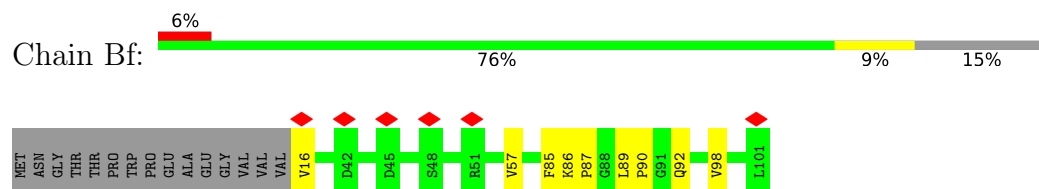
- Molecule 54: 50S ribosomal protein L32e



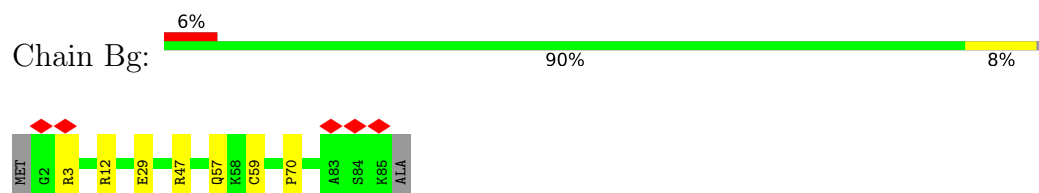
- Molecule 55: 50S ribosomal protein L34e



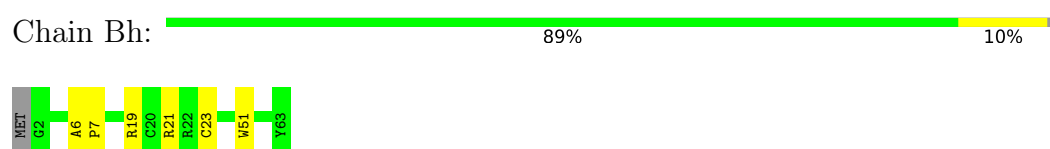
- Molecule 56: Ribosomal protein eL35A



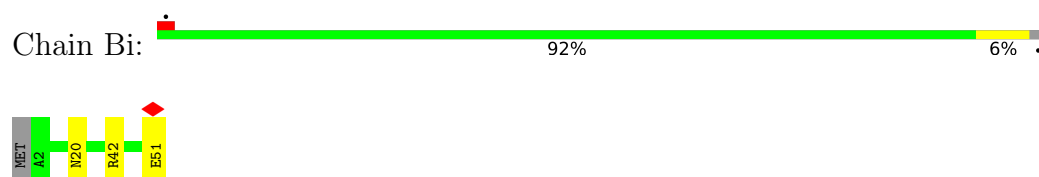
- Molecule 57: 50S ribosomal protein L37Ae



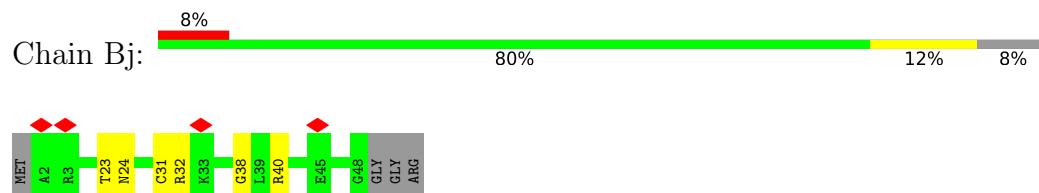
- Molecule 58: 50S ribosomal protein L37e



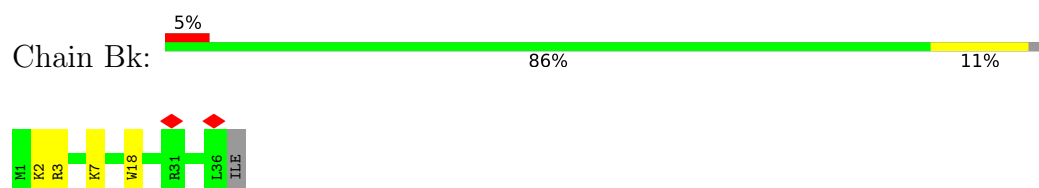
- Molecule 59: 50S ribosomal protein L39e



- Molecule 60: 50S ribosomal protein L40e

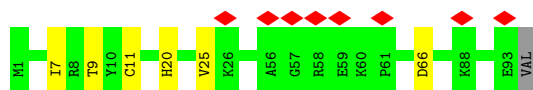


- Molecule 61: LSU ribosomal protein L41E

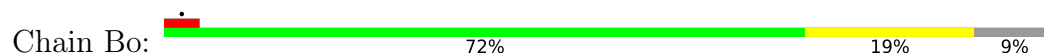


- Molecule 62: 50S ribosomal protein L44e

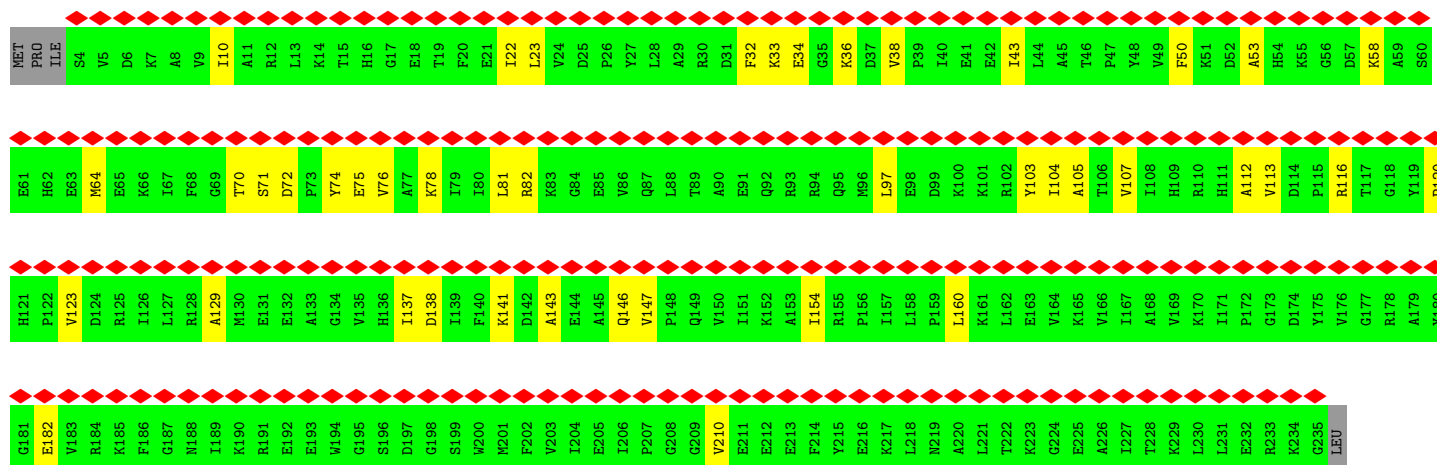
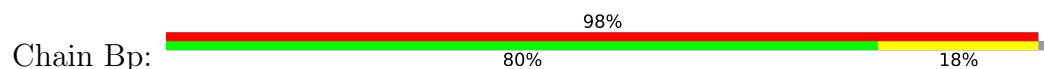




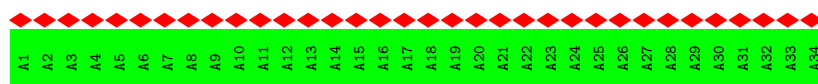
- Molecule 63: Nucleic acid-binding protein, containing C2H2 zinc-finger



- Molecule 64: Predicted exosome subunit, UPF0023 family



- Molecule 65: Unknown ribosomal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	116585	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	29000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.497	Depositor
Minimum map value	-0.266	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LV2, 6MZ, 5MU, 2MG, A2M, OMG, 5MC, MA6, OMC, ZN, 4SU, OMU

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	Aa	0.21	1/33690 (0.0%)	0.38	17/52572 (0.0%)
2	Ab	0.16	0/1611	0.32	0/2179
3	Ac	0.24	0/1558	0.41	0/2089
4	Ad	0.17	0/1578	0.35	0/2119
5	Ae	0.26	0/1477	0.43	0/1980
6	Af	0.20	0/1999	0.36	0/2700
7	Ag	0.19	0/1779	0.37	0/2396
8	Ah	0.32	0/968	0.45	0/1300
9	Ai	0.15	0/1748	0.32	0/2347
10	Aj	0.19	0/1039	0.34	0/1397
11	Ak	0.20	0/991	0.35	0/1322
12	Al	0.17	0/1068	0.39	0/1430
13	Am	0.16	0/810	0.37	0/1087
14	An	0.59	2/971 (0.2%)	0.87	2/1308 (0.2%)
15	Ao	0.18	0/1139	0.35	0/1518
16	Ap	0.27	0/1113	0.47	0/1500
17	Aq	0.24	0/1241	0.38	0/1667
18	Ar	0.15	0/457	0.34	0/602
19	As	0.18	0/899	0.37	0/1214
20	At	0.15	0/545	0.31	0/725
20	Bm	0.18	0/541	0.35	0/720
21	Au	0.15	0/970	0.34	0/1295
22	Av	0.17	0/1249	0.32	0/1687
23	Aw	0.18	0/790	0.36	0/1063
23	Bn	0.17	0/765	0.37	0/1030
24	Ax	0.16	0/469	0.30	0/633
25	Ay	0.15	0/501	0.35	0/672
26	Az	0.17	0/440	0.29	0/599
27	BA	0.24	1/68729 (0.0%)	0.35	10/107278 (0.0%)
28	BB	0.15	0/2993	0.27	0/4668
29	BC	0.29	0/1860	0.45	0/2511
30	BD	0.23	0/2815	0.41	0/3795

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	BE	0.23	0/2066	0.44	0/2785
32	BF	0.19	0/1355	0.45	0/1806
33	BG	0.18	0/1490	0.39	0/2006
34	BH	0.18	0/941	0.33	0/1272
34	BI	0.16	0/941	0.36	0/1272
35	BJ	0.21	0/1429	0.37	0/1921
36	BK	0.24	0/1165	0.44	0/1558
37	BL	0.20	0/1067	0.39	0/1435
38	BM	0.22	0/614	0.41	0/824
38	BN	0.18	0/614	0.45	0/824
39	BO	0.21	0/1188	0.44	0/1585
40	BP	0.30	0/1621	0.50	0/2163
41	BQ	0.18	0/1342	0.38	0/1804
42	BR	0.23	0/971	0.40	0/1301
43	BS	0.25	0/1216	0.47	0/1607
44	BT	0.18	0/636	0.36	0/852
45	BU	0.22	0/806	0.38	0/1080
46	BV	0.22	0/1259	0.38	0/1688
47	BW	0.21	0/690	0.38	0/925
48	BX	0.22	0/1007	0.40	0/1344
49	BY	0.22	0/538	0.39	0/716
50	BZ	0.23	0/506	0.43	0/668
51	Ba	0.29	0/1259	0.45	0/1680
52	Bb	0.17	0/742	0.33	0/1001
53	Bc	0.23	0/736	0.40	0/990
54	Bd	0.24	0/1044	0.40	0/1394
55	Be	0.23	0/746	0.42	0/997
56	Bf	0.23	0/681	0.41	0/919
57	Bg	0.23	0/640	0.41	0/855
58	Bh	0.29	0/524	0.46	0/692
59	Bi	0.25	0/441	0.44	0/588
60	Bj	0.40	0/381	0.69	2/505 (0.4%)
61	Bk	0.69	0/351	1.09	0/454
62	Bl	0.22	0/796	0.40	0/1056
63	Bo	0.21	0/356	0.40	0/474
64	Bp	0.17	0/1899	0.44	0/2559
65	Bq	0.17	0/169	0.27	0/235
All	All	0.23	4/173030 (0.0%)	0.38	31/255238 (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
14	An	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	An	130	ARG	C-N	13.07	1.50	1.33
27	BA	2173	G	O3'-P	5.17	1.69	1.61
1	Aa	352	A2M	O3'-P	5.06	1.61	1.56
14	An	124	ILE	N-CA	5.04	1.49	1.45

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	An	130	ARG	CA-C-N	17.14	137.16	119.85
14	An	130	ARG	C-N-CA	17.14	137.16	119.85
1	Aa	1298	A	C2'-C3'-O3'	11.17	126.26	109.50
1	Aa	439	A	C4'-C3'-O3'	9.18	123.17	109.40
1	Aa	231	A	C2'-C3'-O3'	8.87	122.81	109.50
27	BA	128	U	C2'-C3'-O3'	8.60	122.39	109.50
1	Aa	622	A	C1'-C2'-O2'	-7.77	96.75	108.40
1	Aa	622	A	C4'-C3'-O3'	7.39	124.09	113.00
27	BA	1741	C	C2'-C3'-O3'	7.28	124.62	113.70
1	Aa	621	U	C4'-C3'-O3'	7.09	123.63	113.00
27	BA	2173	G	P-O3'-C3'	7.00	130.70	120.20
1	Aa	453	A	C2'-C3'-O3'	6.99	124.18	113.70
1	Aa	621	U	C1'-C2'-O2'	-6.84	98.14	108.40
1	Aa	1093	G	C2'-C3'-O3'	6.71	123.77	113.70
27	BA	128	U	C4'-C3'-O3'	6.59	119.29	109.40
27	BA	2551	G	C2'-C3'-O3'	6.50	119.25	109.50
27	BA	134	C	C2'-C3'-O3'	6.40	119.09	109.50
60	Bj	38	GLY	CA-C-N	6.39	131.82	123.00
60	Bj	38	GLY	C-N-CA	6.39	131.82	123.00
27	BA	2551	G	C4'-C3'-O3'	6.20	118.69	109.40
1	Aa	661	A	C4'-C3'-O3'	6.18	122.28	113.00
1	Aa	468	C	C4'-C3'-O3'	6.12	122.18	113.00
1	Aa	441	U	C4'-C3'-O3'	5.96	121.94	113.00
1	Aa	231	A	C4'-C3'-O3'	5.90	118.25	109.40
1	Aa	1172	G	C4'-C3'-O3'	-5.67	104.50	113.00
27	BA	1742	G	C2'-C3'-O3'	5.65	122.18	113.70
27	BA	1742	G	C4'-C3'-O3'	5.53	121.29	113.00
1	Aa	622	A	N9-C1'-C2'	-5.22	104.17	112.00
1	Aa	619	G	C4'-C3'-O3'	5.16	120.73	113.00
1	Aa	664	G	C4'-C3'-O3'	5.14	120.71	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	134	C	C4'-C3'-O3'	5.01	116.91	109.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	An	126	HIS	Peptide
14	An	127	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	31531	0	16007	233	0
2	Ab	1580	0	1634	8	0
3	Ac	1536	0	1621	12	0
4	Ad	1550	0	1618	12	0
5	Ae	1454	0	1521	10	0
6	Af	1952	0	2035	18	0
7	Ag	1753	0	1822	14	0
8	Ah	952	0	997	16	0
9	Ai	1715	0	1779	17	0
10	Aj	1020	0	1066	2	0
11	Ak	982	0	1071	7	0
12	Al	1054	0	1105	15	0
13	Am	803	0	854	7	0
14	An	953	0	973	7	0
15	Ao	1122	0	1212	7	0
16	Ap	1090	0	1121	10	0
17	Aq	1217	0	1302	7	0
18	Ar	447	0	469	7	0
19	As	879	0	907	4	0
20	At	538	0	560	4	0
20	Bm	534	0	557	5	0
21	Au	952	0	1000	10	0
22	Av	1216	0	1236	8	0
23	Aw	777	0	797	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	Bn	752	0	767	4	0
24	Ax	461	0	492	1	0
25	Ay	499	0	528	4	0
26	Az	426	0	402	0	0
27	BA	63209	0	32023	485	0
28	BB	2678	0	1361	19	0
29	BC	1820	0	1902	15	0
30	BD	2746	0	2840	27	0
31	BE	2026	0	2128	26	0
32	BF	1338	0	1403	34	0
33	BG	1463	0	1520	12	0
34	BH	928	0	970	8	0
34	BI	928	0	970	12	0
35	BJ	1399	0	1426	11	0
36	BK	1146	0	1213	5	0
37	BL	1055	0	1134	7	0
38	BM	610	0	660	19	0
38	BN	610	0	660	11	0
39	BO	1166	0	1229	13	0
40	BP	1582	0	1677	8	0
41	BQ	1314	0	1359	20	0
42	BR	959	0	1018	11	0
43	BS	1200	0	1298	11	0
44	BT	624	0	647	0	0
45	BU	784	0	821	9	0
46	BV	1234	0	1274	7	0
47	BW	683	0	743	8	0
48	BX	991	0	1053	7	0
49	BY	524	0	512	5	0
50	BZ	506	0	559	1	0
51	Ba	1242	0	1332	9	0
52	Bb	730	0	768	12	0
53	Bc	721	0	776	4	0
54	Bd	1022	0	1106	5	0
55	Be	728	0	786	4	0
56	Bf	669	0	714	6	0
57	Bg	630	0	675	8	0
58	Bh	512	0	527	5	0
59	Bi	432	0	488	2	0
60	Bj	373	0	390	5	0
61	Bk	345	0	407	5	0
62	Bl	778	0	831	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	Bo	349	0	358	7	0
64	Bp	1861	0	1900	30	0
65	Bq	170	0	172	0	0
66	Ag	1	0	0	0	0
66	Ar	1	0	0	0	0
66	As	1	0	0	0	0
66	Ax	1	0	0	0	0
66	Az	2	0	0	0	0
66	BY	1	0	0	0	0
66	Be	2	0	0	0	0
66	Bg	1	0	0	0	0
66	Bh	1	0	0	0	0
66	Bj	1	0	0	0	0
66	Bl	1	0	0	0	0
66	Bo	1	0	0	0	0
67	Aa	266	0	0	31	0
67	Ad	1	0	0	0	0
67	Af	4	0	0	0	0
67	Ag	1	0	0	0	0
67	Ai	1	0	0	0	0
67	Aj	2	0	0	0	0
67	Ak	6	0	0	2	0
67	Al	2	0	0	0	0
67	Am	2	0	0	0	0
67	An	2	0	0	0	0
67	Ao	1	0	0	0	0
67	Ap	3	0	0	0	0
67	Aq	5	0	0	0	0
67	As	2	0	0	2	0
67	Au	1	0	0	0	0
67	Av	1	0	0	0	0
67	Az	1	0	0	0	0
67	BA	2715	0	0	172	0
67	BB	23	0	0	3	0
67	BC	51	0	0	1	0
67	BD	59	0	0	1	0
67	BE	41	0	0	7	0
67	BF	2	0	0	1	0
67	BG	1	0	0	0	0
67	BH	1	0	0	0	0
67	BJ	13	0	0	0	0
67	BK	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	BL	15	0	0	1	0
67	BM	3	0	0	2	0
67	BN	3	0	0	1	0
67	BO	30	0	0	1	0
67	BP	36	0	0	1	0
67	BQ	6	0	0	1	0
67	BR	14	0	0	0	0
67	BS	17	0	0	0	0
67	BT	2	0	0	0	0
67	BU	13	0	0	3	0
67	BV	22	0	0	0	0
67	BW	3	0	0	0	0
67	BX	10	0	0	1	0
67	BY	12	0	0	1	0
67	BZ	7	0	0	0	0
67	Ba	14	0	0	3	0
67	Bb	8	0	0	1	0
67	Bc	10	0	0	1	0
67	Bd	23	0	0	2	0
67	Be	8	0	0	0	0
67	Bf	7	0	0	1	0
67	Bg	15	0	0	6	0
67	Bh	23	0	0	3	0
67	Bi	10	0	0	1	0
67	Bj	3	0	0	2	0
67	Bk	3	0	0	0	0
67	Bl	8	0	0	2	0
67	Bm	1	0	0	0	0
67	Bn	1	0	0	0	0
67	Bo	4	0	0	0	0
All	All	167400	0	119083	1247	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 4.

All (1247) 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)
27:BA:2678:G:OP1	67:BA:3101:HOH:O	1.68	1.09
27:BA:1478:A:OP2	67:BA:3102:HOH:O	1.75	1.04
27:BA:850:U:O4	57:Bg:3:ARG:NH1	1.92	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ac:193:ILE:HD11	20:At:12:THR:HG21	1.42	0.98
27:BA:1137:A:OP2	67:BA:3104:HOH:O	1.83	0.96
51:Ba:120:HIS:NE2	67:Ba:201:HOH:O	1.69	0.96
1:Aa:1174:G:O6	67:Aa:1501:HOH:O	1.83	0.96
1:Aa:761:A:OP1	61:Bk:3:ARG:NH1	1.98	0.96
1:Aa:1257:G:H5''	22:Av:84:GLY:HA2	1.45	0.96
27:BA:1463:C:OP2	67:BA:3103:HOH:O	1.81	0.96
8:Ah:51:PHE:CE2	8:Ah:123:ILE:HD11	2.02	0.95
27:BA:168:G:N7	67:BA:3120:HOH:O	2.00	0.93
27:BA:1030:U:O2'	27:BA:1031:C:OP1	1.84	0.93
27:BA:1635:G:N2	27:BA:1653:A:N7	2.16	0.92
27:BA:341:C:H6	27:BA:341:C:H5'	1.34	0.92
1:Aa:467:C:H41	15:Ao:70:ARG:NH2	1.67	0.91
57:Bg:59:CYS:SG	67:Bg:205:HOH:O	2.28	0.91
1:Aa:738:A:O2'	1:Aa:739:U:OP2	1.89	0.90
27:BA:2318:G:OP1	27:BA:2318:G:N2	2.03	0.90
27:BA:489:G:OP2	67:BA:3105:HOH:O	1.90	0.88
29:BC:100:ALA:O	29:BC:134:ARG:NH2	2.06	0.88
5:Ae:52:ARG:NH2	7:Ag:160:ARG:O	2.07	0.87
27:BA:3023:C:H5''	27:BA:3023:C:H6	1.38	0.87
1:Aa:1006:5MC:H2'	1:Aa:1007:5MC:H5''	1.54	0.87
27:BA:1041:C:OP1	35:BJ:19:ARG:NH2	2.08	0.87
41:BQ:145:ASN:OD1	67:BQ:301:HOH:O	1.91	0.87
27:BA:2125:G:OP2	67:BA:3106:HOH:O	1.91	0.87
57:Bg:3:ARG:NH2	67:Bg:201:HOH:O	2.08	0.86
27:BA:2531:G:N7	67:BA:3161:HOH:O	2.07	0.86
67:BA:3107:HOH:O	63:Bo:22:ARG:O	1.93	0.86
27:BA:2744:G:N7	67:BA:3131:HOH:O	2.10	0.85
32:BF:87:MET:SD	32:BF:90:ARG:NH2	2.50	0.85
2:Ab:81:LYS:NZ	2:Ab:193:ASP:O	2.10	0.84
27:BA:1681:G:O6	27:BA:1685:G:N2	2.11	0.84
27:BA:1759:A:OP1	67:BA:3108:HOH:O	1.94	0.84
27:BA:348:A:N1	67:BA:3178:HOH:O	2.11	0.83
27:BA:2536:A:OP2	67:BA:3109:HOH:O	1.94	0.83
27:BA:2836:G:O2'	27:BA:2837:C:O5'	1.96	0.83
27:BA:1624:A:O2'	27:BA:1625:U:O5'	1.96	0.83
27:BA:189:C:OP2	67:BA:3110:HOH:O	1.96	0.83
59:Bi:51:GLU:OE2	67:Bi:101:HOH:O	1.95	0.83
27:BA:1178:A:O2'	27:BA:1179:G:O5'	1.96	0.82
31:BE:172:ARG:NH1	31:BE:195:LYS:O	2.12	0.82
27:BA:2556:C:N3	67:BA:3185:HOH:O	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2616:C:OP1	30:BD:9:ARG:NH1	2.12	0.82
8:Ah:70:ASP:OD2	8:Ah:83:ARG:NH2	2.13	0.82
27:BA:2835:A:O2'	27:BA:2836:G:O4'	1.96	0.82
1:Aa:1449:6MZ:OP1	67:Aa:1503:HOH:O	1.98	0.81
1:Aa:1275:G:OP2	67:Aa:1502:HOH:O	1.98	0.81
8:Ah:48:SER:HB3	8:Ah:54:GLU:HA	1.60	0.81
27:BA:671:G:N7	67:BA:3186:HOH:O	2.13	0.81
27:BA:3033:C:N4	27:BA:3034:G:O6	2.12	0.81
62:Bl:11:CYS:SG	67:Bl:201:HOH:O	2.36	0.81
28:BB:28:C:O2	28:BB:59:G:N2	2.13	0.81
38:BM:50:VAL:O	52:Bb:29:LYS:NZ	2.14	0.81
27:BA:1008:U:O2'	27:BA:1009:U:O4'	1.99	0.81
1:Aa:1272:C:OP2	67:Aa:1502:HOH:O	1.97	0.81
1:Aa:1231:A:O2'	1:Aa:1233:U:OP2	1.97	0.81
27:BA:2586:A:OP2	67:BA:3112:HOH:O	1.98	0.81
1:Aa:1006:5MC:C2'	1:Aa:1007:5MC:H5''	2.11	0.81
27:BA:1390:U:OP1	67:BA:3111:HOH:O	1.97	0.81
1:Aa:64:G:N7	67:Aa:1511:HOH:O	2.12	0.80
7:Ag:12:LEU:O	7:Ag:26:LYS:NZ	2.14	0.80
27:BA:2987:G:O6	67:BA:3115:HOH:O	1.99	0.80
27:BA:1861:G:N7	67:BA:3191:HOH:O	2.14	0.80
27:BA:317:G:H8	27:BA:317:G:H5''	1.47	0.80
39:BO:82:ASP:OD2	42:BR:74:ARG:NH2	2.15	0.80
54:Bd:49:ARG:NH1	67:Bd:202:HOH:O	2.14	0.80
27:BA:1384:U:OP1	67:BA:3113:HOH:O	1.99	0.80
27:BA:857:C:OP2	67:BA:3114:HOH:O	1.99	0.79
27:BA:2693:A:OP1	67:BA:3117:HOH:O	2.00	0.79
1:Aa:467:C:H41	15:Ao:70:ARG:HH22	1.30	0.79
1:Aa:1164:A:O2'	1:Aa:1165:A:OP2	2.01	0.79
27:BA:235:A:OP2	67:BA:3116:HOH:O	2.00	0.79
27:BA:1520:G:O6	67:BA:3119:HOH:O	2.01	0.79
27:BA:1518:G:OP2	67:BA:3119:HOH:O	2.00	0.79
27:BA:399:C:OP1	63:Bo:35:ARG:NH2	2.16	0.78
27:BA:856:C:OP1	67:BA:3122:HOH:O	2.01	0.78
27:BA:912:OMG:H5'	27:BA:913:G:OP1	1.82	0.78
27:BA:2576:G:N7	67:BA:3208:HOH:O	2.17	0.78
64:Bp:104:ILE:HD12	64:Bp:147:VAL:HG22	1.64	0.78
27:BA:833:OMG:N2	67:BA:3211:HOH:O	2.17	0.78
27:BA:1768:C:O2'	27:BA:1769:C:OP2	2.01	0.78
27:BA:1830:G:OP2	67:BA:3125:HOH:O	2.02	0.78
27:BA:1896:G:N7	67:BA:3203:HOH:O	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:1352:5MC:OP2	67:Aa:1504:HOH:O	2.01	0.78
27:BA:341:C:H5'	27:BA:341:C:C6	2.18	0.78
1:Aa:316:C:OP2	67:Aa:1505:HOH:O	2.02	0.78
27:BA:1558:G:N7	38:BM:16:ARG:NH1	2.32	0.78
38:BM:46:ARG:NH2	67:BM:101:HOH:O	2.17	0.78
46:BV:71:GLN:OE1	46:BV:83:ARG:NH2	2.16	0.78
17:Aq:99:ARG:NH2	17:Aq:119:GLU:OE2	2.17	0.77
19:As:22:TRP:O	67:As:301:HOH:O	2.01	0.77
1:Aa:1454:G:OP1	67:Aa:1506:HOH:O	2.03	0.77
27:BA:231:U:O4	67:BA:3130:HOH:O	2.03	0.77
27:BA:1911:A:OP1	67:BA:3132:HOH:O	2.03	0.77
27:BA:2172:A:N7	67:BA:3213:HOH:O	2.17	0.77
28:BB:36:C:O2	41:BQ:148:HIS:NE2	2.17	0.77
27:BA:191:U:OP2	67:BA:3121:HOH:O	2.01	0.77
27:BA:236:G:N7	67:BA:3116:HOH:O	2.17	0.77
27:BA:1481:C:OP2	67:BA:3127:HOH:O	2.02	0.77
27:BA:1788:G:OP2	67:BA:3123:HOH:O	2.01	0.77
27:BA:959:G:OP2	67:BA:3126:HOH:O	2.02	0.77
1:Aa:1448:A:OP1	67:Aa:1503:HOH:O	2.03	0.77
1:Aa:659:OMG:H2'	1:Aa:660:G:C8	2.20	0.77
27:BA:2053:U:O2'	27:BA:2054:C:OP2	2.00	0.77
27:BA:434:G:O2'	40:BP:91:SER:OG	2.02	0.76
31:BE:109:GLU:OE1	67:BE:301:HOH:O	2.03	0.76
52:Bb:13:ASP:OD1	52:Bb:14:THR:N	2.18	0.76
8:Ah:32:ARG:NH1	8:Ah:36:GLU:OE1	2.18	0.76
62:Bl:20:HIS:NE2	67:Bl:201:HOH:O	2.17	0.76
27:BA:1397:G:N7	67:BA:3202:HOH:O	2.16	0.76
27:BA:629:G:N7	67:BA:3216:HOH:O	2.18	0.76
1:Aa:1268:G:O6	21:Au:35:ARG:NH1	2.18	0.76
27:BA:341:C:H6	27:BA:341:C:C5'	1.97	0.76
27:BA:888:C:OP2	67:BA:3129:HOH:O	2.03	0.76
27:BA:636:U:OP2	34:Bl:41:LYS:NZ	2.17	0.76
27:BA:1409:A:OP2	67:BA:3133:HOH:O	2.03	0.76
27:BA:2371:A:OP1	67:BA:3146:HOH:O	2.04	0.76
27:BA:2678:G:OP2	67:BA:3128:HOH:O	2.02	0.76
27:BA:1691:U:O2'	27:BA:1692:U:OP2	2.03	0.76
27:BA:2743:A:OP2	67:BA:3131:HOH:O	2.03	0.76
38:BM:8:ARG:NH2	38:BM:56:LEU:O	2.19	0.76
1:Aa:105:C:OP1	1:Aa:550:C:O2'	2.02	0.76
1:Aa:1092:G:H5''	1:Aa:1092:G:H8	1.49	0.76
27:BA:823:G:N7	67:BA:3221:HOH:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1323:G:OP2	67:BA:3135:HOH:O	2.04	0.75
27:BA:1819:U:OP2	67:BA:3137:HOH:O	2.04	0.75
27:BA:2012:A:OP2	67:BA:3134:HOH:O	2.03	0.75
27:BA:2524:C:OP1	39:BO:61:ARG:NH2	2.19	0.75
27:BA:2555:A:OP1	67:BA:3144:HOH:O	2.04	0.75
1:Aa:1447:U:O3'	67:Aa:1507:HOH:O	2.04	0.75
27:BA:1807:A:OP2	67:BA:3136:HOH:O	2.04	0.75
27:BA:1141:C:OP2	67:BA:3143:HOH:O	2.04	0.75
27:BA:1322:G:OP1	67:BA:3135:HOH:O	2.04	0.75
27:BA:1758:G:OP1	67:BA:3139:HOH:O	2.04	0.75
27:BA:2681:A:OP1	67:BA:3147:HOH:O	2.04	0.75
27:BA:3002:A:OP1	67:BA:3142:HOH:O	2.04	0.75
23:Bn:24:LEU:HD13	23:Bn:64:VAL:HG22	1.67	0.75
27:BA:195:A:OP1	67:BA:3141:HOH:O	2.04	0.75
27:BA:946:G:OP2	67:BA:3138:HOH:O	2.04	0.75
1:Aa:1397:C:O2'	1:Aa:1398:C:H5'	1.86	0.74
54:Bd:35:ASP:O	67:Bd:201:HOH:O	2.05	0.74
27:BA:1476:U:O2'	67:BA:3149:HOH:O	2.05	0.74
1:Aa:509:U:OP1	67:Aa:1508:HOH:O	2.04	0.74
27:BA:1929:U:OP2	67:BA:3148:HOH:O	2.05	0.74
1:Aa:959:C:OP2	1:Aa:969:G:O2'	2.04	0.74
1:Aa:1288:U:O2'	9:Ai:85:PHE:O	2.06	0.74
27:BA:2083:A:OP2	67:BA:3140:HOH:O	2.04	0.74
27:BA:507:OMG:HM22	27:BA:508:G:H5'	1.68	0.74
27:BA:1107:G:OP2	67:BA:3151:HOH:O	2.06	0.74
27:BA:3023:C:H5''	27:BA:3023:C:C6	2.20	0.74
48:BX:68:GLU:OE1	67:BX:201:HOH:O	2.05	0.74
27:BA:1824:A:OP2	67:BA:3150:HOH:O	2.06	0.74
13:Am:26:ILE:HG23	13:Am:84:GLN:HG3	1.69	0.73
27:BA:2865:G:OP2	67:BA:3154:HOH:O	2.07	0.73
1:Aa:792:G:O2'	4:Ad:180:LYS:O	2.05	0.73
16:Ap:24:TRP:O	16:Ap:27:THR:OG1	2.07	0.73
27:BA:1945:G:OP1	29:BC:54:ARG:NH1	2.20	0.73
27:BA:1605:C:N3	67:BA:3227:HOH:O	2.20	0.73
1:Aa:1466:G:N7	67:Aa:1526:HOH:O	2.22	0.73
18:Ar:32:ARG:HG3	18:Ar:37:MET:HE1	1.70	0.73
49:BY:33:CYS:SG	67:BY:212:HOH:O	2.28	0.73
27:BA:2850:A:OP2	67:BA:3153:HOH:O	2.06	0.73
1:Aa:889:A:H5''	1:Aa:889:A:H8	1.53	0.72
27:BA:921:A:OP1	67:BA:3155:HOH:O	2.07	0.72
27:BA:1901:A:OP1	27:BA:1956:OMG:HM22	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BS:81:LYS:HG2	43:BS:88:ARG:NH1	2.04	0.72
27:BA:120:U:OP1	50:BZ:63:ARG:NH1	2.23	0.72
27:BA:2603:C:OP2	67:BA:3157:HOH:O	2.07	0.72
1:Aa:634:G:OP1	14:An:49:MET:HG2	1.89	0.72
36:BK:94:PHE:O	67:BK:201:HOH:O	2.08	0.72
27:BA:371:A:OP1	31:BE:191:TYR:OH	2.06	0.72
56:Bf:89:LEU:O	67:Bf:201:HOH:O	2.06	0.72
27:BA:2216:G:O2'	27:BA:2217:G:O4'	2.08	0.72
6:Af:184:TYR:OH	6:Af:218:GLU:OE2	2.07	0.72
30:BD:273:GLU:HA	30:BD:301:ASP:OD1	1.90	0.72
40:BP:117:TYR:OH	40:BP:129:GLU:OE1	2.06	0.72
27:BA:905:G:OP2	67:BA:3160:HOH:O	2.07	0.71
27:BA:1812:A:OP2	67:BA:3152:HOH:O	2.06	0.71
28:BB:102:G:N7	67:BB:201:HOH:O	2.22	0.71
1:Aa:928:A:OP1	67:Aa:1509:HOH:O	2.08	0.71
1:Aa:1168:C:OP2	1:Aa:1168:C:H2'	1.89	0.71
27:BA:321:C:OP1	63:Bo:8:LYS:NZ	2.22	0.71
27:BA:585:G:OP2	67:BA:3156:HOH:O	2.07	0.71
27:BA:51:G:N2	27:BA:52:G:O6	2.24	0.71
39:BO:24:LYS:O	67:BO:201:HOH:O	2.08	0.71
58:Bh:19:ARG:O	67:Bh:201:HOH:O	2.08	0.71
1:Aa:340:5MC:H4'	1:Aa:342:G:OP1	1.90	0.71
27:BA:1564:G:OP1	67:BA:3168:HOH:O	2.09	0.71
52:Bb:13:ASP:OD1	52:Bb:14:THR:HG23	1.90	0.71
8:Ah:51:PHE:HE2	8:Ah:123:ILE:HD11	1.54	0.71
27:BA:871:G:OP1	67:BA:3170:HOH:O	2.09	0.71
27:BA:2505:G:O6	67:BA:3159:HOH:O	2.07	0.71
27:BA:1498:G:OP2	67:BA:3158:HOH:O	2.07	0.71
1:Aa:889:A:H8	1:Aa:889:A:C5'	2.04	0.71
27:BA:2750:G:OP2	30:BD:324:ARG:NH2	2.24	0.71
6:Af:126:ARG:NH2	6:Af:128:ASN:OD1	2.23	0.71
27:BA:1153:U:O2'	27:BA:1158:C:N4	2.24	0.71
27:BA:2679:U:OP2	67:BA:3101:HOH:O	2.09	0.71
27:BA:492:A:OP2	67:BA:3163:HOH:O	2.08	0.70
27:BA:2642:OMG:HM22	27:BA:2642:OMG:H4'	1.71	0.70
1:Aa:1133:G:O2'	1:Aa:1134:G:O4'	2.07	0.70
3:Ac:152:ALA:O	3:Ac:158:ALA:HB2	1.92	0.70
27:BA:1956:OMG:OP2	67:BA:3169:HOH:O	2.09	0.70
1:Aa:1217:C:C5'	1:Aa:1217:C:H6	2.04	0.70
27:BA:451:C:OP1	67:BA:3164:HOH:O	2.08	0.70
56:Bf:90:PRO:HB2	56:Bf:92:GLN:OE1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Af:168:VAL:HG23	6:Af:169:PRO:HD3	1.71	0.70
23:Bn:23:VAL:HG11	23:Bn:31:PRO:HG3	1.72	0.70
18:Ar:22:MET:HE2	18:Ar:37:MET:HB2	1.71	0.70
27:BA:2345:U:OP1	67:BA:3165:HOH:O	2.09	0.70
27:BA:2674:G:N7	67:BA:3253:HOH:O	2.24	0.70
31:BE:156:GLN:OE1	67:BE:302:HOH:O	2.10	0.70
1:Aa:930:C:O2	18:Ar:12:ARG:NH1	2.24	0.70
19:As:20:CYS:SG	67:As:301:HOH:O	2.31	0.70
27:BA:814:U:O2	67:BA:3172:HOH:O	2.10	0.70
27:BA:2393:G:N7	67:BA:3262:HOH:O	2.25	0.70
27:BA:2696:G:OP1	67:BA:3167:HOH:O	2.09	0.70
1:Aa:277:C:OP2	67:Aa:1510:HOH:O	2.10	0.69
27:BA:757:G:OP2	67:BA:3171:HOH:O	2.09	0.69
1:Aa:770:OMG:OP2	17:Aq:9:ARG:NH1	2.25	0.69
27:BA:2094:A:OP2	67:BA:3175:HOH:O	2.10	0.69
27:BA:492:A:OP1	67:BA:3177:HOH:O	2.10	0.69
52:Bb:45:ASP:OD1	52:Bb:46:ILE:N	2.26	0.69
58:Bh:23:CYS:SG	67:Bh:223:HOH:O	2.49	0.69
27:BA:153:A:N1	67:BA:3120:HOH:O	2.26	0.69
27:BA:1945:G:O6	67:BA:3162:HOH:O	2.08	0.69
27:BA:630:G:N7	67:BA:3256:HOH:O	2.24	0.69
27:BA:2959:U:O2	30:BD:106:LYS:NZ	2.25	0.69
27:BA:1081:G:N7	67:BA:3257:HOH:O	2.24	0.69
64:Bp:113:VAL:HG12	64:Bp:120:PRO:HA	1.74	0.69
1:Aa:1007:5MC:H6	1:Aa:1007:5MC:H5'	1.57	0.69
27:BA:770:A:N7	67:BA:3254:HOH:O	2.24	0.69
21:Au:48:LEU:HD23	21:Au:71:MET:SD	2.33	0.68
27:BA:2216:G:O2'	27:BA:2217:G:O5'	2.10	0.68
27:BA:2516:G:O6	67:BA:3176:HOH:O	2.10	0.68
27:BA:1392:C:OP2	67:BA:3173:HOH:O	2.10	0.68
12:Al:42:ARG:HG2	12:Al:46:MET:HE2	1.75	0.68
53:Bc:3:ILE:O	53:Bc:83:ARG:NH2	2.27	0.68
27:BA:2490:G:OP1	67:BA:3174:HOH:O	2.10	0.68
31:BE:190:ARG:O	67:BE:303:HOH:O	2.11	0.68
27:BA:36:G:OP2	67:BA:3179:HOH:O	2.11	0.68
1:Aa:1108:G:N7	20:At:44:LYS:NZ	2.41	0.68
27:BA:1482:G:OP2	67:BA:3127:HOH:O	2.11	0.68
51:Ba:71:ARG:NH2	51:Ba:120:HIS:HD2	1.92	0.68
27:BA:2021:G:N2	27:BA:2037:C:O2	2.27	0.68
27:BA:2427:5MU:H3'	27:BA:2428:G:H5''	1.74	0.68
28:BB:99:G:N7	67:BB:202:HOH:O	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:1296:C:OP1	12:Al:129:LYS:NZ	2.27	0.67
27:BA:1470:C:OP2	67:BA:3181:HOH:O	2.12	0.67
1:Aa:687:G:N7	67:Aa:1530:HOH:O	2.27	0.67
27:BA:548:U:OP2	67:BA:3183:HOH:O	2.12	0.67
27:BA:37:A:N1	67:BA:3274:HOH:O	2.28	0.67
1:Aa:523:U:OP1	67:Aa:1512:HOH:O	2.12	0.67
27:BA:2986:G:OP2	67:BA:3180:HOH:O	2.11	0.67
1:Aa:960:C:O2'	1:Aa:961:A:OP1	2.12	0.67
31:BE:233:GLY:O	31:BE:234:THR:OG1	2.09	0.67
45:BU:96:GLN:OE1	67:BU:101:HOH:O	2.11	0.67
27:BA:2462:C:OP2	67:BA:3188:HOH:O	2.13	0.67
27:BA:188:A:OP1	67:BA:3110:HOH:O	2.12	0.67
27:BA:1950:G:N7	67:BA:3277:HOH:O	2.28	0.67
1:Aa:1402:G:H2'	1:Aa:1403:G:O4'	1.94	0.66
27:BA:670:OMG:H4'	27:BA:670:OMG:HM22	1.75	0.66
41:BQ:116:SER:O	41:BQ:120:VAL:HG23	1.95	0.66
64:Bp:143:ALA:O	64:Bp:147:VAL:HG23	1.95	0.66
5:Ae:83:LEU:O	5:Ae:146:ARG:NH2	2.28	0.66
27:BA:2482:A:O2'	27:BA:2483:A:OP1	2.12	0.66
27:BA:2685:G:N7	67:BA:3268:HOH:O	2.27	0.66
1:Aa:1478:5MC:H4'	1:Aa:1479:G:OP2	1.96	0.66
17:Aq:69:LYS:NZ	17:Aq:77:GLU:OE1	2.29	0.66
27:BA:2571:C:H2'	27:BA:2572:G:O4'	1.96	0.66
32:BF:22:ILE:HD12	32:BF:85:TYR:CE1	2.31	0.66
1:Aa:668:G:OP1	4:Ad:102:ARG:NH1	2.29	0.66
27:BA:1136:A:OP2	67:BA:3104:HOH:O	2.12	0.66
1:Aa:63:G:N7	67:Aa:1532:HOH:O	2.29	0.66
23:Aw:49:ASN:O	23:Aw:50:THR:OG1	2.09	0.66
38:BM:8:ARG:NH2	38:BM:58:GLU:O	2.27	0.66
6:Af:55:TYR:OH	6:Af:98:GLU:OE2	2.13	0.66
5:Ae:132:VAL:HG12	5:Ae:133:ASN:H	1.60	0.66
27:BA:2596:U:OP1	67:BA:3192:HOH:O	2.14	0.66
41:BQ:66:GLU:OE1	41:BQ:69:ARG:NH1	2.29	0.66
1:Aa:6:G:N7	7:Ag:191:ARG:NH2	2.44	0.65
1:Aa:1357:G:H2'	1:Aa:1358:OMU:H6	1.77	0.65
27:BA:693:G:N7	42:BR:85:LYS:NZ	2.43	0.65
27:BA:659:U:OP1	67:BA:3195:HOH:O	2.15	0.65
27:BA:2665:A:N7	67:BA:3276:HOH:O	2.28	0.65
6:Af:217:ASP:OD1	6:Af:218:GLU:N	2.29	0.65
27:BA:2160:G:OP1	67:BA:3196:HOH:O	2.15	0.65
1:Aa:1217:C:H6	1:Aa:1217:C:H5''	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2048:G:O6	67:BA:3182:HOH:O	2.12	0.65
27:BA:2817:G:OP2	67:BA:3193:HOH:O	2.14	0.65
31:BE:71:GLU:OE2	67:BE:304:HOH:O	2.14	0.65
38:BN:45:ARG:NH2	38:BN:66:ALA:O	2.30	0.65
38:BM:4:ILE:O	38:BM:4:ILE:HG22	1.97	0.65
58:Bh:21:ARG:NH1	67:Bh:202:HOH:O	2.21	0.65
27:BA:1398:G:O6	67:BA:3189:HOH:O	2.13	0.64
1:Aa:464:5MC:H2'	1:Aa:465:A:O4'	1.97	0.64
23:Aw:16:ARG:NH1	23:Aw:72:TYR:OH	2.29	0.64
27:BA:1180:A:H2	27:BA:2853:G:H22	1.45	0.64
27:BA:719:C:O2'	27:BA:783:U:OP1	2.15	0.64
27:BA:1818:C:OP1	67:BA:3137:HOH:O	2.15	0.64
14:An:110:ARG:NH2	25:Ay:60:GLU:O	2.31	0.64
27:BA:1408:C:OP2	67:BA:3133:HOH:O	2.15	0.64
27:BA:2799:G:N7	67:BA:3284:HOH:O	2.29	0.64
31:BE:33:ARG:NH1	67:BE:301:HOH:O	2.29	0.64
1:Aa:1372:C:O4'	67:Aa:1513:HOH:O	2.15	0.64
27:BA:2369:A:OP2	67:BA:3194:HOH:O	2.14	0.64
27:BA:1747:U:O4	67:BA:3102:HOH:O	2.13	0.64
31:BE:103:GLU:OE1	67:BE:305:HOH:O	2.15	0.64
27:BA:1362:G:N7	67:BA:3290:HOH:O	2.30	0.64
27:BA:160:G:O2'	27:BA:161:U:O4'	2.16	0.64
33:BG:143:ASP:O	33:BG:147:VAL:HG23	1.98	0.64
20:Bm:39:THR:HG22	20:Bm:41:VAL:HG23	1.80	0.63
1:Aa:620:G:OP1	4:Ad:122:ARG:NH1	2.31	0.63
1:Aa:1096:G:H5''	1:Aa:1096:G:H8	1.62	0.63
41:BQ:118:PHE:CD1	41:BQ:137:ILE:HD12	2.34	0.63
1:Aa:724:G:N7	67:Aa:1534:HOH:O	2.31	0.63
27:BA:787:U:O4	67:BA:3166:HOH:O	2.09	0.63
48:BX:87:ASP:OD1	48:BX:88:GLY:N	2.31	0.63
9:Ai:134:GLU:OE2	9:Ai:149:SER:OG	2.15	0.63
23:Aw:72:TYR:OH	23:Aw:82:GLU:OE2	2.17	0.63
35:BJ:19:ARG:NH1	35:BJ:21:GLU:OE2	2.32	0.63
27:BA:1776:OMU:H2'	27:BA:1777:G:O4'	1.99	0.63
45:BU:46:GLU:OE2	45:BU:48:SER:OG	2.16	0.63
57:Bg:70:PRO:O	67:Bg:202:HOH:O	2.16	0.63
59:Bi:20:ASN:ND2	59:Bi:42:ARG:O	2.30	0.63
27:BA:1412:G:OP1	67:BA:3197:HOH:O	2.15	0.62
27:BA:2031:A:N3	27:BA:2032:A:N6	2.46	0.62
52:Bb:81:VAL:HG12	52:Bb:81:VAL:O	1.99	0.62
27:BA:1468:G:OP1	67:BA:3199:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BJ:82:TYR:O	35:BJ:82:TYR:CD1	2.52	0.62
41:BQ:112:THR:OG1	41:BQ:115:SER:OG	2.16	0.62
64:Bp:182:GLU:N	64:Bp:182:GLU:OE1	2.33	0.62
27:BA:1002:G:O2'	27:BA:1003:G:O5'	2.16	0.62
36:BK:9:LEU:HD22	36:BK:118:ALA:O	2.00	0.62
27:BA:36:G:O2'	27:BA:37:A:OP2	2.13	0.62
27:BA:1624:A:HO2'	27:BA:1625:U:C5'	2.10	0.62
1:Aa:548:G:OP2	6:Af:191:LYS:NZ	2.29	0.62
1:Aa:1216:C:H2'	1:Aa:1217:C:H5''	1.80	0.62
1:Aa:1297:U:H2'	1:Aa:1297:U:O2	1.99	0.62
30:BD:5:HIS:NE2	67:BD:402:HOH:O	2.31	0.62
1:Aa:922:G:H5''	1:Aa:923:5MC:HM51	1.81	0.61
4:Ad:42:ASP:OD1	4:Ad:43:ASP:N	2.32	0.61
27:BA:2412:G:O2'	27:BA:2413:A:O4'	2.14	0.61
29:BC:31:VAL:HG12	29:BC:69:LYS:HE3	1.81	0.61
27:BA:1665:G:O6	67:BA:3187:HOH:O	2.13	0.61
34:BI:63:VAL:HG13	34:BI:66:LEU:HD12	1.81	0.61
27:BA:1671:A:H1'	27:BA:1672:U:OP2	2.00	0.61
27:BA:319:G:O2'	63:Bo:34:THR:HG22	2.01	0.61
27:BA:1945:G:OP2	29:BC:29:ARG:NH2	2.32	0.61
27:BA:670:OMG:O3'	27:BA:670:OMG:HM23	1.99	0.60
28:BB:51:G:N3	67:BB:203:HOH:O	2.31	0.60
64:Bp:32:PHE:HB2	64:Bp:43:ILE:HD13	1.83	0.60
1:Aa:917:5MU:H73	1:Aa:917:5MU:OP2	2.02	0.60
22:Av:22:GLU:OE1	22:Av:22:GLU:N	2.34	0.60
27:BA:1849:A:O3'	27:BA:1893:OMG:HM21	2.02	0.60
27:BA:611:G:N7	38:BN:16:ARG:NH1	2.49	0.60
27:BA:1532:U:OP1	67:BA:3205:HOH:O	2.17	0.60
32:BF:42:GLU:OE1	67:BF:201:HOH:O	2.16	0.60
60:Bj:32:ARG:NE	67:Bj:201:HOH:O	2.20	0.60
23:Aw:33:ARG:NH1	23:Aw:90:ASP:OD1	2.34	0.59
43:BS:81:LYS:HG2	43:BS:88:ARG:HH12	1.67	0.59
1:Aa:1320:G:OP2	12:Al:122:SER:OG	2.20	0.59
27:BA:317:G:H5''	27:BA:317:G:C8	2.34	0.59
51:Ba:94:GLU:N	51:Ba:94:GLU:OE1	2.35	0.59
1:Aa:1321:5MC:HM52	12:Al:117:HIS:ND1	2.17	0.59
9:Ai:29:GLU:N	9:Ai:29:GLU:OE2	2.34	0.59
7:Ag:216:ASP:OD1	7:Ag:219:ARG:NH1	2.35	0.59
9:Ai:215:ARG:NH1	25:Ay:58:GLU:OE2	2.35	0.59
27:BA:1150:OMU:OP2	67:BA:3209:HOH:O	2.17	0.59
27:BA:1670:A:H1'	27:BA:1671:A:OP2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2078:C:N3	67:BA:3298:HOH:O	2.31	0.59
64:Bp:138:ASP:OD2	64:Bp:141:LYS:N	2.36	0.59
1:Aa:889:A:C5'	1:Aa:889:A:C8	2.84	0.59
1:Aa:1475:G:N7	14:An:135:ARG:NH1	2.49	0.59
31:BE:180:ARG:NE	31:BE:189:ARG:O	2.36	0.59
27:BA:248:A:OP2	67:BA:3200:HOH:O	2.16	0.59
27:BA:1361:A:OP1	54:Bd:38:TRP:HB3	2.02	0.59
27:BA:2534:A:O2'	27:BA:2535:G:OP2	2.20	0.59
32:BF:45:LEU:O	32:BF:49:VAL:HG22	2.01	0.59
27:BA:196:G:OP2	67:BA:3210:HOH:O	2.17	0.59
30:BD:269:ILE:HD11	30:BD:306:GLU:CG	2.33	0.59
1:Aa:503:C:OP1	67:Aa:1514:HOH:O	2.16	0.59
27:BA:2642:OMG:O3'	27:BA:2642:OMG:HM23	2.03	0.59
39:BO:79:ASN:OD1	39:BO:80:ASP:N	2.35	0.59
1:Aa:293:G:H5''	1:Aa:294:A:OP1	2.03	0.59
1:Aa:917:5MU:H6	1:Aa:917:5MU:O5'	1.85	0.59
1:Aa:1217:C:C5'	1:Aa:1217:C:C6	2.85	0.59
14:An:132:LYS:O	14:An:132:LYS:HG2	2.02	0.59
1:Aa:1096:G:H5''	1:Aa:1096:G:C8	2.38	0.58
6:Af:181:VAL:HG12	6:Af:181:VAL:O	2.04	0.58
3:Ac:64:GLU:OE1	3:Ac:67:ARG:NH2	2.35	0.58
27:BA:1949:U:OP2	67:BA:3204:HOH:O	2.17	0.58
27:BA:3023:C:C6	27:BA:3023:C:C5'	2.85	0.58
45:BU:89:HIS:ND1	45:BU:91:VAL:HG23	2.18	0.58
4:Ad:76:ASP:OD2	4:Ad:78:LYS:NZ	2.35	0.58
30:BD:269:ILE:HD11	30:BD:306:GLU:HG2	1.84	0.58
32:BF:57:ARG:NE	32:BF:70:GLY:O	2.34	0.58
45:BU:9:ARG:NH1	67:BU:102:HOH:O	2.30	0.58
1:Aa:896:G:OP1	67:Aa:1515:HOH:O	2.17	0.58
27:BA:1916:C:OP2	67:BA:3207:HOH:O	2.17	0.58
27:BA:2464:G:OP2	67:BA:3188:HOH:O	2.17	0.58
27:BA:2580:A:H2'	27:BA:2581:4SU:O4'	2.02	0.58
64:Bp:32:PHE:HB2	64:Bp:43:ILE:CD1	2.34	0.58
5:Ae:133:ASN:OD1	5:Ae:134:GLY:N	2.35	0.58
28:BB:40:U:O2'	28:BB:45:A:N6	2.36	0.58
1:Aa:687:G:H5'	17:Aq:98:LEU:HD21	1.86	0.57
27:BA:285:U:O4	67:BA:3206:HOH:O	2.17	0.57
34:BI:6:TYR:OH	34:BI:55:GLU:O	2.22	0.57
1:Aa:1467:MA6:H102	1:Aa:1468:MA6:H103	1.85	0.57
27:BA:1560:C:OP1	38:BM:47:ARG:NH1	2.37	0.57
1:Aa:1084:G:N7	22:Av:2:ALA:HB2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:1383:U:H2'	1:Aa:1384:G:O4'	2.04	0.57
27:BA:147:U:H5''	27:BA:148:G:OP2	2.04	0.57
27:BA:1672:U:OP2	27:BA:1672:U:H4'	2.02	0.57
27:BA:1030:U:HO2'	27:BA:1031:C:P	2.26	0.57
27:BA:257:G:O2'	67:BA:3107:HOH:O	1.92	0.57
27:BA:1381:U:OP1	39:BO:3:ARG:NH1	2.37	0.57
67:BA:3196:HOH:O	46:BV:70:SER:OG	2.15	0.57
32:BF:28:ASN:OD1	32:BF:29:ILE:N	2.37	0.57
1:Aa:269:G:O2'	1:Aa:270:A:OP2	2.17	0.57
13:Am:26:ILE:HG21	13:Am:85:ILE:HG13	1.87	0.57
27:BA:569:G:N7	67:BA:3303:HOH:O	2.32	0.57
31:BE:142:LEU:HD22	31:BE:241:ILE:HG23	1.85	0.57
45:BU:89:HIS:CE1	45:BU:91:VAL:HG23	2.39	0.57
63:Bo:30:ALA:O	63:Bo:34:THR:HG23	2.04	0.57
28:BB:52:A:O2'	28:BB:53:A:O5'	2.22	0.57
1:Aa:1192:U:O2'	9:Ai:91:ARG:O	2.20	0.57
60:Bj:23:THR:O	60:Bj:32:ARG:NH1	2.36	0.57
1:Aa:1163:G:N2	1:Aa:1163:G:OP2	2.38	0.57
57:Bg:29:GLU:OE1	67:Bg:203:HOH:O	2.17	0.56
4:Ad:89:HIS:NE2	4:Ad:192:ILE:HD12	2.20	0.56
6:Af:167:GLN:NE2	6:Af:170:GLU:OE2	2.37	0.56
27:BA:2042:G:OP2	27:BA:2042:G:N2	2.32	0.56
34:BI:39:THR:HG23	34:BI:100:ALA:HB2	1.87	0.56
52:Bb:7:GLU:O	52:Bb:11:VAL:HG23	2.06	0.56
11:Ak:47:ILE:HD11	11:Ak:57:ARG:HG3	1.86	0.56
1:Aa:583:G:O2'	6:Af:203:ARG:NH1	2.37	0.56
3:Ac:171:LEU:HD12	3:Ac:176:ILE:HD12	1.88	0.56
27:BA:564:U:OP1	67:BA:3214:HOH:O	2.17	0.56
1:Aa:351:A:HO2'	1:Aa:352:A2M:P	2.28	0.56
27:BA:55:5MC:HM53	27:BA:205:G:H3'	1.87	0.56
37:BL:84:ARG:NH2	37:BL:121:ALA:O	2.39	0.56
27:BA:2436:A:H5'	27:BA:2438:A:H1'	1.87	0.56
31:BE:123:ASN:OD1	31:BE:124:TYR:N	2.39	0.56
27:BA:2227:G:O2'	27:BA:2229:G:N7	2.24	0.56
4:Ad:26:TYR:O	4:Ad:84:THR:OG1	2.22	0.56
8:Ah:86:ILE:HD11	8:Ah:88:LEU:HD21	1.86	0.56
1:Aa:636:OMG:H2'	1:Aa:637:G:C8	2.40	0.56
35:BJ:163:ARG:NH2	35:BJ:173:THR:HG21	2.20	0.56
7:Ag:49:VAL:HG11	7:Ag:120:ILE:CD1	2.36	0.56
27:BA:1943:U:OP1	67:BA:3212:HOH:O	2.17	0.56
56:Bf:57:VAL:HG22	56:Bf:98:VAL:CG1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:BA:3240:HOH:O	55:Be:28:ARG:NH1	2.38	0.55
46:BV:153:GLU:OE1	46:BV:155:ARG:NH2	2.39	0.55
1:Aa:966:G:OP2	21:Au:65:ARG:NH1	2.39	0.55
29:BC:36:VAL:HG12	29:BC:36:VAL:O	2.07	0.55
51:Ba:51:LYS:NZ	67:Ba:202:HOH:O	2.35	0.55
1:Aa:693:G:O2'	17:Aq:55:ARG:NH2	2.39	0.55
2:Ab:79:VAL:HG12	2:Ab:90:ALA:HB1	1.87	0.55
30:BD:111:ARG:HD2	30:BD:159:LYS:HE3	1.89	0.55
41:BQ:113:ARG:NH1	41:BQ:138:TYR:O	2.31	0.55
1:Aa:840:G:C8	61:Bk:2:LYS:HG3	2.41	0.55
1:Aa:1400:U:H2'	1:Aa:1401:C:C5	2.40	0.55
27:BA:2252:G:N1	27:BA:2264:G:O6	2.40	0.55
23:Bn:50:THR:O	23:Bn:51:THR:OG1	2.22	0.55
27:BA:507:OMG:HM23	31:BE:75:THR:OG1	2.07	0.55
1:Aa:664:G:H2'	1:Aa:665:C:C6	2.42	0.55
2:Ab:170:LEU:O	2:Ab:174:VAL:HG23	2.07	0.55
27:BA:2482:A:HO2'	27:BA:2483:A:P	2.28	0.55
7:Ag:142:PHE:CE1	7:Ag:210:VAL:HG21	2.41	0.55
23:Aw:78:MET:HE1	23:Aw:92:LEU:HD13	1.89	0.55
1:Aa:941:G:O2'	18:Ar:7:ASN:ND2	2.39	0.54
20:At:15:GLU:OE2	20:At:19:ARG:NH1	2.41	0.54
38:BM:2:PRO:O	67:BM:102:HOH:O	2.18	0.54
38:BN:70:GLU:N	38:BN:70:GLU:OE1	2.41	0.54
1:Aa:309:A:N6	1:Aa:317:A:OP2	2.40	0.54
1:Aa:621:U:H2'	1:Aa:622:A:C8	2.43	0.54
1:Aa:962:G:H2'	1:Aa:963:OMG:H5''	1.89	0.54
27:BA:968:G:HO2'	42:BR:2:VAL:N	2.04	0.54
27:BA:2427:5MU:H3'	27:BA:2428:G:C5'	2.35	0.54
27:BA:1671:A:H4'	27:BA:1672:U:O5'	2.07	0.54
37:BL:74:ARG:NH1	67:BL:201:HOH:O	2.30	0.54
27:BA:932:A2M:HM'2	27:BA:934:C:C6	2.43	0.54
27:BA:2687:G:OP2	67:BA:3215:HOH:O	2.18	0.54
51:Ba:8:ARG:NH1	51:Ba:28:LEU:O	2.38	0.54
27:BA:303:U:H1'	27:BA:304:A:OP2	2.08	0.54
1:Aa:1052:G:OP1	3:Ac:153:LYS:N	2.40	0.54
1:Aa:1092:G:H5''	1:Aa:1092:G:C8	2.37	0.54
6:Af:138:VAL:HB	6:Af:150:VAL:HG23	1.90	0.54
23:Aw:53:ILE:HG22	23:Aw:54:GLN:O	2.08	0.54
27:BA:2573:A:N6	27:BA:2585:G:O2'	2.39	0.54
6:Af:195:ARG:NH2	6:Af:221:GLU:OE1	2.41	0.54
11:Ak:4:TRP:NE1	11:Ak:27:GLU:OE1	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Ax:45:THR:HG21	24:Ax:48:GLU:OE2	2.08	0.54
27:BA:434:G:HO2'	40:BP:91:SER:HG	1.51	0.54
27:BA:452:A:OP2	67:BA:3164:HOH:O	2.18	0.54
27:BA:1134:C:OP1	67:BA:3217:HOH:O	2.18	0.54
64:Bp:64:MET:SD	64:Bp:76:VAL:HG21	2.47	0.54
27:BA:2527:OMG:HM22	27:BA:2528:OMG:H5'	1.90	0.54
1:Aa:703:U:H2'	1:Aa:704:G:O4'	2.08	0.53
11:Ak:91:ARG:NH1	67:Ak:202:HOH:O	2.35	0.53
12:Al:131:GLN:OE1	12:Al:133:SER:OG	2.26	0.53
41:BQ:43:HIS:ND1	41:BQ:64:THR:OG1	2.33	0.53
64:Bp:33:LYS:HD3	64:Bp:81:LEU:O	2.08	0.53
1:Aa:863:A:H1'	1:Aa:864:A:OP2	2.09	0.53
23:Aw:54:GLN:HE22	23:Aw:86:ILE:HD13	1.73	0.53
27:BA:315:A:H2'	27:BA:316:G:C8	2.43	0.53
27:BA:471:U:HO2'	27:BA:472:A:P	2.32	0.53
27:BA:2239:G:O2'	27:BA:2240:G:P	2.66	0.53
53:Bc:61:ARG:NH1	67:Bc:101:HOH:O	2.32	0.53
27:BA:1469:C:OP2	67:BA:3219:HOH:O	2.18	0.53
27:BA:1907:U:OP2	27:BA:1912:A:N6	2.38	0.53
1:Aa:904:G:N7	16:Ap:133:ARG:NH1	2.47	0.53
1:Aa:1190:A:N7	1:Aa:1251:A:N6	2.56	0.53
2:Ab:110:GLU:OE2	7:Ag:20:LYS:N	2.40	0.53
7:Ag:149:GLY:O	7:Ag:152:ARG:NH1	2.40	0.53
27:BA:1624:A:O2'	27:BA:1625:U:O4'	2.27	0.53
45:BU:61:ARG:NH2	67:BU:103:HOH:O	2.40	0.53
1:Aa:1006:5MC:H2'	1:Aa:1007:5MC:C5'	2.33	0.53
12:Al:12:THR:HG22	12:Al:12:THR:O	2.09	0.53
1:Aa:884:C:H2'	1:Aa:884:C:O2	2.08	0.53
33:BG:90:LEU:HD23	33:BG:174:ILE:HA	1.91	0.53
1:Aa:622:A:H2'	1:Aa:623:C:H6	1.73	0.53
13:Am:26:ILE:HG21	13:Am:85:ILE:CG1	2.39	0.53
27:BA:2215:G:N1	27:BA:2216:G:O6	2.41	0.53
1:Aa:889:A:H5''	1:Aa:889:A:C8	2.41	0.53
27:BA:872:OMG:HN1	27:BA:881:U:H3	1.57	0.53
27:BA:2297:C:H2'	27:BA:2298:U:N1	2.23	0.53
27:BA:2829:C:OP1	67:BA:3223:HOH:O	2.19	0.53
1:Aa:292:G:H2'	1:Aa:293:G:O4'	2.09	0.52
1:Aa:316:C:H1'	1:Aa:317:A:OP2	2.10	0.52
52:Bb:40:ARG:O	52:Bb:47:LYS:NZ	2.24	0.52
8:Ah:76:PRO:O	8:Ah:110:ASN:ND2	2.39	0.52
9:Ai:98:MET:SD	9:Ai:98:MET:N	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Bg:47:ARG:NH2	57:Bg:57:GLN:OE1	2.43	0.52
20:Bm:39:THR:CG2	20:Bm:41:VAL:HG23	2.40	0.52
1:Aa:960:C:HO2'	1:Aa:961:A:P	2.32	0.52
27:BA:2571:C:O2'	27:BA:2572:G:O5'	2.19	0.52
1:Aa:269:G:O2'	1:Aa:270:A:P	2.68	0.52
18:Ar:24:CYS:SG	18:Ar:25:GLY:N	2.83	0.52
38:BN:4:ILE:HG22	38:BN:4:ILE:O	2.09	0.52
41:BQ:8:ARG:NE	45:BU:22:ARG:O	2.42	0.52
1:Aa:349:5MC:H2'	1:Aa:350:G:O4'	2.10	0.52
1:Aa:451:G:H5''	1:Aa:452:C:H2'	1.92	0.52
1:Aa:1084:G:H21	1:Aa:1085:C:H42	1.56	0.52
15:Ao:54:VAL:HG13	15:Ao:73:VAL:CG2	2.40	0.52
27:BA:437:G:OP2	40:BP:68:ARG:NH2	2.42	0.52
1:Aa:1257:G:H1'	1:Aa:1284:A:N6	2.25	0.52
3:Ac:28:ALA:HB2	3:Ac:53:TYR:HB3	1.91	0.52
12:Al:42:ARG:CG	12:Al:46:MET:HE2	2.39	0.52
15:Ao:100:HIS:O	64:Bp:116:ARG:NH1	2.41	0.52
38:BN:22:VAL:HA	38:BN:37:GLY:HA2	1.90	0.52
1:Aa:1447:U:H1'	1:Aa:1448:A:OP2	2.10	0.52
27:BA:1685:G:O6	43:BS:46:HIS:NE2	2.40	0.52
27:BA:2533:C:OP1	67:BA:3218:HOH:O	2.18	0.52
27:BA:2891:A:O2'	27:BA:3026:G:N2	2.39	0.52
31:BE:123:ASN:O	31:BE:127:VAL:HG23	2.09	0.52
34:BH:61:GLU:OE1	34:BH:61:GLU:N	2.38	0.52
27:BA:2025:A:H62	27:BA:2030:U:H3	1.57	0.52
63:Bo:17:LEU:HD13	63:Bo:26:VAL:HG11	1.92	0.52
1:Aa:467:C:N4	15:Ao:70:ARG:HH22	2.03	0.51
1:Aa:1376:G:H2'	1:Aa:1377:U:O4'	2.10	0.51
19:As:37:VAL:HG13	19:As:46:VAL:HG13	1.92	0.51
27:BA:2496:C:O2'	67:BA:3145:HOH:O	2.04	0.51
1:Aa:525:C:H2'	1:Aa:526:G:O4'	2.09	0.51
23:Aw:47:ASP:OD1	23:Aw:49:ASN:N	2.43	0.51
27:BA:2882:C:H2'	27:BA:2882:C:O2	2.10	0.51
32:BF:25:VAL:CG2	32:BF:84:ALA:HB1	2.40	0.51
34:BH:112:GLU:OE2	34:BH:116:MET:HE3	2.10	0.51
1:Aa:1024:A:OP1	7:Ag:101:HIS:NE2	2.36	0.51
5:Ae:132:VAL:O	5:Ae:134:GLY:N	2.43	0.51
27:BA:314:G:H2'	27:BA:315:A:O4'	2.10	0.51
27:BA:404:G:O2'	27:BA:405:U:P	2.69	0.51
34:BH:10:GLU:O	34:BH:121:LEU:HD21	2.10	0.51
1:Aa:921:C:H4'	1:Aa:923:5MC:HM52	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:341:C:C6	27:BA:341:C:C5'	2.85	0.51
27:BA:1178:A:HO2'	27:BA:1179:G:P	2.31	0.51
27:BA:2562:C:OP2	67:BA:3220:HOH:O	2.19	0.51
29:BC:85:ILE:HG23	29:BC:96:THR:HB	1.93	0.51
37:BL:108:THR:HG22	37:BL:109:PRO:HD2	1.92	0.51
38:BM:22:VAL:HG11	38:BM:35:VAL:CG1	2.40	0.51
60:Bj:24:ASN:HA	67:Bj:201:HOH:O	2.11	0.51
60:Bj:31:CYS:SG	60:Bj:32:ARG:N	2.83	0.51
27:BA:1113:C:OP2	51:Ba:14:ARG:NH1	2.44	0.51
27:BA:482:A:O2'	27:BA:1336:C:O2'	2.12	0.51
34:BI:32:ILE:HG22	34:BI:33:ARG:N	2.26	0.51
47:BW:11:LEU:HD12	47:BW:27:THR:HG22	1.92	0.51
1:Aa:16:G:H2'	1:Aa:17:5MC:C6	2.46	0.51
27:BA:661:G:O6	67:BA:3201:HOH:O	2.16	0.51
27:BA:879:A2M:OP1	67:BA:3108:HOH:O	2.19	0.51
27:BA:1660:U:H2'	27:BA:1661:G:O4'	2.11	0.51
33:BG:155:GLU:OE2	33:BG:174:ILE:N	2.34	0.51
47:BW:12:VAL:HG13	47:BW:12:VAL:O	2.11	0.51
1:Aa:1218:G:N7	22:Av:99:ARG:NH2	2.59	0.51
1:Aa:1321:5MC:HM52	12:Al:117:HIS:CE1	2.46	0.51
5:Ae:50:GLU:OE2	5:Ae:53:ARG:NH1	2.44	0.51
27:BA:2835:A:C2'	27:BA:2836:G:O4'	2.58	0.51
46:BV:70:SER:OG	46:BV:70:SER:O	2.25	0.51
1:Aa:1092:G:H8	1:Aa:1092:G:C5'	2.23	0.51
27:BA:2469:OMG:H8	27:BA:2469:OMG:H5''	1.76	0.51
29:BC:108:VAL:CG1	29:BC:157:ALA:HB1	2.41	0.51
1:Aa:851:A:O5'	1:Aa:851:A:H8	1.94	0.50
27:BA:2268:G:H4'	27:BA:2269:G:OP1	2.11	0.50
30:BD:278:VAL:O	30:BD:334:ARG:NH2	2.44	0.50
40:BP:157:ARG:HA	40:BP:162:LEU:HD12	1.92	0.50
1:Aa:192:A:OP2	67:Aa:1517:HOH:O	2.20	0.50
27:BA:317:G:C8	27:BA:317:G:C5'	2.94	0.50
27:BA:920:G:OP2	67:BA:3224:HOH:O	2.19	0.50
27:BA:2745:OMG:HM22	27:BA:2746:G:H5'	1.93	0.50
27:BA:2892:C:O2'	27:BA:3027:U:OP1	2.28	0.50
27:BA:997:U:H2'	27:BA:998:G:O4'	2.11	0.50
27:BA:2836:G:HO2'	27:BA:2837:C:P	2.29	0.50
41:BQ:106:ILE:HD12	41:BQ:117:ILE:HG21	1.92	0.50
1:Aa:51:A:OP2	1:Aa:340:5MC:HM51	2.11	0.50
8:Ah:51:PHE:CE2	8:Ah:123:ILE:CD1	2.87	0.50
27:BA:1799:G:N2	53:Bc:22:VAL:HG12	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BP:144:PRO:O	67:BP:201:HOH:O	2.18	0.50
27:BA:1683:A:O2'	27:BA:1684:A:O4'	2.27	0.50
27:BA:1691:U:HO2'	27:BA:1692:U:P	2.28	0.50
27:BA:2936:A2M:H5'	67:BA:5614:HOH:O	2.11	0.50
27:BA:365:OMG:HM22	27:BA:366:G:H5'	1.93	0.50
27:BA:621:G:N7	67:BA:3308:HOH:O	2.33	0.50
61:Bk:18:TRP:CE3	61:Bk:18:TRP:HA	2.47	0.50
64:Bp:104:ILE:HD11	64:Bp:143:ALA:HB1	1.94	0.50
1:Aa:1020:OMU:HN3	1:Aa:1025:G:H1	1.59	0.50
1:Aa:1374:G:H2'	1:Aa:1375:G:O4'	2.12	0.50
6:Af:38:SER:O	6:Af:42:SER:OG	2.20	0.50
27:BA:1482:G:O2'	27:BA:1516:A:N3	2.45	0.50
32:BF:49:VAL:HG23	32:BF:50:GLY:N	2.26	0.50
64:Bp:10:ILE:HD11	64:Bp:53:ALA:HB3	1.94	0.50
1:Aa:697:C:H2'	1:Aa:698:G:O4'	2.12	0.50
1:Aa:1097:C:H4'	1:Aa:1098:A:O5'	2.12	0.50
1:Aa:1257:G:H5''	22:Av:84:GLY:CA	2.31	0.50
27:BA:1759:A:N6	46:BV:136:ARG:O	2.45	0.50
30:BD:61:THR:HG22	30:BD:61:THR:O	2.12	0.50
5:Ae:12:GLU:OE1	5:Ae:49:LYS:NZ	2.44	0.49
9:Ai:187:GLU:OE2	9:Ai:198:SER:OG	2.24	0.49
30:BD:45:LYS:O	30:BD:313:PHE:O	2.30	0.49
1:Aa:1297:U:O2	1:Aa:1297:U:C2'	2.60	0.49
1:Aa:1188:A:OP1	67:Aa:1516:HOH:O	2.20	0.49
23:Aw:3:ILE:HD12	23:Aw:39:LYS:HG2	1.95	0.49
27:BA:45:G:OP2	67:BA:3225:HOH:O	2.20	0.49
1:Aa:120:G:H2'	1:Aa:121:OMG:H5''	1.93	0.49
1:Aa:931:C:O2	18:Ar:17:GLY:N	2.41	0.49
3:Ac:193:ILE:CD1	20:At:12:THR:HG21	2.30	0.49
12:Al:27:ARG:NH1	22:Av:6:ASP:OD1	2.43	0.49
27:BA:1670:A:O2'	27:BA:1671:A:OP2	2.29	0.49
27:BA:687:A:H2'	27:BA:688:G:C8	2.47	0.49
1:Aa:316:C:O2	1:Aa:316:C:H2'	2.12	0.49
27:BA:2176:C:H2'	27:BA:2177:C:C6	2.47	0.49
39:BO:32:GLY:O	39:BO:45:GLN:NE2	2.46	0.49
48:BX:96:HIS:CE1	48:BX:98:SER:HG	2.28	0.49
1:Aa:888:A:H2'	1:Aa:889:A:H5''	1.95	0.49
15:Ao:70:ARG:NH2	15:Ao:118:ASP:OD2	2.43	0.49
27:BA:1358:G:N2	27:BA:1360:G:H3'	2.28	0.49
27:BA:2000:U:H2'	27:BA:2001:G:O4'	2.12	0.49
27:BA:2550:OMG:HM22	27:BA:2605:5MC:CM5	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BD:292:PHE:O	30:BD:295:TYR:O	2.31	0.49
1:Aa:661:A:H2'	1:Aa:662:C:C6	2.47	0.49
1:Aa:1430:U:O2'	1:Aa:1431:G:P	2.71	0.49
1:Aa:1430:U:O2'	1:Aa:1431:G:O5'	2.28	0.49
6:Af:118:GLU:OE1	6:Af:118:GLU:N	2.46	0.49
7:Ag:49:VAL:HG11	7:Ag:120:ILE:HD12	1.94	0.49
28:BB:42:U:O2'	32:BF:52:LYS:O	2.27	0.49
32:BF:104:PHE:CD1	32:BF:110:PHE:HB3	2.48	0.49
34:BI:18:LYS:HD2	34:BI:110:LEU:HD12	1.94	0.49
56:Bf:16:VAL:O	56:Bf:16:VAL:HG12	2.12	0.49
64:Bp:72:ASP:OD1	64:Bp:74:TYR:N	2.45	0.49
11:Ak:3:ILE:HD12	11:Ak:3:ILE:H	1.78	0.49
27:BA:2758:C:OP2	37:BL:2:ALA:N	2.46	0.49
38:BN:46:ARG:NH2	67:BN:101:HOH:O	2.29	0.49
1:Aa:63:G:H2'	1:Aa:64:G:C8	2.48	0.49
1:Aa:1082:C:H2'	1:Aa:1083:C:C6	2.48	0.49
27:BA:636:U:H2'	27:BA:637:G:O4'	2.12	0.49
27:BA:2252:G:N2	27:BA:2253:C:H41	2.10	0.49
27:BA:1910:U:OP1	67:BA:3226:HOH:O	2.20	0.48
47:BW:38:ASP:OD1	47:BW:41:ARG:NH1	2.46	0.48
1:Aa:622:A:H2'	1:Aa:623:C:C6	2.48	0.48
1:Aa:840:G:OP2	61:Bk:7:LYS:HE3	2.13	0.48
27:BA:968:G:O2'	42:BR:2:VAL:N	2.46	0.48
27:BA:2529:A:O2'	27:BA:2530:U:OP2	2.22	0.48
41:BQ:67:LEU:HD23	41:BQ:89:LEU:HD11	1.95	0.48
64:Bp:22:ILE:HG22	64:Bp:23:LEU:N	2.28	0.48
64:Bp:210:VAL:HG23	64:Bp:210:VAL:O	2.12	0.48
27:BA:1565:C:O2	67:BA:3198:HOH:O	2.16	0.48
16:Ap:117:ARG:HG2	16:Ap:127:VAL:CG1	2.44	0.48
31:BE:29:ASP:OD1	31:BE:30:LEU:N	2.46	0.48
64:Bp:50:PHE:HA	64:Bp:58:LYS:HA	1.95	0.48
27:BA:2312:C:H6	27:BA:2312:C:O5'	1.95	0.48
27:BA:2571:C:O2'	27:BA:2572:G:P	2.72	0.48
1:Aa:964:C:OP1	21:Au:62:LYS:NZ	2.44	0.48
2:Ab:117:THR:O	2:Ab:157:ASN:ND2	2.43	0.48
27:BA:2252:G:O2'	27:BA:2253:C:O5'	2.30	0.48
27:BA:2260:G:O2'	27:BA:2261:G:O4'	2.26	0.48
29:BC:104:GLU:OE1	29:BC:104:GLU:N	2.44	0.48
34:BI:63:VAL:HG12	34:BI:63:VAL:O	2.13	0.48
42:BR:65:VAL:HG12	42:BR:67:GLY:H	1.78	0.48
61:Bk:18:TRP:HA	61:Bk:18:TRP:HE3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Bm:41:VAL:O	20:Bm:47:ARG:NH2	2.38	0.48
1:Aa:963:OMG:HN1	1:Aa:971:U:H3	1.61	0.48
27:BA:687:A:O2'	27:BA:688:G:P	2.72	0.48
32:BF:25:VAL:HG21	32:BF:84:ALA:HB1	1.96	0.48
8:Ah:85:LYS:HG2	8:Ah:104:LYS:HD2	1.96	0.48
27:BA:690:G:O2'	67:BE:301:HOH:O	2.04	0.48
42:BR:23:SER:OG	42:BR:28:VAL:O	2.31	0.48
1:Aa:1170:C:C2'	1:Aa:1171:C:H5'	2.44	0.48
1:Aa:1358:OMU:O4	67:Aa:1518:HOH:O	2.20	0.48
7:Ag:75:ASP:OD1	7:Ag:75:ASP:N	2.47	0.48
27:BA:1773:G:N2	43:BS:58:GLN:OE1	2.46	0.48
1:Aa:931:C:OP2	67:Aa:1501:HOH:O	2.20	0.48
1:Aa:1302:C:N3	9:Ai:95:SER:OG	2.46	0.48
21:Au:52:ILE:HD13	21:Au:77:MET:SD	2.54	0.48
12:Al:6:THR:HG22	12:Al:7:ALA:N	2.29	0.47
19:As:85:VAL:CG2	19:As:101:VAL:HG13	2.44	0.47
27:BA:2038:U:H2'	27:BA:2038:U:O2	2.13	0.47
28:BB:56:U:H4'	28:BB:57:A:O5'	2.14	0.47
29:BC:185:ARG:O	29:BC:187:ARG:N	2.45	0.47
30:BD:84:ARG:NE	30:BD:98:GLU:OE2	2.47	0.47
41:BQ:104:LEU:HD21	41:BQ:106:ILE:HD11	1.95	0.47
42:BR:33:ASP:HA	42:BR:36:TRP:CD1	2.49	0.47
1:Aa:539:U:H2'	1:Aa:540:A:O4'	2.14	0.47
1:Aa:1087:G:H8	1:Aa:1087:G:H5''	1.79	0.47
13:Am:4:ALA:HB3	13:Am:75:ILE:CG2	2.44	0.47
27:BA:527:G:N2	27:BA:530:A:OP2	2.45	0.47
27:BA:2482:A:O2'	27:BA:2483:A:P	2.72	0.47
46:BV:47:ASP:OD1	46:BV:50:ARG:NH2	2.42	0.47
55:Be:10:TRP:O	55:Be:27:GLU:O	2.32	0.47
27:BA:588:U:H3'	27:BA:589:G:H5'	1.97	0.47
34:BI:25:ILE:O	34:BI:29:THR:HG22	2.15	0.47
1:Aa:519:A:OP2	67:Aa:1519:HOH:O	2.20	0.47
1:Aa:725:C:H2'	1:Aa:726:G:O4'	2.14	0.47
7:Ag:169:VAL:HG21	7:Ag:193:THR:HG23	1.96	0.47
18:Ar:32:ARG:O	18:Ar:32:ARG:HG2	2.14	0.47
27:BA:598:C:H2'	27:BA:599:G:O4'	2.15	0.47
27:BA:1463:C:H2'	27:BA:1464:G:O4'	2.14	0.47
27:BA:1681:G:N2	27:BA:1684:A:H61	2.12	0.47
27:BA:2252:G:HO2'	27:BA:2253:C:C5'	2.28	0.47
67:BA:4123:HOH:O	39:BO:9:ARG:HD3	2.15	0.47
38:BN:26:ASP:OD1	38:BN:27:ILE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:818:C:H2'	1:Aa:819:G:O4'	2.15	0.47
1:Aa:1045:A:H4'	1:Aa:1046:A:O5'	2.15	0.47
6:Af:3:ARG:CZ	6:Af:7:LYS:HE3	2.45	0.47
27:BA:670:OMG:H5'	27:BA:2131:U:H5''	1.97	0.47
37:BL:98:LYS:NZ	49:BY:38:GLU:OE2	2.43	0.47
52:Bb:76:GLY:N	67:Bb:201:HOH:O	2.37	0.47
27:BA:657:OMU:H2'	27:BA:658:C:C6	2.50	0.47
27:BA:1353:G:OP1	67:BA:3229:HOH:O	2.20	0.47
27:BA:1411:A:OP2	67:BA:3230:HOH:O	2.20	0.47
27:BA:2267:U:O2	27:BA:2267:U:H2'	2.14	0.47
13:Am:30:THR:OG1	13:Am:80:ARG:NH1	2.48	0.47
27:BA:1928:C:H1'	27:BA:1929:U:OP2	2.14	0.47
1:Aa:490:C:H2'	1:Aa:491:G:O4'	2.15	0.47
27:BA:1691:U:O2'	27:BA:1692:U:P	2.73	0.47
27:BA:2176:C:H2'	27:BA:2177:C:H6	1.79	0.47
33:BG:6:TRP:O	33:BG:7:ILE:C	2.57	0.47
38:BM:70:GLU:OE1	38:BM:70:GLU:N	2.44	0.47
1:Aa:1270:A:O2'	21:Au:70:ASP:OD2	2.33	0.46
27:BA:996:C:OP2	67:BA:3231:HOH:O	2.21	0.46
27:BA:2297:C:H2'	27:BA:2298:U:C6	2.50	0.46
57:Bg:12:ARG:NH1	67:Bg:203:HOH:O	2.48	0.46
1:Aa:1153:A:H4'	1:Aa:1154:G:H5''	1.98	0.46
27:BA:2250:C:H2'	27:BA:2251:C:C6	2.50	0.46
28:BB:45:A:OP1	32:BF:80:ARG:NH1	2.48	0.46
38:BM:22:VAL:HG11	38:BM:35:VAL:HG13	1.96	0.46
54:Bd:89:GLU:O	54:Bd:90:ALA:HB3	2.15	0.46
63:Bo:4:LEU:HD13	63:Bo:37:VAL:HG13	1.97	0.46
1:Aa:662:C:H2'	1:Aa:663:C:C6	2.50	0.46
1:Aa:942:C:O2	1:Aa:1165:A:N6	2.48	0.46
1:Aa:1361:OMC:H1'	1:Aa:1361:OMC:HM23	1.69	0.46
8:Ah:75:ARG:NH2	8:Ah:92:PRO:O	2.46	0.46
27:BA:1462:U:H5'	27:BA:2124:OMC:HM23	1.96	0.46
27:BA:1671:A:C1'	27:BA:1672:U:OP2	2.64	0.46
32:BF:23:ALA:HB3	32:BF:139:THR:HG23	1.96	0.46
39:BO:41:LYS:O	39:BO:42:ARG:HG2	2.15	0.46
5:Ae:132:VAL:O	5:Ae:133:ASN:C	2.58	0.46
23:Aw:34:GLU:OE1	23:Aw:34:GLU:N	2.42	0.46
33:BG:143:ASP:OD1	33:BG:146:ALA:HB3	2.15	0.46
34:BH:86:LEU:HD21	34:BH:99:VAL:HG23	1.98	0.46
47:BW:3:PRO:O	47:BW:4:TYR:HB2	2.14	0.46
52:Bb:30:VAL:HG12	52:Bb:30:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ag:38:ARG:NH1	7:Ag:122:GLU:OE1	2.38	0.46
9:Ai:25:ASP:OD1	9:Ai:25:ASP:N	2.48	0.46
27:BA:670:OMG:O3'	27:BA:670:OMG:CM2	2.62	0.46
27:BA:1672:U:O2'	27:BA:1673:G:OP2	2.30	0.46
27:BA:2642:OMG:H4'	27:BA:2642:OMG:CM2	2.41	0.46
32:BF:95:VAL:HG11	32:BF:114:ILE:HG22	1.97	0.46
38:BM:27:ILE:HG12	38:BM:33:VAL:HG12	1.98	0.46
43:BS:4:LEU:HA	43:BS:7:GLN:OE1	2.16	0.46
45:BU:31:PHE:HA	45:BU:91:VAL:HG22	1.97	0.46
1:Aa:238:A:H4'	1:Aa:239:G:O5'	2.16	0.46
1:Aa:636:OMG:HM23	1:Aa:636:OMG:H1'	1.50	0.46
1:Aa:891:OMG:HM23	1:Aa:891:OMG:H1'	1.55	0.46
27:BA:2124:OMC:HM23	27:BA:2124:OMC:H1'	1.52	0.46
1:Aa:1006:5MC:O2'	1:Aa:1007:5MC:H5''	2.16	0.46
25:Ay:44:VAL:HG11	25:Ay:48:VAL:HG11	1.98	0.46
27:BA:730:C:H2'	27:BA:731:G:O4'	2.16	0.46
27:BA:2394:U:OP1	27:BA:2486:C:O2'	2.34	0.46
32:BF:44:MET:HE2	32:BF:132:PHE:CB	2.46	0.46
42:BR:12:LEU:HG	42:BR:84:TRP:CZ2	2.50	0.46
64:Bp:143:ALA:HA	64:Bp:146:GLN:HG2	1.98	0.46
1:Aa:1086:U:H1'	1:Aa:1087:G:C8	2.51	0.46
1:Aa:1350:A:OP2	67:Aa:1520:HOH:O	2.20	0.46
1:Aa:1397:C:C2'	1:Aa:1398:C:H5'	2.46	0.46
11:Ak:26:ARG:O	67:Ak:201:HOH:O	2.21	0.46
27:BA:544:A:N3	67:BA:3340:HOH:O	2.36	0.46
28:BB:52:A:HO2'	28:BB:53:A:P	2.39	0.46
1:Aa:1178:C:OP2	16:Ap:132:THR:OG1	2.30	0.46
3:Ac:155:GLY:O	3:Ac:158:ALA:HB3	2.16	0.46
27:BA:149:C:H2'	27:BA:150:C:C6	2.51	0.46
27:BA:1329:OMG:HM22	27:BA:1330:G:O4'	2.16	0.46
32:BF:44:MET:HE2	32:BF:132:PHE:CG	2.51	0.46
1:Aa:1091:A:H2'	1:Aa:1092:G:H5''	1.98	0.45
2:Ab:24:THR:HG22	2:Ab:25:LYS:N	2.32	0.45
27:BA:14:G:H2'	27:BA:15:U:O4'	2.15	0.45
27:BA:2640:OMG:H1'	27:BA:2640:OMG:HM23	1.67	0.45
31:BE:33:ARG:NH1	31:BE:109:GLU:OE1	2.48	0.45
32:BF:104:PHE:HE2	32:BF:169:ILE:HA	1.80	0.45
34:BI:29:THR:HG23	34:BI:30:GLY:N	2.31	0.45
48:BX:48:VAL:O	48:BX:66:VAL:HB	2.15	0.45
1:Aa:243:G:OP2	67:Aa:1522:HOH:O	2.21	0.45
16:Ap:11:VAL:HG12	16:Ap:12:ALA:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:657:OMU:H1'	27:BA:657:OMU:HM23	1.55	0.45
27:BA:1979:U:H2'	27:BA:1980:G:O4'	2.16	0.45
27:BA:2107:OMC:OP2	67:BA:3234:HOH:O	2.21	0.45
27:BA:2958:U:C3'	27:BA:2959:U:H5'	2.45	0.45
51:Ba:82:ASP:OD1	51:Ba:83:GLU:N	2.49	0.45
1:Aa:606:G:H2'	1:Aa:607:G:C8	2.51	0.45
6:Af:237:LYS:HD2	6:Af:238:PRO:O	2.17	0.45
12:Al:6:THR:HG22	12:Al:7:ALA:H	1.81	0.45
27:BA:2035:C:H2'	27:BA:2036:U:O4'	2.16	0.45
27:BA:2338:U:H2'	27:BA:2339:G:O4'	2.17	0.45
38:BM:4:ILE:O	38:BM:4:ILE:CG2	2.64	0.45
38:BM:18:ALA:HB3	55:Be:67:PRO:HG3	1.98	0.45
1:Aa:92:C:H2'	1:Aa:93:U:C6	2.51	0.45
10:Aj:28:LYS:HB3	10:Aj:29:PRO:HD3	1.98	0.45
27:BA:231:U:OP1	67:BA:3233:HOH:O	2.21	0.45
27:BA:1002:G:O2'	27:BA:1003:G:P	2.74	0.45
27:BA:1864:U:H2'	27:BA:1865:G:O4'	2.17	0.45
27:BA:2876:C:H2'	27:BA:2877:G:O4'	2.17	0.45
1:Aa:351:A:O2'	1:Aa:352:A2M:P	2.73	0.45
6:Af:214:THR:HG23	6:Af:224:ASP:OD1	2.16	0.45
27:BA:712:C:OP2	31:BE:110:ARG:NH1	2.49	0.45
27:BA:1145:C:OP1	33:BG:61:ARG:NH2	2.49	0.45
27:BA:3034:G:H2'	27:BA:3035:G:O4'	2.16	0.45
1:Aa:546:C:H2'	1:Aa:547:U:O4'	2.16	0.45
27:BA:1242:G:N3	27:BA:1242:G:H2'	2.31	0.45
27:BA:1969:OMU:H2'	27:BA:1970:G:O4'	2.17	0.45
1:Aa:316:C:O2'	1:Aa:317:A:P	2.74	0.45
1:Aa:703:U:OP1	1:Aa:768:C:O2'	2.35	0.45
9:Ai:47:SER:N	9:Ai:65:GLU:OE1	2.43	0.45
35:BJ:33:ILE:HG22	35:BJ:36:MET:SD	2.57	0.45
46:BV:22:SER:OG	46:BV:24:ARG:NE	2.49	0.45
52:Bb:19:MET:HB2	52:Bb:81:VAL:HG13	1.99	0.45
1:Aa:1092:G:C8	1:Aa:1092:G:C5'	2.98	0.45
27:BA:1750:C:H2'	27:BA:1751:G:O4'	2.16	0.45
27:BA:2220:G:H2'	27:BA:2221:U:O4'	2.17	0.45
27:BA:2642:OMG:CM2	27:BA:2642:OMG:C4'	2.95	0.45
28:BB:4:A:H2	28:BB:22:G:H21	1.63	0.45
38:BN:22:VAL:HB	38:BN:35:VAL:HG22	1.98	0.45
1:Aa:621:U:H2'	1:Aa:622:A:H8	1.80	0.45
27:BA:1524:C:OP1	67:BA:3235:HOH:O	2.21	0.45
27:BA:2650:U:OP1	67:BA:3232:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BF:176:LEU:O	32:BF:177:LYS:CG	2.64	0.45
34:BH:93:GLU:OE1	34:BH:93:GLU:N	2.50	0.45
1:Aa:54:C:O5'	1:Aa:54:C:H6	2.00	0.45
1:Aa:1020:OMU:HM23	1:Aa:1020:OMU:H1'	1.76	0.45
27:BA:42:U:OP2	31:BE:186:MET:HG2	2.18	0.45
27:BA:699:A:H2'	27:BA:700:A:C8	2.52	0.45
27:BA:2171:A:H2'	27:BA:2172:A:O4'	2.17	0.45
27:BA:2219:G:N1	27:BA:2295:C:O2	2.50	0.45
27:BA:2231:A:H3'	27:BA:2232:G:H5''	1.98	0.45
30:BD:244:ALA:O	30:BD:245:ARG:HG3	2.17	0.45
54:Bd:27:TRP:HA	54:Bd:33:LYS:HD3	1.98	0.45
5:Ae:132:VAL:HG12	5:Ae:133:ASN:N	2.30	0.44
27:BA:55:5MC:HM51	27:BA:205:G:H8	1.82	0.44
27:BA:974:A:H1'	27:BA:975:G:OP2	2.17	0.44
27:BA:2642:OMG:HM22	27:BA:2642:OMG:C4'	2.44	0.44
64:Bp:32:PHE:CD2	64:Bp:81:LEU:HD13	2.52	0.44
8:Ah:68:ASP:HA	8:Ah:116:ILE:HA	2.00	0.44
27:BA:739:C:H2'	27:BA:740:G:O4'	2.17	0.44
27:BA:1337:C:H5''	31:BE:189:ARG:HD3	1.98	0.44
27:BA:1360:G:H2'	27:BA:1361:A:C8	2.52	0.44
27:BA:1882:C:N3	27:BA:2819:C:O2'	2.51	0.44
27:BA:1993:A:H2'	27:BA:1994:A:O4'	2.17	0.44
27:BA:2039:U:H3	27:BA:2042:G:H22	1.65	0.44
27:BA:2412:G:H2'	27:BA:2413:A:C8	2.51	0.44
33:BG:5:ALA:O	33:BG:58:GLU:O	2.34	0.44
1:Aa:1324:C:O2	9:Ai:95:SER:HB3	2.16	0.44
27:BA:1014:G:H22	27:BA:1024:U:H3	1.66	0.44
27:BA:2420:C:H2'	27:BA:2421:G:O4'	2.18	0.44
32:BF:176:LEU:O	32:BF:177:LYS:HG2	2.17	0.44
35:BJ:18:THR:O	35:BJ:19:ARG:CG	2.65	0.44
42:BR:7:PRO:O	42:BR:13:ARG:NE	2.50	0.44
51:Ba:120:HIS:HB2	51:Ba:121:PRO:HD2	1.98	0.44
1:Aa:542:G:OP2	67:Aa:1523:HOH:O	2.21	0.44
4:Ad:95:TYR:OH	4:Ad:186:ARG:NH2	2.49	0.44
17:Aq:60:ILE:HG23	17:Aq:66:ILE:HD12	1.99	0.44
27:BA:2053:U:C2'	27:BA:2054:C:OP2	2.65	0.44
32:BF:68:ARG:HD2	32:BF:71:GLU:HB3	1.99	0.44
32:BF:142:ARG:HB3	32:BF:143:PRO:HD2	1.99	0.44
39:BO:82:ASP:OD1	39:BO:120:THR:OG1	2.36	0.44
39:BO:122:ALA:HB1	39:BO:142:GLY:O	2.18	0.44
43:BS:9:ARG:HG3	43:BS:10:ILE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:1352:5MC:H6	1:Aa:1352:5MC:O5'	2.01	0.44
21:Au:31:SER:HA	21:Au:34:ARG:HB3	2.00	0.44
27:BA:2239:G:O2'	27:BA:2240:G:O5'	2.36	0.44
30:BD:151:PRO:O	30:BD:154:ILE:O	2.35	0.44
31:BE:82:PHE:O	31:BE:82:PHE:CD1	2.71	0.44
32:BF:166:GLU:HA	32:BF:169:ILE:HD12	1.99	0.44
1:Aa:1070:U:H5	13:Am:5:ARG:NH2	2.15	0.44
1:Aa:1445:C:H2'	1:Aa:1446:G:O4'	2.17	0.44
1:Aa:1475:G:C8	14:An:135:ARG:NH1	2.85	0.44
27:BA:808:U:H3	27:BA:923:G:H1	1.66	0.44
27:BA:1587:G:H5''	43:BS:96:MET:HE1	1.99	0.44
27:BA:2159:C:O2'	27:BA:2949:A:N1	2.45	0.44
27:BA:2263:C:H2'	27:BA:2264:G:C8	2.53	0.44
1:Aa:449:G:OP2	1:Aa:479:OMU:HM22	2.18	0.44
16:Ap:116:TYR:O	16:Ap:120:ARG:HG2	2.17	0.44
27:BA:1147:A:N1	27:BA:1272:U:O2'	2.40	0.44
27:BA:1151:G:OP2	67:BA:3209:HOH:O	2.21	0.44
31:BE:188:GLY:O	31:BE:190:ARG:N	2.50	0.44
32:BF:166:GLU:O	32:BF:170:VAL:HG13	2.18	0.44
35:BJ:82:TYR:O	35:BJ:82:TYR:CG	2.71	0.44
47:BW:85:LEU:HD23	47:BW:85:LEU:H	1.83	0.44
4:Ad:14:LYS:O	4:Ad:18:LYS:HG2	2.18	0.44
21:Au:29:LEU:O	21:Au:34:ARG:NH1	2.51	0.44
22:Av:32:ALA:N	22:Av:33:PRO:HD2	2.32	0.44
27:BA:2853:G:OP1	27:BA:2853:G:N2	2.49	0.44
29:BC:182:ALA:O	29:BC:185:ARG:O	2.35	0.44
34:BI:41:LYS:O	34:BI:45:ARG:HG2	2.18	0.44
20:Bm:7:THR:O	20:Bm:10:LYS:HG2	2.18	0.44
1:Aa:314:G:OP1	11:Ak:50:TYR:O	2.36	0.44
1:Aa:1094:A:H8	1:Aa:1094:A:H5''	1.82	0.44
9:Ai:130:SER:OG	9:Ai:200:ALA:HB1	2.17	0.44
16:Ap:70:PRO:HB2	16:Ap:75:ILE:HG21	1.99	0.44
17:Aq:113:ARG:O	17:Aq:117:LEU:HG	2.17	0.44
27:BA:879:A2M:O5'	27:BA:879:A2M:H8	2.18	0.44
27:BA:1406:A:N3	27:BA:2116:G:O2'	2.47	0.44
27:BA:2216:G:C2'	27:BA:2217:G:O4'	2.65	0.44
27:BA:2835:A:HO2'	27:BA:2836:G:C4'	2.18	0.44
1:Aa:1415:C:H2'	1:Aa:1416:G:O4'	2.17	0.43
8:Ah:87:LEU:HD11	8:Ah:102:ARG:HB3	1.99	0.43
27:BA:692:C:H2'	27:BA:693:G:O4'	2.18	0.43
27:BA:2688:5MC:H2'	27:BA:2689:U:H2'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Ba:14:ARG:NH1	67:Ba:203:HOH:O	2.51	0.43
1:Aa:924:OMC:O3'	1:Aa:924:OMC:HM23	2.17	0.43
4:Ad:76:ASP:OD1	4:Ad:77:VAL:N	2.51	0.43
5:Ae:107:THR:O	5:Ae:111:ARG:HG2	2.17	0.43
12:Al:55:GLU:O	12:Al:59:ARG:NH1	2.51	0.43
23:Aw:93:VAL:HG12	23:Aw:94:GLN:N	2.33	0.43
27:BA:2053:U:H1'	27:BA:2054:C:OP2	2.18	0.43
27:BA:2162:U:H2'	27:BA:2163:G:O4'	2.17	0.43
27:BA:2379:OMG:OP2	67:BA:3236:HOH:O	2.21	0.43
33:BG:58:GLU:O	33:BG:59:PHE:CD2	2.71	0.43
34:BI:31:ARG:HB2	34:BI:102:ILE:O	2.18	0.43
36:BK:84:PRO:O	36:BK:90:GLY:HA3	2.18	0.43
42:BR:96:GLU:O	42:BR:97:ALA:HB3	2.18	0.43
7:Ag:94:TYR:CE1	7:Ag:122:GLU:HG2	2.53	0.43
27:BA:2728:OMG:HM23	27:BA:2728:OMG:H1'	1.73	0.43
30:BD:324:ARG:O	30:BD:324:ARG:HG2	2.18	0.43
31:BE:37:ALA:O	31:BE:40:THR:OG1	2.30	0.43
32:BF:95:VAL:HG11	32:BF:114:ILE:CG2	2.48	0.43
52:Bb:19:MET:HE1	52:Bb:77:ARG:CZ	2.47	0.43
64:Bp:129:ALA:HB3	64:Bp:154:ILE:HD11	2.00	0.43
1:Aa:147:OMG:HM23	8:Ah:9:SER:HB3	2.00	0.43
10:Aj:55:ASP:OD1	10:Aj:58:ALA:O	2.37	0.43
27:BA:1676:C:H2'	27:BA:1677:U:O4'	2.18	0.43
34:BH:31:ARG:HB3	34:BH:102:ILE:O	2.19	0.43
2:Ab:102:ASN:O	2:Ab:105:VAL:HG22	2.19	0.43
27:BA:2431:A:H2'	27:BA:2432:G:C8	2.53	0.43
30:BD:49:THR:HG22	30:BD:72:ILE:HD11	2.00	0.43
41:BQ:133:HIS:NE2	41:BQ:135:GLU:OE2	2.51	0.43
62:Bl:7:ILE:HD12	62:Bl:9:THR:HG21	1.99	0.43
64:Bp:70:THR:HG21	64:Bp:75:GLU:HB2	2.00	0.43
1:Aa:1266:5MC:C2	1:Aa:1267:U:C5	3.06	0.43
27:BA:410:C:O2'	27:BA:411:U:P	2.77	0.43
39:BO:91:ALA:O	39:BO:93:ILE:N	2.44	0.43
53:Bc:6:GLY:O	53:Bc:7:GLU:C	2.60	0.43
27:BA:715:A:H2'	27:BA:715:A:N3	2.33	0.43
27:BA:2578:C:O2	27:BA:2578:C:H2'	2.18	0.43
28:BB:52:A:O2'	28:BB:53:A:H8	2.02	0.43
31:BE:140:ILE:O	31:BE:140:ILE:HG22	2.19	0.43
34:BI:18:LYS:HG3	34:BI:114:ILE:HD11	2.01	0.43
35:BJ:171:ASP:OD1	35:BJ:173:THR:HG22	2.19	0.43
38:BN:22:VAL:HG21	38:BN:35:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:179:G:N3	1:Aa:179:G:H2'	2.34	0.43
1:Aa:850:A:H2'	1:Aa:851:A:C8	2.54	0.43
1:Aa:1007:5MC:H6	1:Aa:1007:5MC:C5'	2.29	0.43
1:Aa:1007:5MC:HM52	1:Aa:1008:G:O2'	2.19	0.43
27:BA:1995:OMC:HM23	27:BA:1995:OMC:H1'	1.71	0.43
27:BA:2032:A:H2'	27:BA:2032:A:N3	2.34	0.43
27:BA:2805:C:OP2	43:BS:62:ARG:NH2	2.41	0.43
29:BC:36:VAL:O	29:BC:37:GLN:C	2.62	0.43
41:BQ:104:LEU:CD2	41:BQ:106:ILE:HD11	2.49	0.43
60:Bj:40:ARG:O	60:Bj:40:ARG:HG3	2.18	0.43
1:Aa:598:U:O4	1:Aa:698:G:O2'	2.34	0.43
1:Aa:1427:C:H2'	1:Aa:1428:C:C6	2.53	0.43
4:Ad:96:ILE:O	4:Ad:100:VAL:HG12	2.19	0.43
12:Al:10:ARG:HG3	12:Al:11:LYS:H	1.84	0.43
27:BA:91:OMC:H1'	27:BA:91:OMC:HM23	1.44	0.43
27:BA:288:OMG:H1'	27:BA:288:OMG:HM23	1.53	0.43
27:BA:1014:G:N1	27:BA:1024:U:O4	2.51	0.43
27:BA:1160:A:H2'	27:BA:1161:A:C8	2.54	0.43
27:BA:1937:A:H2'	27:BA:1938:A:C8	2.54	0.43
30:BD:61:THR:HG21	30:BD:66:ILE:HG21	2.00	0.43
30:BD:269:ILE:HD11	30:BD:306:GLU:HG3	2.01	0.43
33:BG:50:ASP:OD1	33:BG:51:GLY:N	2.47	0.43
3:Ac:18:ASP:OD1	3:Ac:30:TYR:OH	2.34	0.43
11:Ak:40:ASP:OD1	11:Ak:40:ASP:N	2.51	0.43
23:Aw:82:GLU:OE1	23:Aw:86:ILE:HD11	2.18	0.43
27:BA:770:A:H2'	27:BA:771:A:O4'	2.18	0.43
27:BA:873:C:H2'	27:BA:874:G:O4'	2.18	0.43
27:BA:1293:C:H2'	27:BA:1294:G:O4'	2.18	0.43
27:BA:1669:G:OP2	27:BA:1670:A:O2'	2.30	0.43
27:BA:2426:G:O2'	27:BA:2427:5MU:H5''	2.18	0.43
27:BA:2430:A:H2'	27:BA:2431:A:C8	2.53	0.43
48:BX:52:VAL:CG1	48:BX:100:VAL:HG21	2.49	0.43
49:BY:26:ASP:OD2	49:BY:28:ARG:NE	2.49	0.43
23:Bn:33:ARG:NH2	23:Bn:53:ILE:O	2.49	0.43
1:Aa:1094:A:H5''	1:Aa:1094:A:C8	2.54	0.42
1:Aa:1231:A:C5'	1:Aa:1232:A:OP1	2.67	0.42
28:BB:39:G:O2'	28:BB:40:U:O4'	2.34	0.42
64:Bp:70:THR:HG22	64:Bp:71:SER:N	2.33	0.42
4:Ad:113:ILE:HD13	4:Ad:150:TYR:CD1	2.54	0.42
6:Af:167:GLN:O	6:Af:171:ARG:N	2.52	0.42
27:BA:2080:U:O2	27:BA:2080:U:O4'	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BG:6:TRP:O	33:BG:6:TRP:CD1	2.71	0.42
40:BP:119:VAL:HG22	40:BP:119:VAL:O	2.18	0.42
57:Bg:12:ARG:NE	67:Bg:203:HOH:O	2.51	0.42
27:BA:986:G:O2'	27:BA:987:G:H5'	2.19	0.42
27:BA:2565:C:H2'	27:BA:2566:U:C6	2.54	0.42
27:BA:2958:U:C4'	27:BA:2959:U:H5'	2.49	0.42
32:BF:22:ILE:HD12	32:BF:85:TYR:CD1	2.53	0.42
32:BF:131:ILE:H	32:BF:131:ILE:HD12	1.85	0.42
38:BN:38:ALA:HB3	38:BN:40:LEU:HD13	2.00	0.42
39:BO:14:SER:O	39:BO:15:HIS:HB3	2.19	0.42
41:BQ:87:GLY:HA2	41:BQ:90:ILE:HG22	2.01	0.42
52:Bb:19:MET:HE1	52:Bb:77:ARG:NE	2.35	0.42
20:Bm:41:VAL:HG12	20:Bm:42:THR:N	2.34	0.42
1:Aa:1324:C:H2'	1:Aa:1325:G:O4'	2.20	0.42
9:Ai:44:LEU:HD11	12:Al:40:ILE:HG13	2.01	0.42
16:Ap:86:TYR:HA	21:Au:10:ARG:NH2	2.35	0.42
27:BA:956:C:N4	67:BA:3507:HOH:O	2.50	0.42
27:BA:1109:A:OP1	67:BA:3151:HOH:O	2.21	0.42
27:BA:1684:A:OP1	43:BS:43:ARG:NE	2.52	0.42
27:BA:2069:G:C8	27:BA:2070:5MC:HM52	2.55	0.42
27:BA:2410:A:H2'	27:BA:2411:G:C4	2.54	0.42
28:BB:56:U:H5''	32:BF:15:HIS:NE2	2.34	0.42
29:BC:238:ARG:NH2	67:BC:307:HOH:O	2.50	0.42
35:BJ:18:THR:HG22	35:BJ:92:GLN:HA	2.00	0.42
56:Bf:85:PHE:O	56:Bf:87:PRO:O	2.38	0.42
1:Aa:1266:5MC:HM52	21:Au:35:ARG:HD2	2.01	0.42
9:Ai:99:LYS:O	9:Ai:103:VAL:HG23	2.19	0.42
27:BA:849:A2M:HM'2	27:BA:850:U:O4'	2.19	0.42
27:BA:2186:U:H2'	27:BA:2187:U:C6	2.54	0.42
27:BA:2373:G:OP2	67:BA:3228:HOH:O	2.20	0.42
34:BH:53:ILE:HG22	34:BH:54:ALA:N	2.34	0.42
41:BQ:99:ILE:O	41:BQ:99:ILE:HG13	2.19	0.42
56:Bf:85:PHE:O	56:Bf:86:LYS:C	2.62	0.42
64:Bp:32:PHE:HD1	64:Bp:38:VAL:HB	1.85	0.42
1:Aa:753:OMU:HM23	1:Aa:753:OMU:H1'	1.59	0.42
1:Aa:851:A:C5	1:Aa:852:OMG:H1'	2.55	0.42
1:Aa:1131:A:H2'	1:Aa:1132:A:O4'	2.20	0.42
25:Ay:30:ILE:HB	25:Ay:35:ASP:O	2.19	0.42
27:BA:230:U:H2'	27:BA:231:U:O4'	2.20	0.42
27:BA:1238:C:H2'	27:BA:1239:G:C8	2.54	0.42
27:BA:2521:OMG:H1'	27:BA:2521:OMG:HM23	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2595:OMC:O2'	27:BA:2596:U:P	2.78	0.42
62:Bl:25:VAL:HG23	62:Bl:66:ASP:O	2.20	0.42
15:Ao:133:SER:O	15:Ao:137:LEU:HD23	2.20	0.42
27:BA:65:OMG:H1'	27:BA:65:OMG:HM23	1.78	0.42
27:BA:1088:A:H2'	27:BA:1089:A:C8	2.54	0.42
27:BA:2222:G:H4'	27:BA:2223:C:OP2	2.19	0.42
27:BA:2423:A:H2'	27:BA:2423:A:N3	2.35	0.42
34:BH:26:ALA:HB3	34:BH:32:ILE:HD11	2.02	0.42
42:BR:34:ILE:HD13	42:BR:64:ILE:HD13	2.00	0.42
1:Aa:140:A:H2'	1:Aa:141:A:O4'	2.20	0.42
1:Aa:232:U:O4	1:Aa:856:G:H1'	2.19	0.42
1:Aa:1304:C:H2'	1:Aa:1305:G:C8	2.55	0.42
8:Ah:38:ILE:HD11	8:Ah:63:ILE:HD11	2.01	0.42
27:BA:541:A:H4'	27:BA:542:A:OP1	2.20	0.42
27:BA:1488:A:H2'	27:BA:1489:A:C8	2.55	0.42
33:BG:61:ARG:O	33:BG:65:VAL:HG23	2.19	0.42
27:BA:1860:C:H2'	27:BA:1861:G:O4'	2.20	0.42
45:BU:31:PHE:CD2	45:BU:91:VAL:HG21	2.54	0.42
3:Ac:87:ASN:N	3:Ac:88:PRO:CD	2.82	0.42
9:Ai:18:MET:HE2	9:Ai:101:TYR:CE1	2.54	0.42
14:An:73:GLU:O	14:An:77:LYS:HG2	2.20	0.42
27:BA:153:A:N6	67:BA:3120:HOH:O	2.45	0.42
27:BA:670:OMG:HM22	27:BA:670:OMG:C4'	2.48	0.42
27:BA:1776:OMU:HM23	27:BA:1776:OMU:H1'	1.52	0.42
27:BA:2124:OMC:H2'	27:BA:2125:G:O4'	2.20	0.42
27:BA:2140:C:H2'	27:BA:2141:G:O4'	2.20	0.42
27:BA:2250:C:N3	27:BA:2266:G:N2	2.68	0.42
27:BA:2483:A:H2'	27:BA:2484:A:C8	2.55	0.42
27:BA:2551:G:O4'	27:BA:2605:5MC:HM53	2.20	0.42
35:BJ:4:ARG:NH1	35:BJ:9:ASP:OD1	2.53	0.42
48:BX:27:MET:SD	48:BX:71:LEU:HD23	2.59	0.42
64:Bp:103:TYR:O	64:Bp:107:VAL:HG23	2.20	0.42
1:Aa:316:C:O2'	1:Aa:317:A:OP2	2.29	0.41
1:Aa:1112:G:C2	1:Aa:1113:C:C6	3.08	0.41
2:Ab:6:VAL:HG13	2:Ab:7:PRO:HD2	2.02	0.41
8:Ah:86:ILE:CD1	8:Ah:88:LEU:HD21	2.48	0.41
9:Ai:70:LYS:HA	9:Ai:70:LYS:HD3	1.88	0.41
16:Ap:11:VAL:HG12	16:Ap:12:ALA:N	2.35	0.41
16:Ap:17:ASP:OD1	16:Ap:18:GLY:N	2.53	0.41
27:BA:93:A:OP2	48:BX:47:ARG:NH2	2.53	0.41
27:BA:1270:G:OP2	36:BK:52:ARG:NH2	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1386:C:O2	27:BA:1386:C:O5'	2.38	0.41
27:BA:2053:U:O2'	27:BA:2054:C:P	2.78	0.41
27:BA:2543:A:H4'	27:BA:2545:OMC:OP2	2.20	0.41
32:BF:141:GLU:HG3	32:BF:142:ARG:N	2.35	0.41
1:Aa:534:G:OP2	67:Aa:1521:HOH:O	2.21	0.41
1:Aa:664:G:H2'	1:Aa:665:C:H6	1.83	0.41
14:An:109:SER:HB3	14:An:115:ILE:HD12	2.02	0.41
27:BA:993:G:H2'	27:BA:994:C:C6	2.55	0.41
27:BA:2545:OMC:H1'	27:BA:2545:OMC:HM23	1.56	0.41
30:BD:78:LEU:HD13	30:BD:147:VAL:HG11	2.02	0.41
32:BF:45:LEU:O	32:BF:49:VAL:HG13	2.21	0.41
1:Aa:863:A:O2'	1:Aa:864:A:OP2	2.27	0.41
27:BA:345:U:H2'	27:BA:346:G:O4'	2.21	0.41
27:BA:912:OMG:C5'	27:BA:913:G:OP1	2.63	0.41
27:BA:1285:C:H2'	27:BA:1286:G:O4'	2.20	0.41
47:BW:30:VAL:HG12	47:BW:31:ASP:N	2.35	0.41
64:Bp:105:ALA:HB1	64:Bp:123:VAL:HG23	2.02	0.41
1:Aa:92:C:H1'	1:Aa:342:G:H5'	2.03	0.41
8:Ah:75:ARG:NH2	8:Ah:88:LEU:HD13	2.35	0.41
27:BA:392:C:H2'	27:BA:393:G:O4'	2.19	0.41
27:BA:1828:U:H2'	27:BA:1829:G:O4'	2.20	0.41
27:BA:2413:A:N7	27:BA:2414:A:C8	2.89	0.41
27:BA:2414:A:H2'	27:BA:2415:U:O4'	2.20	0.41
27:BA:2673:G:N7	30:BD:3:LYS:HE3	2.35	0.41
30:BD:84:ARG:HD2	30:BD:146:LEU:HD21	2.02	0.41
30:BD:154:ILE:O	30:BD:156:LEU:N	2.52	0.41
41:BQ:60:VAL:HG12	41:BQ:61:SER:N	2.35	0.41
23:Aw:3:ILE:HD12	23:Aw:39:LYS:CG	2.50	0.41
27:BA:925:C:O2'	58:Bh:51:TRP:O	2.39	0.41
27:BA:1030:U:O2'	27:BA:1031:C:P	2.74	0.41
27:BA:1944:U:O2	27:BA:1944:U:O4'	2.39	0.41
27:BA:2640:OMG:H5''	27:BA:2640:OMG:H8	1.86	0.41
28:BB:83:U:H2'	28:BB:84:G:C8	2.56	0.41
31:BE:73:ILE:HG22	31:BE:75:THR:H	1.85	0.41
64:Bp:10:ILE:HA	64:Bp:22:ILE:O	2.21	0.41
9:Ai:93:ILE:O	9:Ai:93:ILE:HG13	2.21	0.41
13:Am:26:ILE:HD13	13:Am:29:ARG:NH2	2.36	0.41
27:BA:1272:U:H4'	27:BA:1274:A:O4'	2.21	0.41
32:BF:145:PHE:CD1	32:BF:157:ILE:HG13	2.55	0.41
27:BA:314:G:H2'	27:BA:315:A:C1'	2.50	0.41
27:BA:561:C:H2'	27:BA:562:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BB:10:G:O6	41:BQ:12:ARG:NH1	2.54	0.41
28:BB:18:G:H2'	28:BB:19:G:O4'	2.21	0.41
32:BF:40:LYS:O	32:BF:43:THR:N	2.53	0.41
32:BF:88:LEU:HD21	32:BF:138:VAL:HG21	2.03	0.41
33:BG:6:TRP:O	33:BG:6:TRP:HD1	2.04	0.41
38:BM:22:VAL:CG1	38:BM:35:VAL:HG13	2.51	0.41
64:Bp:38:VAL:O	64:Bp:38:VAL:HG23	2.19	0.41
64:Bp:78:LYS:O	64:Bp:82:ARG:HG2	2.21	0.41
1:Aa:147:OMG:HM23	1:Aa:147:OMG:H1'	1.62	0.41
1:Aa:351:A:O2'	1:Aa:352:A2M:OP1	2.30	0.41
27:BA:2238:A:O3'	27:BA:2239:G:O4'	2.38	0.41
36:BK:22:LEU:O	36:BK:96:ARG:NH1	2.43	0.41
1:Aa:1009:U:H4'	1:Aa:1010:C:O5'	2.19	0.41
1:Aa:1420:C:H2'	1:Aa:1421:U:O4'	2.20	0.41
3:Ac:75:LEU:HD23	3:Ac:75:LEU:HA	1.98	0.41
27:BA:493:A:H4'	27:BA:494:C:OP2	2.21	0.41
27:BA:1241:C:OP2	27:BA:1242:G:N2	2.54	0.41
27:BA:1820:OMC:H2'	27:BA:1821:G:O4'	2.21	0.41
27:BA:2021:G:H3'	27:BA:2022:G:C8	2.56	0.41
27:BA:2127:A:H2'	27:BA:2128:A:C8	2.56	0.41
27:BA:2172:A:O2'	27:BA:2173:G:H3'	2.21	0.41
27:BA:2173:G:H5'	27:BA:2174:A:C2	2.56	0.41
27:BA:2264:G:H2'	27:BA:2265:G:C8	2.56	0.41
29:BC:54:ARG:O	29:BC:55:THR:CG2	2.69	0.41
30:BD:25:PRO:HB2	30:BD:202:ILE:HG22	2.02	0.41
37:BL:138:SER:C	37:BL:139:ILE:HG13	2.46	0.41
38:BM:33:VAL:HG23	38:BM:35:VAL:HG23	2.03	0.41
38:BM:54:GLU:OE2	55:Be:85:ARG:NH2	2.49	0.41
38:BM:67:SER:HB3	38:BM:69:GLU:OE1	2.21	0.41
43:BS:132:PHE:O	43:BS:133:LYS:HB2	2.20	0.41
58:Bh:6:ALA:HB3	58:Bh:7:PRO:HD3	2.03	0.41
64:Bp:97:LEU:HD11	64:Bp:137:ILE:HB	2.02	0.41
1:Aa:344:A:O2'	1:Aa:356:U:O2'	2.32	0.41
1:Aa:1257:G:H1'	1:Aa:1284:A:H61	1.86	0.41
27:BA:2720:C:H2'	27:BA:2721:U:O4'	2.21	0.41
27:BA:2858:U:H4'	27:BA:2859:A:OP1	2.20	0.41
49:BY:3:ARG:HA	49:BY:3:ARG:NE	2.36	0.41
1:Aa:889:A:H2	1:Aa:1328:U:O2	2.04	0.40
1:Aa:1129:G:H2'	1:Aa:1130:G:O4'	2.21	0.40
1:Aa:1352:5MC:H4'	1:Aa:1353:G:OP2	2.22	0.40
3:Ac:152:ALA:O	3:Ac:153:LYS:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:185:G:H2'	27:BA:186:A:O4'	2.21	0.40
27:BA:233:G:O2'	27:BA:245:G:O6	2.36	0.40
27:BA:312:C:H2'	27:BA:313:G:O4'	2.21	0.40
27:BA:982:A:H2'	27:BA:983:G:O4'	2.21	0.40
27:BA:1534:U:O2	27:BA:1534:U:H2'	2.20	0.40
27:BA:1946:U:O2'	29:BC:121:TYR:HA	2.20	0.40
27:BA:2550:OMG:HM22	27:BA:2605:5MC:HM52	2.01	0.40
27:BA:2824:A:OP1	67:BA:3237:HOH:O	2.22	0.40
27:BA:3032:C:H2'	27:BA:3033:C:C6	2.56	0.40
29:BC:186:ASN:O	29:BC:186:ASN:CG	2.64	0.40
31:BE:137:VAL:HG12	31:BE:138:VAL:N	2.36	0.40
37:BL:119:ARG:HB3	37:BL:119:ARG:HH11	1.87	0.40
40:BP:180:GLU:OE1	40:BP:180:GLU:N	2.46	0.40
41:BQ:140:GLU:OE1	41:BQ:140:GLU:N	2.53	0.40
1:Aa:101:A:H61	1:Aa:227:G:H1	1.68	0.40
1:Aa:1398:C:H2'	1:Aa:1399:U:O4'	2.21	0.40
1:Aa:1442:A:O2'	1:Aa:1443:G:H8	2.04	0.40
23:Aw:52:VAL:HG13	23:Aw:78:MET:CE	2.51	0.40
27:BA:143:C:H2'	27:BA:144:U:O4'	2.21	0.40
27:BA:471:U:O2'	27:BA:472:A:P	2.77	0.40
27:BA:754:C:H2'	27:BA:755:G:O4'	2.21	0.40
27:BA:2075:5MC:OP2	27:BA:2075:5MC:H6	2.04	0.40
27:BA:2998:G:OP1	49:BY:63:ARG:NH1	2.50	0.40
30:BD:111:ARG:HG3	30:BD:160:PRO:O	2.21	0.40
64:Bp:34:GLU:HG2	64:Bp:36:LYS:NZ	2.37	0.40
1:Aa:738:A:C2'	1:Aa:739:U:OP2	2.66	0.40
12:Al:70:GLY:O	12:Al:74:GLN:HG3	2.22	0.40
27:BA:1907:U:H5	27:BA:1912:A:N7	2.20	0.40
31:BE:61:ILE:HG23	31:BE:62:GLY:N	2.36	0.40
43:BS:30:GLU:HG2	43:BS:31:ASP:N	2.36	0.40
47:BW:30:VAL:CG1	47:BW:31:ASP:N	2.84	0.40
1:Aa:630:G:H2'	1:Aa:631:G:C8	2.56	0.40
1:Aa:891:OMG:H2'	1:Aa:892:G:O4'	2.21	0.40
27:BA:1033:C:C6	27:BA:1033:C:H5''	2.56	0.40
27:BA:2224:G:N3	27:BA:2224:G:H2'	2.35	0.40
27:BA:2595:OMC:HM23	27:BA:2595:OMC:H1'	1.50	0.40
30:BD:84:ARG:NH1	30:BD:98:GLU:OE2	2.55	0.40
32:BF:66:GLY:HA2	32:BF:73:ILE:HG13	2.02	0.40
35:BJ:69:VAL:HG13	35:BJ:148:ALA:HB1	2.04	0.40
38:BM:36:THR:O	38:BM:36:THR:HG23	2.22	0.40
38:BN:37:GLY:O	38:BN:38:ALA:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BQ:37:VAL:O	41:BQ:38:ARG:NH1	2.54	0.40
1:Aa:361:A:C2	1:Aa:362:A:C8	3.10	0.40
1:Aa:451:G:H5''	1:Aa:451:G:H8	1.86	0.40
1:Aa:757:U:O2'	1:Aa:851:A:N1	2.55	0.40
1:Aa:1013:C:OP2	67:Aa:1525:HOH:O	2.22	0.40
6:Af:181:VAL:O	6:Af:181:VAL:CG1	2.69	0.40
22:Av:74:ARG:NE	22:Av:93:ALA:O	2.48	0.40
27:BA:934:C:OP2	39:BO:26:ARG:NH1	2.54	0.40
27:BA:1520:G:OP2	67:BA:3240:HOH:O	2.22	0.40
28:BB:24:G:N7	28:BB:56:U:O2'	2.29	0.40
30:BD:111:ARG:HD2	30:BD:111:ARG:HA	1.82	0.40
32:BF:145:PHE:O	32:BF:145:PHE:CG	2.74	0.40
47:BW:44:GLU:O	47:BW:48:ASN:N	2.50	0.40
64:Bp:112:ALA:HB1	64:Bp:160:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ab	194/201 (96%)	181 (93%)	13 (7%)	0	100	100
3	Ac	193/209 (92%)	185 (96%)	8 (4%)	0	100	100
4	Ad	188/200 (94%)	175 (93%)	13 (7%)	0	100	100
5	Ae	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
6	Af	240/243 (99%)	234 (98%)	6 (2%)	0	100	100
7	Ag	221/235 (94%)	209 (95%)	12 (5%)	0	100	100
8	Ah	121/125 (97%)	118 (98%)	3 (2%)	0	100	100
9	Ai	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
10	Aj	127/130 (98%)	119 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	Ak	123/130 (95%)	116 (94%)	7 (6%)	0	100	100
12	Al	131/135 (97%)	123 (94%)	8 (6%)	0	100	100
13	Am	98/102 (96%)	94 (96%)	4 (4%)	0	100	100
14	An	125/140 (89%)	118 (94%)	6 (5%)	1 (1%)	16	27
15	Ao	141/147 (96%)	135 (96%)	6 (4%)	0	100	100
16	Ap	133/149 (89%)	118 (89%)	15 (11%)	0	100	100
17	Aq	147/151 (97%)	141 (96%)	6 (4%)	0	100	100
18	Ar	52/56 (93%)	46 (88%)	6 (12%)	0	100	100
19	As	106/114 (93%)	102 (96%)	4 (4%)	0	100	100
20	At	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
20	Bm	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
21	Au	114/133 (86%)	111 (97%)	3 (3%)	0	100	100
22	Av	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
23	Aw	93/98 (95%)	87 (94%)	6 (6%)	0	100	100
23	Bn	90/98 (92%)	85 (94%)	5 (6%)	0	100	100
24	Ax	59/65 (91%)	56 (95%)	3 (5%)	0	100	100
25	Ay	62/70 (89%)	60 (97%)	2 (3%)	0	100	100
26	Az	53/62 (86%)	51 (96%)	2 (4%)	0	100	100
29	BC	235/239 (98%)	221 (94%)	14 (6%)	0	100	100
30	BD	342/346 (99%)	322 (94%)	20 (6%)	0	100	100
31	BE	253/255 (99%)	241 (95%)	12 (5%)	0	100	100
32	BF	162/183 (88%)	132 (82%)	30 (18%)	0	100	100
33	BG	181/184 (98%)	169 (93%)	12 (7%)	0	100	100
34	BH	119/123 (97%)	113 (95%)	6 (5%)	0	100	100
34	BI	119/123 (97%)	108 (91%)	11 (9%)	0	100	100
35	BJ	167/182 (92%)	157 (94%)	10 (6%)	0	100	100
36	BK	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
37	BL	138/141 (98%)	128 (93%)	10 (7%)	0	100	100
38	BM	79/83 (95%)	70 (89%)	9 (11%)	0	100	100
38	BN	79/83 (95%)	72 (91%)	7 (9%)	0	100	100
39	BO	146/148 (99%)	134 (92%)	12 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BP	191/194 (98%)	182 (95%)	9 (5%)	0	100	100
41	BQ	158/201 (79%)	149 (94%)	9 (6%)	0	100	100
42	BR	118/121 (98%)	112 (95%)	6 (5%)	0	100	100
43	BS	144/150 (96%)	139 (96%)	5 (4%)	0	100	100
44	BT	72/77 (94%)	70 (97%)	2 (3%)	0	100	100
45	BU	94/98 (96%)	91 (97%)	3 (3%)	0	100	100
46	BV	152/156 (97%)	149 (98%)	3 (2%)	0	100	100
47	BW	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
48	BX	118/121 (98%)	113 (96%)	5 (4%)	0	100	100
49	BY	60/67 (90%)	60 (100%)	0	0	100	100
50	BZ	56/66 (85%)	54 (96%)	2 (4%)	0	100	100
51	Ba	152/155 (98%)	147 (97%)	5 (3%)	0	100	100
52	Bb	94/102 (92%)	87 (93%)	7 (7%)	0	100	100
53	Bc	87/90 (97%)	80 (92%)	7 (8%)	0	100	100
54	Bd	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
55	Be	87/90 (97%)	82 (94%)	5 (6%)	0	100	100
56	Bf	84/101 (83%)	80 (95%)	4 (5%)	0	100	100
57	Bg	82/86 (95%)	77 (94%)	5 (6%)	0	100	100
58	Bh	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
59	Bi	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
60	Bj	45/51 (88%)	43 (96%)	2 (4%)	0	100	100
61	Bk	34/37 (92%)	34 (100%)	0	0	100	100
62	Bl	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
63	Bo	41/47 (87%)	38 (93%)	3 (7%)	0	100	100
64	Bp	230/236 (98%)	213 (93%)	17 (7%)	0	100	100
65	Bq	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
All	All	8160/8603 (95%)	7713 (94%)	446 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	An	133	GLY

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	Ab	170/175 (97%)	170 (100%)	0	100	100
3	Ac	156/168 (93%)	156 (100%)	0	100	100
4	Ad	162/169 (96%)	162 (100%)	0	100	100
5	Ae	153/156 (98%)	153 (100%)	0	100	100
6	Af	211/212 (100%)	211 (100%)	0	100	100
7	Ag	185/197 (94%)	185 (100%)	0	100	100
8	Ah	104/105 (99%)	104 (100%)	0	100	100
9	Ai	183/184 (100%)	183 (100%)	0	100	100
10	Aj	106/107 (99%)	106 (100%)	0	100	100
11	Ak	101/105 (96%)	101 (100%)	0	100	100
12	Al	110/112 (98%)	110 (100%)	0	100	100
13	Am	89/91 (98%)	89 (100%)	0	100	100
14	An	95/108 (88%)	94 (99%)	1 (1%)	65	80
15	Ao	117/120 (98%)	117 (100%)	0	100	100
16	Ap	111/123 (90%)	111 (100%)	0	100	100
17	Aq	129/131 (98%)	129 (100%)	0	100	100
18	Ar	45/46 (98%)	45 (100%)	0	100	100
19	As	96/101 (95%)	96 (100%)	0	100	100
20	At	58/61 (95%)	58 (100%)	0	100	100
20	Bm	58/61 (95%)	58 (100%)	0	100	100
21	Au	104/117 (89%)	104 (100%)	0	100	100
22	Av	125/126 (99%)	125 (100%)	0	100	100
23	Aw	85/88 (97%)	85 (100%)	0	100	100
23	Bn	82/88 (93%)	82 (100%)	0	100	100
24	Ax	53/56 (95%)	53 (100%)	0	100	100
25	Ay	53/59 (90%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	Az	49/55 (89%)	49 (100%)	0	100	100
29	BC	185/187 (99%)	185 (100%)	0	100	100
30	BD	288/289 (100%)	288 (100%)	0	100	100
31	BE	212/212 (100%)	212 (100%)	0	100	100
32	BF	140/155 (90%)	140 (100%)	0	100	100
33	BG	158/159 (99%)	158 (100%)	0	100	100
34	BH	99/100 (99%)	99 (100%)	0	100	100
34	BI	99/100 (99%)	99 (100%)	0	100	100
35	BJ	145/153 (95%)	145 (100%)	0	100	100
36	BK	120/120 (100%)	120 (100%)	0	100	100
37	BL	104/105 (99%)	104 (100%)	0	100	100
38	BM	63/65 (97%)	63 (100%)	0	100	100
38	BN	63/65 (97%)	63 (100%)	0	100	100
39	BO	116/116 (100%)	116 (100%)	0	100	100
40	BP	161/162 (99%)	161 (100%)	0	100	100
41	BQ	138/167 (83%)	138 (100%)	0	100	100
42	BR	101/102 (99%)	101 (100%)	0	100	100
43	BS	120/124 (97%)	120 (100%)	0	100	100
44	BT	69/72 (96%)	69 (100%)	0	100	100
45	BU	84/85 (99%)	84 (100%)	0	100	100
46	BV	129/131 (98%)	129 (100%)	0	100	100
47	BW	75/76 (99%)	75 (100%)	0	100	100
48	BX	109/109 (100%)	109 (100%)	0	100	100
49	BY	54/58 (93%)	54 (100%)	0	100	100
50	BZ	57/61 (93%)	57 (100%)	0	100	100
51	Ba	132/133 (99%)	132 (100%)	0	100	100
52	Bb	76/80 (95%)	76 (100%)	0	100	100
53	Bc	75/76 (99%)	75 (100%)	0	100	100
54	Bd	106/107 (99%)	106 (100%)	0	100	100
55	Be	80/80 (100%)	80 (100%)	0	100	100
56	Bf	71/83 (86%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	Bg	62/63 (98%)	62 (100%)	0	100	100
58	Bh	50/51 (98%)	50 (100%)	0	100	100
59	Bi	45/46 (98%)	45 (100%)	0	100	100
60	Bj	36/38 (95%)	36 (100%)	0	100	100
61	Bk	34/35 (97%)	34 (100%)	0	100	100
62	Bl	83/84 (99%)	83 (100%)	0	100	100
63	Bo	36/39 (92%)	36 (100%)	0	100	100
64	Bp	196/200 (98%)	196 (100%)	0	100	100
All	All	6961/7209 (97%)	6960 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	An	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
3	Ac	95	GLN
8	Ah	13	ASN
9	Ai	117	GLN
10	Aj	44	ASN
11	Ak	53	ASN
16	Ap	7	HIS
17	Aq	104	GLN
18	Ar	7	ASN
18	Ar	34	HIS
20	At	6	GLN
23	Aw	54	GLN
29	BC	201	ASN
29	BC	229	HIS
30	BD	88	GLN
30	BD	260	HIS
31	BE	139	GLN
31	BE	214	HIS
32	BF	161	HIS
35	BJ	138	ASN
35	BJ	141	HIS

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Mol	Chain	Res	Type
37	BL	75	HIS
38	BN	61	ASN
39	BO	25	HIS
42	BR	44	GLN
43	BS	20	ASN
45	BU	42	HIS
46	BV	12	ASN
46	BV	101	ASN
48	BX	7	GLN
51	Ba	77	ASN
53	Bc	16	ASN
55	Be	25	HIS
55	Be	83	GLN
56	Bf	34	ASN
59	Bi	43	HIS
20	Bm	6	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	1457/1498 (97%)	241 (16%)	0
27	BA	2929/3037 (96%)	491 (16%)	36 (1%)
28	BB	124/126 (98%)	15 (12%)	3 (2%)
All	All	4510/4661 (96%)	747 (16%)	39 (0%)

All (747) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Aa	4	C
1	Aa	17	5MC
1	Aa	33	U
1	Aa	42	G
1	Aa	45	U
1	Aa	47	A
1	Aa	54	C
1	Aa	60	A
1	Aa	65	G
1	Aa	70	C
1	Aa	77	C
1	Aa	95	A
1	Aa	99	A

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Mol	Chain	Res	Type
1	Aa	100	C
1	Aa	109	A
1	Aa	111	C
1	Aa	121	OMG
1	Aa	137	G
1	Aa	143	C
1	Aa	179	G
1	Aa	188	G
1	Aa	192	A
1	Aa	194	A
1	Aa	195	G
1	Aa	214	G
1	Aa	219	OMG
1	Aa	228	C
1	Aa	231	A
1	Aa	232	U
1	Aa	233	U
1	Aa	235	G
1	Aa	239	G
1	Aa	254	G
1	Aa	255	C
1	Aa	268	A
1	Aa	270	A
1	Aa	277	C
1	Aa	289	G
1	Aa	291	G
1	Aa	294	A
1	Aa	316	C
1	Aa	317	A
1	Aa	318	C
1	Aa	320	OMG
1	Aa	335	G
1	Aa	337	G
1	Aa	340	5MC
1	Aa	341	A
1	Aa	342	G
1	Aa	350	G
1	Aa	352	A2M
1	Aa	355	C
1	Aa	360	C
1	Aa	372	C
1	Aa	381	OMG

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Mol	Chain	Res	Type
1	Aa	385	A
1	Aa	386	C
1	Aa	391	A
1	Aa	394	G
1	Aa	428	A
1	Aa	440	A
1	Aa	441	U
1	Aa	442	A
1	Aa	443	A
1	Aa	453	A
1	Aa	454	A
1	Aa	456	G
1	Aa	457	5MC
1	Aa	463	G
1	Aa	466	G
1	Aa	469	G
1	Aa	472	G
1	Aa	477	A
1	Aa	478	A
1	Aa	492	A
1	Aa	498	OMG
1	Aa	506	U
1	Aa	509	U
1	Aa	517	A
1	Aa	518	A
1	Aa	521	C
1	Aa	522	G
1	Aa	526	G
1	Aa	541	A
1	Aa	564	U
1	Aa	578	U
1	Aa	579	G
1	Aa	599	U
1	Aa	611	A
1	Aa	620	G
1	Aa	621	U
1	Aa	634	G
1	Aa	647	A
1	Aa	649	A
1	Aa	662	C
1	Aa	663	C
1	Aa	664	G

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Mol	Chain	Res	Type
1	Aa	669	U
1	Aa	670	OMG
1	Aa	677	G
1	Aa	679	G
1	Aa	694	G
1	Aa	695	U
1	Aa	701	G
1	Aa	707	G
1	Aa	719	G
1	Aa	723	A
1	Aa	727	A
1	Aa	738	A
1	Aa	739	U
1	Aa	761	A
1	Aa	763	G
1	Aa	774	A
1	Aa	787	G
1	Aa	793	A
1	Aa	822	A
1	Aa	840	G
1	Aa	864	A
1	Aa	869	A
1	Aa	876	G
1	Aa	877	G
1	Aa	884	C
1	Aa	886	A
1	Aa	889	A
1	Aa	890	G
1	Aa	911	U
1	Aa	917	5MU
1	Aa	919	A
1	Aa	920	A
1	Aa	922	G
1	Aa	925	G
1	Aa	926	G
1	Aa	927	G
1	Aa	928	A
1	Aa	929	A
1	Aa	941	G
1	Aa	943	G
1	Aa	944	A
1	Aa	947	G

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Mol	Chain	Res	Type
1	Aa	959	C
1	Aa	961	A
1	Aa	963	OMG
1	Aa	968	A
1	Aa	969	G
1	Aa	970	G
1	Aa	975	G
1	Aa	979	G
1	Aa	987	G
1	Aa	988	A
1	Aa	997	G
1	Aa	1004	5MC
1	Aa	1007	5MC
1	Aa	1009	U
1	Aa	1010	C
1	Aa	1038	G
1	Aa	1039	U
1	Aa	1044	U
1	Aa	1045	A
1	Aa	1069	U
1	Aa	1070	U
1	Aa	1076	U
1	Aa	1077	C
1	Aa	1084	G
1	Aa	1085	C
1	Aa	1086	U
1	Aa	1088	G
1	Aa	1092	G
1	Aa	1093	G
1	Aa	1094	A
1	Aa	1096	G
1	Aa	1098	A
1	Aa	1107	OMG
1	Aa	1111	C
1	Aa	1119	A
1	Aa	1120	U
1	Aa	1127	G
1	Aa	1136	G
1	Aa	1147	U
1	Aa	1148	A
1	Aa	1149	G
1	Aa	1154	G

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Mol	Chain	Res	Type
1	Aa	1157	U
1	Aa	1158	G
1	Aa	1164	A
1	Aa	1165	A
1	Aa	1168	C
1	Aa	1169	C
1	Aa	1171	C
1	Aa	1176	U
1	Aa	1179	A
1	Aa	1190	A
1	Aa	1193	G
1	Aa	1208	A
1	Aa	1209	U
1	Aa	1212	G
1	Aa	1217	C
1	Aa	1221	A
1	Aa	1222	G
1	Aa	1231	A
1	Aa	1232	A
1	Aa	1252	G
1	Aa	1253	U
1	Aa	1254	U
1	Aa	1255	C
1	Aa	1272	C
1	Aa	1288	U
1	Aa	1299	G
1	Aa	1305	G
1	Aa	1306	5MC
1	Aa	1311	C
1	Aa	1312	A
1	Aa	1316	U
1	Aa	1322	G
1	Aa	1328	U
1	Aa	1331	G
1	Aa	1334	C
1	Aa	1349	C
1	Aa	1350	A
1	Aa	1352	5MC
1	Aa	1355	C
1	Aa	1371	G
1	Aa	1376	G
1	Aa	1400	U

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Mol	Chain	Res	Type
1	Aa	1401	C
1	Aa	1402	G
1	Aa	1403	G
1	Aa	1407	G
1	Aa	1423	G
1	Aa	1431	G
1	Aa	1434	G
1	Aa	1436	G
1	Aa	1442	A
1	Aa	1446	G
1	Aa	1448	A
1	Aa	1451	A
1	Aa	1452	A
1	Aa	1453	G
1	Aa	1455	U
1	Aa	1466	G
1	Aa	1478	5MC
1	Aa	1479	G
27	BA	12	C
27	BA	15	U
27	BA	18	C
27	BA	19	A
27	BA	21	C
27	BA	32	G
27	BA	33	G
27	BA	37	A
27	BA	43	C
27	BA	51	G
27	BA	55	5MC
27	BA	64	G
27	BA	73	A
27	BA	80	A
27	BA	83	A
27	BA	84	G
27	BA	94	G
27	BA	100	G
27	BA	108	U
27	BA	109	C
27	BA	126	A
27	BA	127	A
27	BA	128	U
27	BA	129	G

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Mol	Chain	Res	Type
27	BA	132	A
27	BA	133	C
27	BA	134	C
27	BA	135	U
27	BA	136	C
27	BA	148	G
27	BA	153	A
27	BA	159	A
27	BA	160	G
27	BA	161	U
27	BA	162	C
27	BA	172	A
27	BA	187	A
27	BA	190	A
27	BA	206	G
27	BA	207	A
27	BA	208	A
27	BA	212	A
27	BA	213	A
27	BA	217	A
27	BA	219	A
27	BA	220	A
27	BA	221	G
27	BA	224	A
27	BA	239	G
27	BA	257	G
27	BA	277	C
27	BA	278	G
27	BA	287	G
27	BA	301	U
27	BA	302	G
27	BA	303	U
27	BA	304	A
27	BA	314	G
27	BA	316	G
27	BA	317	G
27	BA	318	A
27	BA	323	U
27	BA	331	A
27	BA	332	A
27	BA	340	U
27	BA	341	C

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Mol	Chain	Res	Type
27	BA	342	OMC
27	BA	343	G
27	BA	350	C
27	BA	360	G
27	BA	365	OMG
27	BA	368	G
27	BA	369	A
27	BA	372	G
27	BA	377	G
27	BA	398	C
27	BA	401	G
27	BA	405	U
27	BA	408	C
27	BA	411	U
27	BA	414	G
27	BA	429	U
27	BA	430	A
27	BA	440	A
27	BA	445	G
27	BA	453	OMU
27	BA	456	G
27	BA	460	C
27	BA	472	A
27	BA	476	C
27	BA	495	U
27	BA	496	A
27	BA	506	G
27	BA	518	A
27	BA	519	A
27	BA	520	G
27	BA	531	G
27	BA	540	A
27	BA	542	A
27	BA	543	G
27	BA	546	C
27	BA	567	G
27	BA	568	A
27	BA	569	G
27	BA	570	G
27	BA	574	C
27	BA	581	A
27	BA	584	OMG

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Mol	Chain	Res	Type
27	BA	589	G
27	BA	616	C
27	BA	622	A
27	BA	623	G
27	BA	654	C
27	BA	666	A
27	BA	674	OMG
27	BA	677	A
27	BA	688	G
27	BA	694	A
27	BA	707	C
27	BA	708	A
27	BA	729	C
27	BA	733	C
27	BA	734	A
27	BA	736	G
27	BA	801	A
27	BA	802	A
27	BA	803	G
27	BA	812	U
27	BA	835	C
27	BA	840	A
27	BA	841	A
27	BA	842	C
27	BA	844	G
27	BA	846	G
27	BA	849	A2M
27	BA	852	G
27	BA	853	A
27	BA	856	C
27	BA	870	U
27	BA	875	5MU
27	BA	891	G
27	BA	892	A
27	BA	893	C
27	BA	903	G
27	BA	904	G
27	BA	910	A
27	BA	912	OMG
27	BA	913	G
27	BA	920	G
27	BA	933	G

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Mol	Chain	Res	Type
27	BA	940	C
27	BA	950	U
27	BA	951	A
27	BA	955	C
27	BA	956	C
27	BA	974	A
27	BA	975	G
27	BA	983	G
27	BA	988	G
27	BA	995	A
27	BA	998	G
27	BA	1001	U
27	BA	1003	G
27	BA	1006	G
27	BA	1008	U
27	BA	1012	G
27	BA	1014	G
27	BA	1016	C
27	BA	1017	G
27	BA	1018	A
27	BA	1019	A
27	BA	1021	G
27	BA	1022	C
27	BA	1023	C
27	BA	1026	C
27	BA	1031	C
27	BA	1036	U
27	BA	1039	A
27	BA	1041	C
27	BA	1048	C
27	BA	1066	G
27	BA	1076	G
27	BA	1077	G
27	BA	1102	G
27	BA	1103	A
27	BA	1117	G
27	BA	1119	C
27	BA	1129	G
27	BA	1130	G
27	BA	1136	A
27	BA	1139	U
27	BA	1140	G

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Mol	Chain	Res	Type
27	BA	1144	G
27	BA	1149	G
27	BA	1158	C
27	BA	1159	A
27	BA	1165	U
27	BA	1175	C
27	BA	1177	U
27	BA	1179	G
27	BA	1180	A
27	BA	1183	G
27	BA	1184	C
27	BA	1238	C
27	BA	1239	G
27	BA	1243	A
27	BA	1244	G
27	BA	1249	G
27	BA	1250	G
27	BA	1266	C
27	BA	1270	G
27	BA	1275	A
27	BA	1307	A
27	BA	1309	U
27	BA	1310	G
27	BA	1318	A
27	BA	1320	C
27	BA	1322	G
27	BA	1331	G
27	BA	1336	C
27	BA	1361	A
27	BA	1362	G
27	BA	1372	A
27	BA	1373	C
27	BA	1388	G
27	BA	1391	C
27	BA	1409	A
27	BA	1410	U
27	BA	1436	U
27	BA	1437	A
27	BA	1438	G
27	BA	1474	G
27	BA	1490	C
27	BA	1503	U

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Mol	Chain	Res	Type
27	BA	1515	A
27	BA	1517	A
27	BA	1521	A
27	BA	1533	A
27	BA	1556	G
27	BA	1563	C
27	BA	1568	G
27	BA	1581	C
27	BA	1606	A
27	BA	1608	A
27	BA	1623	U
27	BA	1638	U
27	BA	1639	G
27	BA	1640	C
27	BA	1664	A
27	BA	1671	A
27	BA	1672	U
27	BA	1673	G
27	BA	1680	C
27	BA	1681	G
27	BA	1683	A
27	BA	1685	G
27	BA	1692	U
27	BA	1693	C
27	BA	1696	C
27	BA	1699	A
27	BA	1706	G
27	BA	1715	A
27	BA	1734	U
27	BA	1741	C
27	BA	1742	G
27	BA	1743	A
27	BA	1752	A
27	BA	1754	A
27	BA	1755	A
27	BA	1762	C
27	BA	1764	G
27	BA	1767	G
27	BA	1768	C
27	BA	1769	C
27	BA	1785	U
27	BA	1792	U

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Mol	Chain	Res	Type
27	BA	1793	G
27	BA	1795	C
27	BA	1801	A
27	BA	1811	G
27	BA	1822	G
27	BA	1848	A
27	BA	1859	G
27	BA	1861	G
27	BA	1884	G
27	BA	1891	G
27	BA	1892	G
27	BA	1901	A
27	BA	1904	G
27	BA	1908	A
27	BA	1914	A
27	BA	1928	C
27	BA	1929	U
27	BA	1945	G
27	BA	1957	A
27	BA	1967	A
27	BA	1991	A
27	BA	2002	A
27	BA	2014	A
27	BA	2016	OMG
27	BA	2020	G
27	BA	2021	G
27	BA	2023	G
27	BA	2024	U
27	BA	2025	A
27	BA	2026	A
27	BA	2027	C
27	BA	2028	U
27	BA	2029	A
27	BA	2031	A
27	BA	2033	C
27	BA	2034	C
27	BA	2036	U
27	BA	2037	C
27	BA	2039	U
27	BA	2043	G
27	BA	2050	A
27	BA	2053	U

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Mol	Chain	Res	Type
27	BA	2054	C
27	BA	2067	A
27	BA	2068	U
27	BA	2076	U
27	BA	2080	U
27	BA	2083	A
27	BA	2084	U
27	BA	2085	G
27	BA	2104	U
27	BA	2133	U
27	BA	2139	G
27	BA	2142	C
27	BA	2143	A
27	BA	2144	U
27	BA	2145	A
27	BA	2167	A
27	BA	2174	A
27	BA	2175	C
27	BA	2181	G
27	BA	2205	G
27	BA	2207	C
27	BA	2219	G
27	BA	2220	G
27	BA	2222	G
27	BA	2223	C
27	BA	2224	G
27	BA	2225	C
27	BA	2226	A
27	BA	2227	G
27	BA	2228	C
27	BA	2229	G
27	BA	2230	U
27	BA	2234	C
27	BA	2237	G
27	BA	2238	A
27	BA	2240	G
27	BA	2242	G
27	BA	2243	U
27	BA	2244	C
27	BA	2245	G
27	BA	2248	G
27	BA	2249	C

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Mol	Chain	Res	Type
27	BA	2257	C
27	BA	2260	G
27	BA	2261	G
27	BA	2269	G
27	BA	2270	A
27	BA	2271	G
27	BA	2275	C
27	BA	2278	A
27	BA	2281	A
27	BA	2282	G
27	BA	2283	A
27	BA	2286	C
27	BA	2288	G
27	BA	2292	A
27	BA	2299	G
27	BA	2310	A
27	BA	2311	A
27	BA	2317	G
27	BA	2318	G
27	BA	2321	G
27	BA	2327	A
27	BA	2328	C
27	BA	2336	G
27	BA	2337	G
27	BA	2340	G
27	BA	2353	OMG
27	BA	2360	A
27	BA	2369	A
27	BA	2382	G
27	BA	2385	G
27	BA	2386	C
27	BA	2390	A
27	BA	2391	A
27	BA	2409	C
27	BA	2412	G
27	BA	2414	A
27	BA	2415	U
27	BA	2423	A
27	BA	2425	A
27	BA	2428	G
27	BA	2438	A
27	BA	2448	G

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Mol	Chain	Res	Type
27	BA	2450	C
27	BA	2453	G
27	BA	2460	A
27	BA	2469	OMG
27	BA	2483	A
27	BA	2489	G
27	BA	2491	C
27	BA	2498	A
27	BA	2527	OMG
27	BA	2531	G
27	BA	2534	A
27	BA	2535	G
27	BA	2536	A
27	BA	2542	OMU
27	BA	2545	OMC
27	BA	2551	G
27	BA	2552	A
27	BA	2557	A
27	BA	2572	G
27	BA	2573	A
27	BA	2574	G
27	BA	2579	C
27	BA	2580	A
27	BA	2595	OMC
27	BA	2596	U
27	BA	2602	C
27	BA	2606	G
27	BA	2609	G
27	BA	2622	A
27	BA	2633	G
27	BA	2638	A
27	BA	2640	OMG
27	BA	2642	OMG
27	BA	2670	A
27	BA	2671	G
27	BA	2677	C
27	BA	2682	G
27	BA	2686	G
27	BA	2703	G
27	BA	2706	A
27	BA	2707	G
27	BA	2713	A

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Mol	Chain	Res	Type
27	BA	2717	U
27	BA	2718	A
27	BA	2719	U
27	BA	2733	U
27	BA	2744	G
27	BA	2749	A
27	BA	2750	G
27	BA	2766	G
27	BA	2768	G
27	BA	2776	G
27	BA	2787	U
27	BA	2794	U
27	BA	2808	C
27	BA	2809	A
27	BA	2815	U
27	BA	2817	G
27	BA	2829	C
27	BA	2836	G
27	BA	2837	C
27	BA	2850	A
27	BA	2853	G
27	BA	2860	A
27	BA	2862	G
27	BA	2864	C
27	BA	2867	A
27	BA	2878	A
27	BA	2879	A
27	BA	2882	C
27	BA	2884	G
27	BA	2937	G
27	BA	2944	G
27	BA	2959	U
27	BA	2960	G
27	BA	2961	A
27	BA	2982	G
27	BA	2988	A
27	BA	2995	C
27	BA	3001	C
27	BA	3007	G
27	BA	3008	C
27	BA	3017	A
27	BA	3021	C

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Mol	Chain	Res	Type
27	BA	3023	C
27	BA	3024	G
27	BA	3026	G
27	BA	3032	C
27	BA	3034	G
28	BB	4	A
28	BB	11	C
28	BB	13	A
28	BB	27	A
28	BB	35	U
28	BB	41	U
28	BB	44	G
28	BB	47	C
28	BB	50	G
28	BB	53	A
28	BB	57	A
28	BB	79	G
28	BB	89	C
28	BB	95	G
28	BB	115	G

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	108	U
27	BA	128	U
27	BA	134	C
27	BA	303	U
27	BA	317	G
27	BA	404	G
27	BA	410	C
27	BA	471	U
27	BA	687	A
27	BA	912	OMG
27	BA	974	A
27	BA	1002	G
27	BA	1030	U
27	BA	1178	A
27	BA	1360	G
27	BA	1670	A
27	BA	1671	A
27	BA	1691	U

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Mol	Chain	Res	Type
27	BA	1741	C
27	BA	1742	G
27	BA	1754	A
27	BA	1767	G
27	BA	1928	C
27	BA	2053	U
27	BA	2173	G
27	BA	2174	A
27	BA	2239	G
27	BA	2268	G
27	BA	2482	A
27	BA	2534	A
27	BA	2551	G
27	BA	2571	C
27	BA	2595	OMC
27	BA	2605	5MC
27	BA	2836	G
27	BA	3023	C
28	BB	34	G
28	BB	52	A
28	BB	56	U

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

145 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
27	OMG	BA	2016	27	23,26,27	2.34	8 (34%)	33,38,41	1.84	8 (24%)
1	5MC	Aa	1004	1	18,22,23	3.59	7 (38%)	26,32,35	1.01	2 (7%)
27	5MU	BA	1854	27	19,22,23	4.88	7 (36%)	28,32,35	3.73	9 (32%)
27	OMG	BA	2672	27	23,26,27	2.33	8 (34%)	33,38,41	1.85	8 (24%)
27	OMG	BA	912	27	23,26,27	2.33	8 (34%)	33,38,41	1.86	8 (24%)
27	OMG	BA	674	27	23,26,27	2.33	9 (39%)	33,38,41	1.81	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	Aa	457	1	18,22,23	3.58	7 (38%)	26,32,35	1.01	2 (7%)
27	OMU	BA	2656	27	19,22,23	3.03	8 (42%)	26,31,34	1.70	4 (15%)
27	OMG	BA	2010	27	23,26,27	2.32	8 (34%)	33,38,41	1.86	8 (24%)
1	MA6	Aa	1468	1	23,26,27	1.33	4 (17%)	34,38,41	3.45	12 (35%)
27	OMG	BA	2353	27	23,26,27	1.25	3 (13%)	33,38,41	2.02	6 (18%)
1	OMG	Aa	770	1	23,26,27	2.34	9 (39%)	33,38,41	1.85	8 (24%)
27	OMC	BA	2545	27	19,22,23	3.02	8 (42%)	26,31,34	0.76	0
1	6MZ	Aa	1449	1	22,25,26	1.45	4 (18%)	30,36,39	2.15	8 (26%)
27	OMU	BA	1776	27	19,22,23	3.02	8 (42%)	26,31,34	1.65	4 (15%)
27	OMG	BA	2870	27	23,26,27	2.32	9 (39%)	33,38,41	1.79	8 (24%)
1	5MC	Aa	854	1	18,22,23	3.55	7 (38%)	26,32,35	1.05	2 (7%)
27	OMC	BA	91	27	19,22,23	2.99	8 (42%)	26,31,34	0.69	0
1	5MC	Aa	464	1	18,22,23	3.59	7 (38%)	26,32,35	1.03	2 (7%)
27	OMC	BA	66	27	19,22,23	2.97	8 (42%)	26,31,34	0.76	0
1	OMG	Aa	147	1	23,26,27	2.35	8 (34%)	33,38,41	1.83	8 (24%)
27	OMC	BA	342	27	19,22,23	0.84	0	26,31,34	0.98	1 (3%)
1	5MC	Aa	349	1	18,22,23	3.54	7 (38%)	26,32,35	1.04	2 (7%)
27	OMG	BA	2640	27	23,26,27	2.35	8 (34%)	33,38,41	1.90	9 (27%)
1	5MC	Aa	923	1	18,22,23	3.54	7 (38%)	26,32,35	1.08	2 (7%)
27	5MC	BA	2075	27	18,22,23	3.51	7 (38%)	26,32,35	1.04	2 (7%)
27	4SU	BA	2553	27	18,21,22	1.75	4 (22%)	26,30,33	2.19	5 (19%)
1	5MC	Aa	1006	1	18,22,23	3.57	7 (38%)	26,32,35	1.04	2 (7%)
27	OMC	BA	2124	27	19,22,23	2.97	8 (42%)	26,31,34	0.66	0
1	2MG	Aa	995	1	23,26,27	1.25	4 (17%)	32,38,41	2.19	7 (21%)
1	OMU	Aa	479	1	19,22,23	3.07	8 (42%)	26,31,34	1.70	4 (15%)
27	A2M	BA	505	27	22,25,26	3.40	9 (40%)	31,36,39	2.54	12 (38%)
27	5MC	BA	1965	27	18,22,23	3.55	7 (38%)	26,32,35	1.04	2 (7%)
27	OMC	BA	869	27	19,22,23	2.97	8 (42%)	26,31,34	0.70	0
1	5MC	Aa	1306	1	18,22,23	3.55	7 (38%)	26,32,35	1.01	2 (7%)
27	OMG	BA	1956	27	23,26,27	2.35	8 (34%)	33,38,41	1.88	8 (24%)
27	A2M	BA	879	27	22,25,26	3.40	9 (40%)	31,36,39	2.55	11 (35%)
27	OMG	BA	288	27	23,26,27	2.36	8 (34%)	33,38,41	1.85	8 (24%)
1	OMG	Aa	574	1	23,26,27	2.36	8 (34%)	33,38,41	1.84	8 (24%)
1	OMG	Aa	121	1	23,26,27	2.34	8 (34%)	33,38,41	1.85	8 (24%)
1	OMG	Aa	1223	1	23,26,27	2.36	8 (34%)	33,38,41	1.86	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	Aa	473	1	18,22,23	3.54	7 (38%)	26,32,35	1.07	2 (7%)
27	A2M	BA	849	27	22,25,26	3.39	9 (40%)	31,36,39	2.51	10 (32%)
27	5MC	BA	2688	27	18,22,23	3.55	7 (38%)	26,32,35	1.04	1 (3%)
27	4SU	BA	2581	27	18,21,22	4.24	8 (44%)	26,30,33	2.23	5 (19%)
1	OMU	Aa	1020	1	19,22,23	3.04	8 (42%)	26,31,34	1.67	5 (19%)
1	5MC	Aa	672	1	18,22,23	3.54	7 (38%)	26,32,35	1.02	2 (7%)
27	OMG	BA	872	27	23,26,27	2.31	8 (34%)	33,38,41	1.85	9 (27%)
27	5MU	BA	2427	27	19,22,23	4.92	7 (36%)	28,32,35	3.62	9 (32%)
27	OMG	BA	215	27	23,26,27	2.33	8 (34%)	33,38,41	1.86	8 (24%)
27	OMG	BA	65	27	23,26,27	2.33	8 (34%)	33,38,41	1.83	8 (24%)
1	OMG	Aa	532	1	23,26,27	2.33	9 (39%)	33,38,41	1.82	8 (24%)
27	OMG	BA	670	27	23,26,27	2.32	8 (34%)	33,38,41	1.91	9 (27%)
1	OMU	Aa	8	1	19,22,23	3.02	8 (42%)	26,31,34	1.71	5 (19%)
1	OMG	Aa	852	1	23,26,27	1.22	3 (13%)	33,38,41	2.10	8 (24%)
1	OMG	Aa	963	1	23,26,27	2.37	8 (34%)	33,38,41	1.81	8 (24%)
27	OMG	BA	2379	27	23,26,27	2.33	8 (34%)	33,38,41	1.86	8 (24%)
27	OMC	BA	2107	27	19,22,23	2.99	8 (42%)	26,31,34	0.77	0
1	OMC	Aa	1361	1	19,22,23	3.02	8 (42%)	26,31,34	0.74	0
1	OMG	Aa	495	1	23,26,27	2.34	8 (34%)	33,38,41	1.85	8 (24%)
1	OMC	Aa	825	1	19,22,23	2.97	8 (42%)	26,31,34	0.73	0
1	OMU	Aa	753	1	19,22,23	3.05	8 (42%)	26,31,34	1.70	4 (15%)
1	OMG	Aa	219	1	23,26,27	2.33	8 (34%)	33,38,41	1.82	8 (24%)
1	5MC	Aa	1184	1	18,22,23	3.56	7 (38%)	26,32,35	1.01	2 (7%)
1	5MC	Aa	1478	1	18,22,23	3.58	7 (38%)	26,32,35	1.11	2 (7%)
27	OMG	BA	2745	27	23,26,27	2.31	9 (39%)	33,38,41	1.84	8 (24%)
1	OMG	Aa	836	1	23,26,27	2.35	8 (34%)	33,38,41	1.88	8 (24%)
1	OMG	Aa	450	1	23,26,27	1.23	3 (13%)	33,38,41	2.05	8 (24%)
1	OMG	Aa	1107	1	23,26,27	2.36	8 (34%)	33,38,41	1.85	8 (24%)
27	OMU	BA	453	27	19,22,23	3.03	8 (42%)	26,31,34	1.72	4 (15%)
1	5MC	Aa	1321	1	18,22,23	3.51	7 (38%)	26,32,35	1.15	2 (7%)
1	OMG	Aa	446	1	23,26,27	2.33	8 (34%)	33,38,41	1.86	8 (24%)
1	5MC	Aa	1476	1	18,22,23	3.52	7 (38%)	26,32,35	0.99	2 (7%)
1	5MC	Aa	17	1	18,22,23	3.51	7 (38%)	26,32,35	1.01	2 (7%)
1	5MC	Aa	340	1	18,22,23	3.56	7 (38%)	26,32,35	1.11	2 (7%)
1	OMG	Aa	629	1	23,26,27	2.35	8 (34%)	33,38,41	1.87	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	OMC	BA	2047	27	19,22,23	2.96	8 (42%)	26,31,34	0.74	0
27	5MU	BA	875	27	19,22,23	4.92	7 (36%)	28,32,35	3.63	10 (35%)
27	OMU	BA	1480	27	19,22,23	3.04	8 (42%)	26,31,34	1.70	4 (15%)
27	OMG	BA	1893	27	23,26,27	2.35	8 (34%)	33,38,41	1.88	8 (24%)
27	OMU	BA	2542	27	19,22,23	3.01	8 (42%)	26,31,34	1.66	4 (15%)
27	OMC	BA	2967	27	19,22,23	3.00	8 (42%)	26,31,34	0.73	0
1	LV2	Aa	918	1	20,23,24	0.89	0	26,33,36	0.81	0
27	5MC	BA	2055	27	18,22,23	3.57	7 (38%)	26,32,35	1.00	1 (3%)
1	5MC	Aa	1266	1	18,22,23	3.56	7 (38%)	26,32,35	1.02	2 (7%)
1	OMG	Aa	670	1	23,26,27	2.35	8 (34%)	33,38,41	1.90	8 (24%)
1	5MC	Aa	685	1	18,22,23	3.53	7 (38%)	26,32,35	1.04	2 (7%)
27	OMC	BA	2169	27	19,22,23	2.98	8 (42%)	26,31,34	0.75	0
1	A2M	Aa	352	1	22,25,26	3.39	9 (40%)	31,36,39	2.53	10 (32%)
27	OMU	BA	2389	27	19,22,23	1.33	4 (21%)	26,31,34	2.01	7 (26%)
1	OMG	Aa	498	1	23,26,27	2.35	8 (34%)	33,38,41	1.87	8 (24%)
27	A2M	BA	2091	27	22,25,26	1.40	4 (18%)	31,36,39	2.21	10 (32%)
27	5MC	BA	2605	27	18,22,23	3.55	7 (38%)	26,32,35	1.12	2 (7%)
27	OMG	BA	2521	27	23,26,27	2.33	9 (39%)	33,38,41	1.86	8 (24%)
27	OMG	BA	833	27	23,26,27	2.35	8 (34%)	33,38,41	1.85	8 (24%)
27	OMG	BA	2550	27	23,26,27	1.27	3 (13%)	33,38,41	1.99	7 (21%)
27	OMG	BA	2469	27	23,26,27	2.33	8 (34%)	33,38,41	1.85	9 (27%)
1	OMU	Aa	1358	1	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
27	5MC	BA	1345	27	18,22,23	3.55	7 (38%)	26,32,35	1.02	1 (3%)
27	OMG	BA	1508	27	23,26,27	2.35	8 (34%)	33,38,41	1.86	8 (24%)
27	OMG	BA	2168	27	23,26,27	2.33	8 (34%)	33,38,41	1.85	8 (24%)
27	A2M	BA	2936	27	22,25,26	3.42	9 (40%)	31,36,39	2.50	12 (38%)
27	OMG	BA	1525	27	23,26,27	2.33	8 (34%)	33,38,41	1.82	8 (24%)
1	5MC	Aa	1352	1	18,22,23	3.59	7 (38%)	26,32,35	0.98	1 (3%)
1	5MC	Aa	1003	1	18,22,23	3.57	7 (38%)	26,32,35	1.01	2 (7%)
1	OMG	Aa	994	1	23,26,27	2.36	8 (34%)	33,38,41	1.85	8 (24%)
27	OMU	BA	1402	27	19,22,23	3.06	8 (42%)	26,31,34	1.67	4 (15%)
1	OMC	Aa	1354	1	19,22,23	2.97	8 (42%)	26,31,34	0.77	0
27	A2M	BA	932	27	22,25,26	3.43	9 (40%)	31,36,39	2.50	11 (35%)
27	OMG	BA	1953	27	23,26,27	2.31	9 (39%)	33,38,41	1.79	8 (24%)
27	OMC	BA	1995	27	19,22,23	3.00	8 (42%)	26,31,34	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	Aa	381	1	23,26,27	2.36	8 (34%)	33,38,41	1.85	8 (24%)
27	OMC	BA	1820	27	19,22,23	3.00	8 (42%)	26,31,34	0.71	0
1	OMC	Aa	924	1	19,22,23	3.01	8 (42%)	26,31,34	0.73	0
27	A2M	BA	2329	27	22,25,26	1.44	3 (13%)	31,36,39	2.08	8 (25%)
1	OMC	Aa	229	1	19,22,23	3.00	8 (42%)	26,31,34	0.78	0
1	OMC	Aa	752	1	19,22,23	3.01	8 (42%)	26,31,34	0.71	0
27	OMG	BA	63	27	23,26,27	2.35	8 (34%)	33,38,41	1.87	8 (24%)
27	5MU	BA	1766	27	19,22,23	4.88	7 (36%)	28,32,35	3.67	9 (32%)
27	OMG	BA	584	27	23,26,27	2.35	8 (34%)	33,38,41	1.86	8 (24%)
27	OMU	BA	1969	27	19,22,23	3.05	8 (42%)	26,31,34	1.73	5 (19%)
1	5MU	Aa	917	1	19,22,23	1.36	4 (21%)	28,32,35	2.15	6 (21%)
27	5MC	BA	2070	27	18,22,23	3.50	7 (38%)	26,32,35	1.01	2 (7%)
27	5MC	BA	55	27	18,22,23	3.48	7 (38%)	26,32,35	1.17	3 (11%)
27	OMG	BA	365	27	23,26,27	2.33	8 (34%)	33,38,41	1.87	9 (27%)
27	OMG	BA	2527	27	23,26,27	2.33	8 (34%)	33,38,41	1.80	8 (24%)
27	OMG	BA	2642	27	23,26,27	2.32	8 (34%)	33,38,41	1.90	9 (27%)
1	OMG	Aa	891	1	23,26,27	2.34	8 (34%)	33,38,41	1.82	8 (24%)
27	OMC	BA	2595	27	19,22,23	3.03	8 (42%)	26,31,34	0.92	1 (3%)
27	OMG	BA	507	27	23,26,27	2.33	9 (39%)	33,38,41	1.83	8 (24%)
1	OMG	Aa	636	1	23,26,27	2.36	8 (34%)	33,38,41	1.88	9 (27%)
1	OMG	Aa	659	1	23,26,27	2.34	8 (34%)	33,38,41	1.83	8 (24%)
1	OMC	Aa	112	1	19,22,23	2.99	8 (42%)	26,31,34	0.74	0
1	MA6	Aa	1467	1	23,26,27	1.33	4 (17%)	34,38,41	3.39	11 (32%)
27	5MU	BA	829	27	19,22,23	4.86	7 (36%)	28,32,35	3.68	10 (35%)
27	OMU	BA	1150	27	19,22,23	3.03	8 (42%)	26,31,34	1.70	4 (15%)
1	OMG	Aa	320	1	23,26,27	2.33	8 (34%)	33,38,41	1.85	8 (24%)
1	OMG	Aa	913	1	23,26,27	2.35	8 (34%)	33,38,41	1.83	8 (24%)
27	OMG	BA	2528	27	23,26,27	2.32	9 (39%)	33,38,41	1.81	8 (24%)
1	5MC	Aa	1007	1	18,22,23	3.57	7 (38%)	26,32,35	1.05	1 (3%)
27	OMG	BA	2466	27	23,26,27	2.32	8 (34%)	33,38,41	1.78	8 (24%)
27	OMG	BA	2728	27	23,26,27	2.32	8 (34%)	33,38,41	1.83	8 (24%)
27	OMG	BA	1329	27	23,26,27	2.33	8 (34%)	33,38,41	1.89	8 (24%)
27	OMU	BA	657	27	19,22,23	3.01	8 (42%)	26,31,34	1.70	4 (15%)
27	OMG	BA	800	27	23,26,27	2.33	8 (34%)	33,38,41	1.85	8 (24%)

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
27	OMG	BA	2016	27	-	2/9/27/28	0/3/3/3
1	5MC	Aa	1004	1	-	3/7/25/26	0/2/2/2
27	5MU	BA	1854	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	2672	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	912	27	-	1/9/27/28	0/3/3/3
27	OMG	BA	674	27	-	2/9/27/28	0/3/3/3
1	5MC	Aa	457	1	-	2/7/25/26	0/2/2/2
27	OMU	BA	2656	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	2010	27	-	0/9/27/28	0/3/3/3
1	MA6	Aa	1468	1	-	1/11/29/30	0/3/3/3
27	OMG	BA	2353	27	-	2/9/27/28	0/3/3/3
1	OMG	Aa	770	1	-	0/9/27/28	0/3/3/3
27	OMC	BA	2545	27	-	3/9/27/28	0/2/2/2
1	6MZ	Aa	1449	1	-	2/9/27/28	0/3/3/3
27	OMU	BA	1776	27	-	1/9/27/28	0/2/2/2
27	OMG	BA	2870	27	-	0/9/27/28	0/3/3/3
1	5MC	Aa	854	1	-	0/7/25/26	0/2/2/2
27	OMC	BA	91	27	-	1/9/27/28	0/2/2/2
1	5MC	Aa	464	1	-	0/7/25/26	0/2/2/2
27	OMC	BA	66	27	-	1/9/27/28	0/2/2/2
1	OMG	Aa	147	1	-	1/9/27/28	0/3/3/3
27	OMC	BA	342	27	-	2/9/27/28	0/2/2/2
1	5MC	Aa	349	1	-	0/7/25/26	0/2/2/2
27	OMG	BA	2640	27	-	3/9/27/28	0/3/3/3
1	5MC	Aa	923	1	-	0/7/25/26	0/2/2/2
27	5MC	BA	2075	27	-	0/7/25/26	0/2/2/2
27	4SU	BA	2553	27	-	0/7/25/26	0/2/2/2
1	5MC	Aa	1006	1	-	0/7/25/26	0/2/2/2
27	OMC	BA	2124	27	-	1/9/27/28	0/2/2/2
1	2MG	Aa	995	1	-	0/9/27/28	0/3/3/3
1	OMU	Aa	479	1	-	0/9/27/28	0/2/2/2
27	A2M	BA	505	27	-	0/9/27/28	0/3/3/3
27	5MC	BA	1965	27	-	0/7/25/26	0/2/2/2
27	OMC	BA	869	27	-	0/9/27/28	0/2/2/2
1	5MC	Aa	1306	1	-	3/7/25/26	0/2/2/2
27	OMG	BA	1956	27	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	A2M	BA	879	27	-	1/9/27/28	0/3/3/3
27	OMG	BA	288	27	-	1/9/27/28	0/3/3/3
1	OMG	Aa	574	1	-	1/9/27/28	0/3/3/3
1	OMG	Aa	121	1	-	2/9/27/28	0/3/3/3
1	OMG	Aa	1223	1	-	0/9/27/28	0/3/3/3
1	5MC	Aa	473	1	-	0/7/25/26	0/2/2/2
27	A2M	BA	849	27	-	2/9/27/28	0/3/3/3
27	5MC	BA	2688	27	-	0/7/25/26	0/2/2/2
27	4SU	BA	2581	27	-	1/7/25/26	0/2/2/2
1	OMU	Aa	1020	1	-	1/9/27/28	0/2/2/2
1	5MC	Aa	672	1	-	0/7/25/26	0/2/2/2
27	OMG	BA	872	27	-	0/9/27/28	0/3/3/3
27	5MU	BA	2427	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	215	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	65	27	-	1/9/27/28	0/3/3/3
1	OMG	Aa	532	1	-	0/9/27/28	0/3/3/3
27	OMG	BA	670	27	-	1/9/27/28	0/3/3/3
1	OMU	Aa	8	1	-	6/9/27/28	0/2/2/2
1	OMG	Aa	852	1	-	0/9/27/28	0/3/3/3
1	OMG	Aa	963	1	-	2/9/27/28	0/3/3/3
27	OMG	BA	2379	27	-	2/9/27/28	0/3/3/3
27	OMC	BA	2107	27	-	0/9/27/28	0/2/2/2
1	OMC	Aa	1361	1	-	1/9/27/28	0/2/2/2
1	OMG	Aa	495	1	-	2/9/27/28	0/3/3/3
1	OMC	Aa	825	1	-	0/9/27/28	0/2/2/2
1	OMU	Aa	753	1	-	1/9/27/28	0/2/2/2
1	OMG	Aa	219	1	-	2/9/27/28	0/3/3/3
1	5MC	Aa	1184	1	-	0/7/25/26	0/2/2/2
1	5MC	Aa	1478	1	-	5/7/25/26	0/2/2/2
27	OMG	BA	2745	27	-	0/9/27/28	0/3/3/3
1	OMG	Aa	836	1	-	0/9/27/28	0/3/3/3
1	OMG	Aa	450	1	-	0/9/27/28	0/3/3/3
1	OMG	Aa	1107	1	-	2/9/27/28	0/3/3/3
27	OMU	BA	453	27	-	2/9/27/28	0/2/2/2
1	5MC	Aa	1321	1	-	0/7/25/26	0/2/2/2
1	OMG	Aa	446	1	-	0/9/27/28	0/3/3/3
1	5MC	Aa	1476	1	-	0/7/25/26	0/2/2/2
1	5MC	Aa	17	1	-	2/7/25/26	0/2/2/2
1	5MC	Aa	340	1	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	Aa	629	1	-	0/9/27/28	0/3/3/3
27	OMC	BA	2047	27	-	3/9/27/28	0/2/2/2
27	5MU	BA	875	27	-	0/7/25/26	0/2/2/2
27	OMU	BA	1480	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	1893	27	-	2/9/27/28	0/3/3/3
27	OMU	BA	2542	27	-	2/9/27/28	0/2/2/2
27	OMC	BA	2967	27	-	0/9/27/28	0/2/2/2
1	LV2	Aa	918	1	-	0/9/29/30	0/2/2/2
27	5MC	BA	2055	27	-	0/7/25/26	0/2/2/2
1	5MC	Aa	1266	1	-	0/7/25/26	0/2/2/2
1	OMG	Aa	670	1	-	2/9/27/28	0/3/3/3
1	5MC	Aa	685	1	-	0/7/25/26	0/2/2/2
27	OMC	BA	2169	27	-	0/9/27/28	0/2/2/2
1	A2M	Aa	352	1	-	2/9/27/28	0/3/3/3
27	OMU	BA	2389	27	-	2/9/27/28	0/2/2/2
1	OMG	Aa	498	1	-	2/9/27/28	0/3/3/3
27	A2M	BA	2091	27	-	0/9/27/28	0/3/3/3
27	5MC	BA	2605	27	-	4/7/25/26	0/2/2/2
27	OMG	BA	2521	27	-	1/9/27/28	0/3/3/3
27	OMG	BA	833	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	2550	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	2469	27	-	4/9/27/28	0/3/3/3
1	OMU	Aa	1358	1	-	0/9/27/28	0/2/2/2
27	5MC	BA	1345	27	-	1/7/25/26	0/2/2/2
27	OMG	BA	1508	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	2168	27	-	0/9/27/28	0/3/3/3
27	A2M	BA	2936	27	-	1/9/27/28	0/3/3/3
27	OMG	BA	1525	27	-	2/9/27/28	0/3/3/3
1	5MC	Aa	1352	1	-	2/7/25/26	0/2/2/2
1	5MC	Aa	1003	1	-	0/7/25/26	0/2/2/2
1	OMG	Aa	994	1	-	0/9/27/28	0/3/3/3
27	OMU	BA	1402	27	-	2/9/27/28	0/2/2/2
1	OMC	Aa	1354	1	-	0/9/27/28	0/2/2/2
27	A2M	BA	932	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	1953	27	-	1/9/27/28	0/3/3/3
27	OMC	BA	1995	27	-	1/9/27/28	0/2/2/2
1	OMG	Aa	381	1	-	2/9/27/28	0/3/3/3
27	OMC	BA	1820	27	-	1/9/27/28	0/2/2/2
1	OMC	Aa	924	1	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	A2M	BA	2329	27	-	2/9/27/28	0/3/3/3
1	OMC	Aa	229	1	-	1/9/27/28	0/2/2/2
1	OMC	Aa	752	1	-	0/9/27/28	0/2/2/2
27	OMG	BA	63	27	-	0/9/27/28	0/3/3/3
27	5MU	BA	1766	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	584	27	-	0/9/27/28	0/3/3/3
27	OMU	BA	1969	27	-	0/9/27/28	0/2/2/2
1	5MU	Aa	917	1	-	2/7/25/26	0/2/2/2
27	5MC	BA	2070	27	-	0/7/25/26	0/2/2/2
27	5MC	BA	55	27	-	3/7/25/26	0/2/2/2
27	OMG	BA	365	27	-	3/9/27/28	0/3/3/3
27	OMG	BA	2527	27	-	2/9/27/28	0/3/3/3
27	OMG	BA	2642	27	-	3/9/27/28	0/3/3/3
1	OMG	Aa	891	1	-	1/9/27/28	0/3/3/3
27	OMC	BA	2595	27	-	1/9/27/28	0/2/2/2
27	OMG	BA	507	27	-	0/9/27/28	0/3/3/3
1	OMG	Aa	636	1	-	1/9/27/28	0/3/3/3
1	OMG	Aa	659	1	-	1/9/27/28	0/3/3/3
1	OMC	Aa	112	1	-	0/9/27/28	0/2/2/2
1	MA6	Aa	1467	1	-	0/11/29/30	0/3/3/3
27	5MU	BA	829	27	-	0/7/25/26	0/2/2/2
27	OMU	BA	1150	27	-	2/9/27/28	0/2/2/2
1	OMG	Aa	320	1	-	3/9/27/28	0/3/3/3
1	OMG	Aa	913	1	-	2/9/27/28	0/3/3/3
27	OMG	BA	2528	27	-	0/9/27/28	0/3/3/3
1	5MC	Aa	1007	1	-	2/7/25/26	0/2/2/2
27	OMG	BA	2466	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	2728	27	-	1/9/27/28	0/3/3/3
27	OMG	BA	1329	27	-	0/9/27/28	0/3/3/3
27	OMU	BA	657	27	-	1/9/27/28	0/2/2/2
27	OMG	BA	800	27	-	1/9/27/28	0/3/3/3

All (1068) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	875	5MU	C2-N1	11.41	1.56	1.38
27	BA	2427	5MU	C2-N1	11.33	1.56	1.38
27	BA	1854	5MU	C2-N1	11.29	1.56	1.38
27	BA	829	5MU	C2-N1	11.25	1.56	1.38
27	BA	1766	5MU	C2-N1	11.22	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	875	5MU	C6-N1	10.84	1.56	1.38
27	BA	2427	5MU	C6-N1	10.81	1.56	1.38
27	BA	1766	5MU	C6-N1	10.65	1.56	1.38
27	BA	829	5MU	C6-N1	10.63	1.56	1.38
27	BA	1854	5MU	C6-N1	10.60	1.56	1.38
27	BA	875	5MU	C4-C5	10.00	1.61	1.44
27	BA	829	5MU	C4-C5	9.93	1.61	1.44
27	BA	1766	5MU	C4-C5	9.90	1.61	1.44
27	BA	2427	5MU	C4-C5	9.89	1.61	1.44
27	BA	1854	5MU	C4-C5	9.88	1.61	1.44
27	BA	2581	4SU	C2-N1	9.25	1.53	1.38
27	BA	1965	5MC	C6-C5	9.24	1.49	1.34
1	Aa	1004	5MC	C6-C5	9.23	1.49	1.34
27	BA	2055	5MC	C6-C5	9.22	1.49	1.34
27	BA	2605	5MC	C6-C5	9.21	1.49	1.34
1	Aa	1352	5MC	C6-C5	9.20	1.49	1.34
1	Aa	854	5MC	C6-C5	9.17	1.49	1.34
1	Aa	1007	5MC	C6-C5	9.17	1.49	1.34
1	Aa	1003	5MC	C6-C5	9.15	1.49	1.34
1	Aa	1478	5MC	C6-C5	9.15	1.49	1.34
27	BA	2688	5MC	C6-C5	9.15	1.49	1.34
27	BA	1345	5MC	C6-C5	9.14	1.49	1.34
1	Aa	457	5MC	C6-C5	9.11	1.49	1.34
1	Aa	1006	5MC	C6-C5	9.09	1.49	1.34
1	Aa	1184	5MC	C6-C5	9.08	1.49	1.34
1	Aa	464	5MC	C6-C5	9.07	1.49	1.34
1	Aa	672	5MC	C6-C5	9.07	1.49	1.34
1	Aa	685	5MC	C6-C5	9.05	1.49	1.34
1	Aa	340	5MC	C6-C5	9.05	1.49	1.34
1	Aa	923	5MC	C6-C5	9.04	1.49	1.34
1	Aa	473	5MC	C6-C5	9.04	1.49	1.34
1	Aa	1306	5MC	C6-C5	9.03	1.49	1.34
1	Aa	1266	5MC	C6-C5	9.01	1.49	1.34
1	Aa	1476	5MC	C6-C5	9.00	1.49	1.34
27	BA	2075	5MC	C6-C5	8.97	1.49	1.34
1	Aa	349	5MC	C6-C5	8.96	1.49	1.34
27	BA	2070	5MC	C6-C5	8.96	1.49	1.34
27	BA	55	5MC	C6-C5	8.94	1.49	1.34
1	Aa	17	5MC	C6-C5	8.93	1.49	1.34
1	Aa	1321	5MC	C6-C5	8.92	1.49	1.34
27	BA	932	A2M	O4'-C1'	8.69	1.62	1.42
27	BA	2936	A2M	C2'-C1'	-8.65	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	879	A2M	O4'-C1'	8.62	1.62	1.42
27	BA	2936	A2M	O4'-C1'	8.61	1.62	1.42
27	BA	505	A2M	O4'-C1'	8.55	1.62	1.42
27	BA	505	A2M	C2'-C1'	-8.54	1.31	1.53
27	BA	849	A2M	C2'-C1'	-8.53	1.31	1.53
1	Aa	352	A2M	O4'-C1'	8.50	1.62	1.42
27	BA	879	A2M	C2'-C1'	-8.49	1.31	1.53
27	BA	849	A2M	O4'-C1'	8.49	1.62	1.42
27	BA	932	A2M	C2'-C1'	-8.48	1.31	1.53
1	Aa	352	A2M	C2'-C1'	-8.45	1.31	1.53
27	BA	2581	4SU	C4-N3	8.37	1.46	1.37
27	BA	1854	5MU	C4-N3	-7.50	1.24	1.38
27	BA	2427	5MU	C4-N3	-7.44	1.25	1.38
27	BA	1766	5MU	C4-N3	-7.42	1.25	1.38
27	BA	829	5MU	C4-N3	-7.31	1.25	1.38
1	Aa	479	OMU	C2-N1	7.22	1.50	1.38
27	BA	875	5MU	C4-N3	-7.21	1.25	1.38
1	Aa	753	OMU	C2-N1	7.16	1.49	1.38
27	BA	1480	OMU	C2-N1	7.16	1.49	1.38
27	BA	2656	OMU	C2-N1	7.16	1.49	1.38
27	BA	1150	OMU	C2-N1	7.15	1.49	1.38
27	BA	1402	OMU	C2-N1	7.14	1.49	1.38
27	BA	453	OMU	C2-N1	7.14	1.49	1.38
27	BA	2542	OMU	C2-N1	7.11	1.49	1.38
1	Aa	1020	OMU	C2-N1	7.10	1.49	1.38
27	BA	1776	OMU	C2-N1	7.09	1.49	1.38
1	Aa	8	OMU	C2-N1	7.05	1.49	1.38
27	BA	657	OMU	C2-N1	7.04	1.49	1.38
27	BA	1969	OMU	C2-N1	7.03	1.49	1.38
1	Aa	1358	OMU	C2-N1	6.99	1.49	1.38
27	BA	2581	4SU	C2-N3	6.89	1.50	1.38
27	BA	2581	4SU	C5-C4	6.82	1.51	1.42
1	Aa	1020	OMU	C2-N3	6.76	1.50	1.38
27	BA	1969	OMU	C2-N3	6.75	1.50	1.38
27	BA	1402	OMU	C2-N3	6.75	1.50	1.38
1	Aa	753	OMU	C2-N3	6.74	1.50	1.38
1	Aa	479	OMU	C2-N3	6.74	1.50	1.38
27	BA	453	OMU	C2-N3	6.68	1.49	1.38
27	BA	1776	OMU	C2-N3	6.67	1.49	1.38
27	BA	2656	OMU	C2-N3	6.64	1.49	1.38
1	Aa	1358	OMU	C2-N3	6.62	1.49	1.38
1	Aa	8	OMU	C2-N3	6.62	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	464	5MC	C4-N3	6.60	1.45	1.34
27	BA	1480	OMU	C2-N3	6.59	1.49	1.38
1	Aa	1352	5MC	C4-N3	6.59	1.45	1.34
27	BA	657	OMU	C2-N3	6.59	1.49	1.38
27	BA	2542	OMU	C2-N3	6.57	1.49	1.38
1	Aa	457	5MC	C4-N3	6.55	1.45	1.34
27	BA	2427	5MU	C6-C5	6.53	1.45	1.34
27	BA	875	5MU	C6-C5	6.51	1.45	1.34
27	BA	1150	OMU	C2-N3	6.51	1.49	1.38
1	Aa	1266	5MC	C4-N3	6.49	1.45	1.34
1	Aa	1006	5MC	C4-N3	6.47	1.45	1.34
1	Aa	1184	5MC	C4-N3	6.46	1.45	1.34
1	Aa	340	5MC	C4-N3	6.46	1.45	1.34
1	Aa	1306	5MC	C4-N3	6.46	1.45	1.34
1	Aa	1003	5MC	C4-N3	6.46	1.45	1.34
1	Aa	1004	5MC	C4-N3	6.46	1.45	1.34
1	Aa	923	5MC	C4-N3	6.44	1.45	1.34
1	Aa	1321	5MC	C4-N3	6.44	1.45	1.34
27	BA	1345	5MC	C4-N3	6.43	1.45	1.34
1	Aa	1478	5MC	C4-N3	6.43	1.45	1.34
1	Aa	349	5MC	C4-N3	6.43	1.45	1.34
1	Aa	1361	OMC	C2-N3	6.41	1.49	1.36
27	BA	2967	OMC	C2-N3	6.40	1.49	1.36
27	BA	2581	4SU	C6-C5	6.38	1.49	1.35
27	BA	91	OMC	C2-N3	6.38	1.49	1.36
27	BA	932	A2M	O4'-C4'	-6.37	1.30	1.45
1	Aa	473	5MC	C4-N3	6.37	1.44	1.34
1	Aa	112	OMC	C2-N3	6.36	1.49	1.36
1	Aa	1007	5MC	C4-N3	6.36	1.44	1.34
27	BA	2055	5MC	C4-N3	6.36	1.44	1.34
1	Aa	352	A2M	O4'-C4'	-6.36	1.30	1.45
1	Aa	924	OMC	C2-N3	6.35	1.49	1.36
27	BA	2688	5MC	C4-N3	6.35	1.44	1.34
27	BA	2595	OMC	C2-N3	6.35	1.49	1.36
27	BA	2545	OMC	C2-N3	6.35	1.49	1.36
1	Aa	17	5MC	C4-N3	6.35	1.44	1.34
27	BA	1995	OMC	C2-N3	6.35	1.49	1.36
27	BA	2075	5MC	C4-N3	6.34	1.44	1.34
1	Aa	672	5MC	C4-N3	6.34	1.44	1.34
27	BA	1820	OMC	C2-N3	6.34	1.49	1.36
1	Aa	1476	5MC	C4-N3	6.33	1.44	1.34
27	BA	505	A2M	O4'-C4'	-6.33	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	229	OMC	C2-N3	6.33	1.49	1.36
1	Aa	685	5MC	C4-N3	6.32	1.44	1.34
1	Aa	752	OMC	C2-N3	6.31	1.49	1.36
1	Aa	854	5MC	C4-N3	6.31	1.44	1.34
27	BA	1766	5MU	C6-C5	6.31	1.45	1.34
27	BA	2070	5MC	C4-N3	6.30	1.44	1.34
27	BA	869	OMC	C2-N3	6.30	1.49	1.36
27	BA	2107	OMC	C2-N3	6.29	1.49	1.36
27	BA	2169	OMC	C2-N3	6.28	1.49	1.36
27	BA	1854	5MU	C6-C5	6.28	1.44	1.34
27	BA	2124	OMC	C2-N3	6.27	1.49	1.36
27	BA	55	5MC	C4-N3	6.25	1.44	1.34
27	BA	2605	5MC	C4-N3	6.25	1.44	1.34
1	Aa	963	OMG	C4-N3	6.24	1.49	1.34
1	Aa	994	OMG	C4-N3	6.24	1.49	1.34
1	Aa	495	OMG	C4-N3	6.23	1.49	1.34
1	Aa	1107	OMG	C4-N3	6.23	1.49	1.34
27	BA	2047	OMC	C2-N3	6.23	1.49	1.36
1	Aa	1223	OMG	C4-N3	6.23	1.49	1.34
1	Aa	629	OMG	C4-N3	6.23	1.49	1.34
27	BA	288	OMG	C4-N3	6.23	1.49	1.34
27	BA	833	OMG	C4-N3	6.23	1.49	1.34
1	Aa	574	OMG	C4-N3	6.22	1.49	1.34
1	Aa	636	OMG	C4-N3	6.21	1.49	1.34
27	BA	879	A2M	O4'-C4'	-6.21	1.31	1.45
1	Aa	147	OMG	C4-N3	6.21	1.49	1.34
1	Aa	381	OMG	C4-N3	6.21	1.49	1.34
1	Aa	1354	OMC	C2-N3	6.20	1.48	1.36
27	BA	2016	OMG	C4-N3	6.20	1.49	1.34
27	BA	66	OMC	C2-N3	6.20	1.48	1.36
1	Aa	825	OMC	C2-N3	6.20	1.48	1.36
27	BA	584	OMG	C4-N3	6.20	1.49	1.34
27	BA	2936	A2M	O4'-C4'	-6.20	1.31	1.45
1	Aa	498	OMG	C4-N3	6.19	1.49	1.34
27	BA	1508	OMG	C4-N3	6.19	1.49	1.34
27	BA	1965	5MC	C4-N3	6.19	1.44	1.34
1	Aa	836	OMG	C4-N3	6.19	1.49	1.34
1	Aa	670	OMG	C4-N3	6.19	1.49	1.34
1	Aa	659	OMG	C4-N3	6.19	1.49	1.34
27	BA	849	A2M	O4'-C4'	-6.19	1.31	1.45
27	BA	63	OMG	C4-N3	6.19	1.49	1.34
27	BA	1525	OMG	C4-N3	6.18	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	365	OMG	C4-N3	6.18	1.49	1.34
1	Aa	913	OMG	C4-N3	6.18	1.49	1.34
1	Aa	320	OMG	C4-N3	6.18	1.48	1.34
27	BA	2642	OMG	C4-N3	6.18	1.48	1.34
1	Aa	457	5MC	C2-N3	6.17	1.48	1.36
27	BA	829	5MU	C6-C5	6.17	1.44	1.34
27	BA	2640	OMG	C4-N3	6.17	1.48	1.34
27	BA	2466	OMG	C4-N3	6.17	1.48	1.34
27	BA	2469	OMG	C4-N3	6.17	1.48	1.34
1	Aa	464	5MC	C2-N3	6.17	1.48	1.36
27	BA	912	OMG	C4-N3	6.17	1.48	1.34
1	Aa	121	OMG	C4-N3	6.16	1.48	1.34
27	BA	2672	OMG	C4-N3	6.16	1.48	1.34
27	BA	1956	OMG	C4-N3	6.16	1.48	1.34
1	Aa	891	OMG	C4-N3	6.15	1.48	1.34
27	BA	215	OMG	C4-N3	6.15	1.48	1.34
27	BA	800	OMG	C4-N3	6.15	1.48	1.34
1	Aa	219	OMG	C4-N3	6.15	1.48	1.34
27	BA	65	OMG	C4-N3	6.15	1.48	1.34
27	BA	2527	OMG	C4-N3	6.15	1.48	1.34
27	BA	1893	OMG	C4-N3	6.14	1.48	1.34
1	Aa	770	OMG	C4-N3	6.14	1.48	1.34
27	BA	2010	OMG	C4-N3	6.14	1.48	1.34
27	BA	2168	OMG	C4-N3	6.14	1.48	1.34
1	Aa	532	OMG	C4-N3	6.13	1.48	1.34
27	BA	2528	OMG	C4-N3	6.13	1.48	1.34
1	Aa	1266	5MC	C2-N3	6.13	1.48	1.36
27	BA	1329	OMG	C4-N3	6.13	1.48	1.34
1	Aa	446	OMG	C4-N3	6.12	1.48	1.34
27	BA	2595	OMC	C6-C5	6.12	1.49	1.35
1	Aa	1006	5MC	C2-N3	6.12	1.48	1.36
27	BA	674	OMG	C4-N3	6.11	1.48	1.34
27	BA	670	OMG	C4-N3	6.11	1.48	1.34
27	BA	2745	OMG	C4-N3	6.11	1.48	1.34
27	BA	2870	OMG	C4-N3	6.11	1.48	1.34
27	BA	2379	OMG	C4-N3	6.10	1.48	1.34
27	BA	2545	OMC	C6-C5	6.10	1.49	1.35
27	BA	507	OMG	C4-N3	6.10	1.48	1.34
27	BA	2521	OMG	C4-N3	6.09	1.48	1.34
1	Aa	1352	5MC	C2-N3	6.09	1.48	1.36
1	Aa	1184	5MC	C2-N3	6.09	1.48	1.36
27	BA	2728	OMG	C4-N3	6.08	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	340	5MC	C2-N3	6.08	1.48	1.36
1	Aa	924	OMC	C6-C5	6.05	1.49	1.35
1	Aa	349	5MC	C2-N3	6.05	1.48	1.36
1	Aa	1004	5MC	C2-N3	6.05	1.48	1.36
1	Aa	923	5MC	C2-N3	6.04	1.48	1.36
27	BA	872	OMG	C4-N3	6.04	1.48	1.34
27	BA	2055	5MC	C2-N3	6.03	1.48	1.36
1	Aa	1478	5MC	C2-N3	6.02	1.48	1.36
1	Aa	1306	5MC	C2-N3	6.02	1.48	1.36
1	Aa	229	OMC	C6-C5	6.02	1.49	1.35
1	Aa	17	5MC	C2-N3	6.01	1.48	1.36
1	Aa	1007	5MC	C2-N3	6.01	1.48	1.36
1	Aa	854	5MC	C2-N3	6.01	1.48	1.36
1	Aa	752	OMC	C6-C5	6.01	1.49	1.35
1	Aa	1354	OMC	C6-C5	6.01	1.49	1.35
27	BA	2075	5MC	C2-N3	6.00	1.48	1.36
1	Aa	1003	5MC	C2-N3	6.00	1.48	1.36
1	Aa	473	5MC	C2-N3	6.00	1.48	1.36
1	Aa	1361	OMC	C6-C5	6.00	1.49	1.35
1	Aa	672	5MC	C2-N3	5.99	1.48	1.36
27	BA	1995	OMC	C6-C5	5.98	1.49	1.35
27	BA	1820	OMC	C6-C5	5.98	1.49	1.35
1	Aa	825	OMC	C6-C5	5.98	1.48	1.35
27	BA	1953	OMG	C4-N3	5.97	1.48	1.34
1	Aa	1476	5MC	C2-N3	5.97	1.48	1.36
1	Aa	112	OMC	C6-C5	5.97	1.48	1.35
27	BA	2047	OMC	C6-C5	5.96	1.48	1.35
27	BA	2688	5MC	C2-N3	5.96	1.48	1.36
27	BA	869	OMC	C6-C5	5.95	1.48	1.35
27	BA	1345	5MC	C2-N3	5.95	1.48	1.36
27	BA	1965	5MC	C2-N3	5.95	1.48	1.36
27	BA	2107	OMC	C6-C5	5.94	1.48	1.35
1	Aa	1321	5MC	C2-N3	5.94	1.48	1.36
27	BA	2169	OMC	C6-C5	5.94	1.48	1.35
27	BA	2124	OMC	C6-C5	5.94	1.48	1.35
27	BA	91	OMC	C6-C5	5.93	1.48	1.35
27	BA	2605	5MC	C2-N3	5.92	1.48	1.36
27	BA	2967	OMC	C6-C5	5.92	1.48	1.35
27	BA	66	OMC	C6-C5	5.91	1.48	1.35
1	Aa	685	5MC	C2-N3	5.91	1.48	1.36
27	BA	2070	5MC	C2-N3	5.90	1.48	1.36
27	BA	55	5MC	C2-N3	5.85	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	479	OMU	C6-C5	5.78	1.48	1.35
27	BA	1150	OMU	C6-C5	5.72	1.48	1.35
1	Aa	1020	OMU	C6-C5	5.72	1.48	1.35
1	Aa	8	OMU	C6-C5	5.71	1.48	1.35
27	BA	1969	OMU	C6-C5	5.69	1.48	1.35
1	Aa	1358	OMU	C6-C5	5.69	1.48	1.35
27	BA	1402	OMU	C6-C5	5.68	1.48	1.35
27	BA	1480	OMU	C6-C5	5.65	1.48	1.35
1	Aa	636	OMG	C2-N3	5.65	1.46	1.33
1	Aa	963	OMG	C2-N3	5.64	1.46	1.33
1	Aa	1223	OMG	C2-N3	5.64	1.46	1.33
1	Aa	670	OMG	C2-N3	5.64	1.46	1.33
1	Aa	753	OMU	C6-C5	5.64	1.48	1.35
1	Aa	1107	OMG	C2-N3	5.63	1.46	1.33
27	BA	2656	OMU	C6-C5	5.63	1.48	1.35
27	BA	2640	OMG	C2-N3	5.61	1.46	1.33
1	Aa	994	OMG	C2-N3	5.60	1.46	1.33
27	BA	2542	OMU	C6-C5	5.60	1.48	1.35
27	BA	1508	OMG	C2-N3	5.60	1.46	1.33
1	Aa	147	OMG	C2-N3	5.59	1.46	1.33
27	BA	288	OMG	C2-N3	5.59	1.46	1.33
1	Aa	659	OMG	C2-N3	5.59	1.46	1.33
27	BA	1776	OMU	C6-C5	5.59	1.48	1.35
1	Aa	629	OMG	C2-N3	5.58	1.46	1.33
1	Aa	381	OMG	C2-N3	5.57	1.46	1.33
27	BA	584	OMG	C2-N3	5.57	1.46	1.33
27	BA	1893	OMG	C2-N3	5.57	1.46	1.33
27	BA	657	OMU	C6-C5	5.56	1.48	1.35
1	Aa	574	OMG	C2-N3	5.56	1.46	1.33
1	Aa	913	OMG	C2-N3	5.55	1.46	1.33
27	BA	670	OMG	C2-N3	5.55	1.46	1.33
27	BA	453	OMU	C6-C5	5.54	1.47	1.35
27	BA	1956	OMG	C2-N3	5.54	1.46	1.33
27	BA	365	OMG	C2-N3	5.54	1.46	1.33
1	Aa	498	OMG	C2-N3	5.53	1.46	1.33
1	Aa	121	OMG	C2-N3	5.53	1.46	1.33
1	Aa	836	OMG	C2-N3	5.52	1.46	1.33
27	BA	833	OMG	C2-N3	5.52	1.46	1.33
1	Aa	770	OMG	C2-N3	5.52	1.46	1.33
1	Aa	891	OMG	C2-N3	5.52	1.46	1.33
27	BA	215	OMG	C2-N3	5.51	1.46	1.33
27	BA	2527	OMG	C2-N3	5.51	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2469	OMG	C2-N3	5.51	1.46	1.33
1	Aa	219	OMG	C2-N3	5.50	1.46	1.33
27	BA	2016	OMG	C2-N3	5.50	1.46	1.33
1	Aa	446	OMG	C2-N3	5.49	1.46	1.33
1	Aa	495	OMG	C2-N3	5.49	1.46	1.33
27	BA	2672	OMG	C2-N3	5.49	1.46	1.33
27	BA	872	OMG	C2-N3	5.49	1.46	1.33
27	BA	912	OMG	C2-N3	5.48	1.46	1.33
27	BA	2642	OMG	C2-N3	5.48	1.46	1.33
27	BA	65	OMG	C2-N3	5.48	1.46	1.33
27	BA	1329	OMG	C2-N3	5.48	1.46	1.33
1	Aa	532	OMG	C2-N3	5.48	1.46	1.33
1	Aa	320	OMG	C2-N3	5.47	1.46	1.33
27	BA	1525	OMG	C2-N3	5.47	1.46	1.33
27	BA	2466	OMG	C2-N3	5.46	1.46	1.33
27	BA	63	OMG	C2-N3	5.46	1.46	1.33
27	BA	2168	OMG	C2-N3	5.44	1.46	1.33
27	BA	2010	OMG	C2-N3	5.44	1.46	1.33
27	BA	2728	OMG	C2-N3	5.44	1.46	1.33
27	BA	2379	OMG	C2-N3	5.43	1.46	1.33
27	BA	800	OMG	C2-N3	5.43	1.46	1.33
27	BA	1953	OMG	C2-N3	5.42	1.46	1.33
27	BA	2528	OMG	C2-N3	5.42	1.46	1.33
27	BA	2870	OMG	C2-N3	5.42	1.46	1.33
27	BA	2521	OMG	C2-N3	5.40	1.46	1.33
27	BA	674	OMG	C2-N3	5.40	1.46	1.33
27	BA	507	OMG	C2-N3	5.40	1.46	1.33
27	BA	2745	OMG	C2-N3	5.39	1.46	1.33
1	Aa	752	OMC	C4-N3	5.19	1.44	1.34
1	Aa	1361	OMC	C4-N3	5.18	1.44	1.34
27	BA	2967	OMC	C4-N3	5.17	1.44	1.34
1	Aa	924	OMC	C4-N3	5.16	1.44	1.34
27	BA	1820	OMC	C4-N3	5.15	1.44	1.34
27	BA	2595	OMC	C4-N3	5.14	1.44	1.34
27	BA	1995	OMC	C4-N3	5.10	1.44	1.34
1	Aa	229	OMC	C4-N3	5.09	1.44	1.34
1	Aa	112	OMC	C4-N3	5.08	1.44	1.34
27	BA	91	OMC	C4-N3	5.07	1.44	1.34
27	BA	2107	OMC	C4-N3	5.07	1.44	1.34
27	BA	2169	OMC	C4-N3	5.06	1.44	1.34
27	BA	2545	OMC	C4-N3	5.05	1.44	1.34
27	BA	2124	OMC	C4-N3	5.05	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	66	OMC	C4-N3	5.04	1.44	1.34
1	Aa	825	OMC	C4-N3	5.02	1.44	1.34
1	Aa	1354	OMC	C4-N3	5.00	1.44	1.34
27	BA	869	OMC	C4-N3	4.97	1.44	1.34
27	BA	2047	OMC	C4-N3	4.96	1.44	1.34
1	Aa	1361	OMC	C4-N4	4.92	1.45	1.33
27	BA	1995	OMC	C4-N4	4.89	1.45	1.33
1	Aa	825	OMC	C4-N4	4.88	1.45	1.33
27	BA	2107	OMC	C4-N4	4.88	1.45	1.33
27	BA	2595	OMC	C4-N4	4.88	1.45	1.33
1	Aa	924	OMC	C4-N4	4.87	1.45	1.33
27	BA	2967	OMC	C4-N4	4.87	1.45	1.33
27	BA	91	OMC	C4-N4	4.85	1.45	1.33
1	Aa	752	OMC	C4-N4	4.84	1.45	1.33
1	Aa	229	OMC	C4-N4	4.84	1.45	1.33
27	BA	2545	OMC	C4-N4	4.84	1.45	1.33
1	Aa	1354	OMC	C4-N4	4.83	1.45	1.33
1	Aa	112	OMC	C4-N4	4.83	1.45	1.33
27	BA	2047	OMC	C4-N4	4.82	1.45	1.33
27	BA	2169	OMC	C4-N4	4.82	1.45	1.33
27	BA	66	OMC	C4-N4	4.81	1.45	1.33
27	BA	1820	OMC	C4-N4	4.78	1.45	1.33
27	BA	869	OMC	C4-N4	4.77	1.45	1.33
27	BA	2124	OMC	C4-N4	4.75	1.45	1.33
1	Aa	1478	5MC	C6-N1	4.60	1.45	1.38
1	Aa	464	5MC	C6-N1	4.58	1.45	1.38
27	BA	2055	5MC	C6-N1	4.57	1.45	1.38
27	BA	2595	OMC	C2-N1	4.56	1.49	1.40
27	BA	1965	5MC	C6-N1	4.55	1.45	1.38
1	Aa	1004	5MC	C6-N1	4.55	1.45	1.38
1	Aa	1449	6MZ	C5-C4	4.55	1.47	1.39
1	Aa	672	5MC	C6-N1	4.53	1.45	1.38
1	Aa	1306	5MC	C6-N1	4.53	1.45	1.38
27	BA	66	OMC	C2-N1	4.53	1.49	1.40
1	Aa	1007	5MC	C6-N1	4.52	1.45	1.38
1	Aa	1476	5MC	C6-N1	4.51	1.45	1.38
1	Aa	1006	5MC	C6-N1	4.51	1.45	1.38
27	BA	2605	5MC	C6-N1	4.51	1.45	1.38
27	BA	932	A2M	C6-N6	4.51	1.45	1.34
1	Aa	685	5MC	C6-N1	4.51	1.45	1.38
27	BA	1820	OMC	C2-N1	4.50	1.49	1.40
1	Aa	1184	5MC	C6-N1	4.49	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2688	5MC	C6-N1	4.49	1.45	1.38
1	Aa	1352	5MC	C6-N1	4.49	1.45	1.38
1	Aa	1361	OMC	C2-N1	4.49	1.49	1.40
1	Aa	457	5MC	C6-N1	4.49	1.45	1.38
27	BA	2545	OMC	C2-N1	4.48	1.49	1.40
1	Aa	229	OMC	C2-N1	4.48	1.49	1.40
27	BA	2936	A2M	C6-N6	4.48	1.45	1.34
1	Aa	473	5MC	C6-N1	4.47	1.45	1.38
1	Aa	112	OMC	C2-N1	4.47	1.49	1.40
1	Aa	854	5MC	C6-N1	4.47	1.45	1.38
27	BA	849	A2M	C6-N6	4.46	1.45	1.34
1	Aa	340	5MC	C6-N1	4.46	1.45	1.38
27	BA	1345	5MC	C6-N1	4.46	1.45	1.38
1	Aa	752	OMC	C2-N1	4.45	1.49	1.40
27	BA	2967	OMC	C2-N1	4.45	1.49	1.40
1	Aa	1266	5MC	C6-N1	4.45	1.45	1.38
1	Aa	349	5MC	C6-N1	4.45	1.45	1.38
27	BA	879	A2M	C6-N6	4.44	1.45	1.34
1	Aa	1003	5MC	C6-N1	4.43	1.45	1.38
27	BA	2070	5MC	C6-N1	4.42	1.45	1.38
1	Aa	352	A2M	C6-N6	4.42	1.45	1.34
1	Aa	923	5MC	C6-N1	4.42	1.45	1.38
27	BA	2047	OMC	C2-N1	4.41	1.49	1.40
1	Aa	825	OMC	C2-N1	4.41	1.49	1.40
1	Aa	924	OMC	C2-N1	4.41	1.49	1.40
27	BA	1995	OMC	C2-N1	4.41	1.49	1.40
27	BA	2107	OMC	C2-N1	4.40	1.49	1.40
27	BA	869	OMC	C2-N1	4.40	1.49	1.40
1	Aa	1352	5MC	C4-N4	4.39	1.45	1.34
27	BA	2169	OMC	C2-N1	4.39	1.49	1.40
1	Aa	17	5MC	C6-N1	4.39	1.45	1.38
27	BA	2581	4SU	C4-S4	-4.37	1.60	1.68
27	BA	91	OMC	C2-N1	4.37	1.49	1.40
27	BA	2124	OMC	C2-N1	4.37	1.49	1.40
1	Aa	1478	5MC	C2-N1	4.36	1.49	1.40
1	Aa	1266	5MC	C4-N4	4.36	1.45	1.34
1	Aa	1003	5MC	C4-N4	4.36	1.45	1.34
1	Aa	464	5MC	C4-N4	4.35	1.45	1.34
1	Aa	457	5MC	C4-N4	4.35	1.45	1.34
27	BA	2688	5MC	C4-N4	4.35	1.45	1.34
1	Aa	1004	5MC	C4-N4	4.35	1.45	1.34
27	BA	2605	5MC	C4-N4	4.35	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2075	5MC	C6-N1	4.34	1.45	1.38
1	Aa	923	5MC	C4-N4	4.34	1.45	1.34
27	BA	505	A2M	C6-N6	4.34	1.45	1.34
1	Aa	1006	5MC	C4-N4	4.34	1.45	1.34
1	Aa	464	5MC	C2-N1	4.33	1.49	1.40
1	Aa	1306	5MC	C4-N4	4.33	1.45	1.34
1	Aa	349	5MC	C4-N4	4.33	1.45	1.34
1	Aa	473	5MC	C4-N4	4.33	1.45	1.34
27	BA	2553	4SU	C4-S4	-4.33	1.60	1.68
27	BA	1345	5MC	C4-N4	4.33	1.45	1.34
1	Aa	1007	5MC	C4-N4	4.32	1.45	1.34
27	BA	2055	5MC	C4-N4	4.32	1.45	1.34
1	Aa	1321	5MC	C4-N4	4.32	1.45	1.34
1	Aa	854	5MC	C4-N4	4.31	1.45	1.34
1	Aa	340	5MC	C2-N1	4.31	1.49	1.40
27	BA	1965	5MC	C4-N4	4.30	1.45	1.34
1	Aa	1321	5MC	C6-N1	4.30	1.45	1.38
1	Aa	1184	5MC	C4-N4	4.30	1.45	1.34
27	BA	2070	5MC	C4-N4	4.30	1.45	1.34
27	BA	2075	5MC	C4-N4	4.30	1.45	1.34
1	Aa	685	5MC	C4-N4	4.30	1.45	1.34
1	Aa	1354	OMC	C2-N1	4.29	1.49	1.40
1	Aa	17	5MC	C4-N4	4.29	1.45	1.34
1	Aa	340	5MC	C4-N4	4.28	1.45	1.34
27	BA	55	5MC	C6-N1	4.28	1.45	1.38
1	Aa	1476	5MC	C4-N4	4.28	1.45	1.34
1	Aa	1478	5MC	C4-N4	4.27	1.45	1.34
1	Aa	479	OMU	C4-N3	4.27	1.46	1.38
1	Aa	457	5MC	C2-N1	4.26	1.49	1.40
1	Aa	1003	5MC	C2-N1	4.26	1.49	1.40
1	Aa	1007	5MC	C2-N1	4.26	1.49	1.40
27	BA	55	5MC	C4-N4	4.25	1.45	1.34
1	Aa	1004	5MC	C2-N1	4.25	1.49	1.40
1	Aa	1321	5MC	C2-N1	4.24	1.49	1.40
1	Aa	672	5MC	C4-N4	4.24	1.45	1.34
27	BA	55	5MC	C2-N1	4.24	1.49	1.40
1	Aa	349	5MC	C2-N1	4.24	1.49	1.40
1	Aa	473	5MC	C2-N1	4.23	1.49	1.40
1	Aa	923	5MC	C2-N1	4.23	1.49	1.40
1	Aa	1006	5MC	C2-N1	4.23	1.49	1.40
1	Aa	1306	5MC	C2-N1	4.22	1.49	1.40
1	Aa	1266	5MC	C2-N1	4.22	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2055	5MC	C2-N1	4.21	1.49	1.40
1	Aa	672	5MC	C2-N1	4.20	1.49	1.40
27	BA	2329	A2M	C5-C4	4.20	1.46	1.39
1	Aa	685	5MC	C2-N1	4.20	1.49	1.40
1	Aa	1352	5MC	C2-N1	4.20	1.49	1.40
27	BA	2075	5MC	C2-N1	4.19	1.49	1.40
27	BA	1965	5MC	C2-N1	4.19	1.49	1.40
27	BA	1480	OMU	C4-N3	4.18	1.46	1.38
1	Aa	753	OMU	C4-N3	4.18	1.46	1.38
27	BA	2688	5MC	C2-N1	4.17	1.49	1.40
1	Aa	1184	5MC	C2-N1	4.17	1.49	1.40
27	BA	1345	5MC	C2-N1	4.17	1.49	1.40
1	Aa	854	5MC	C2-N1	4.17	1.49	1.40
1	Aa	17	5MC	C2-N1	4.17	1.49	1.40
27	BA	1969	OMU	C4-N3	4.13	1.46	1.38
1	Aa	1476	5MC	C2-N1	4.12	1.48	1.40
27	BA	2605	5MC	C2-N1	4.12	1.48	1.40
27	BA	453	OMU	C4-N3	4.12	1.45	1.38
1	Aa	1020	OMU	C4-N3	4.11	1.45	1.38
27	BA	2070	5MC	C2-N1	4.10	1.48	1.40
27	BA	2656	OMU	C4-N3	4.09	1.45	1.38
1	Aa	963	OMG	C2-N2	4.07	1.43	1.34
27	BA	1402	OMU	C4-N3	4.06	1.45	1.38
1	Aa	994	OMG	C2-N2	4.05	1.43	1.34
1	Aa	1107	OMG	C2-N2	4.05	1.43	1.34
1	Aa	574	OMG	C2-N2	4.04	1.43	1.34
1	Aa	1223	OMG	C2-N2	4.04	1.43	1.34
1	Aa	1358	OMU	C4-N3	4.04	1.45	1.38
1	Aa	636	OMG	C2-N2	4.03	1.43	1.34
27	BA	1508	OMG	C2-N2	4.02	1.43	1.34
27	BA	1150	OMU	C4-N3	4.02	1.45	1.38
1	Aa	836	OMG	C2-N2	4.02	1.43	1.34
1	Aa	913	OMG	C2-N2	4.02	1.43	1.34
1	Aa	498	OMG	C2-N2	4.02	1.43	1.34
1	Aa	147	OMG	C2-N2	4.02	1.43	1.34
1	Aa	629	OMG	C2-N2	4.01	1.43	1.34
1	Aa	532	OMG	C2-N2	4.01	1.43	1.34
27	BA	288	OMG	C2-N2	4.01	1.43	1.34
1	Aa	8	OMU	C4-N3	4.00	1.45	1.38
27	BA	2542	OMU	C4-N3	4.00	1.45	1.38
27	BA	833	OMG	C2-N2	3.99	1.43	1.34
27	BA	2728	OMG	C2-N2	3.99	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2521	OMG	C2-N2	3.99	1.43	1.34
1	Aa	891	OMG	C2-N2	3.98	1.43	1.34
1	Aa	495	OMG	C2-N2	3.98	1.43	1.34
1	Aa	670	OMG	C2-N2	3.98	1.43	1.34
27	BA	2379	OMG	C2-N2	3.98	1.43	1.34
1	Aa	121	OMG	C2-N2	3.98	1.43	1.34
1	Aa	770	OMG	C2-N2	3.98	1.43	1.34
27	BA	912	OMG	C2-N2	3.97	1.43	1.34
27	BA	1776	OMU	C4-N3	3.97	1.45	1.38
27	BA	1953	OMG	C2-N2	3.97	1.43	1.34
27	BA	2640	OMG	C2-N2	3.97	1.43	1.34
1	Aa	446	OMG	C2-N2	3.96	1.43	1.34
1	Aa	219	OMG	C2-N2	3.96	1.43	1.34
1	Aa	381	OMG	C2-N2	3.96	1.43	1.34
27	BA	2672	OMG	C2-N2	3.96	1.43	1.34
27	BA	2091	A2M	C5-C4	3.96	1.46	1.39
1	Aa	659	OMG	C2-N2	3.96	1.43	1.34
27	BA	1956	OMG	C2-N2	3.95	1.43	1.34
27	BA	584	OMG	C2-N2	3.95	1.43	1.34
27	BA	2010	OMG	C2-N2	3.95	1.43	1.34
27	BA	2016	OMG	C2-N2	3.95	1.43	1.34
27	BA	215	OMG	C2-N2	3.94	1.43	1.34
27	BA	657	OMU	C4-N3	3.94	1.45	1.38
27	BA	674	OMG	C2-N2	3.94	1.43	1.34
27	BA	800	OMG	C2-N2	3.93	1.43	1.34
27	BA	1525	OMG	C2-N2	3.93	1.43	1.34
27	BA	2466	OMG	C2-N2	3.93	1.43	1.34
27	BA	2870	OMG	C2-N2	3.93	1.43	1.34
1	Aa	320	OMG	C2-N2	3.93	1.43	1.34
27	BA	1893	OMG	C2-N2	3.93	1.43	1.34
27	BA	1329	OMG	C2-N2	3.92	1.43	1.34
27	BA	872	OMG	C2-N2	3.92	1.43	1.34
27	BA	2168	OMG	C2-N2	3.91	1.43	1.34
27	BA	365	OMG	C2-N2	3.91	1.43	1.34
27	BA	2528	OMG	C2-N2	3.91	1.43	1.34
27	BA	2745	OMG	C2-N2	3.90	1.43	1.34
27	BA	507	OMG	C2-N2	3.90	1.43	1.34
27	BA	2527	OMG	C2-N2	3.90	1.43	1.34
27	BA	63	OMG	C2-N2	3.89	1.43	1.34
27	BA	65	OMG	C2-N2	3.88	1.43	1.34
27	BA	2642	OMG	C2-N2	3.88	1.43	1.34
27	BA	2469	OMG	C2-N2	3.88	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	670	OMG	C2-N2	3.84	1.43	1.34
1	Aa	1467	MA6	C6-N6	3.61	1.47	1.36
27	BA	2553	4SU	C4-N3	-3.61	1.33	1.37
1	Aa	1468	MA6	C6-N6	3.58	1.47	1.36
27	BA	2595	OMC	C6-N1	3.27	1.45	1.38
27	BA	2545	OMC	C6-N1	3.25	1.45	1.38
27	BA	1820	OMC	C6-N1	3.23	1.45	1.38
1	Aa	924	OMC	C6-N1	3.23	1.45	1.38
1	Aa	825	OMC	C6-N1	3.22	1.45	1.38
27	BA	2124	OMC	C6-N1	3.22	1.45	1.38
27	BA	1995	OMC	C6-N1	3.21	1.45	1.38
27	BA	869	OMC	C6-N1	3.20	1.45	1.38
27	BA	66	OMC	C6-N1	3.20	1.45	1.38
1	Aa	752	OMC	C6-N1	3.19	1.45	1.38
27	BA	91	OMC	C6-N1	3.19	1.45	1.38
27	BA	2107	OMC	C6-N1	3.19	1.45	1.38
1	Aa	1361	OMC	C6-N1	3.19	1.45	1.38
27	BA	2047	OMC	C6-N1	3.18	1.45	1.38
1	Aa	229	OMC	C6-N1	3.18	1.45	1.38
27	BA	2169	OMC	C6-N1	3.18	1.45	1.38
1	Aa	112	OMC	C6-N1	3.17	1.45	1.38
27	BA	657	OMU	O4-C4	-3.15	1.18	1.24
27	BA	2967	OMC	C6-N1	3.15	1.45	1.38
27	BA	1854	5MU	O4-C4	-3.13	1.17	1.23
1	Aa	1354	OMC	C6-N1	3.13	1.45	1.38
27	BA	1402	OMU	O4-C4	-3.13	1.18	1.24
27	BA	2656	OMU	O4-C4	-3.12	1.18	1.24
27	BA	932	A2M	O3'-C3'	-3.12	1.35	1.43
27	BA	1480	OMU	O4-C4	-3.11	1.18	1.24
27	BA	1776	OMU	O4-C4	-3.10	1.18	1.24
1	Aa	8	OMU	O4-C4	-3.09	1.18	1.24
27	BA	829	5MU	O4-C4	-3.08	1.17	1.23
27	BA	1969	OMU	O4-C4	-3.08	1.18	1.24
27	BA	2542	OMU	O4-C4	-3.06	1.18	1.24
27	BA	1766	5MU	O4-C4	-3.05	1.17	1.23
1	Aa	995	2MG	C5-C4	3.05	1.47	1.38
27	BA	2550	OMG	C6-N1	-3.04	1.33	1.38
27	BA	453	OMU	O4-C4	-3.04	1.18	1.24
27	BA	1150	OMU	O4-C4	-3.04	1.18	1.24
1	Aa	1020	OMU	O4-C4	-3.03	1.18	1.24
27	BA	1329	OMG	O6-C6	-3.03	1.17	1.23
27	BA	1956	OMG	O6-C6	-3.03	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2427	5MU	O4-C4	-3.02	1.17	1.23
27	BA	1956	OMG	C5-N7	-3.00	1.33	1.39
1	Aa	636	OMG	C5-N7	-3.00	1.33	1.39
1	Aa	753	OMU	O4-C4	-3.00	1.18	1.24
27	BA	912	OMG	C5-N7	-3.00	1.33	1.39
27	BA	1893	OMG	C5-N7	-3.00	1.33	1.39
27	BA	63	OMG	O6-C6	-2.99	1.17	1.23
27	BA	584	OMG	O6-C6	-2.99	1.17	1.23
27	BA	215	OMG	O6-C6	-2.99	1.17	1.23
27	BA	1525	OMG	C5-N7	-2.97	1.33	1.39
1	Aa	17	5MC	O2-C2	-2.97	1.18	1.23
27	BA	65	OMG	O6-C6	-2.97	1.17	1.23
27	BA	1965	5MC	O2-C2	-2.97	1.18	1.23
27	BA	1402	OMU	C6-N1	2.97	1.45	1.38
27	BA	2672	OMG	O6-C6	-2.96	1.17	1.23
27	BA	2016	OMG	C5-N7	-2.96	1.33	1.39
27	BA	2469	OMG	C5-N7	-2.96	1.33	1.39
27	BA	2640	OMG	C5-N7	-2.96	1.33	1.39
27	BA	507	OMG	O6-C6	-2.95	1.18	1.23
27	BA	63	OMG	C5-N7	-2.95	1.33	1.39
27	BA	2936	A2M	O3'-C3'	-2.95	1.36	1.43
1	Aa	1476	5MC	O2-C2	-2.95	1.18	1.23
27	BA	2070	5MC	O2-C2	-2.95	1.18	1.23
27	BA	674	OMG	O6-C6	-2.95	1.18	1.23
1	Aa	659	OMG	C5-N7	-2.95	1.33	1.39
1	Aa	672	5MC	O2-C2	-2.95	1.18	1.23
27	BA	365	OMG	O6-C6	-2.94	1.18	1.23
27	BA	2168	OMG	C5-N7	-2.94	1.33	1.39
27	BA	1953	OMG	O6-C6	-2.94	1.18	1.23
27	BA	1480	OMU	C6-N1	2.94	1.45	1.38
27	BA	2870	OMG	O6-C6	-2.93	1.18	1.23
27	BA	507	OMG	C5-N7	-2.93	1.33	1.39
27	BA	872	OMG	C5-N7	-2.93	1.33	1.39
1	Aa	1321	5MC	O2-C2	-2.93	1.18	1.23
1	Aa	1358	OMU	O4-C4	-2.93	1.18	1.24
27	BA	365	OMG	C5-N7	-2.93	1.33	1.39
27	BA	2075	5MC	O2-C2	-2.93	1.18	1.23
1	Aa	917	5MU	C4-N3	-2.93	1.33	1.38
27	BA	2521	OMG	O6-C6	-2.92	1.18	1.23
27	BA	2168	OMG	O6-C6	-2.92	1.18	1.23
27	BA	1525	OMG	O6-C6	-2.92	1.18	1.23
27	BA	55	5MC	O2-C2	-2.91	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2055	5MC	O2-C2	-2.91	1.18	1.23
27	BA	1329	OMG	C5-N7	-2.91	1.33	1.39
27	BA	1893	OMG	O6-C6	-2.91	1.18	1.23
27	BA	2379	OMG	O6-C6	-2.91	1.18	1.23
1	Aa	1007	5MC	O2-C2	-2.91	1.18	1.23
27	BA	2605	5MC	O2-C2	-2.91	1.18	1.23
27	BA	912	OMG	O6-C6	-2.90	1.18	1.23
27	BA	2469	OMG	O6-C6	-2.90	1.18	1.23
27	BA	1345	5MC	O2-C2	-2.90	1.18	1.23
27	BA	670	OMG	O6-C6	-2.90	1.18	1.23
27	BA	1150	OMU	C6-N1	2.90	1.45	1.38
27	BA	2010	OMG	C5-N7	-2.90	1.33	1.39
1	Aa	1306	5MC	O2-C2	-2.90	1.18	1.23
27	BA	833	OMG	O6-C6	-2.90	1.18	1.23
27	BA	849	A2M	O3'-C3'	-2.90	1.36	1.43
27	BA	657	OMU	C6-N1	2.90	1.45	1.38
1	Aa	770	OMG	O6-C6	-2.90	1.18	1.23
27	BA	1776	OMU	C6-N1	2.90	1.45	1.38
1	Aa	852	OMG	C6-N1	-2.90	1.33	1.38
1	Aa	685	5MC	O2-C2	-2.90	1.18	1.23
27	BA	2010	OMG	O6-C6	-2.90	1.18	1.23
27	BA	1508	OMG	C5-N7	-2.90	1.33	1.39
1	Aa	670	OMG	C5-N7	-2.90	1.33	1.39
27	BA	2656	OMU	C6-N1	2.89	1.45	1.38
27	BA	674	OMG	C5-N7	-2.89	1.33	1.39
27	BA	2016	OMG	O6-C6	-2.89	1.18	1.23
1	Aa	854	5MC	O2-C2	-2.89	1.18	1.23
1	Aa	479	OMU	O4-C4	-2.89	1.18	1.24
27	BA	65	OMG	C5-N7	-2.89	1.33	1.39
27	BA	879	A2M	C5-C4	-2.89	1.33	1.39
27	BA	2353	OMG	C6-N1	-2.89	1.33	1.38
27	BA	875	5MU	O4-C4	-2.89	1.18	1.23
27	BA	2688	5MC	O2-C2	-2.89	1.18	1.23
27	BA	1969	OMU	C6-N1	2.88	1.45	1.38
1	Aa	670	OMG	O6-C6	-2.88	1.18	1.23
27	BA	2466	OMG	O6-C6	-2.88	1.18	1.23
27	BA	584	OMG	C5-N7	-2.88	1.33	1.39
27	BA	872	OMG	O6-C6	-2.88	1.18	1.23
27	BA	2728	OMG	O6-C6	-2.88	1.18	1.23
1	Aa	479	OMU	C6-N1	2.88	1.44	1.38
27	BA	670	OMG	C5-N7	-2.88	1.33	1.39
27	BA	2870	OMG	C5-N7	-2.88	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	8	OMU	C6-N1	2.88	1.44	1.38
27	BA	800	OMG	O6-C6	-2.88	1.18	1.23
1	Aa	473	5MC	O2-C2	-2.88	1.18	1.23
1	Aa	1184	5MC	O2-C2	-2.88	1.18	1.23
27	BA	1953	OMG	C5-N7	-2.88	1.33	1.39
27	BA	2642	OMG	O6-C6	-2.88	1.18	1.23
1	Aa	994	OMG	C5-N7	-2.87	1.33	1.39
1	Aa	1478	5MC	O2-C2	-2.87	1.18	1.23
27	BA	2640	OMG	O6-C6	-2.87	1.18	1.23
27	BA	2542	OMU	C6-N1	2.87	1.44	1.38
1	Aa	219	OMG	C5-N7	-2.87	1.33	1.39
1	Aa	574	OMG	O6-C6	-2.87	1.18	1.23
1	Aa	349	5MC	O2-C2	-2.87	1.18	1.23
1	Aa	836	OMG	O6-C6	-2.87	1.18	1.23
27	BA	2550	OMG	C5-C4	2.87	1.46	1.38
1	Aa	1107	OMG	C5-N7	-2.87	1.33	1.39
27	BA	833	OMG	C5-N7	-2.87	1.33	1.39
27	BA	2745	OMG	O6-C6	-2.87	1.18	1.23
1	Aa	446	OMG	O6-C6	-2.87	1.18	1.23
1	Aa	1003	5MC	O2-C2	-2.86	1.18	1.23
27	BA	2672	OMG	C5-N7	-2.86	1.33	1.39
1	Aa	770	OMG	C5-N7	-2.86	1.33	1.39
27	BA	2107	OMC	O2-C2	-2.86	1.18	1.23
1	Aa	320	OMG	O6-C6	-2.86	1.18	1.23
27	BA	800	OMG	C5-N7	-2.86	1.33	1.39
1	Aa	532	OMG	O6-C6	-2.86	1.18	1.23
1	Aa	753	OMU	C6-N1	2.86	1.44	1.38
27	BA	215	OMG	C5-N7	-2.86	1.33	1.39
1	Aa	1006	5MC	O2-C2	-2.85	1.18	1.23
1	Aa	913	OMG	C5-N7	-2.85	1.33	1.39
1	Aa	1004	5MC	O2-C2	-2.85	1.18	1.23
1	Aa	629	OMG	C5-N7	-2.85	1.33	1.39
27	BA	2728	OMG	C5-N7	-2.85	1.33	1.39
1	Aa	1266	5MC	O2-C2	-2.85	1.18	1.23
27	BA	2527	OMG	O6-C6	-2.85	1.18	1.23
27	BA	2528	OMG	O6-C6	-2.85	1.18	1.23
1	Aa	340	5MC	O2-C2	-2.85	1.18	1.23
27	BA	453	OMU	C6-N1	2.85	1.44	1.38
1	Aa	891	OMG	O6-C6	-2.85	1.18	1.23
1	Aa	381	OMG	O6-C6	-2.84	1.18	1.23
27	BA	879	A2M	O2'-C2'	2.84	1.49	1.42
1	Aa	659	OMG	O6-C6	-2.84	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	288	OMG	C5-N7	-2.84	1.33	1.39
27	BA	2528	OMG	C5-N7	-2.84	1.33	1.39
1	Aa	352	A2M	C5-C4	-2.84	1.33	1.39
27	BA	505	A2M	O3'-C3'	-2.84	1.36	1.43
1	Aa	1352	5MC	O2-C2	-2.84	1.18	1.23
1	Aa	836	OMG	C5-N7	-2.84	1.33	1.39
27	BA	849	A2M	C5-C4	-2.84	1.33	1.39
27	BA	2379	OMG	C5-N7	-2.84	1.33	1.39
27	BA	869	OMC	O2-C2	-2.83	1.18	1.23
1	Aa	446	OMG	C5-N7	-2.83	1.33	1.39
1	Aa	219	OMG	O6-C6	-2.83	1.18	1.23
27	BA	2124	OMC	O2-C2	-2.83	1.18	1.23
1	Aa	498	OMG	C5-N7	-2.83	1.33	1.39
1	Aa	629	OMG	O6-C6	-2.83	1.18	1.23
1	Aa	1020	OMU	C6-N1	2.83	1.44	1.38
1	Aa	450	OMG	C5-C4	2.83	1.46	1.38
27	BA	2353	OMG	C5-C4	2.83	1.46	1.38
1	Aa	913	OMG	O6-C6	-2.83	1.18	1.23
27	BA	2389	OMU	C4-N3	-2.83	1.33	1.38
1	Aa	498	OMG	O6-C6	-2.83	1.18	1.23
27	BA	2936	A2M	C5-C4	-2.83	1.33	1.39
1	Aa	352	A2M	O2'-C2'	2.83	1.49	1.42
1	Aa	121	OMG	C5-N7	-2.82	1.33	1.39
1	Aa	147	OMG	C5-N7	-2.82	1.33	1.39
27	BA	879	A2M	O3'-C3'	-2.82	1.36	1.43
1	Aa	320	OMG	C5-N7	-2.82	1.33	1.39
27	BA	2169	OMC	O2-C2	-2.82	1.18	1.23
1	Aa	495	OMG	C5-N7	-2.82	1.33	1.39
1	Aa	381	OMG	C5-N7	-2.81	1.33	1.39
1	Aa	1467	MA6	C5-C4	-2.81	1.33	1.39
1	Aa	1223	OMG	O6-C6	-2.81	1.18	1.23
1	Aa	1468	MA6	C5-C4	-2.81	1.33	1.39
27	BA	1508	OMG	O6-C6	-2.81	1.18	1.23
27	BA	288	OMG	O6-C6	-2.81	1.18	1.23
1	Aa	1354	OMC	O2-C2	-2.81	1.18	1.23
1	Aa	891	OMG	C5-N7	-2.81	1.33	1.39
1	Aa	450	OMG	C6-N1	-2.81	1.33	1.38
1	Aa	495	OMG	O6-C6	-2.81	1.18	1.23
1	Aa	963	OMG	C5-N7	-2.80	1.33	1.39
27	BA	849	A2M	O2'-C2'	2.80	1.49	1.42
27	BA	2091	A2M	C5-N7	-2.80	1.33	1.39
1	Aa	994	OMG	O6-C6	-2.80	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	574	OMG	C5-N7	-2.79	1.33	1.39
27	BA	2545	OMC	O2-C2	-2.79	1.18	1.23
1	Aa	852	OMG	C5-C4	2.79	1.46	1.38
27	BA	2527	OMG	C5-N7	-2.79	1.33	1.39
1	Aa	121	OMG	O6-C6	-2.79	1.18	1.23
27	BA	1820	OMC	O2-C2	-2.79	1.18	1.23
27	BA	932	A2M	C5-C4	-2.79	1.33	1.39
27	BA	932	A2M	O2'-C2'	2.79	1.49	1.42
27	BA	2936	A2M	O2'-C2'	2.79	1.49	1.42
1	Aa	636	OMG	O6-C6	-2.79	1.18	1.23
1	Aa	923	5MC	O2-C2	-2.79	1.18	1.23
27	BA	2521	OMG	C5-N7	-2.78	1.33	1.39
1	Aa	1223	OMG	C5-N7	-2.78	1.33	1.39
1	Aa	457	5MC	O2-C2	-2.78	1.18	1.23
1	Aa	752	OMC	O2-C2	-2.78	1.18	1.23
1	Aa	532	OMG	C5-N7	-2.77	1.33	1.39
1	Aa	1358	OMU	C6-N1	2.76	1.44	1.38
27	BA	2745	OMG	C5-N7	-2.76	1.33	1.39
1	Aa	963	OMG	O6-C6	-2.76	1.18	1.23
1	Aa	464	5MC	O2-C2	-2.76	1.18	1.23
27	BA	66	OMC	O2-C2	-2.76	1.18	1.23
1	Aa	147	OMG	O6-C6	-2.76	1.18	1.23
27	BA	2466	OMG	C5-N7	-2.74	1.33	1.39
27	BA	505	A2M	C5-C4	-2.74	1.33	1.39
1	Aa	352	A2M	O3'-C3'	-2.74	1.36	1.43
27	BA	2642	OMG	C5-N7	-2.73	1.33	1.39
27	BA	505	A2M	O2'-C2'	2.73	1.49	1.42
27	BA	2047	OMC	O2-C2	-2.73	1.18	1.23
1	Aa	1107	OMG	O6-C6	-2.73	1.18	1.23
27	BA	1766	5MU	O2-C2	-2.72	1.18	1.23
1	Aa	112	OMC	O2-C2	-2.72	1.18	1.23
27	BA	505	A2M	C5-N7	-2.72	1.33	1.39
27	BA	91	OMC	O2-C2	-2.71	1.18	1.23
1	Aa	229	OMC	O2-C2	-2.71	1.18	1.23
1	Aa	825	OMC	O2-C2	-2.70	1.18	1.23
1	Aa	924	OMC	O2-C2	-2.69	1.18	1.23
27	BA	1995	OMC	O2-C2	-2.68	1.18	1.23
27	BA	2595	OMC	O2-C2	-2.67	1.18	1.23
27	BA	2329	A2M	C5-N7	-2.66	1.34	1.39
27	BA	2967	OMC	O2-C2	-2.65	1.18	1.23
27	BA	2581	4SU	O2-C2	-2.65	1.18	1.23
1	Aa	1361	OMC	O2-C2	-2.63	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	849	A2M	C5-N7	-2.60	1.34	1.39
27	BA	2427	5MU	O2-C2	-2.60	1.18	1.23
1	Aa	963	OMG	C6-N1	2.59	1.43	1.38
27	BA	2595	OMC	C5-C4	2.58	1.48	1.42
27	BA	932	A2M	C5-N7	-2.57	1.34	1.39
1	Aa	913	OMG	C6-N1	2.57	1.43	1.38
27	BA	2550	OMG	C5-N7	-2.57	1.34	1.39
27	BA	1854	5MU	O2-C2	-2.57	1.18	1.23
27	BA	829	5MU	O2-C2	-2.57	1.18	1.23
27	BA	879	A2M	C5-N7	-2.56	1.34	1.39
1	Aa	1449	6MZ	C5-C6	2.56	1.48	1.41
27	BA	1150	OMU	O2-C2	-2.56	1.18	1.23
27	BA	657	OMU	O2-C2	-2.56	1.18	1.23
1	Aa	352	A2M	C5-N7	-2.55	1.34	1.39
27	BA	1776	OMU	O2-C2	-2.55	1.18	1.23
27	BA	1402	OMU	O2-C2	-2.55	1.18	1.23
1	Aa	995	2MG	C6-N1	-2.54	1.34	1.38
1	Aa	381	OMG	C6-N1	2.54	1.43	1.38
27	BA	2169	OMC	C5-C4	2.54	1.48	1.42
27	BA	2521	OMG	C6-N1	2.53	1.43	1.38
1	Aa	495	OMG	C6-N1	2.53	1.43	1.38
27	BA	2642	OMG	C5-C6	2.53	1.53	1.44
1	Aa	574	OMG	C6-N1	2.53	1.43	1.38
1	Aa	836	OMG	C6-N1	2.53	1.43	1.38
1	Aa	1354	OMC	C5-C4	2.53	1.48	1.42
27	BA	1508	OMG	C6-N1	2.52	1.43	1.38
27	BA	2581	4SU	C6-N1	2.52	1.44	1.38
1	Aa	320	OMG	C6-N1	2.51	1.43	1.38
1	Aa	994	OMG	C2-N1	2.51	1.43	1.37
27	BA	1995	OMC	C5-C4	2.51	1.48	1.42
27	BA	1480	OMU	O2-C2	-2.51	1.18	1.23
1	Aa	636	OMG	C6-N1	2.51	1.43	1.38
27	BA	2545	OMC	C5-C4	2.51	1.48	1.42
1	Aa	532	OMG	C6-N1	2.51	1.43	1.38
27	BA	1969	OMU	O2-C2	-2.51	1.18	1.23
1	Aa	963	OMG	C2-N1	2.51	1.43	1.37
1	Aa	994	OMG	C6-N1	2.50	1.43	1.38
1	Aa	1107	OMG	C6-N1	2.50	1.43	1.38
1	Aa	913	OMG	C2-N1	2.50	1.43	1.37
1	Aa	381	OMG	C2-N1	2.50	1.43	1.37
27	BA	2936	A2M	C5-N7	-2.50	1.34	1.39
1	Aa	1107	OMG	C2-N1	2.49	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	875	5MU	O2-C2	-2.49	1.18	1.23
1	Aa	479	OMU	C5-C4	2.49	1.49	1.43
1	Aa	836	OMG	C2-N1	2.49	1.43	1.37
1	Aa	1223	OMG	C6-N1	2.49	1.43	1.38
27	BA	584	OMG	C6-N1	2.49	1.43	1.38
27	BA	2329	A2M	C5-C6	2.49	1.48	1.41
1	Aa	924	OMC	C5-C4	2.49	1.48	1.42
1	Aa	1358	OMU	O2-C2	-2.48	1.18	1.23
27	BA	872	OMG	C5-C6	2.48	1.53	1.44
1	Aa	1223	OMG	C2-N1	2.48	1.43	1.37
27	BA	2091	A2M	C5-C6	2.48	1.48	1.41
27	BA	2379	OMG	C6-N1	2.48	1.43	1.38
1	Aa	574	OMG	C5-C6	2.48	1.53	1.44
1	Aa	1361	OMC	C5-C4	2.48	1.48	1.42
1	Aa	147	OMG	C6-N1	2.48	1.43	1.38
1	Aa	629	OMG	C6-N1	2.47	1.43	1.38
27	BA	2466	OMG	C5-C6	2.47	1.53	1.44
27	BA	2640	OMG	C2-N1	2.47	1.43	1.37
27	BA	2107	OMC	C5-C4	2.47	1.48	1.42
27	BA	2527	OMG	C5-C6	2.47	1.53	1.44
1	Aa	381	OMG	C5-C6	2.47	1.53	1.44
1	Aa	836	OMG	C5-C6	2.47	1.53	1.44
1	Aa	121	OMG	C2-N1	2.47	1.43	1.37
1	Aa	498	OMG	C2-N1	2.47	1.43	1.37
27	BA	288	OMG	C6-N1	2.47	1.43	1.38
1	Aa	825	OMC	C5-C4	2.47	1.48	1.42
27	BA	2353	OMG	C5-N7	-2.46	1.34	1.39
27	BA	1969	OMU	C5-C4	2.46	1.49	1.43
27	BA	63	OMG	C2-N1	2.46	1.43	1.37
27	BA	2521	OMG	C5-C6	2.46	1.53	1.44
27	BA	2728	OMG	C6-N1	2.46	1.43	1.38
27	BA	800	OMG	C5-C6	2.45	1.53	1.44
1	Aa	636	OMG	C2-N1	2.45	1.43	1.37
1	Aa	1223	OMG	C5-C6	2.45	1.53	1.44
27	BA	670	OMG	C5-C6	2.45	1.53	1.44
1	Aa	994	OMG	C5-C6	2.45	1.53	1.44
1	Aa	219	OMG	C5-C6	2.45	1.53	1.44
1	Aa	495	OMG	C5-C6	2.45	1.53	1.44
27	BA	453	OMU	O2-C2	-2.45	1.18	1.23
1	Aa	498	OMG	C5-C6	2.45	1.53	1.44
1	Aa	219	OMG	C2-N1	2.45	1.43	1.37
1	Aa	770	OMG	C2-N1	2.45	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	147	OMG	C2-N1	2.45	1.43	1.37
27	BA	288	OMG	C5-C6	2.45	1.53	1.44
1	Aa	670	OMG	C5-C6	2.45	1.53	1.44
27	BA	1820	OMC	C5-C4	2.45	1.48	1.42
1	Aa	498	OMG	C6-N1	2.45	1.43	1.38
1	Aa	574	OMG	C2-N1	2.45	1.43	1.37
27	BA	2528	OMG	C5-C6	2.45	1.53	1.44
1	Aa	121	OMG	C6-N1	2.45	1.43	1.38
27	BA	2728	OMG	C5-C6	2.45	1.53	1.44
1	Aa	229	OMC	C5-C4	2.44	1.48	1.42
27	BA	507	OMG	C5-C6	2.44	1.53	1.44
27	BA	2379	OMG	C5-C6	2.44	1.53	1.44
1	Aa	147	OMG	C5-C6	2.44	1.53	1.44
1	Aa	320	OMG	C2-N1	2.44	1.43	1.37
1	Aa	659	OMG	C2-N1	2.44	1.43	1.37
1	Aa	752	OMC	C5-C4	2.44	1.48	1.42
1	Aa	446	OMG	C6-N1	2.44	1.43	1.38
27	BA	2521	OMG	C2-N1	2.44	1.43	1.37
1	Aa	670	OMG	C2-N1	2.44	1.43	1.37
1	Aa	112	OMC	C5-C4	2.44	1.48	1.42
27	BA	584	OMG	C5-C6	2.44	1.53	1.44
27	BA	2745	OMG	C5-C6	2.44	1.53	1.44
1	Aa	963	OMG	C5-C6	2.43	1.53	1.44
27	BA	912	OMG	C5-C6	2.43	1.53	1.44
27	BA	833	OMG	C2-N1	2.43	1.43	1.37
27	BA	91	OMC	C5-C4	2.43	1.48	1.42
1	Aa	891	OMG	C2-N1	2.43	1.43	1.37
27	BA	2010	OMG	C2-N1	2.43	1.43	1.37
1	Aa	1107	OMG	C5-C6	2.43	1.53	1.44
27	BA	2640	OMG	C5-C6	2.43	1.53	1.44
27	BA	2672	OMG	C5-C6	2.43	1.53	1.44
1	Aa	753	OMU	C5-C4	2.43	1.49	1.43
27	BA	1508	OMG	C2-N1	2.43	1.43	1.37
27	BA	63	OMG	C6-N1	2.43	1.43	1.38
27	BA	2016	OMG	C2-N1	2.42	1.43	1.37
27	BA	2047	OMC	C5-C4	2.42	1.48	1.42
1	Aa	495	OMG	C2-N1	2.42	1.43	1.37
27	BA	2728	OMG	C2-N1	2.42	1.43	1.37
1	Aa	891	OMG	C5-C6	2.42	1.53	1.44
27	BA	1953	OMG	C2-N1	2.42	1.43	1.37
1	Aa	8	OMU	O2-C2	-2.42	1.18	1.23
27	BA	2016	OMG	C5-C6	2.42	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2528	OMG	C2-N1	2.42	1.43	1.37
27	BA	2168	OMG	C6-N1	2.42	1.43	1.38
27	BA	2967	OMC	C5-C4	2.42	1.48	1.42
1	Aa	636	OMG	C5-C6	2.42	1.53	1.44
1	Aa	770	OMG	C5-C6	2.42	1.53	1.44
27	BA	869	OMC	C5-C4	2.42	1.48	1.42
27	BA	1953	OMG	C5-C6	2.42	1.53	1.44
27	BA	1525	OMG	C2-N1	2.42	1.43	1.37
1	Aa	659	OMG	C5-C6	2.42	1.53	1.44
1	Aa	446	OMG	C2-N1	2.42	1.43	1.37
27	BA	1893	OMG	C5-C6	2.42	1.53	1.44
1	Aa	629	OMG	C5-C6	2.42	1.53	1.44
27	BA	288	OMG	C2-N1	2.42	1.43	1.37
1	Aa	891	OMG	C6-N1	2.41	1.43	1.38
27	BA	674	OMG	C2-N1	2.41	1.43	1.37
1	Aa	219	OMG	C6-N1	2.41	1.43	1.38
27	BA	2656	OMU	O2-C2	-2.41	1.18	1.23
1	Aa	913	OMG	C5-C6	2.41	1.53	1.44
1	Aa	121	OMG	C5-C6	2.41	1.53	1.44
1	Aa	446	OMG	C5-C6	2.41	1.53	1.44
1	Aa	670	OMG	C6-N1	2.41	1.43	1.38
1	Aa	532	OMG	C2-N1	2.41	1.43	1.37
27	BA	2870	OMG	C2-N1	2.41	1.43	1.37
1	Aa	629	OMG	C2-N1	2.41	1.43	1.37
27	BA	2469	OMG	C6-N1	2.41	1.43	1.38
27	BA	800	OMG	C2-N1	2.41	1.43	1.37
27	BA	833	OMG	C5-C6	2.41	1.53	1.44
27	BA	365	OMG	C5-C6	2.41	1.53	1.44
27	BA	2870	OMG	C5-C6	2.40	1.53	1.44
1	Aa	1020	OMU	O2-C2	-2.40	1.18	1.23
27	BA	63	OMG	C5-C6	2.40	1.53	1.44
1	Aa	532	OMG	C5-C6	2.40	1.53	1.44
27	BA	1508	OMG	C5-C6	2.40	1.53	1.44
27	BA	800	OMG	C6-N1	2.40	1.43	1.38
27	BA	2640	OMG	C6-N1	2.40	1.43	1.38
27	BA	2466	OMG	C2-N1	2.40	1.43	1.37
27	BA	1150	OMU	C5-C4	2.40	1.48	1.43
1	Aa	659	OMG	C6-N1	2.40	1.43	1.38
1	Aa	320	OMG	C5-C6	2.40	1.53	1.44
27	BA	2642	OMG	C2-N1	2.40	1.43	1.37
27	BA	674	OMG	C5-C6	2.40	1.53	1.44
27	BA	507	OMG	C2-N1	2.39	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	65	OMG	C5-C6	2.39	1.53	1.44
27	BA	2168	OMG	C2-N1	2.39	1.43	1.37
27	BA	507	OMG	C6-N1	2.39	1.43	1.38
27	BA	1956	OMG	C6-N1	2.39	1.43	1.38
27	BA	2124	OMC	C5-C4	2.39	1.48	1.42
1	Aa	917	5MU	C6-C5	2.39	1.38	1.34
27	BA	912	OMG	C2-N1	2.39	1.43	1.37
1	Aa	753	OMU	O2-C2	-2.39	1.18	1.23
27	BA	1956	OMG	C2-N1	2.39	1.43	1.37
1	Aa	770	OMG	C6-N1	2.39	1.43	1.38
27	BA	833	OMG	C6-N1	2.38	1.43	1.38
27	BA	2527	OMG	C6-N1	2.38	1.43	1.38
27	BA	674	OMG	C6-N1	2.38	1.43	1.38
27	BA	2528	OMG	C6-N1	2.38	1.43	1.38
27	BA	2553	4SU	C2-N3	-2.38	1.33	1.38
27	BA	2672	OMG	C2-N1	2.38	1.43	1.37
27	BA	2389	OMU	C2-N3	-2.38	1.33	1.38
27	BA	66	OMC	C5-C4	2.38	1.48	1.42
27	BA	2010	OMG	C5-C6	2.38	1.53	1.44
27	BA	2379	OMG	C2-N1	2.38	1.43	1.37
27	BA	2168	OMG	C5-C6	2.38	1.53	1.44
27	BA	1953	OMG	C6-N1	2.38	1.43	1.38
27	BA	1956	OMG	C5-C6	2.37	1.53	1.44
27	BA	657	OMU	C5-C4	2.37	1.48	1.43
27	BA	1329	OMG	C5-C6	2.37	1.53	1.44
1	Aa	8	OMU	C5-C4	2.37	1.48	1.43
27	BA	2542	OMU	O2-C2	-2.36	1.18	1.23
27	BA	2553	4SU	C5-C4	-2.36	1.39	1.42
1	Aa	852	OMG	C5-N7	-2.36	1.34	1.39
27	BA	215	OMG	C6-N1	2.36	1.43	1.38
1	Aa	1358	OMU	C5-C4	2.36	1.48	1.43
27	BA	2542	OMU	C5-C4	2.36	1.48	1.43
27	BA	2469	OMG	C2-N1	2.36	1.43	1.37
27	BA	2469	OMG	C5-C6	2.36	1.53	1.44
1	Aa	917	5MU	C6-N1	-2.35	1.34	1.38
27	BA	65	OMG	C2-N1	2.35	1.43	1.37
27	BA	2870	OMG	C6-N1	2.35	1.43	1.38
27	BA	2745	OMG	C6-N1	2.35	1.43	1.38
27	BA	1329	OMG	C6-N1	2.35	1.43	1.38
1	Aa	1020	OMU	C5-C4	2.34	1.48	1.43
27	BA	2527	OMG	C2-N1	2.34	1.43	1.37
27	BA	215	OMG	C2-N1	2.34	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2010	OMG	C6-N1	2.34	1.43	1.38
27	BA	670	OMG	C6-N1	2.34	1.43	1.38
27	BA	365	OMG	C2-N1	2.34	1.43	1.37
27	BA	584	OMG	C2-N1	2.34	1.43	1.37
1	Aa	1449	6MZ	C5-N7	-2.34	1.34	1.39
27	BA	215	OMG	C5-C6	2.34	1.53	1.44
27	BA	1893	OMG	C2-N1	2.33	1.43	1.37
27	BA	1480	OMU	C5-C4	2.33	1.48	1.43
27	BA	1402	OMU	C5-C4	2.33	1.48	1.43
27	BA	872	OMG	C2-N1	2.33	1.43	1.37
27	BA	1525	OMG	C5-C6	2.32	1.53	1.44
27	BA	65	OMG	C6-N1	2.32	1.43	1.38
27	BA	1525	OMG	C6-N1	2.32	1.43	1.38
27	BA	2642	OMG	C6-N1	2.32	1.43	1.38
27	BA	1893	OMG	C6-N1	2.32	1.43	1.38
27	BA	2745	OMG	C2-N1	2.31	1.43	1.37
27	BA	1329	OMG	C2-N1	2.31	1.43	1.37
27	BA	2466	OMG	C6-N1	2.31	1.43	1.38
27	BA	2016	OMG	C6-N1	2.31	1.43	1.38
27	BA	453	OMU	C5-C4	2.30	1.48	1.43
27	BA	912	OMG	C6-N1	2.29	1.43	1.38
1	Aa	1467	MA6	C5-N7	-2.29	1.34	1.39
1	Aa	479	OMU	O2-C2	-2.29	1.18	1.23
27	BA	2656	OMU	C5-C4	2.28	1.48	1.43
1	Aa	1468	MA6	C5-N7	-2.27	1.34	1.39
27	BA	670	OMG	C2-N1	2.27	1.43	1.37
1	Aa	450	OMG	C5-N7	-2.27	1.34	1.39
27	BA	1776	OMU	C5-C4	2.26	1.48	1.43
27	BA	872	OMG	C6-N1	2.26	1.43	1.38
27	BA	2672	OMG	C6-N1	2.24	1.43	1.38
27	BA	365	OMG	C6-N1	2.23	1.43	1.38
1	Aa	917	5MU	C2-N3	-2.22	1.34	1.38
27	BA	2389	OMU	C5-C4	-2.22	1.38	1.43
27	BA	505	A2M	C8-N9	-2.21	1.33	1.37
1	Aa	995	2MG	C5-N7	-2.20	1.34	1.39
1	Aa	1449	6MZ	C8-N7	2.18	1.35	1.31
27	BA	879	A2M	C8-N9	-2.17	1.33	1.37
1	Aa	352	A2M	C8-N9	-2.13	1.33	1.37
1	Aa	1467	MA6	C8-N9	-2.13	1.33	1.37
1	Aa	995	2MG	C2-N3	2.12	1.36	1.31
27	BA	2936	A2M	C8-N9	-2.11	1.33	1.37
27	BA	849	A2M	C8-N9	-2.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	932	A2M	C8-N9	-2.07	1.33	1.37
27	BA	674	OMG	C4-N9	-2.07	1.32	1.38
27	BA	2521	OMG	C4-N9	-2.06	1.32	1.38
27	BA	2091	A2M	C8-N9	-2.04	1.33	1.37
1	Aa	532	OMG	C4-N9	-2.04	1.32	1.38
27	BA	1953	OMG	C4-N9	-2.03	1.32	1.38
27	BA	2745	OMG	C4-N9	-2.03	1.32	1.38
27	BA	2870	OMG	C4-N9	-2.02	1.32	1.38
27	BA	507	OMG	C4-N9	-2.02	1.32	1.38
1	Aa	1468	MA6	C8-N9	-2.02	1.33	1.37
27	BA	2389	OMU	C2-N1	2.01	1.41	1.38
1	Aa	770	OMG	C4-N9	-2.01	1.32	1.38
27	BA	2528	OMG	C4-N9	-2.00	1.32	1.38

All (792) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1468	MA6	N1-C6-N6	-14.01	101.77	117.08
1	Aa	1467	MA6	N1-C6-N6	-13.58	102.23	117.08
27	BA	1854	5MU	C5-C4-N3	12.41	125.90	115.31
27	BA	1766	5MU	C5-C4-N3	12.21	125.73	115.31
27	BA	829	5MU	C5-C4-N3	12.09	125.63	115.31
27	BA	2427	5MU	C5-C4-N3	12.06	125.61	115.31
27	BA	875	5MU	C5-C4-N3	11.95	125.51	115.31
27	BA	1854	5MU	C5-C6-N1	-10.39	112.65	123.34
27	BA	1766	5MU	C5-C6-N1	-10.17	112.87	123.34
27	BA	2427	5MU	C5-C6-N1	-9.98	113.07	123.34
27	BA	829	5MU	C5-C6-N1	-9.87	113.18	123.34
27	BA	875	5MU	C5-C6-N1	-9.86	113.20	123.34
27	BA	2581	4SU	C4-N3-C2	-7.90	119.66	127.34
1	Aa	1468	MA6	C5-C6-N6	7.37	138.13	125.30
1	Aa	995	2MG	C2-N3-C4	7.22	121.00	112.04
1	Aa	1467	MA6	C5-C6-N6	7.14	137.74	125.30
27	BA	2553	4SU	C4-N3-C2	-6.63	120.90	127.34
27	BA	2329	A2M	C5-C4-N3	-6.49	118.28	126.75
1	Aa	1449	6MZ	C5-C4-N3	-6.40	118.40	126.75
27	BA	2091	A2M	C5-C4-N3	-6.26	118.58	126.75
1	Aa	450	OMG	C5-C4-N3	-6.26	118.30	128.46
27	BA	2550	OMG	C5-C4-N3	-6.21	118.38	128.46
1	Aa	995	2MG	C5-C4-N3	-6.18	118.44	128.46
27	BA	2353	OMG	C5-C4-N3	-6.10	118.57	128.46
1	Aa	852	OMG	C5-C4-N3	-6.02	118.69	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	352	A2M	N6-C6-N1	-5.89	105.45	118.35
27	BA	849	A2M	N6-C6-N1	-5.83	105.58	118.35
27	BA	879	A2M	N6-C6-N1	-5.79	105.68	118.35
27	BA	932	A2M	N6-C6-N1	-5.75	105.75	118.35
27	BA	505	A2M	N6-C6-N1	-5.71	105.84	118.35
27	BA	2936	A2M	N6-C6-N1	-5.66	105.95	118.35
1	Aa	1467	MA6	N1-C2-N3	-5.56	119.90	128.60
27	BA	879	A2M	N3-C2-N1	-5.55	119.92	128.60
1	Aa	1468	MA6	N1-C2-N3	-5.55	119.92	128.60
27	BA	849	A2M	N3-C2-N1	-5.53	119.96	128.60
27	BA	505	A2M	C5-C4-N3	-5.52	119.55	126.75
1	Aa	352	A2M	N3-C2-N1	-5.51	119.98	128.60
27	BA	932	A2M	N3-C2-N1	-5.50	120.01	128.60
27	BA	2936	A2M	N3-C2-N1	-5.41	120.13	128.60
27	BA	932	A2M	C5-C4-N3	-5.40	119.71	126.75
27	BA	879	A2M	C5-C4-N3	-5.40	119.71	126.75
27	BA	2581	4SU	C5-C4-N3	5.38	119.68	114.69
1	Aa	636	OMG	C5-C4-N3	-5.36	119.77	128.46
27	BA	657	OMU	C4-N3-C2	-5.34	119.53	126.58
27	BA	2640	OMG	C5-C4-N3	-5.33	119.81	128.46
1	Aa	1467	MA6	C5-C4-N3	-5.33	119.80	126.75
27	BA	849	A2M	C5-C4-N3	-5.32	119.81	126.75
27	BA	2091	A2M	N3-C4-N9	5.31	135.84	127.08
27	BA	505	A2M	N3-C2-N1	-5.30	120.31	128.60
1	Aa	8	OMU	C4-N3-C2	-5.30	119.59	126.58
1	Aa	352	A2M	C5-C4-N3	-5.30	119.84	126.75
27	BA	829	5MU	O4-C4-C5	-5.29	118.77	124.90
27	BA	1969	OMU	C4-N3-C2	-5.28	119.61	126.58
27	BA	2936	A2M	C5-C4-N3	-5.27	119.87	126.75
27	BA	1150	OMU	C4-N3-C2	-5.26	119.64	126.58
27	BA	2656	OMU	C4-N3-C2	-5.24	119.66	126.58
27	BA	912	OMG	C5-C4-N3	-5.24	119.97	128.46
27	BA	453	OMU	C4-N3-C2	-5.24	119.67	126.58
27	BA	872	OMG	C5-C4-N3	-5.22	119.99	128.46
1	Aa	479	OMU	C4-N3-C2	-5.22	119.69	126.58
27	BA	365	OMG	C5-C4-N3	-5.21	120.00	128.46
1	Aa	670	OMG	C5-C4-N3	-5.21	120.01	128.46
1	Aa	753	OMU	C4-N3-C2	-5.21	119.71	126.58
27	BA	1480	OMU	C4-N3-C2	-5.20	119.72	126.58
27	BA	1956	OMG	C5-C4-N3	-5.20	120.02	128.46
1	Aa	450	OMG	C2-N3-C4	5.20	121.56	112.30
1	Aa	917	5MU	C4-N3-C2	-5.19	120.63	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	2542	OMU	C4-N3-C2	-5.17	119.76	126.58
27	BA	1508	OMG	C5-C4-N3	-5.16	120.09	128.46
27	BA	1893	OMG	C5-C4-N3	-5.12	120.15	128.46
27	BA	2469	OMG	C5-C4-N3	-5.12	120.15	128.46
27	BA	875	5MU	O4-C4-C5	-5.12	118.96	124.90
1	Aa	1107	OMG	C5-C4-N3	-5.12	120.16	128.46
1	Aa	1020	OMU	C4-N3-C2	-5.12	119.83	126.58
27	BA	2016	OMG	C5-C4-N3	-5.11	120.17	128.46
1	Aa	836	OMG	C5-C4-N3	-5.11	120.17	128.46
1	Aa	1358	OMU	C4-N3-C2	-5.11	119.84	126.58
1	Aa	659	OMG	C5-C4-N3	-5.09	120.21	128.46
1	Aa	1468	MA6	C5-C4-N3	-5.08	120.12	126.75
27	BA	2550	OMG	C2-N3-C4	5.08	121.35	112.30
1	Aa	629	OMG	C5-C4-N3	-5.07	120.23	128.46
27	BA	1402	OMU	C4-N3-C2	-5.06	119.90	126.58
1	Aa	1223	OMG	C5-C4-N3	-5.05	120.26	128.46
27	BA	584	OMG	C5-C4-N3	-5.05	120.27	128.46
1	Aa	994	OMG	C5-C4-N3	-5.05	120.27	128.46
27	BA	849	A2M	C5-C6-N6	5.04	134.40	123.43
27	BA	2353	OMG	C2-N3-C4	5.03	121.27	112.30
27	BA	1329	OMG	C5-C4-N3	-5.02	120.31	128.46
1	Aa	352	A2M	C5-C6-N6	5.02	134.35	123.43
27	BA	2010	OMG	C5-C4-N3	-5.02	120.33	128.46
27	BA	2379	OMG	C5-C4-N3	-5.02	120.33	128.46
1	Aa	121	OMG	C5-C4-N3	-5.01	120.33	128.46
27	BA	2672	OMG	C5-C4-N3	-5.01	120.34	128.46
27	BA	670	OMG	C5-C4-N3	-5.01	120.34	128.46
1	Aa	1449	6MZ	N3-C4-N9	5.00	135.33	127.08
27	BA	2168	OMG	C5-C4-N3	-5.00	120.35	128.46
27	BA	65	OMG	C5-C4-N3	-5.00	120.35	128.46
27	BA	1854	5MU	O4-C4-C5	-4.99	119.12	124.90
27	BA	1776	OMU	C4-N3-C2	-4.99	120.00	126.58
1	Aa	147	OMG	C5-C4-N3	-4.99	120.37	128.46
1	Aa	498	OMG	C5-C4-N3	-4.99	120.37	128.46
27	BA	2728	OMG	C5-C4-N3	-4.98	120.38	128.46
27	BA	1525	OMG	C5-C4-N3	-4.98	120.39	128.46
27	BA	800	OMG	C5-C4-N3	-4.98	120.39	128.46
27	BA	932	A2M	C5-C6-N6	4.97	134.25	123.43
27	BA	215	OMG	C5-C4-N3	-4.97	120.40	128.46
27	BA	833	OMG	C5-C4-N3	-4.97	120.40	128.46
27	BA	2553	4SU	N3-C2-N1	4.97	121.48	114.89
27	BA	829	5MU	C4-N3-C2	-4.96	120.93	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	2329	A2M	N3-C4-N9	4.96	135.26	127.08
1	Aa	574	OMG	C5-C4-N3	-4.96	120.41	128.46
1	Aa	219	OMG	C5-C4-N3	-4.96	120.42	128.46
1	Aa	495	OMG	C5-C4-N3	-4.96	120.42	128.46
27	BA	1854	5MU	C4-N3-C2	-4.96	120.93	127.35
27	BA	288	OMG	C5-C4-N3	-4.96	120.42	128.46
27	BA	1766	5MU	C4-N3-C2	-4.96	120.93	127.35
1	Aa	852	OMG	C2-N3-C4	4.95	121.13	112.30
27	BA	1766	5MU	O4-C4-C5	-4.94	119.18	124.90
1	Aa	913	OMG	C5-C4-N3	-4.93	120.46	128.46
27	BA	2466	OMG	C5-C4-N3	-4.93	120.46	128.46
27	BA	2553	4SU	C5-C4-N3	4.93	119.26	114.69
1	Aa	446	OMG	C5-C4-N3	-4.93	120.46	128.46
27	BA	63	OMG	C5-C4-N3	-4.93	120.47	128.46
27	BA	507	OMG	C5-C4-N3	-4.92	120.48	128.46
27	BA	2527	OMG	C5-C4-N3	-4.91	120.50	128.46
27	BA	2642	OMG	C5-C4-N3	-4.90	120.50	128.46
1	Aa	963	OMG	C5-C4-N3	-4.90	120.51	128.46
27	BA	879	A2M	C5-C6-N6	4.90	134.09	123.43
1	Aa	381	OMG	C5-C4-N3	-4.90	120.51	128.46
27	BA	2870	OMG	C5-C4-N3	-4.90	120.52	128.46
27	BA	2528	OMG	C5-C4-N3	-4.89	120.52	128.46
1	Aa	770	OMG	C5-C4-N3	-4.87	120.55	128.46
1	Aa	891	OMG	C5-C4-N3	-4.87	120.56	128.46
1	Aa	917	5MU	N3-C2-N1	4.87	121.35	114.89
27	BA	505	A2M	C5-C6-N6	4.86	134.00	123.43
1	Aa	320	OMG	C5-C4-N3	-4.85	120.59	128.46
27	BA	2745	OMG	C5-C4-N3	-4.83	120.63	128.46
27	BA	2936	A2M	C5-C6-N6	4.82	133.93	123.43
27	BA	2389	OMU	C4-N3-C2	-4.82	120.22	126.58
27	BA	2521	OMG	C5-C4-N3	-4.81	120.65	128.46
27	BA	1953	OMG	C5-C4-N3	-4.80	120.67	128.46
1	Aa	532	OMG	C5-C4-N3	-4.80	120.67	128.46
27	BA	674	OMG	C5-C4-N3	-4.80	120.68	128.46
27	BA	875	5MU	C4-N3-C2	-4.76	121.19	127.35
1	Aa	917	5MU	C5-C4-N3	4.70	119.32	115.31
27	BA	2550	OMG	N9-C4-N3	4.70	135.37	125.94
27	BA	2427	5MU	O4-C4-C5	-4.67	119.49	124.90
27	BA	2427	5MU	C4-N3-C2	-4.66	121.32	127.35
1	Aa	450	OMG	N9-C4-N3	4.64	135.26	125.94
1	Aa	852	OMG	C2'-C1'-N9	-4.60	105.29	114.22
1	Aa	995	2MG	N9-C4-N3	4.60	135.18	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1468	MA6	N9-C8-N7	-4.56	107.68	113.91
27	BA	2379	OMG	C2-N3-C4	4.53	120.37	112.30
27	BA	1956	OMG	C2-N3-C4	4.53	120.37	112.30
1	Aa	917	5MU	O4-C4-C5	-4.52	119.67	124.90
1	Aa	836	OMG	C2-N3-C4	4.49	120.31	112.30
27	BA	912	OMG	C2-N3-C4	4.48	120.29	112.30
1	Aa	670	OMG	C2-N3-C4	4.48	120.28	112.30
27	BA	1329	OMG	C2-N3-C4	4.48	120.28	112.30
1	Aa	852	OMG	N9-C4-N3	4.48	134.93	125.94
27	BA	2353	OMG	N9-C4-N3	4.47	134.91	125.94
27	BA	2640	OMG	C2-N3-C4	4.47	120.26	112.30
1	Aa	446	OMG	C2-N3-C4	4.46	120.24	112.30
1	Aa	498	OMG	C2-N3-C4	4.45	120.22	112.30
27	BA	2728	OMG	C2-N3-C4	4.45	120.22	112.30
1	Aa	636	OMG	C2-N3-C4	4.44	120.22	112.30
27	BA	2010	OMG	C2-N3-C4	4.44	120.20	112.30
27	BA	2168	OMG	C2-N3-C4	4.44	120.20	112.30
27	BA	800	OMG	C2-N3-C4	4.43	120.19	112.30
1	Aa	495	OMG	C2-N3-C4	4.43	120.19	112.30
1	Aa	770	OMG	C2-N3-C4	4.42	120.17	112.30
27	BA	670	OMG	C2-N3-C4	4.41	120.16	112.30
27	BA	872	OMG	C2-N3-C4	4.41	120.16	112.30
1	Aa	629	OMG	C2-N3-C4	4.40	120.14	112.30
27	BA	2389	OMU	N3-C2-N1	4.40	120.73	114.89
27	BA	1508	OMG	C2-N3-C4	4.40	120.14	112.30
27	BA	584	OMG	C2-N3-C4	4.39	120.13	112.30
1	Aa	994	OMG	C2-N3-C4	4.39	120.13	112.30
1	Aa	121	OMG	C2-N3-C4	4.39	120.12	112.30
27	BA	1893	OMG	C2-N3-C4	4.39	120.12	112.30
27	BA	507	OMG	C2-N3-C4	4.39	120.12	112.30
27	BA	63	OMG	C2-N3-C4	4.38	120.11	112.30
27	BA	1766	5MU	N3-C2-N1	4.38	120.71	114.89
1	Aa	381	OMG	C2-N3-C4	4.38	120.10	112.30
27	BA	2745	OMG	C2-N3-C4	4.38	120.10	112.30
27	BA	2016	OMG	C2-N3-C4	4.38	120.10	112.30
27	BA	65	OMG	C2-N3-C4	4.38	120.10	112.30
1	Aa	913	OMG	C2-N3-C4	4.37	120.09	112.30
27	BA	2672	OMG	C2-N3-C4	4.37	120.09	112.30
27	BA	2936	A2M	N9-C8-N7	-4.37	107.94	113.91
1	Aa	1107	OMG	C2-N3-C4	4.36	120.07	112.30
1	Aa	147	OMG	C2-N3-C4	4.36	120.07	112.30
27	BA	215	OMG	C2-N3-C4	4.36	120.06	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	574	OMG	C2-N3-C4	4.36	120.06	112.30
27	BA	365	OMG	C2-N3-C4	4.35	120.06	112.30
27	BA	288	OMG	C2-N3-C4	4.35	120.05	112.30
27	BA	829	5MU	N3-C2-N1	4.34	120.66	114.89
27	BA	875	5MU	N3-C2-N1	4.34	120.66	114.89
27	BA	829	5MU	C5M-C5-C6	-4.34	117.05	122.85
1	Aa	659	OMG	C2-N3-C4	4.34	120.03	112.30
27	BA	2521	OMG	C2-N3-C4	4.34	120.03	112.30
27	BA	833	OMG	C2-N3-C4	4.34	120.03	112.30
27	BA	1953	OMG	C2-N3-C4	4.33	120.01	112.30
27	BA	674	OMG	C2-N3-C4	4.33	120.01	112.30
27	BA	2528	OMG	C2-N3-C4	4.33	120.01	112.30
1	Aa	532	OMG	C2-N3-C4	4.32	120.00	112.30
27	BA	2642	OMG	C2-N3-C4	4.32	120.00	112.30
27	BA	1854	5MU	C5M-C5-C6	-4.32	117.08	122.85
1	Aa	219	OMG	C2-N3-C4	4.31	119.98	112.30
1	Aa	1223	OMG	C2-N3-C4	4.31	119.98	112.30
1	Aa	352	A2M	N9-C8-N7	-4.31	108.02	113.91
1	Aa	891	OMG	C2-N3-C4	4.31	119.97	112.30
1	Aa	1467	MA6	N9-C8-N7	-4.30	108.03	113.91
27	BA	2466	OMG	C2-N3-C4	4.30	119.96	112.30
27	BA	2469	OMG	C2-N3-C4	4.29	119.95	112.30
1	Aa	963	OMG	C2-N3-C4	4.29	119.95	112.30
1	Aa	320	OMG	C2-N3-C4	4.29	119.94	112.30
27	BA	2527	OMG	C2-N3-C4	4.28	119.93	112.30
27	BA	1525	OMG	C2-N3-C4	4.26	119.89	112.30
27	BA	879	A2M	N9-C8-N7	-4.25	108.10	113.91
27	BA	2870	OMG	C2-N3-C4	4.25	119.86	112.30
27	BA	932	A2M	N9-C8-N7	-4.22	108.15	113.91
27	BA	2427	5MU	N3-C2-N1	4.21	120.48	114.89
27	BA	849	A2M	N9-C8-N7	-4.21	108.16	113.91
27	BA	829	5MU	C5M-C5-C4	4.19	123.38	118.77
27	BA	1766	5MU	C5M-C5-C6	-4.16	117.29	122.85
27	BA	1854	5MU	C5M-C5-C4	4.14	123.32	118.77
27	BA	1854	5MU	N3-C2-N1	4.13	120.37	114.89
27	BA	2427	5MU	C5M-C5-C6	-4.11	117.36	122.85
27	BA	875	5MU	C5M-C5-C6	-4.11	117.36	122.85
27	BA	505	A2M	N9-C8-N7	-4.10	108.31	113.91
27	BA	1150	OMU	N3-C2-N1	4.08	120.30	114.89
1	Aa	1358	OMU	N3-C2-N1	4.03	120.25	114.89
27	BA	55	5MC	C5-C6-N1	-4.01	119.21	123.34
27	BA	2427	5MU	C5M-C5-C4	4.01	123.18	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1766	5MU	C5M-C5-C4	3.96	123.13	118.77
27	BA	875	5MU	C5M-C5-C4	3.95	123.12	118.77
27	BA	2581	4SU	N3-C2-N1	3.89	120.06	114.89
27	BA	2091	A2M	C2-N3-C4	3.89	120.95	111.75
1	Aa	1449	6MZ	C2-N3-C4	3.87	120.90	111.75
27	BA	2329	A2M	C2-N3-C4	3.87	120.90	111.75
1	Aa	8	OMU	N3-C2-N1	3.87	120.03	114.89
27	BA	2389	OMU	C5-C4-N3	3.85	120.60	114.84
27	BA	657	OMU	N3-C2-N1	3.85	120.00	114.89
27	BA	1969	OMU	N3-C2-N1	3.84	119.99	114.89
27	BA	453	OMU	N3-C2-N1	3.81	119.95	114.89
1	Aa	479	OMU	N3-C2-N1	3.80	119.94	114.89
27	BA	1402	OMU	N3-C2-N1	3.80	119.93	114.89
27	BA	1480	OMU	N3-C2-N1	3.78	119.91	114.89
1	Aa	1020	OMU	N3-C2-N1	3.78	119.91	114.89
27	BA	2656	OMU	N3-C2-N1	3.75	119.87	114.89
27	BA	1776	OMU	N3-C2-N1	3.74	119.86	114.89
1	Aa	753	OMU	N3-C2-N1	3.72	119.83	114.89
1	Aa	1467	MA6	C4-C5-C6	3.71	120.03	115.88
27	BA	879	A2M	C2-N3-C4	3.66	120.40	111.75
1	Aa	917	5MU	C5-C6-N1	-3.66	119.57	123.34
27	BA	2542	OMU	N3-C2-N1	3.65	119.74	114.89
27	BA	2605	5MC	C5-C6-N1	-3.62	119.61	123.34
1	Aa	923	5MC	C5-C6-N1	-3.59	119.64	123.34
1	Aa	1321	5MC	C5-C6-N1	-3.59	119.64	123.34
1	Aa	1467	MA6	C2-N3-C4	3.59	120.24	111.75
1	Aa	352	A2M	C2-N3-C4	3.59	120.23	111.75
27	BA	2688	5MC	C5-C6-N1	-3.57	119.66	123.34
27	BA	932	A2M	C2-N3-C4	3.56	120.16	111.75
27	BA	849	A2M	C2-N3-C4	3.55	120.13	111.75
27	BA	505	A2M	C2-N3-C4	3.54	120.12	111.75
1	Aa	1468	MA6	C2-N3-C4	3.52	120.07	111.75
1	Aa	1468	MA6	C2-N1-C6	3.52	120.06	111.75
27	BA	2936	A2M	C2-N3-C4	3.51	120.05	111.75
1	Aa	1007	5MC	C5-C6-N1	-3.51	119.73	123.34
27	BA	657	OMU	C5-C4-N3	3.49	120.07	114.84
1	Aa	1467	MA6	C2-N1-C6	3.49	120.00	111.75
27	BA	505	A2M	N3-C4-N9	3.49	132.84	127.08
27	BA	2542	OMU	C5-C4-N3	3.46	120.01	114.84
27	BA	2656	OMU	C5-C4-N3	3.45	120.00	114.84
1	Aa	854	5MC	C5-C6-N1	-3.44	119.80	123.34
1	Aa	1468	MA6	C4-C5-C6	3.43	119.72	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1345	5MC	C5-C6-N1	-3.43	119.81	123.34
1	Aa	8	OMU	C5-C4-N3	3.43	119.97	114.84
27	BA	1480	OMU	C5-C4-N3	3.42	119.96	114.84
1	Aa	685	5MC	C5-C6-N1	-3.39	119.85	123.34
27	BA	1969	OMU	C5-C4-N3	3.38	119.90	114.84
27	BA	1965	5MC	C5-C6-N1	-3.37	119.87	123.34
27	BA	2091	A2M	C2'-C1'-N9	-3.37	107.85	113.53
1	Aa	852	OMG	C6-C5-N7	3.37	136.51	130.25
27	BA	2353	OMG	C6-C5-N7	3.37	136.51	130.25
27	BA	2055	5MC	C5-C6-N1	-3.36	119.88	123.34
1	Aa	1467	MA6	N3-C4-N9	3.36	132.61	127.08
27	BA	2329	A2M	C4-C5-N7	-3.35	106.54	110.62
1	Aa	1004	5MC	C5-C6-N1	-3.35	119.89	123.34
1	Aa	753	OMU	C5-C4-N3	3.34	119.84	114.84
27	BA	453	OMU	C5-C4-N3	3.34	119.84	114.84
27	BA	879	A2M	N3-C4-N9	3.34	132.59	127.08
27	BA	2550	OMG	C6-C5-N7	3.33	136.44	130.25
27	BA	2581	4SU	C5-C4-S4	-3.33	120.18	124.47
27	BA	1150	OMU	C5-C4-N3	3.32	119.81	114.84
1	Aa	450	OMG	C6-C5-N7	3.32	136.41	130.25
1	Aa	636	OMG	N9-C4-N3	3.30	132.56	125.94
27	BA	2640	OMG	N9-C4-N3	3.30	132.56	125.94
1	Aa	479	OMU	C5-C4-N3	3.30	119.77	114.84
27	BA	1402	OMU	C5-C4-N3	3.28	119.75	114.84
27	BA	2075	5MC	C5-C6-N1	-3.28	119.96	123.34
1	Aa	672	5MC	C5-C6-N1	-3.28	119.97	123.34
1	Aa	473	5MC	C5-C6-N1	-3.27	119.97	123.34
27	BA	1776	OMU	C5-C4-N3	3.27	119.73	114.84
1	Aa	1449	6MZ	C4-C5-N7	-3.27	106.64	110.62
27	BA	2521	OMG	N9-C8-N7	-3.25	107.27	113.39
27	BA	365	OMG	N9-C4-N3	3.25	132.46	125.94
27	BA	932	A2M	N3-C4-N9	3.24	132.43	127.08
27	BA	2389	OMU	O4-C4-C5	-3.24	119.46	125.16
1	Aa	1468	MA6	C5-N7-C8	3.24	108.11	103.51
1	Aa	340	5MC	C5-C6-N1	-3.24	120.01	123.34
1	Aa	1003	5MC	C5-C6-N1	-3.23	120.01	123.34
27	BA	2936	A2M	N3-C4-N9	3.23	132.41	127.08
1	Aa	349	5MC	C5-C6-N1	-3.23	120.02	123.34
1	Aa	532	OMG	N9-C8-N7	-3.23	107.31	113.39
1	Aa	1020	OMU	C5-C4-N3	3.21	119.64	114.84
27	BA	2353	OMG	C2'-C1'-N9	-3.21	107.99	114.22
1	Aa	770	OMG	N9-C8-N7	-3.19	107.38	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1006	5MC	C5-C6-N1	-3.19	120.06	123.34
27	BA	879	A2M	C5-N7-C8	3.19	108.04	103.51
1	Aa	320	OMG	N9-C8-N7	-3.18	107.39	113.39
27	BA	1956	OMG	N9-C4-N3	3.18	132.33	125.94
27	BA	2642	OMG	N9-C8-N7	-3.18	107.40	113.39
1	Aa	1306	5MC	C5-C6-N1	-3.18	120.07	123.34
27	BA	288	OMG	N9-C8-N7	-3.18	107.40	113.39
1	Aa	457	5MC	C5-C6-N1	-3.18	120.07	123.34
1	Aa	381	OMG	N9-C8-N7	-3.17	107.41	113.39
1	Aa	464	5MC	C5-C6-N1	-3.17	120.07	123.34
27	BA	2091	A2M	N3-C2-N1	-3.17	123.64	128.60
1	Aa	352	A2M	N3-C4-N9	3.16	132.29	127.08
1	Aa	1107	OMG	N9-C4-N3	3.16	132.28	125.94
27	BA	849	A2M	C5-N7-C8	3.16	108.00	103.51
1	Aa	670	OMG	N9-C4-N3	3.16	132.28	125.94
1	Aa	352	A2M	C5-N7-C8	3.16	108.00	103.51
27	BA	833	OMG	N9-C8-N7	-3.15	107.45	113.39
27	BA	505	A2M	C5-N7-C8	3.15	107.99	103.51
27	BA	63	OMG	N9-C8-N7	-3.15	107.45	113.39
1	Aa	1476	5MC	C5-C6-N1	-3.15	120.10	123.34
1	Aa	1184	5MC	C5-C6-N1	-3.15	120.10	123.34
1	Aa	636	OMG	C2-N1-C6	-3.14	119.36	125.10
27	BA	932	A2M	C5-N7-C8	3.14	107.97	103.51
27	BA	1508	OMG	N9-C4-N3	3.13	132.23	125.94
27	BA	2936	A2M	C5-N7-C8	3.13	107.96	103.51
27	BA	1329	OMG	N9-C8-N7	-3.13	107.50	113.39
27	BA	584	OMG	N9-C8-N7	-3.13	107.50	113.39
27	BA	1508	OMG	C2-N1-C6	-3.12	119.41	125.10
27	BA	2469	OMG	N9-C4-N3	3.12	132.20	125.94
27	BA	1893	OMG	C2-N1-C6	-3.12	119.42	125.10
1	Aa	1223	OMG	N9-C8-N7	-3.12	107.52	113.39
1	Aa	670	OMG	C2-N1-C6	-3.11	119.42	125.10
27	BA	2640	OMG	C2-N1-C6	-3.11	119.42	125.10
1	Aa	1358	OMU	C5-C4-N3	3.11	119.50	114.84
1	Aa	836	OMG	C2-N1-C6	-3.11	119.43	125.10
1	Aa	1449	6MZ	C6-C5-N7	3.11	135.75	132.39
27	BA	2010	OMG	N9-C8-N7	-3.10	107.54	113.39
1	Aa	836	OMG	N9-C8-N7	-3.10	107.55	113.39
27	BA	670	OMG	N9-C8-N7	-3.10	107.55	113.39
1	Aa	498	OMG	N9-C8-N7	-3.10	107.55	113.39
1	Aa	574	OMG	N9-C8-N7	-3.10	107.55	113.39
27	BA	2672	OMG	N9-C8-N7	-3.10	107.56	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	121	OMG	N9-C8-N7	-3.10	107.56	113.39
1	Aa	495	OMG	N9-C8-N7	-3.10	107.56	113.39
27	BA	2379	OMG	N9-C8-N7	-3.10	107.56	113.39
27	BA	849	A2M	N3-C4-N9	3.10	132.18	127.08
1	Aa	995	2MG	C6-C5-N7	3.09	136.00	130.25
1	Aa	446	OMG	N9-C8-N7	-3.09	107.57	113.39
1	Aa	1352	5MC	C5-C6-N1	-3.09	120.16	123.34
27	BA	2070	5MC	C5-C6-N1	-3.09	120.16	123.34
27	BA	2745	OMG	N9-C8-N7	-3.09	107.57	113.39
1	Aa	1468	MA6	N3-C4-N9	3.09	132.17	127.08
1	Aa	891	OMG	N9-C8-N7	-3.09	107.58	113.39
27	BA	800	OMG	N9-C8-N7	-3.08	107.59	113.39
1	Aa	659	OMG	N9-C4-N3	3.08	132.12	125.94
27	BA	2016	OMG	N9-C4-N3	3.08	132.12	125.94
27	BA	2091	A2M	C4-C5-N7	-3.07	106.87	110.62
1	Aa	913	OMG	N9-C8-N7	-3.07	107.61	113.39
1	Aa	994	OMG	N9-C8-N7	-3.07	107.62	113.39
27	BA	507	OMG	N9-C8-N7	-3.07	107.62	113.39
1	Aa	629	OMG	N9-C8-N7	-3.07	107.62	113.39
1	Aa	994	OMG	N9-C4-N3	3.06	132.09	125.94
27	BA	215	OMG	N9-C8-N7	-3.06	107.62	113.39
27	BA	584	OMG	N9-C4-N3	3.06	132.09	125.94
27	BA	2168	OMG	N9-C4-N3	3.06	132.08	125.94
1	Aa	121	OMG	N9-C4-N3	3.06	132.07	125.94
27	BA	1893	OMG	N9-C4-N3	3.06	132.07	125.94
27	BA	65	OMG	N9-C8-N7	-3.05	107.64	113.39
27	BA	63	OMG	C2-N1-C6	-3.05	119.54	125.10
27	BA	1525	OMG	N9-C4-N3	3.05	132.06	125.94
27	BA	2527	OMG	N9-C8-N7	-3.04	107.66	113.39
1	Aa	1107	OMG	C2-N1-C6	-3.04	119.55	125.10
1	Aa	147	OMG	N9-C8-N7	-3.04	107.66	113.39
27	BA	1893	OMG	N9-C8-N7	-3.04	107.66	113.39
1	Aa	670	OMG	N9-C8-N7	-3.04	107.66	113.39
27	BA	872	OMG	C2-N1-C6	-3.04	119.55	125.10
1	Aa	1223	OMG	N9-C4-N3	3.04	132.04	125.94
27	BA	365	OMG	C2-N1-C6	-3.04	119.56	125.10
1	Aa	1449	6MZ	N1-C2-N3	-3.04	123.85	128.60
27	BA	912	OMG	N9-C4-N3	3.04	132.04	125.94
1	Aa	219	OMG	N9-C8-N7	-3.04	107.67	113.39
27	BA	1329	OMG	C2-N1-C6	-3.04	119.56	125.10
27	BA	2168	OMG	N9-C8-N7	-3.04	107.67	113.39
1	Aa	1266	5MC	C5-C6-N1	-3.03	120.22	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	215	OMG	N9-C4-N3	3.03	132.03	125.94
1	Aa	994	OMG	C2-N1-C6	-3.03	119.58	125.10
27	BA	2528	OMG	N9-C8-N7	-3.03	107.69	113.39
27	BA	2010	OMG	C2-N1-C6	-3.03	119.58	125.10
27	BA	2521	OMG	C2-N1-C6	-3.03	119.58	125.10
1	Aa	629	OMG	N9-C4-N3	3.02	132.01	125.94
1	Aa	1478	5MC	C5-C6-N1	-3.02	120.23	123.34
27	BA	1953	OMG	N9-C8-N7	-3.02	107.70	113.39
27	BA	215	OMG	C2-N1-C6	-3.02	119.59	125.10
1	Aa	963	OMG	N9-C8-N7	-3.02	107.70	113.39
1	Aa	1467	MA6	C5-N7-C8	3.02	107.80	103.51
1	Aa	1223	OMG	C2-N1-C6	-3.02	119.59	125.10
27	BA	1525	OMG	C2-N1-C6	-3.02	119.59	125.10
27	BA	1508	OMG	N9-C8-N7	-3.02	107.71	113.39
1	Aa	836	OMG	N9-C4-N3	3.02	132.00	125.94
1	Aa	629	OMG	C2-N1-C6	-3.02	119.60	125.10
1	Aa	320	OMG	C2-N1-C6	-3.02	119.60	125.10
1	Aa	446	OMG	C2-N1-C6	-3.01	119.61	125.10
27	BA	2728	OMG	N9-C8-N7	-3.01	107.73	113.39
27	BA	2469	OMG	C2-N1-C6	-3.00	119.64	125.10
27	BA	2379	OMG	C2-N1-C6	-3.00	119.64	125.10
1	Aa	147	OMG	C2-N1-C6	-2.99	119.64	125.10
27	BA	1329	OMG	N9-C4-N3	2.99	131.95	125.94
27	BA	833	OMG	N9-C4-N3	2.99	131.95	125.94
27	BA	2870	OMG	N9-C8-N7	-2.99	107.75	113.39
27	BA	65	OMG	C2-N1-C6	-2.99	119.64	125.10
27	BA	453	OMU	O4-C4-C5	-2.99	119.90	125.16
1	Aa	659	OMG	C2-N1-C6	-2.99	119.65	125.10
27	BA	2329	A2M	N3-C2-N1	-2.99	123.93	128.60
1	Aa	495	OMG	C2-N1-C6	-2.99	119.65	125.10
27	BA	584	OMG	C2-N1-C6	-2.99	119.65	125.10
27	BA	872	OMG	N9-C4-N3	2.98	131.92	125.94
1	Aa	963	OMG	N9-C4-N3	2.98	131.92	125.94
1	Aa	219	OMG	C2-N1-C6	-2.98	119.67	125.10
1	Aa	498	OMG	N9-C4-N3	2.98	131.92	125.94
1	Aa	574	OMG	C2-N1-C6	-2.97	119.68	125.10
27	BA	2016	OMG	N9-C8-N7	-2.97	107.79	113.39
27	BA	365	OMG	N9-C8-N7	-2.97	107.80	113.39
1	Aa	498	OMG	C2-N1-C6	-2.97	119.68	125.10
27	BA	670	OMG	C2-N1-C6	-2.97	119.68	125.10
27	BA	2527	OMG	C2-N1-C6	-2.97	119.68	125.10
27	BA	288	OMG	C2-N1-C6	-2.97	119.69	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	912	OMG	C2-N1-C6	-2.97	119.69	125.10
1	Aa	1107	OMG	N9-C8-N7	-2.97	107.80	113.39
27	BA	1525	OMG	N9-C8-N7	-2.96	107.81	113.39
27	BA	2642	OMG	C2-N1-C6	-2.96	119.70	125.10
27	BA	1953	OMG	C2-N1-C6	-2.96	119.70	125.10
27	BA	65	OMG	N9-C4-N3	2.96	131.89	125.94
27	BA	2091	A2M	C5-N7-C8	2.96	107.72	103.51
27	BA	288	OMG	N9-C4-N3	2.96	131.88	125.94
1	Aa	147	OMG	N9-C4-N3	2.96	131.88	125.94
1	Aa	121	OMG	C2-N1-C6	-2.96	119.70	125.10
1	Aa	381	OMG	C2-N1-C6	-2.96	119.70	125.10
27	BA	2870	OMG	C2-N1-C6	-2.96	119.71	125.10
1	Aa	913	OMG	N9-C4-N3	2.96	131.88	125.94
27	BA	1956	OMG	N9-C8-N7	-2.96	107.82	113.39
27	BA	670	OMG	N9-C4-N3	2.96	131.87	125.94
27	BA	2466	OMG	N9-C8-N7	-2.96	107.82	113.39
27	BA	2016	OMG	C2-N1-C6	-2.95	119.71	125.10
27	BA	2672	OMG	N9-C4-N3	2.95	131.87	125.94
1	Aa	219	OMG	N9-C4-N3	2.95	131.86	125.94
27	BA	2168	OMG	C2-N1-C6	-2.95	119.72	125.10
27	BA	800	OMG	C2-N1-C6	-2.95	119.73	125.10
1	Aa	770	OMG	C2-N1-C6	-2.94	119.73	125.10
27	BA	2010	OMG	N9-C4-N3	2.94	131.85	125.94
27	BA	674	OMG	C2-N1-C6	-2.94	119.74	125.10
1	Aa	532	OMG	C2-N1-C6	-2.94	119.75	125.10
27	BA	2469	OMG	N9-C8-N7	-2.93	107.87	113.39
27	BA	2728	OMG	C2-N1-C6	-2.93	119.75	125.10
27	BA	2466	OMG	C2-N1-C6	-2.93	119.76	125.10
27	BA	2379	OMG	N9-C4-N3	2.93	131.82	125.94
1	Aa	913	OMG	C2-N1-C6	-2.93	119.76	125.10
27	BA	674	OMG	N9-C8-N7	-2.92	107.89	113.39
27	BA	833	OMG	C2-N1-C6	-2.92	119.77	125.10
1	Aa	495	OMG	N9-C4-N3	2.92	131.80	125.94
1	Aa	574	OMG	N9-C4-N3	2.92	131.79	125.94
1	Aa	659	OMG	N9-C8-N7	-2.91	107.90	113.39
27	BA	2672	OMG	C2-N1-C6	-2.91	119.79	125.10
1	Aa	891	OMG	C2-N1-C6	-2.91	119.79	125.10
27	BA	1956	OMG	C2-N1-C6	-2.91	119.80	125.10
27	BA	2528	OMG	C2-N1-C6	-2.91	119.80	125.10
27	BA	507	OMG	C2-N1-C6	-2.90	119.80	125.10
27	BA	2640	OMG	N9-C8-N7	-2.90	107.94	113.39
1	Aa	381	OMG	N9-C4-N3	2.89	131.75	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	912	OMG	N9-C8-N7	-2.89	107.95	113.39
27	BA	505	A2M	C2'-C1'-N9	-2.89	108.67	113.53
27	BA	2745	OMG	C2-N1-C6	-2.88	119.85	125.10
27	BA	1480	OMU	O4-C4-C5	-2.88	120.10	125.16
27	BA	2728	OMG	N9-C4-N3	2.88	131.71	125.94
27	BA	2656	OMU	O4-C4-C5	-2.87	120.11	125.16
1	Aa	479	OMU	O4-C4-C5	-2.87	120.11	125.16
1	Aa	770	OMG	N9-C4-N3	2.87	131.70	125.94
1	Aa	320	OMG	N9-C4-N3	2.86	131.68	125.94
1	Aa	963	OMG	C2-N1-C6	-2.86	119.89	125.10
27	BA	63	OMG	N9-C4-N3	2.86	131.68	125.94
27	BA	800	OMG	N9-C4-N3	2.86	131.67	125.94
27	BA	2527	OMG	N9-C4-N3	2.85	131.67	125.94
1	Aa	753	OMU	O4-C4-C5	-2.85	120.15	125.16
1	Aa	446	OMG	N9-C4-N3	2.85	131.66	125.94
1	Aa	891	OMG	N9-C4-N3	2.84	131.65	125.94
1	Aa	1020	OMU	O4-C4-C5	-2.84	120.16	125.16
27	BA	2870	OMG	N9-C4-N3	2.84	131.65	125.94
27	BA	1329	OMG	C5-C6-N1	2.84	120.40	113.19
27	BA	2642	OMG	N9-C4-N3	2.83	131.62	125.94
27	BA	2542	OMU	O4-C4-C5	-2.83	120.18	125.16
27	BA	872	OMG	N9-C8-N7	-2.82	108.07	113.39
1	Aa	532	OMG	N9-C4-N3	2.82	131.60	125.94
27	BA	2329	A2M	C5-N7-C8	2.82	107.51	103.51
1	Aa	17	5MC	C5-C6-N1	-2.80	120.46	123.34
27	BA	215	OMG	C5-C6-N1	2.80	120.30	113.19
27	BA	1893	OMG	C5-C6-N1	2.79	120.28	113.19
27	BA	63	OMG	C5-C6-N1	2.79	120.28	113.19
1	Aa	670	OMG	C5-C6-N1	2.79	120.28	113.19
27	BA	1969	OMU	O4-C4-C5	-2.79	120.25	125.16
1	Aa	446	OMG	C5-C6-N1	2.79	120.27	113.19
27	BA	2010	OMG	C5-C6-N1	2.78	120.24	113.19
1	Aa	770	OMG	C5-C6-N1	2.78	120.24	113.19
1	Aa	836	OMG	C5-C6-N1	2.77	120.23	113.19
1	Aa	8	OMU	O4-C4-C5	-2.77	120.29	125.16
27	BA	2091	A2M	C4-N9-C8	2.77	108.72	105.73
27	BA	2528	OMG	N9-C4-N3	2.76	131.49	125.94
27	BA	65	OMG	C5-C6-N1	2.76	120.20	113.19
27	BA	2379	OMG	C5-C6-N1	2.76	120.19	113.19
1	Aa	495	OMG	C5-C6-N1	2.76	120.19	113.19
27	BA	342	OMC	C2'-C1'-N1	-2.75	108.88	114.22
1	Aa	498	OMG	C5-C6-N1	2.75	120.19	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	629	OMG	C5-C6-N1	2.75	120.18	113.19
1	Aa	1449	6MZ	C5-N7-C8	2.75	107.42	103.51
27	BA	670	OMG	C5-C6-N1	2.75	120.17	113.19
27	BA	1508	OMG	C5-C6-N1	2.75	120.17	113.19
1	Aa	994	OMG	C5-C6-N1	2.75	120.17	113.19
27	BA	674	OMG	C5-C6-N1	2.75	120.16	113.19
27	BA	1525	OMG	C5-C6-N1	2.74	120.16	113.19
27	BA	1776	OMU	O4-C4-C5	-2.74	120.34	125.16
27	BA	1953	OMG	N9-C4-N3	2.74	131.44	125.94
1	Aa	320	OMG	C5-C6-N1	2.74	120.14	113.19
27	BA	288	OMG	C5-C6-N1	2.73	120.13	113.19
1	Aa	147	OMG	C5-C6-N1	2.73	120.13	113.19
27	BA	2745	OMG	C5-C6-N1	2.73	120.12	113.19
27	BA	657	OMU	O4-C4-C5	-2.73	120.37	125.16
27	BA	507	OMG	N9-C4-N3	2.72	131.41	125.94
27	BA	2642	OMG	C5-C6-N1	2.72	120.11	113.19
27	BA	2427	5MU	O4-C4-N3	-2.72	114.90	120.12
27	BA	584	OMG	C5-C6-N1	2.72	120.10	113.19
1	Aa	1107	OMG	C5-C6-N1	2.72	120.10	113.19
27	BA	1402	OMU	O4-C4-C5	-2.72	120.38	125.16
1	Aa	1321	5MC	CM5-C5-C6	-2.72	119.22	122.85
1	Aa	381	OMG	C5-C6-N1	2.72	120.09	113.19
27	BA	365	OMG	C5-C6-N1	2.72	120.08	113.19
27	BA	2672	OMG	C5-C6-N1	2.72	120.08	113.19
27	BA	800	OMG	C5-C6-N1	2.71	120.08	113.19
1	Aa	532	OMG	C5-C6-N1	2.71	120.08	113.19
27	BA	2640	OMG	C5-C6-N1	2.71	120.08	113.19
27	BA	2168	OMG	C5-C6-N1	2.71	120.07	113.19
1	Aa	636	OMG	C5-C6-N1	2.71	120.07	113.19
1	Aa	121	OMG	C5-C6-N1	2.70	120.06	113.19
27	BA	2527	OMG	C5-C6-N1	2.70	120.06	113.19
27	BA	2521	OMG	C5-C6-N1	2.70	120.06	113.19
27	BA	833	OMG	C5-C6-N1	2.70	120.05	113.19
1	Aa	574	OMG	C5-C6-N1	2.70	120.05	113.19
1	Aa	636	OMG	N9-C8-N7	-2.70	108.30	113.39
1	Aa	659	OMG	C5-C6-N1	2.70	120.04	113.19
1	Aa	891	OMG	C5-C6-N1	2.70	120.03	113.19
27	BA	2745	OMG	N9-C4-N3	2.69	131.34	125.94
1	Aa	1223	OMG	C5-C6-N1	2.69	120.02	113.19
27	BA	2466	OMG	C5-C6-N1	2.69	120.02	113.19
27	BA	2466	OMG	N9-C4-N3	2.69	131.34	125.94
27	BA	2016	OMG	C5-C6-N1	2.69	120.02	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1953	OMG	C5-C6-N1	2.69	120.02	113.19
1	Aa	913	OMG	C5-C6-N1	2.69	120.01	113.19
27	BA	1956	OMG	C5-C6-N1	2.68	120.00	113.19
27	BA	1854	5MU	O4-C4-N3	-2.68	114.98	120.12
1	Aa	219	OMG	C5-C6-N1	2.68	119.98	113.19
27	BA	2728	OMG	C5-C6-N1	2.67	119.98	113.19
27	BA	912	OMG	C5-C6-N1	2.67	119.97	113.19
27	BA	872	OMG	C5-C6-N1	2.67	119.97	113.19
27	BA	2870	OMG	C5-C6-N1	2.67	119.96	113.19
27	BA	2521	OMG	N9-C4-N3	2.66	131.29	125.94
27	BA	2528	OMG	C5-C6-N1	2.66	119.94	113.19
27	BA	507	OMG	C5-C6-N1	2.66	119.94	113.19
27	BA	2469	OMG	C5-C6-N1	2.65	119.93	113.19
27	BA	674	OMG	N9-C4-N3	2.64	131.24	125.94
1	Aa	1358	OMU	O4-C4-C5	-2.64	120.53	125.16
1	Aa	963	OMG	C5-C6-N1	2.63	119.88	113.19
27	BA	1766	5MU	O4-C4-N3	-2.62	115.09	120.12
27	BA	2353	OMG	C4-C5-N7	-2.60	106.60	110.72
27	BA	2553	4SU	C5-C4-S4	-2.59	121.13	124.47
27	BA	2389	OMU	O4'-C1'-C2'	-2.59	102.03	106.57
27	BA	1508	OMG	O6-C6-C5	-2.57	119.79	126.60
27	BA	2168	OMG	O6-C6-C5	-2.57	119.79	126.60
1	Aa	995	2MG	C4-C5-N7	-2.56	106.67	110.72
1	Aa	381	OMG	O6-C6-C5	-2.56	119.81	126.60
1	Aa	450	OMG	C2'-C1'-N9	-2.55	109.27	114.22
1	Aa	1107	OMG	O6-C6-C5	-2.55	119.83	126.60
1	Aa	450	OMG	C4-C5-N7	-2.55	106.69	110.72
27	BA	1329	OMG	O6-C6-C5	-2.55	119.84	126.60
27	BA	2640	OMG	O6-C6-C5	-2.54	119.86	126.60
27	BA	215	OMG	O6-C6-C5	-2.53	119.88	126.60
1	Aa	917	5MU	O2-C2-N1	-2.53	119.42	122.79
1	Aa	852	OMG	C4-C5-N7	-2.53	106.72	110.72
27	BA	2010	OMG	O6-C6-C5	-2.52	119.92	126.60
1	Aa	636	OMG	O6-C6-C5	-2.51	119.94	126.60
1	Aa	498	OMG	O6-C6-C5	-2.50	119.95	126.60
1	Aa	670	OMG	O6-C6-C5	-2.50	119.96	126.60
27	BA	1525	OMG	O6-C6-C5	-2.50	119.96	126.60
27	BA	1150	OMU	O4-C4-C5	-2.50	120.77	125.16
27	BA	63	OMG	O6-C6-C5	-2.50	119.97	126.60
1	Aa	532	OMG	O6-C6-C5	-2.50	119.98	126.60
1	Aa	629	OMG	O6-C6-C5	-2.49	119.99	126.60
1	Aa	963	OMG	O6-C6-C5	-2.49	119.99	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	994	OMG	O6-C6-C5	-2.49	120.00	126.60
1	Aa	1468	MA6	C4-N9-C8	2.49	108.42	105.73
1	Aa	320	OMG	O6-C6-C5	-2.48	120.01	126.60
27	BA	2550	OMG	C4-C5-N7	-2.48	106.79	110.72
1	Aa	770	OMG	O6-C6-C5	-2.48	120.01	126.60
1	Aa	1223	OMG	O6-C6-C5	-2.48	120.02	126.60
1	Aa	446	OMG	O6-C6-C5	-2.47	120.05	126.60
1	Aa	495	OMG	O6-C6-C5	-2.47	120.05	126.60
27	BA	829	5MU	O2-C2-N1	-2.46	119.51	122.79
1	Aa	836	OMG	O6-C6-C5	-2.46	120.08	126.60
27	BA	1956	OMG	O6-C6-C5	-2.46	120.09	126.60
27	BA	1893	OMG	O6-C6-C5	-2.45	120.09	126.60
27	BA	288	OMG	O6-C6-C5	-2.45	120.10	126.60
1	Aa	121	OMG	O6-C6-C5	-2.44	120.12	126.60
27	BA	584	OMG	O6-C6-C5	-2.44	120.13	126.60
27	BA	674	OMG	O6-C6-C5	-2.44	120.14	126.60
27	BA	2469	OMG	O6-C6-C5	-2.44	120.14	126.60
1	Aa	913	OMG	O6-C6-C5	-2.43	120.14	126.60
27	BA	2553	4SU	O2-C2-N1	-2.43	119.56	122.79
1	Aa	574	OMG	O6-C6-C5	-2.43	120.16	126.60
27	BA	65	OMG	O6-C6-C5	-2.43	120.16	126.60
27	BA	2521	OMG	O6-C6-C5	-2.42	120.18	126.60
1	Aa	659	OMG	O6-C6-C5	-2.41	120.20	126.60
1	Aa	219	OMG	O6-C6-C5	-2.41	120.21	126.60
1	Aa	340	5MC	CM5-C5-C6	-2.41	119.63	122.85
27	BA	2075	5MC	CM5-C5-C6	-2.40	119.64	122.85
27	BA	2379	OMG	O6-C6-C5	-2.40	120.23	126.60
27	BA	875	5MU	O4-C4-N3	-2.40	115.53	120.12
27	BA	2728	OMG	O6-C6-C5	-2.39	120.25	126.60
1	Aa	891	OMG	O6-C6-C5	-2.39	120.26	126.60
27	BA	800	OMG	O6-C6-C5	-2.39	120.26	126.60
27	BA	833	OMG	O6-C6-C5	-2.39	120.26	126.60
27	BA	365	OMG	O6-C6-C5	-2.37	120.30	126.60
1	Aa	147	OMG	O6-C6-C5	-2.37	120.31	126.60
27	BA	2672	OMG	O6-C6-C5	-2.37	120.31	126.60
27	BA	2936	A2M	C2'-C1'-N9	-2.37	109.54	113.53
27	BA	2550	OMG	C2'-C1'-N9	-2.37	109.63	114.22
27	BA	670	OMG	O6-C6-C5	-2.36	120.33	126.60
27	BA	2016	OMG	O6-C6-C5	-2.36	120.34	126.60
27	BA	912	OMG	O6-C6-C5	-2.36	120.35	126.60
27	BA	829	5MU	O4-C4-N3	-2.36	115.60	120.12
1	Aa	1467	MA6	C4-N9-C8	2.35	108.28	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	670	OMG	CM2-O2'-C2'	2.35	120.68	114.52
27	BA	1953	OMG	O6-C6-C5	-2.34	120.38	126.60
27	BA	2870	OMG	O6-C6-C5	-2.34	120.38	126.60
27	BA	2527	OMG	O6-C6-C5	-2.34	120.39	126.60
27	BA	2528	OMG	O6-C6-C5	-2.34	120.39	126.60
27	BA	2936	A2M	C4-N9-C8	2.33	108.26	105.73
27	BA	2389	OMU	O3'-C3'-C4'	-2.32	104.34	111.05
27	BA	2642	OMG	CM2-O2'-C2'	2.32	120.60	114.52
27	BA	2745	OMG	O6-C6-C5	-2.30	120.49	126.60
1	Aa	852	OMG	O6-C6-C5	-2.30	120.51	126.60
27	BA	507	OMG	O6-C6-C5	-2.28	120.54	126.60
27	BA	2642	OMG	O6-C6-C5	-2.28	120.55	126.60
27	BA	2521	OMG	C8-N7-C5	2.28	108.37	104.24
27	BA	879	A2M	C2'-C1'-N9	-2.28	109.69	113.53
27	BA	2642	OMG	C8-N7-C5	2.27	108.35	104.24
27	BA	1766	5MU	O2-C2-N1	-2.27	119.77	122.79
27	BA	63	OMG	C8-N7-C5	2.26	108.33	104.24
27	BA	800	OMG	C8-N7-C5	2.26	108.33	104.24
1	Aa	923	5MC	CM5-C5-C6	-2.25	119.84	122.85
1	Aa	17	5MC	CM5-C5-C6	-2.25	119.84	122.85
1	Aa	1449	6MZ	C4-N9-C8	2.25	108.16	105.73
27	BA	2672	OMG	C8-N7-C5	2.24	108.29	104.24
1	Aa	836	OMG	C8-N7-C5	2.23	108.28	104.24
1	Aa	349	5MC	CM5-C5-C6	-2.23	119.87	122.85
1	Aa	1266	5MC	CM5-C5-C6	-2.23	119.87	122.85
27	BA	2010	OMG	C8-N7-C5	2.23	108.28	104.24
27	BA	584	OMG	C8-N7-C5	2.23	108.27	104.24
27	BA	2605	5MC	CM5-C5-C6	-2.22	119.88	122.85
1	Aa	636	OMG	C1'-N9-C8	-2.22	120.37	126.70
27	BA	507	OMG	C8-N7-C5	2.22	108.26	104.24
1	Aa	473	5MC	CM5-C5-C6	-2.22	119.88	122.85
27	BA	670	OMG	C8-N7-C5	2.21	108.24	104.24
1	Aa	320	OMG	C8-N7-C5	2.21	108.24	104.24
1	Aa	381	OMG	C8-N7-C5	2.21	108.24	104.24
27	BA	2070	5MC	CM5-C5-C6	-2.21	119.90	122.85
1	Aa	770	OMG	C8-N7-C5	2.20	108.23	104.24
1	Aa	1223	OMG	C8-N7-C5	2.20	108.23	104.24
27	BA	875	5MU	C1'-N1-C2	2.20	121.56	117.57
1	Aa	994	OMG	C8-N7-C5	2.20	108.23	104.24
27	BA	288	OMG	C8-N7-C5	2.20	108.23	104.24
27	BA	833	OMG	C8-N7-C5	2.20	108.22	104.24
27	BA	872	OMG	O6-C6-C5	-2.20	120.77	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	498	OMG	C8-N7-C5	2.19	108.21	104.24
1	Aa	1006	5MC	CM5-C5-C6	-2.19	119.92	122.85
27	BA	872	OMG	C8-N7-C5	2.19	108.21	104.24
27	BA	2379	OMG	C8-N7-C5	2.19	108.20	104.24
1	Aa	532	OMG	C8-N7-C5	2.19	108.20	104.24
1	Aa	670	OMG	C8-N7-C5	2.19	108.20	104.24
1	Aa	352	A2M	C4-N9-C8	2.19	108.10	105.73
27	BA	65	OMG	C8-N7-C5	2.18	108.19	104.24
27	BA	1508	OMG	C8-N7-C5	2.18	108.19	104.24
27	BA	849	A2M	C4-C5-N7	-2.18	107.96	110.62
27	BA	1329	OMG	C8-N7-C5	2.18	108.19	104.24
27	BA	2745	OMG	C8-N7-C5	2.17	108.18	104.24
27	BA	2389	OMU	C1'-N1-C2	2.17	121.51	117.57
1	Aa	891	OMG	C8-N7-C5	2.17	108.17	104.24
27	BA	1969	OMU	O2-C2-N1	-2.17	119.90	122.79
1	Aa	854	5MC	CM5-C5-C6	-2.17	119.95	122.85
1	Aa	446	OMG	C8-N7-C5	2.17	108.17	104.24
1	Aa	495	OMG	C8-N7-C5	2.17	108.16	104.24
27	BA	505	A2M	C6-C5-C4	2.16	120.09	117.18
27	BA	879	A2M	C4-N9-C8	2.16	108.07	105.73
27	BA	55	5MC	CM5-C5-C6	-2.16	119.96	122.85
1	Aa	629	OMG	C8-N7-C5	2.16	108.15	104.24
1	Aa	1306	5MC	CM5-C5-C6	-2.16	119.96	122.85
27	BA	2527	OMG	C8-N7-C5	2.16	108.15	104.24
27	BA	2728	OMG	C8-N7-C5	2.16	108.15	104.24
27	BA	2427	5MU	C1'-N1-C2	2.16	121.48	117.57
1	Aa	574	OMG	C8-N7-C5	2.16	108.14	104.24
1	Aa	1358	OMU	O2-C2-N1	-2.16	119.92	122.79
27	BA	1956	OMG	C8-N7-C5	2.15	108.14	104.24
1	Aa	913	OMG	C8-N7-C5	2.15	108.14	104.24
27	BA	912	OMG	C8-N7-C5	2.15	108.14	104.24
1	Aa	121	OMG	C8-N7-C5	2.15	108.14	104.24
27	BA	2466	OMG	O6-C6-C5	-2.15	120.90	126.60
1	Aa	1003	5MC	CM5-C5-C6	-2.15	119.98	122.85
27	BA	1893	OMG	C8-N7-C5	2.15	108.13	104.24
1	Aa	147	OMG	C8-N7-C5	2.14	108.12	104.24
27	BA	365	OMG	C8-N7-C5	2.14	108.12	104.24
27	BA	2469	OMG	C8-N7-C5	2.14	108.11	104.24
1	Aa	352	A2M	C4-C5-N7	-2.14	108.01	110.62
1	Aa	219	OMG	C8-N7-C5	2.14	108.11	104.24
1	Aa	659	OMG	C8-N7-C5	2.14	108.11	104.24
1	Aa	450	OMG	C5-C6-N1	2.14	118.62	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	2595	OMC	O3'-C3'-C2'	2.13	117.22	111.17
27	BA	2528	OMG	C8-N7-C5	2.13	108.09	104.24
27	BA	932	A2M	C6-C5-C4	2.13	120.04	117.18
27	BA	2329	A2M	C4-N9-C8	2.12	108.03	105.73
27	BA	2016	OMG	C8-N7-C5	2.12	108.08	104.24
27	BA	2640	OMG	C8-N7-C5	2.12	108.08	104.24
27	BA	875	5MU	O2-C2-N1	-2.12	119.97	122.79
1	Aa	995	2MG	O6-C6-C5	-2.12	120.97	126.60
1	Aa	8	OMU	O2-C2-N1	-2.12	119.97	122.79
1	Aa	457	5MC	CM5-C5-C6	-2.11	120.03	122.85
1	Aa	450	OMG	O6-C6-C5	-2.11	121.00	126.60
1	Aa	1184	5MC	CM5-C5-C6	-2.11	120.04	122.85
1	Aa	685	5MC	CM5-C5-C6	-2.10	120.04	122.85
27	BA	674	OMG	C8-N7-C5	2.10	108.05	104.24
27	BA	2466	OMG	C8-N7-C5	2.10	108.04	104.24
27	BA	1953	OMG	C8-N7-C5	2.09	108.03	104.24
27	BA	932	A2M	C4-C5-N7	-2.09	108.07	110.62
1	Aa	1468	MA6	C4-C5-N7	-2.09	108.07	110.62
27	BA	829	5MU	C1'-N1-C2	2.09	121.36	117.57
1	Aa	464	5MC	CM5-C5-C6	-2.09	120.06	122.85
1	Aa	1107	OMG	C8-N7-C5	2.09	108.02	104.24
27	BA	2168	OMG	C8-N7-C5	2.08	108.01	104.24
27	BA	879	A2M	C4-C5-N7	-2.08	108.09	110.62
1	Aa	1004	5MC	CM5-C5-C6	-2.07	120.08	122.85
27	BA	505	A2M	C4-N9-C8	2.07	107.97	105.73
1	Aa	963	OMG	C8-N7-C5	2.07	107.98	104.24
27	BA	215	OMG	C8-N7-C5	2.06	107.97	104.24
27	BA	2091	A2M	N9-C8-N7	-2.06	111.09	113.91
27	BA	2870	OMG	C8-N7-C5	2.06	107.97	104.24
27	BA	2091	A2M	C6-C5-N7	2.06	135.85	132.02
1	Aa	672	5MC	CM5-C5-C6	-2.06	120.10	122.85
27	BA	2936	A2M	C4-C5-N7	-2.05	108.12	110.62
1	Aa	1476	5MC	CM5-C5-C6	-2.05	120.11	122.85
1	Aa	852	OMG	C5-C6-N1	2.05	118.40	113.19
27	BA	505	A2M	C4-C5-N7	-2.05	108.12	110.62
27	BA	932	A2M	C4-N9-C8	2.05	107.95	105.73
27	BA	2640	OMG	C1'-N9-C8	-2.04	120.88	126.70
27	BA	2936	A2M	C6-C5-C4	2.04	119.93	117.18
27	BA	2550	OMG	C5-C6-N1	2.04	118.37	113.19
1	Aa	1020	OMU	O2-C2-N1	-2.04	120.08	122.79
27	BA	872	OMG	C1'-N9-C8	-2.03	120.91	126.70
27	BA	2469	OMG	C1'-N9-C8	-2.03	120.92	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	365	OMG	C1'-N9-C8	-2.03	120.92	126.70
27	BA	849	A2M	C6-C5-C4	2.03	119.91	117.18
27	BA	2329	A2M	C6-C5-N7	2.03	135.79	132.02
27	BA	1525	OMG	C8-N7-C5	2.02	107.89	104.24
1	Aa	995	2MG	C2-N1-C6	-2.02	122.16	124.48
1	Aa	1478	5MC	CM5-C5-C6	-2.01	120.16	122.85
27	BA	2581	4SU	O2-C2-N1	-2.01	120.11	122.79
27	BA	55	5MC	C5-C4-N3	-2.01	119.50	121.67
27	BA	1854	5MU	O2-C2-N1	-2.01	120.12	122.79
1	Aa	636	OMG	C8-N7-C5	2.01	107.87	104.24
27	BA	1965	5MC	CM5-C5-C6	-2.00	120.17	122.85

There are no chirality outliers.

All (144) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Aa	147	OMG	C1'-C2'-O2'-CM2
1	Aa	320	OMG	C3'-C4'-C5'-O5'
1	Aa	352	A2M	C1'-C2'-O2'-CM'
1	Aa	381	OMG	O4'-C4'-C5'-O5'
1	Aa	381	OMG	C3'-C4'-C5'-O5'
1	Aa	498	OMG	O4'-C4'-C5'-O5'
1	Aa	498	OMG	C3'-C4'-C5'-O5'
1	Aa	636	OMG	C1'-C2'-O2'-CM2
1	Aa	659	OMG	C1'-C2'-O2'-CM2
1	Aa	753	OMU	C1'-C2'-O2'-CM2
1	Aa	891	OMG	C1'-C2'-O2'-CM2
1	Aa	917	5MU	C3'-C4'-C5'-O5'
1	Aa	917	5MU	O4'-C4'-C5'-O5'
1	Aa	924	OMC	C3'-C2'-O2'-CM2
1	Aa	963	OMG	C3'-C4'-C5'-O5'
1	Aa	1004	5MC	O4'-C4'-C5'-O5'
1	Aa	1004	5MC	C3'-C4'-C5'-O5'
1	Aa	1020	OMU	C1'-C2'-O2'-CM2
1	Aa	1107	OMG	C3'-C4'-C5'-O5'
1	Aa	1306	5MC	O4'-C4'-C5'-O5'
1	Aa	1306	5MC	C3'-C4'-C5'-O5'
1	Aa	1361	OMC	C1'-C2'-O2'-CM2
1	Aa	1449	6MZ	C5-C6-N6-C9
1	Aa	1449	6MZ	N1-C6-N6-C9
27	BA	66	OMC	C1'-C2'-O2'-CM2
27	BA	91	OMC	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
27	BA	288	OMG	C1'-C2'-O2'-CM2
27	BA	342	OMC	C3'-C4'-C5'-O5'
27	BA	342	OMC	O4'-C4'-C5'-O5'
27	BA	453	OMU	C3'-C4'-C5'-O5'
27	BA	453	OMU	O4'-C4'-C5'-O5'
27	BA	657	OMU	C1'-C2'-O2'-CM2
27	BA	670	OMG	C3'-C2'-O2'-CM2
27	BA	674	OMG	O4'-C4'-C5'-O5'
27	BA	674	OMG	C3'-C4'-C5'-O5'
27	BA	849	A2M	C3'-C4'-C5'-O5'
27	BA	879	A2M	C1'-C2'-O2'-CM'
27	BA	1525	OMG	C1'-C2'-O2'-CM2
27	BA	1776	OMU	C1'-C2'-O2'-CM2
27	BA	1820	OMC	C1'-C2'-O2'-CM2
27	BA	1995	OMC	C1'-C2'-O2'-CM2
27	BA	2016	OMG	O4'-C4'-C5'-O5'
27	BA	2016	OMG	C3'-C4'-C5'-O5'
27	BA	2124	OMC	C1'-C2'-O2'-CM2
27	BA	2353	OMG	O4'-C4'-C5'-O5'
27	BA	2353	OMG	C3'-C4'-C5'-O5'
27	BA	2469	OMG	C3'-C4'-C5'-O5'
27	BA	2521	OMG	C1'-C2'-O2'-CM2
27	BA	2527	OMG	C3'-C4'-C5'-O5'
27	BA	2542	OMU	C3'-C4'-C5'-O5'
27	BA	2542	OMU	O4'-C4'-C5'-O5'
27	BA	2545	OMC	C1'-C2'-O2'-CM2
27	BA	2545	OMC	C3'-C4'-C5'-O5'
27	BA	2545	OMC	O4'-C4'-C5'-O5'
27	BA	2595	OMC	C1'-C2'-O2'-CM2
27	BA	2640	OMG	C1'-C2'-O2'-CM2
27	BA	2642	OMG	C3'-C2'-O2'-CM2
27	BA	2728	OMG	C1'-C2'-O2'-CM2
1	Aa	17	5MC	O4'-C4'-C5'-O5'
1	Aa	121	OMG	O4'-C4'-C5'-O5'
1	Aa	121	OMG	C3'-C4'-C5'-O5'
1	Aa	495	OMG	C3'-C4'-C5'-O5'
1	Aa	670	OMG	O4'-C4'-C5'-O5'
1	Aa	913	OMG	C3'-C4'-C5'-O5'
1	Aa	963	OMG	O4'-C4'-C5'-O5'
1	Aa	1007	5MC	O4'-C4'-C5'-O5'
1	Aa	1107	OMG	O4'-C4'-C5'-O5'
1	Aa	1352	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
27	BA	55	5MC	O4'-C4'-C5'-O5'
27	BA	55	5MC	C3'-C4'-C5'-O5'
27	BA	2527	OMG	O4'-C4'-C5'-O5'
27	BA	2640	OMG	O4'-C4'-C5'-O5'
27	BA	2640	OMG	C3'-C4'-C5'-O5'
27	BA	2642	OMG	O4'-C4'-C5'-O5'
1	Aa	17	5MC	C3'-C4'-C5'-O5'
1	Aa	219	OMG	C3'-C4'-C5'-O5'
1	Aa	340	5MC	O4'-C4'-C5'-O5'
1	Aa	340	5MC	C3'-C4'-C5'-O5'
1	Aa	495	OMG	O4'-C4'-C5'-O5'
1	Aa	670	OMG	C3'-C4'-C5'-O5'
1	Aa	913	OMG	O4'-C4'-C5'-O5'
27	BA	849	A2M	O4'-C4'-C5'-O5'
27	BA	1150	OMU	O4'-C4'-C5'-O5'
27	BA	2642	OMG	C3'-C4'-C5'-O5'
1	Aa	320	OMG	O4'-C4'-C5'-O5'
1	Aa	1352	5MC	C3'-C4'-C5'-O5'
1	Aa	8	OMU	C2'-C1'-N1-C6
27	BA	365	OMG	C3'-C4'-C5'-O5'
27	BA	1893	OMG	C3'-C4'-C5'-O5'
1	Aa	1007	5MC	C3'-C4'-C5'-O5'
27	BA	1150	OMU	C3'-C4'-C5'-O5'
27	BA	2047	OMC	O4'-C4'-C5'-O5'
27	BA	2389	OMU	C3'-C4'-C5'-O5'
27	BA	2389	OMU	O4'-C4'-C5'-O5'
27	BA	2469	OMG	O4'-C4'-C5'-O5'
27	BA	1893	OMG	O4'-C4'-C5'-O5'
27	BA	2379	OMG	C4'-C5'-O5'-P
1	Aa	219	OMG	O4'-C4'-C5'-O5'
27	BA	2329	A2M	O4'-C4'-C5'-O5'
1	Aa	8	OMU	O4'-C4'-C5'-O5'
1	Aa	229	OMC	C1'-C2'-O2'-CM2
27	BA	65	OMG	C1'-C2'-O2'-CM2
27	BA	2469	OMG	C1'-C2'-O2'-CM2
1	Aa	8	OMU	O4'-C1'-N1-C6
27	BA	365	OMG	O4'-C4'-C5'-O5'
27	BA	1956	OMG	O4'-C4'-C5'-O5'
27	BA	800	OMG	C3'-C2'-O2'-CM2
27	BA	2936	A2M	C3'-C2'-O2'-CM2
1	Aa	1478	5MC	C4'-C5'-O5'-P
1	Aa	8	OMU	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
27	BA	2605	5MC	C2'-C1'-N1-C6
27	BA	55	5MC	C4'-C5'-O5'-P
1	Aa	1478	5MC	O4'-C1'-N1-C6
1	Aa	320	OMG	C4'-C5'-O5'-P
1	Aa	574	OMG	C3'-C4'-C5'-O5'
27	BA	1345	5MC	O4'-C4'-C5'-O5'
27	BA	2329	A2M	C3'-C4'-C5'-O5'
1	Aa	1478	5MC	C2'-C1'-N1-C2
1	Aa	1478	5MC	C2'-C1'-N1-C6
1	Aa	8	OMU	O4'-C1'-N1-C2
1	Aa	352	A2M	O4'-C4'-C5'-O5'
27	BA	2047	OMC	C3'-C4'-C5'-O5'
27	BA	1402	OMU	C2'-C1'-N1-C6
1	Aa	8	OMU	C3'-C2'-O2'-CM2
27	BA	365	OMG	C3'-C2'-O2'-CM2
27	BA	2469	OMG	C3'-C2'-O2'-CM2
27	BA	2605	5MC	O4'-C1'-N1-C6
1	Aa	340	5MC	C4'-C5'-O5'-P
1	Aa	1468	MA6	O4'-C4'-C5'-O5'
27	BA	912	OMG	C3'-C4'-C5'-O5'
27	BA	1525	OMG	O4'-C4'-C5'-O5'
27	BA	2379	OMG	C3'-C4'-C5'-O5'
27	BA	2581	4SU	O4'-C4'-C5'-O5'
27	BA	1953	OMG	C3'-C4'-C5'-O5'
27	BA	1956	OMG	C3'-C4'-C5'-O5'
27	BA	1402	OMU	C2'-C1'-N1-C2
1	Aa	1478	5MC	O4'-C1'-N1-C2
27	BA	2605	5MC	O4'-C1'-N1-C2
1	Aa	457	5MC	C2'-C1'-N1-C2
1	Aa	1004	5MC	C2'-C1'-N1-C2
27	BA	2047	OMC	C2'-C1'-N1-C2
1	Aa	1306	5MC	C2'-C1'-N1-C2
27	BA	2605	5MC	C2'-C1'-N1-C2
1	Aa	457	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

73 monomers are involved in 114 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	BA	912	OMG	2	0
1	Aa	1468	MA6	1	0
1	Aa	770	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	BA	2545	OMC	2	0
1	Aa	1449	6MZ	1	0
27	BA	1776	OMU	2	0
27	BA	91	OMC	1	0
1	Aa	464	5MC	1	0
1	Aa	147	OMG	2	0
1	Aa	349	5MC	1	0
27	BA	2640	OMG	2	0
1	Aa	923	5MC	2	0
27	BA	2075	5MC	1	0
1	Aa	1006	5MC	4	0
27	BA	2124	OMC	3	0
1	Aa	479	OMU	1	0
27	BA	1956	OMG	2	0
27	BA	879	A2M	2	0
27	BA	288	OMG	1	0
1	Aa	121	OMG	1	0
27	BA	849	A2M	1	0
27	BA	2688	5MC	1	0
27	BA	2581	4SU	1	0
1	Aa	1020	OMU	2	0
27	BA	872	OMG	1	0
27	BA	2427	5MU	3	0
27	BA	65	OMG	1	0
27	BA	670	OMG	5	0
1	Aa	852	OMG	1	0
1	Aa	963	OMG	2	0
27	BA	2379	OMG	1	0
27	BA	2107	OMC	1	0
1	Aa	1361	OMC	1	0
1	Aa	753	OMU	1	0
1	Aa	1478	5MC	1	0
27	BA	2745	OMG	1	0
1	Aa	1321	5MC	2	0
1	Aa	17	5MC	1	0
1	Aa	340	5MC	2	0
27	BA	1893	OMG	1	0
1	Aa	1266	5MC	2	0
1	Aa	352	A2M	3	0
27	BA	2605	5MC	3	0
27	BA	2521	OMG	1	0
27	BA	833	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	BA	2550	OMG	2	0
27	BA	2469	OMG	1	0
1	Aa	1358	OMU	2	0
27	BA	2936	A2M	1	0
1	Aa	1352	5MC	3	0
27	BA	932	A2M	1	0
27	BA	1995	OMC	1	0
27	BA	1820	OMC	1	0
1	Aa	924	OMC	1	0
27	BA	1969	OMU	1	0
1	Aa	917	5MU	2	0
27	BA	2070	5MC	1	0
27	BA	55	5MC	2	0
27	BA	365	OMG	1	0
27	BA	2527	OMG	1	0
27	BA	2642	OMG	5	0
1	Aa	891	OMG	2	0
27	BA	2595	OMC	2	0
27	BA	507	OMG	2	0
1	Aa	636	OMG	2	0
1	Aa	659	OMG	1	0
1	Aa	1467	MA6	1	0
27	BA	1150	OMU	1	0
27	BA	2528	OMG	1	0
1	Aa	1007	5MC	7	0
27	BA	2728	OMG	1	0
27	BA	1329	OMG	1	0
27	BA	657	OMU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

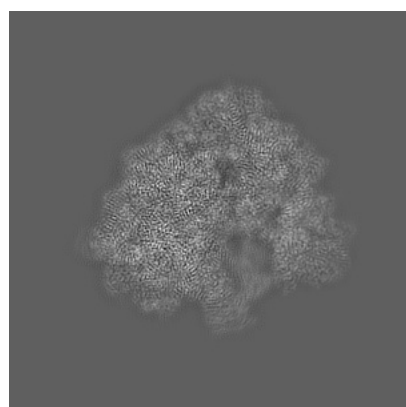
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10224. These allow visual inspection of the internal detail of the map and identification of artifacts.

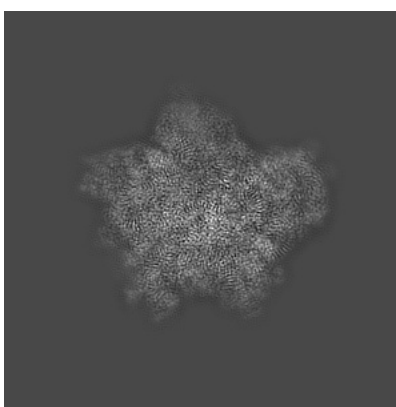
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

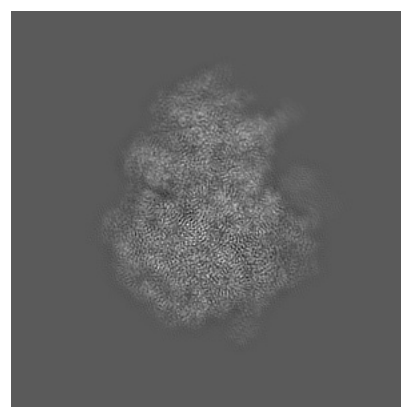
6.1.1 Primary map



X



Y



Z

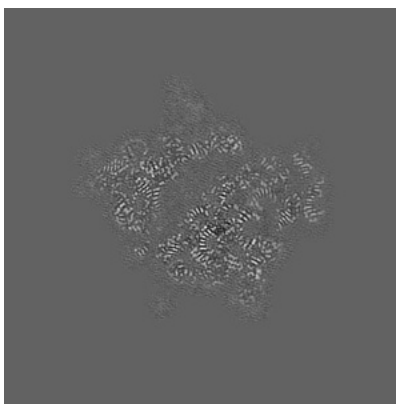
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

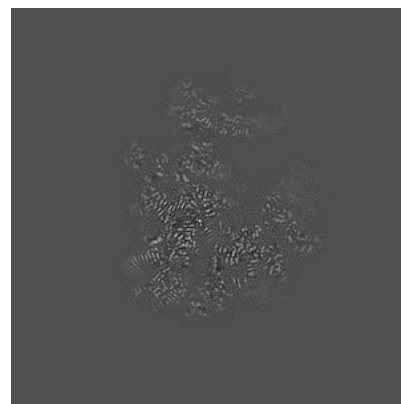
6.2.1 Primary map



X Index: 240



Y Index: 240

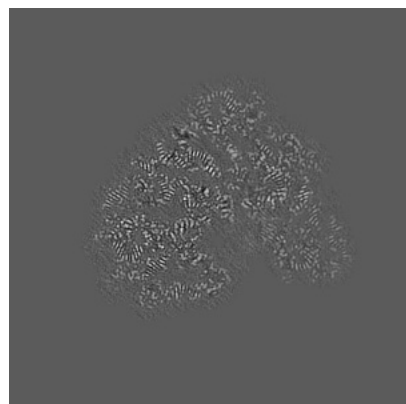


Z Index: 240

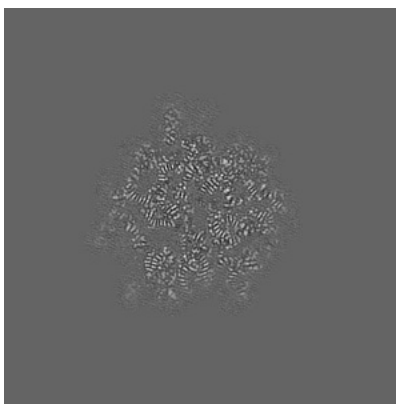
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

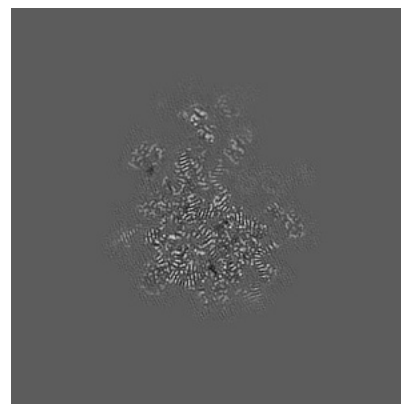
6.3.1 Primary map



X Index: 231



Y Index: 182

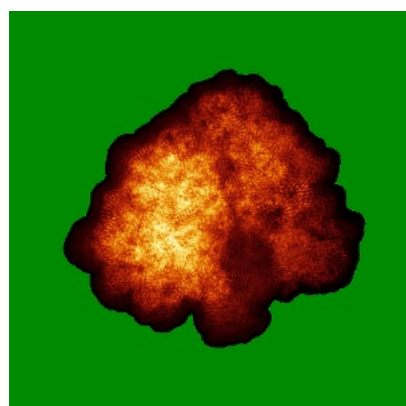


Z Index: 264

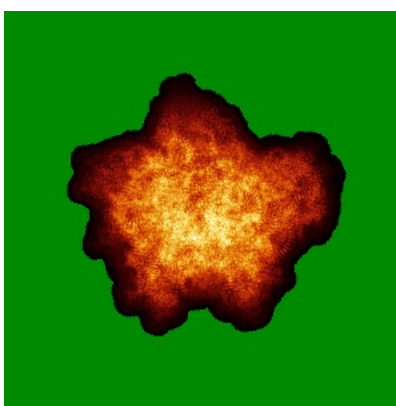
The images above show the largest variance slices of the map in three orthogonal directions.

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

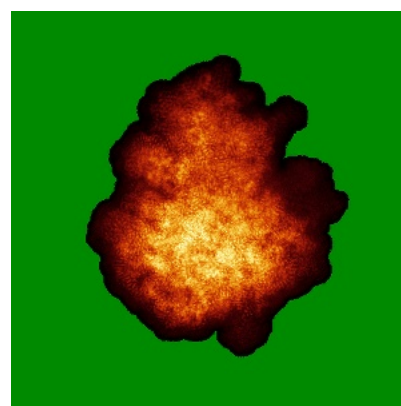
6.4.1 Primary map



X



Y

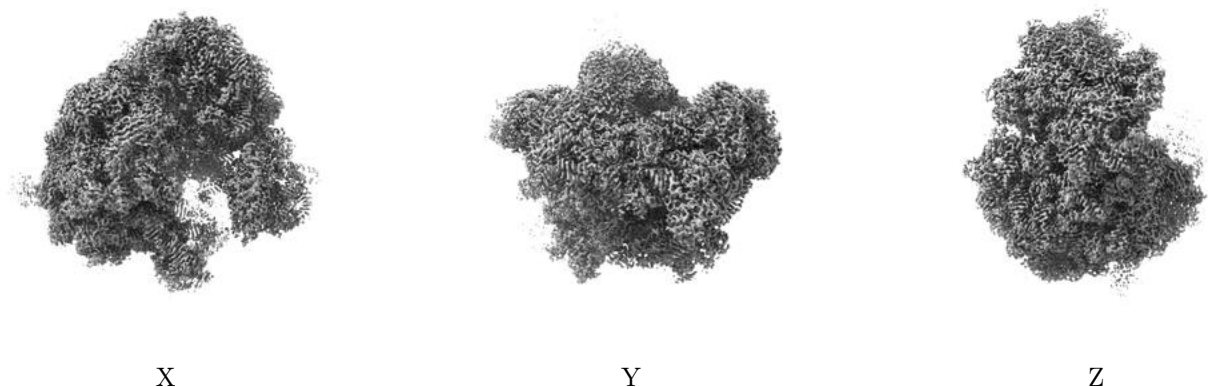


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

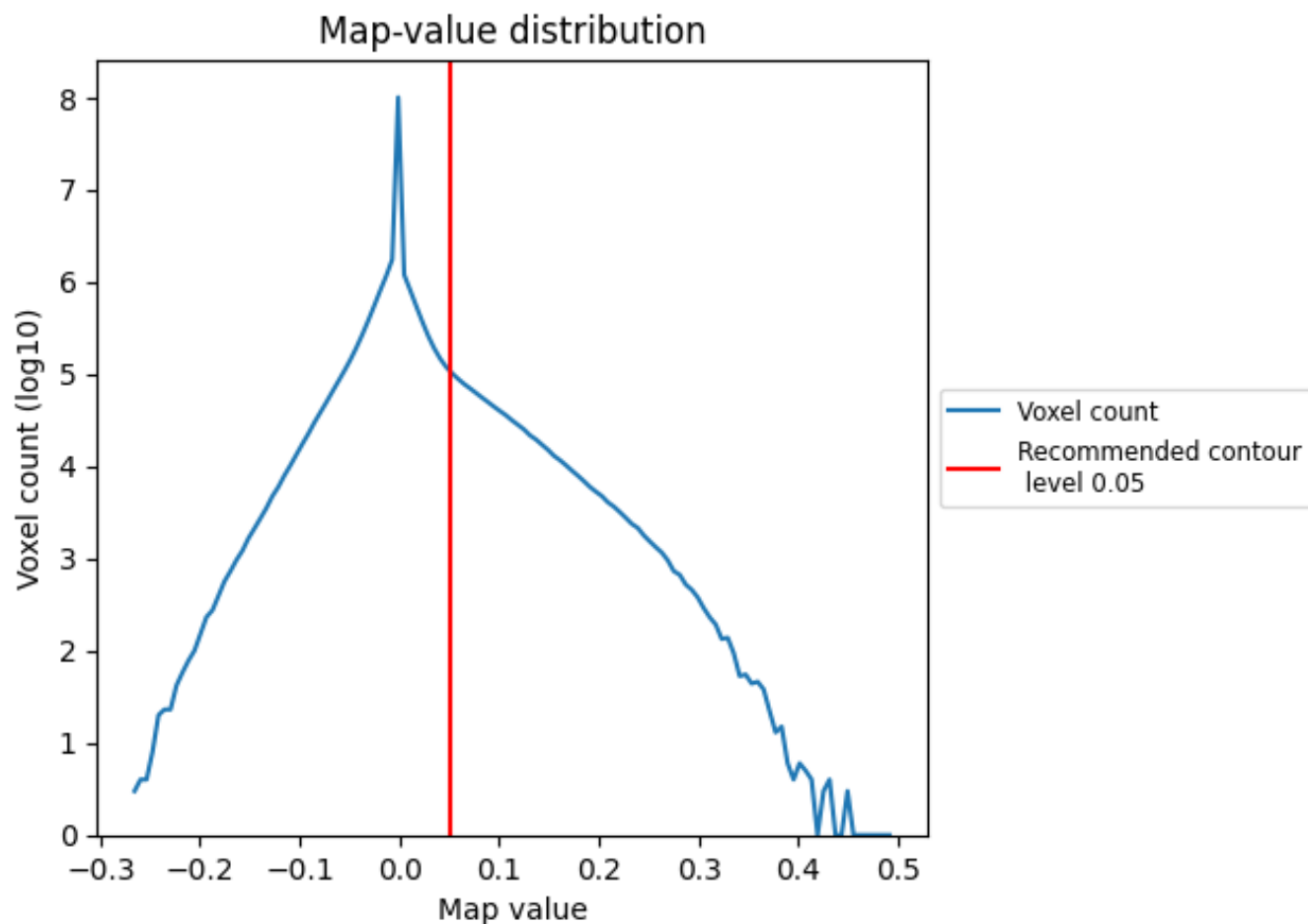
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

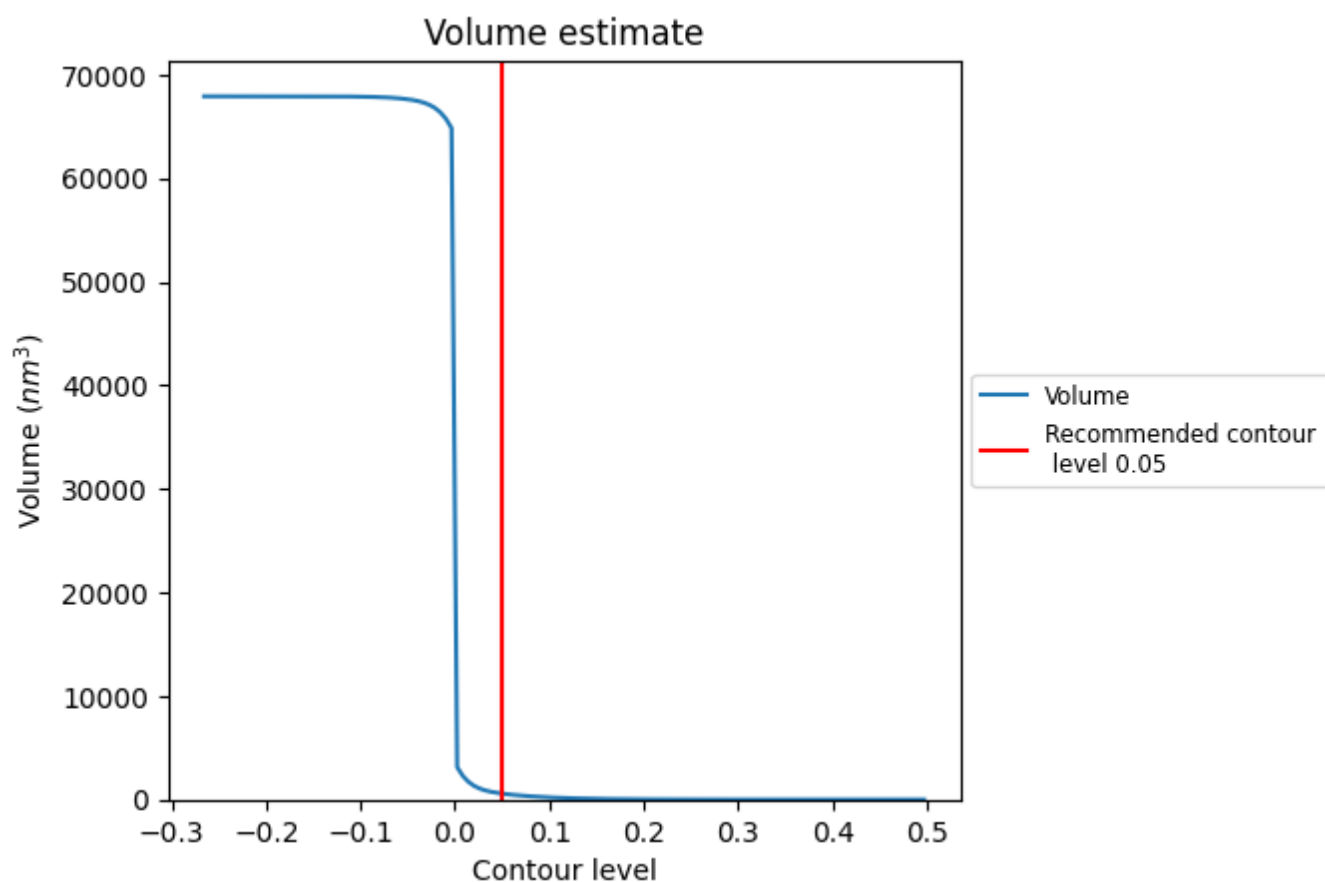
This section contains the results of statistical analysis of the map.

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.

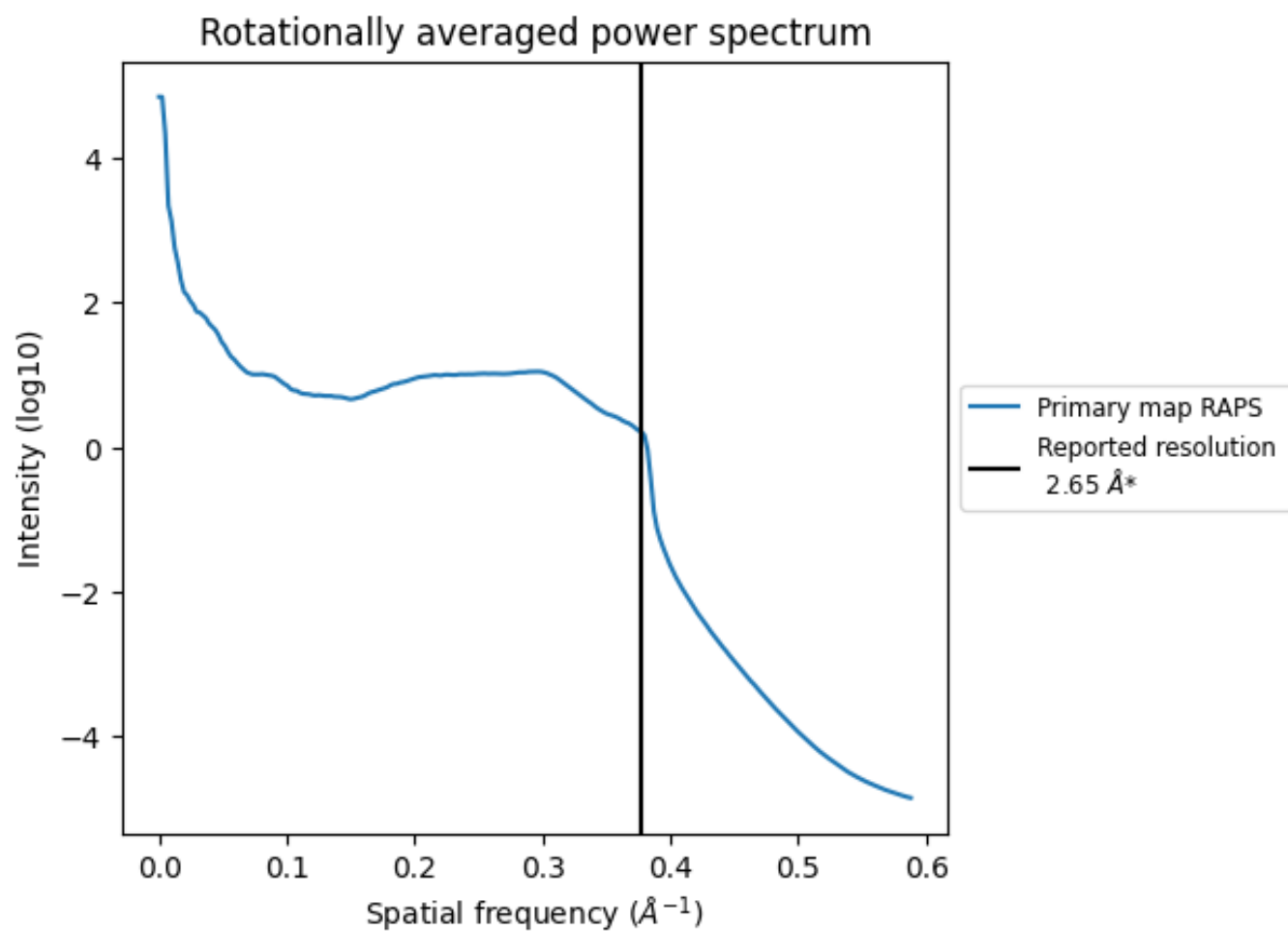
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 576 nm³; this corresponds to an approximate mass of 520 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 0.377 Å⁻¹

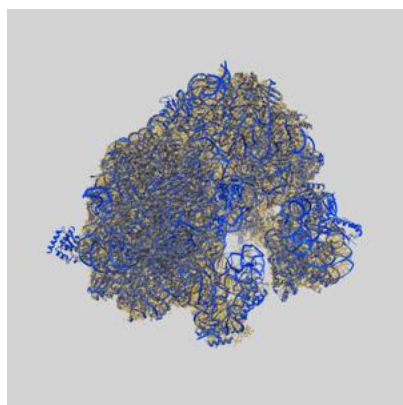
8 Fourier-Shell correlation

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

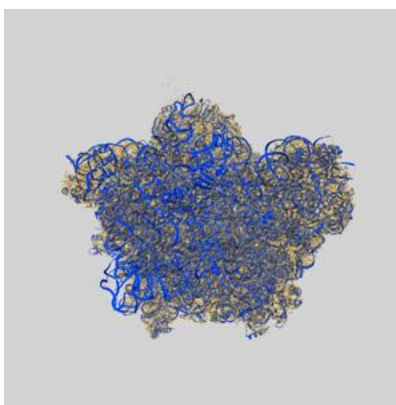
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10224 and PDB model 6SKG. Per-residue inclusion information can be found in section 3 on page 19.

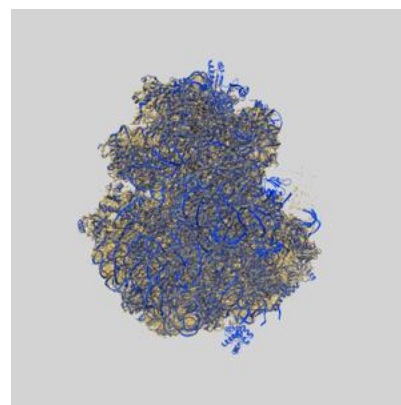
9.1 Map-model overlay [i](#)



X



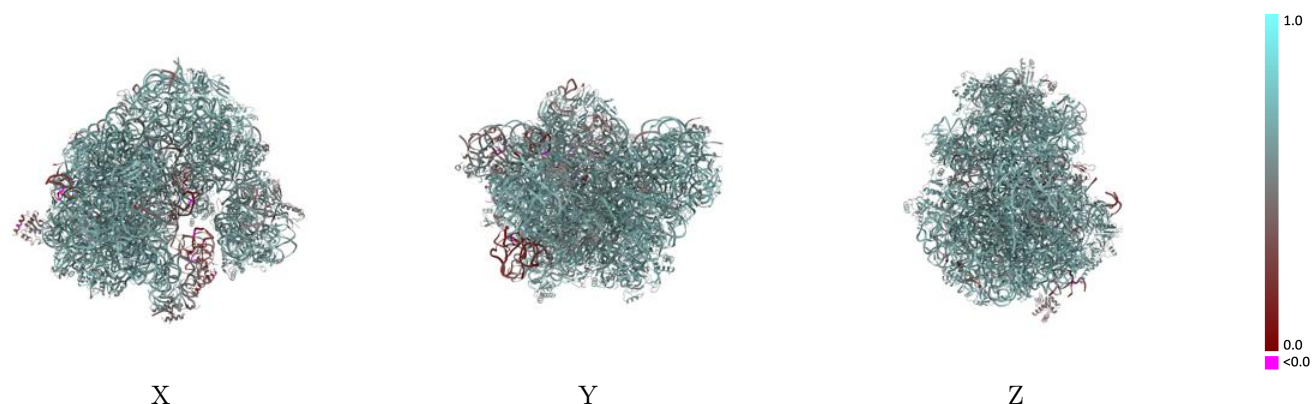
Y



Z

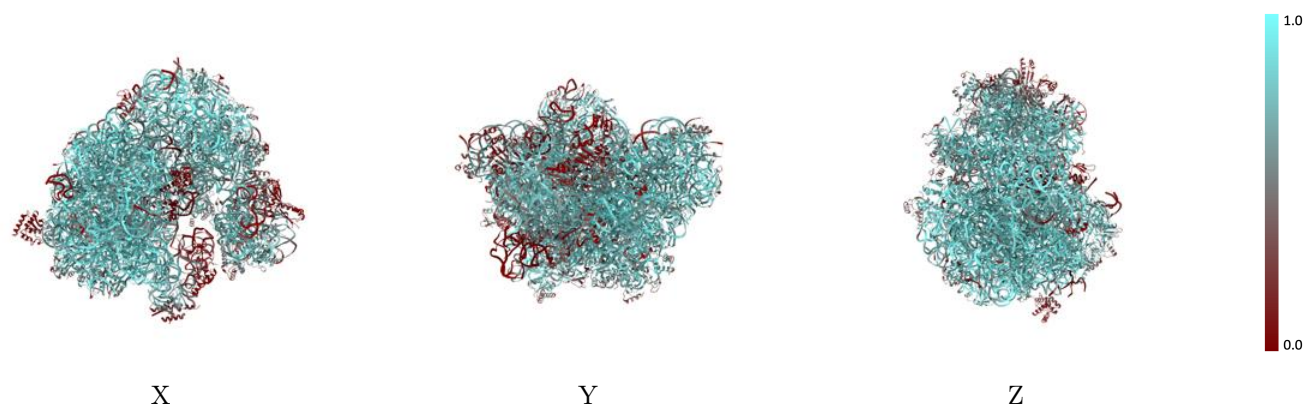
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



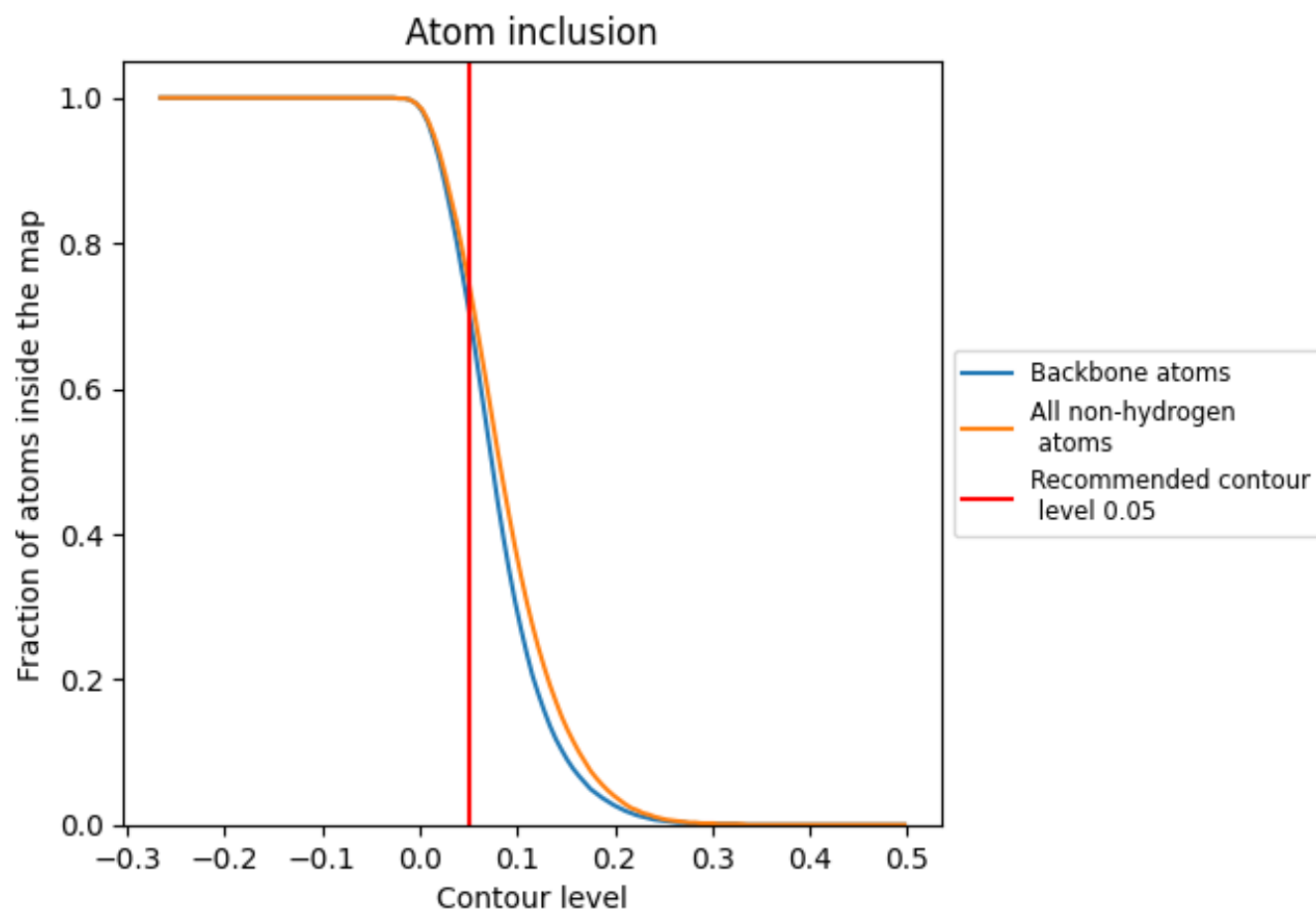
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 75% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.6140
Aa	 0.7930	 0.6280
Ab	 0.5920	 0.6100
Ac	 0.2460	 0.5360
Ad	 0.5660	 0.5980
Ae	 0.6810	 0.6190
Af	 0.7270	 0.6350
Ag	 0.7100	 0.6200
Ah	 0.4000	 0.5690
Ai	 0.4940	 0.5990
Aj	 0.7550	 0.6300
Ak	 0.7110	 0.6310
Al	 0.5270	 0.5990
Am	 0.2700	 0.5380
An	 0.6040	 0.6020
Ao	 0.6920	 0.6310
Ap	 0.5220	 0.5790
Aq	 0.6910	 0.6190
Ar	 0.4750	 0.5880
As	 0.7240	 0.6360
At	 0.3020	 0.5440
Au	 0.5400	 0.6000
Av	 0.5910	 0.6110
Aw	 0.6090	 0.5970
Ax	 0.5550	 0.5970
Ay	 0.3010	 0.5600
Az	 0.7260	 0.6200
BA	 0.8480	 0.6220
BB	 0.6380	 0.5600
BC	 0.8460	 0.6450
BD	 0.8390	 0.6530
BE	 0.8160	 0.6360
BF	 0.1500	 0.3600
BG	 0.6960	 0.6090
BH	 0.5730	 0.5750



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Chain	Atom inclusion	Q-score
BI	 0.0570	 0.3850
BJ	 0.7460	 0.6240
BK	 0.8160	 0.6490
BL	 0.7820	 0.6350
BM	 0.5860	 0.5680
BN	 0.6080	 0.5780
BO	 0.6680	 0.6110
BP	 0.8950	 0.6670
BQ	 0.5270	 0.5510
BR	 0.8240	 0.6440
BS	 0.8030	 0.6340
BT	 0.6930	 0.6170
BU	 0.8370	 0.6540
BV	 0.8380	 0.6560
BW	 0.7220	 0.6220
BX	 0.7980	 0.6320
BY	 0.7940	 0.6420
BZ	 0.6170	 0.5890
Ba	 0.8070	 0.6440
Bb	 0.6500	 0.5960
Bc	 0.7730	 0.6340
Bd	 0.8350	 0.6530
Be	 0.8230	 0.6360
Bf	 0.7600	 0.6300
Bg	 0.7890	 0.6300
Bh	 0.9500	 0.6770
Bi	 0.8500	 0.6450
Bj	 0.7640	 0.6420
Bk	 0.8020	 0.6360
Bl	 0.7510	 0.6440
Bm	 0.5270	 0.5600
Bn	 0.5290	 0.6000
Bo	 0.8140	 0.6430
Bp	 0.0130	 0.3680
Bq	 0.0240	 0.4650