



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 08:40 PM EST

PDB ID : 7MPJ
EMDB ID : EMD-23935
Title : Stm1 bound vacant 80S structure isolated from nop1-D243A
Authors : Rai, J.; Zhao, Y.; Li, H.
Deposited on : 2021-05-04
Resolution : 2.70 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

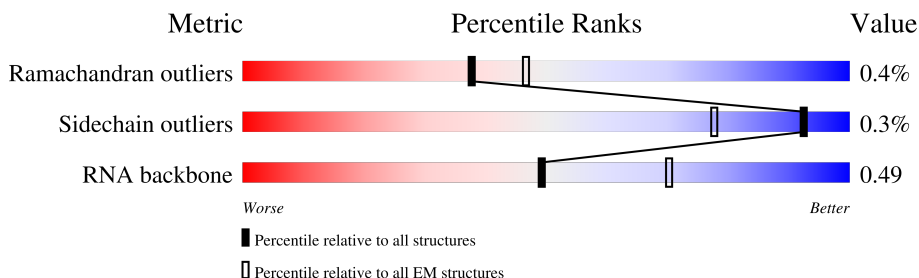
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	BA	206	
2	BB	214	
3	BC	217	
4	BD	223	
5	BE	260	
6	BF	206	
7	BG	226	
8	BH	184	

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Mol	Chain	Length	Quality of chain
9	BI	188	
10	BJ	185	
11	BK	96	
12	BL	155	
13	BM	121	
14	BN	150	
15	BO	127	
16	BP	124	
17	BQ	141	
18	BR	121	
19	BS	145	
20	BT	141	
21	BU	107	
22	BV	87	
23	BW	129	
24	BX	144	
25	BY	134	
26	BZ	69	
27	Ba	97	
28	Bb	81	
29	Bc	63	
30	Bd	53	
31	Be	60	
32	Bf	57	
33	Bg	312	

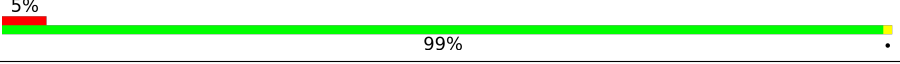
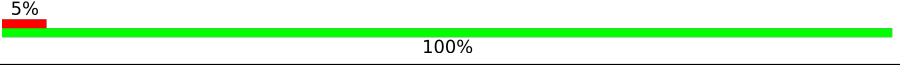
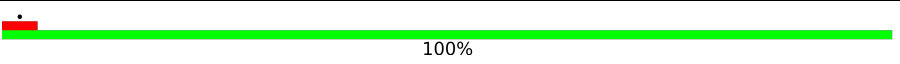
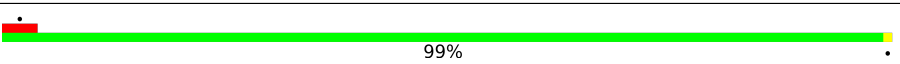
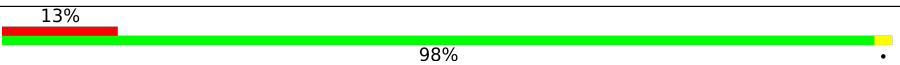
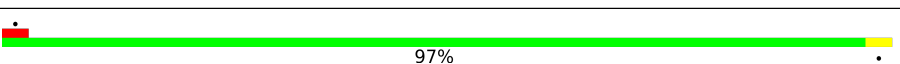
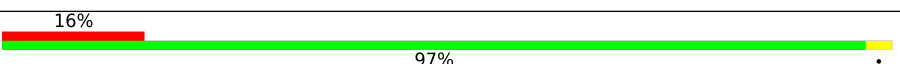
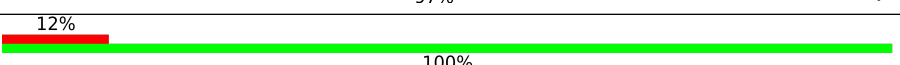
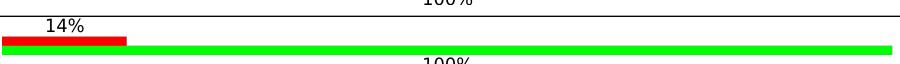
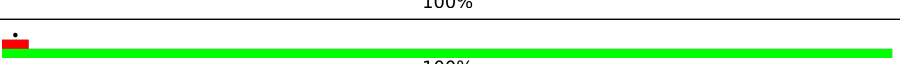
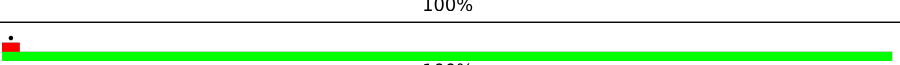
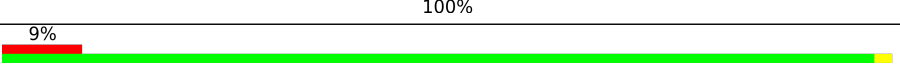
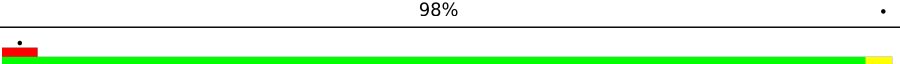
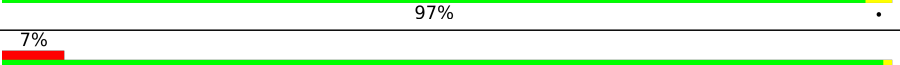
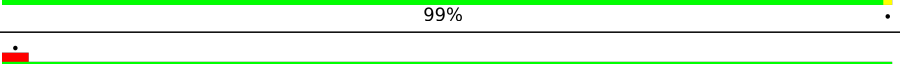
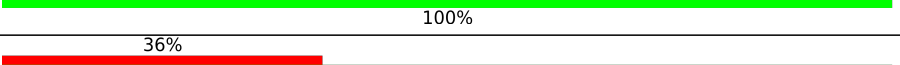
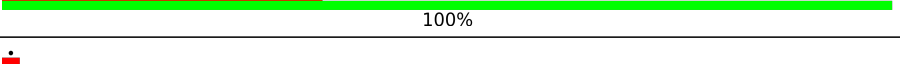
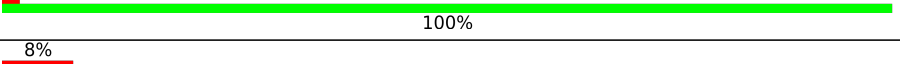
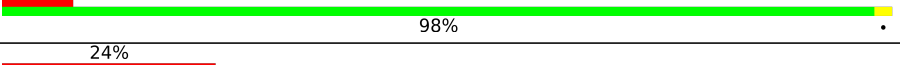
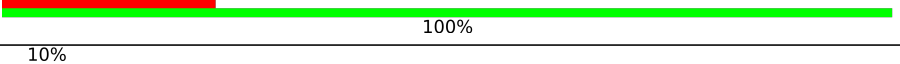
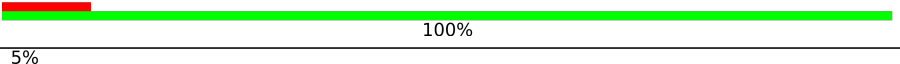
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Mol	Chain	Length	Quality of chain
34	Bh	89	
35	B5	1781	
36	A1	3137	
37	A3	121	
38	A4	158	
39	AA	247	
40	AB	386	
41	AC	361	
42	AD	292	
43	AE	156	
44	AF	222	
45	AG	230	
46	AH	190	
47	AI	205	
48	AJ	169	
49	AL	193	
50	AM	136	
51	AN	203	
52	AO	197	
53	AP	175	
54	AQ	185	
55	AR	188	
56	AS	172	
57	AT	159	
58	AU	100	

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Mol	Chain	Length	Quality of chain
59	AV	136	
60	AW	63	
61	AX	121	
62	AY	126	
63	AZ	135	
64	Aa	148	
65	Ab	58	
66	Ac	97	
67	Ad	109	
68	Ae	127	
69	Af	106	
70	Ag	112	
71	Ah	119	
72	Ai	99	
73	Aj	87	
74	Ak	77	
75	Al	50	
76	Am	52	
77	An	25	
78	Ao	105	
79	Ap	91	

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
35	G7M	B5	1575	X	-	-	-

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 199813 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 protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BA	206	Total	C	N	O	S	0	0
			1612	1034	285	291	2		

- Molecule 2 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 7 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BG	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BH	184	Total	C	N	O	S	0	0
			1481	951	265	265			

- Molecule 9 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	?	-	LYS	deletion	UNP P0CX39
BI	?	-	LYS	deletion	UNP P0CX39
BI	?	-	ASN	deletion	UNP P0CX39
BI	?	-	VAL	deletion	UNP P0CX39
BI	?	-	LYS	deletion	UNP P0CX39
BI	?	-	GLU	deletion	UNP P0CX39
BI	?	-	GLU	deletion	UNP P0CX39
BI	?	-	GLU	deletion	UNP P0CX39
BI	?	-	THR	deletion	UNP P0CX39
BI	?	-	VAL	deletion	UNP P0CX39
BI	?	-	ALA	deletion	UNP P0CX39

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 11 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BK	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 12 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BL	155	Total	C	N	O	S	0	0
			1244	798	235	208	3		

- Molecule 13 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BM	121	Total	C	N	O	S	0	0
			913	574	162	175	2		

- Molecule 14 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 15 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 16 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BP	124	Total	C	N	O	S	0	0
			991	631	187	166	7		

- Molecule 17 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	BQ	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 18 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BR	121	Total	C	N	O	S	0	0
			975	611	183	179	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BR	?	-	SER	deletion	UNP P02407
BR	?	-	ASN	deletion	UNP P02407
BR	?	-	GLY	deletion	UNP P02407
BR	?	-	VAL	deletion	UNP P02407

- Molecule 19 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 20 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BT	141	Total	C	N	O	S	0	0
			1095	685	206	202	2		

- Molecule 21 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 22 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 23 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 24 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 25 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	BY	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 26 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	BZ	69	Total	C	N	O	0	0
			558	357	103	98		

- Molecule 27 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ba	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 28 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Bb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 29 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 30 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bd	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 31 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Be	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 32 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bf	57	Total	C	N	O	S	0	0
			454	288	86	77	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bf	97	ALA	LYS	conflict	UNP P05759
Bf	?	-	CYS	deletion	UNP P05759
Bf	?	-	GLY	deletion	UNP P05759
Bf	?	-	ALA	deletion	UNP P05759

- Molecule 33 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bg	312	Total	C	N	O	S	0	0
			2401	1522	410	461	8		

- Molecule 34 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bh	89	Total	C	N	O		0	0
			675	391	137	147			

- Molecule 35 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B5	1781	Total	C	N	O	P	1	0
			37850	16932	6657	12480	1781		

- Molecule 36 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	A1	3137	Total	C	N	O	P	0	0
			67139	30012	12094	21896	3137		

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	A3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 38 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AA	247	Total	C	N	O	S	0	0
			1878	1170	381	326	1		

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AB	386	Total	C	N	O	S	0	0
			3078	1953	584	533	8		

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AD	292	Total	C	N	O	S	0	0
			2341	1478	408	453	2		

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AE	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AF	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AG	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AI	205	Total	C	N	O	S	0	0
			1672	1063	316	288	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	?	-	MET	deletion	UNP P41805
AI	?	-	LEU	deletion	UNP P41805
AI	?	-	SER	deletion	UNP P41805
AI	?	-	CYS	deletion	UNP P41805
AI	?	-	ALA	deletion	UNP P41805
AI	?	-	GLY	deletion	UNP P41805
AI	?	-	ALA	deletion	UNP P41805
AI	?	-	ASP	deletion	UNP P41805
AI	?	-	ARG	deletion	UNP P41805
AI	?	-	LEU	deletion	UNP P41805
AI	?	-	GLN	deletion	UNP P41805
AI	?	-	GLN	deletion	UNP P41805

- Molecule 48 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	AL	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AM	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AO	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AP	175	Total	C	N	O	S	0	0
			1388	862	277	249			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	VAL	deletion	UNP P05740
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	LYS	deletion	UNP P05740
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	GLU	deletion	UNP P05740
AP	?	-	LYS	deletion	UNP P05740

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	AR	188	Total	C	N	O		
			1521	935	326	260	0	0

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	AS	172	Total	C	N	O	S	
			1445	930	267	244	4	0

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	AT	159	Total	C	N	O	S	
			1276	805	246	221	4	0

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	AU	100	Total	C	N	O		
			796	516	131	149		0

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	AV	136	Total	C	N	O	S	
			1003	628	189	179	7	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
60	AW	63	Total	C	N	O	S	
			521	336	102	82	1	0

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	AX	121	Total	C	N	O	S	
			968	623	170	173	2	0

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	AY	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	AZ	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Aa	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	Ab	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ac	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ad	109	Total	C	N	O	S	0	0
			890	565	168	156	1		

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Ae	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Af	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ag	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ah	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Ai	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Aj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	Ak	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Al	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 76 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Am	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	An	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ao	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ap	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	BJ	1	Total	Mg	0
			1	1	
80	BT	1	Total	Mg	0
			1	1	
80	Be	1	Total	Mg	0
			1	1	
80	B5	122	Total	Mg	0
			122	122	
80	A1	541	Total	Mg	0
			541	541	
80	A3	3	Total	Mg	0
			3	3	
80	A4	18	Total	Mg	0
			18	18	
80	AA	2	Total	Mg	0
			2	2	
80	AB	5	Total	Mg	0
			5	5	

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Mol	Chain	Residues	Atoms		AltConf
80	AC	6	Total 6	Mg 6	0
80	AF	1	Total 1	Mg 1	0
80	AG	1	Total 1	Mg 1	0
80	AI	2	Total 2	Mg 2	0
80	AL	2	Total 2	Mg 2	0
80	AM	1	Total 1	Mg 1	0
80	AN	5	Total 5	Mg 5	0
80	AO	2	Total 2	Mg 2	0
80	AP	2	Total 2	Mg 2	0
80	AQ	3	Total 3	Mg 3	0
80	AR	3	Total 3	Mg 3	0
80	AS	3	Total 3	Mg 3	0
80	AY	1	Total 1	Mg 1	0
80	Aa	3	Total 3	Mg 3	0
80	Ad	2	Total 2	Mg 2	0
80	Ae	3	Total 3	Mg 3	0
80	Af	2	Total 2	Mg 2	0
80	Ai	1	Total 1	Mg 1	0
80	Aj	5	Total 5	Mg 5	0
80	Am	1	Total 1	Mg 1	0
80	Ao	2	Total 2	Mg 2	0

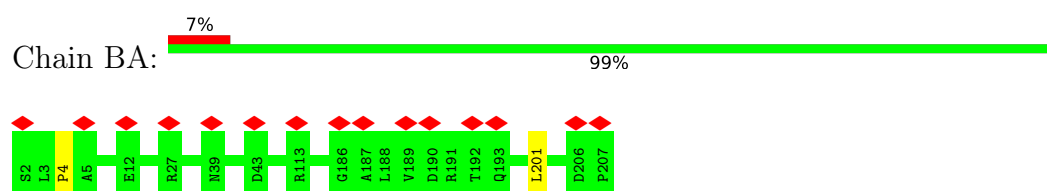
- Molecule 81 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	Bb	1	Total 1	Zn 1	0
81	Ao	1	Total 1	Zn 1	0

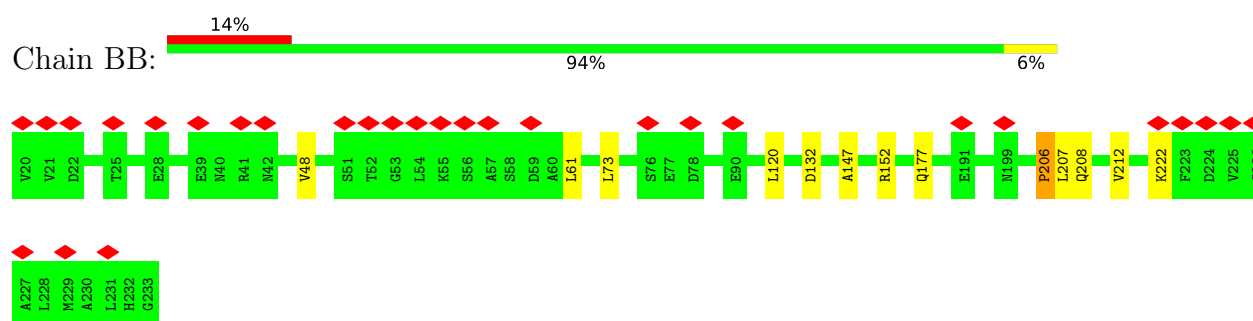
3 Residue-property plots [i](#)

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.

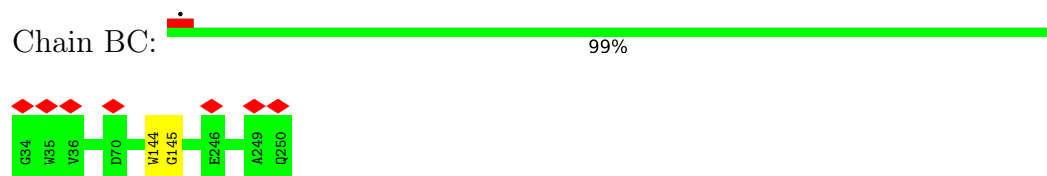
- Molecule 1: 40S ribosomal protein S0-A



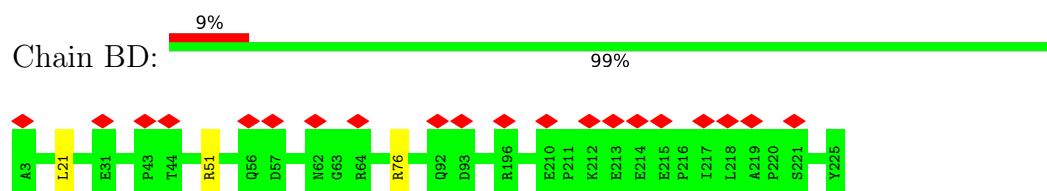
- Molecule 2: 40S ribosomal protein S1-A



- Molecule 3: 40S ribosomal protein S2

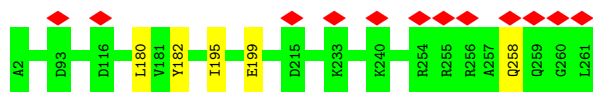


- Molecule 4: 40S ribosomal protein S3



- Molecule 5: 40S ribosomal protein S4-A

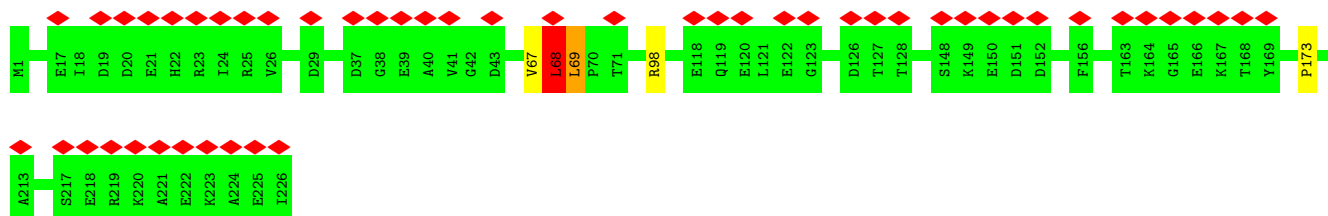




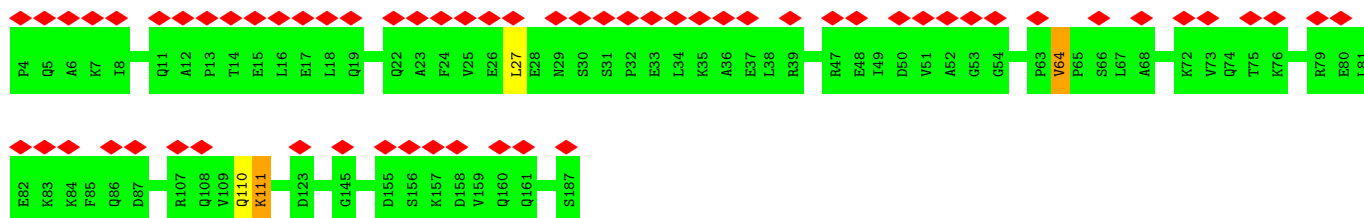
- Molecule 6: 40S ribosomal protein S5



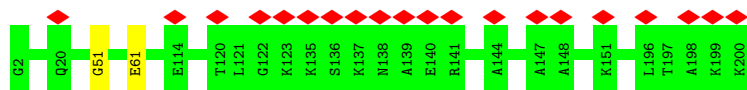
- Molecule 7: 40S ribosomal protein S6-A



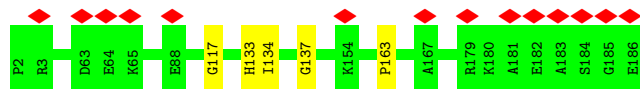
- Molecule 8: 40S ribosomal protein S7-A



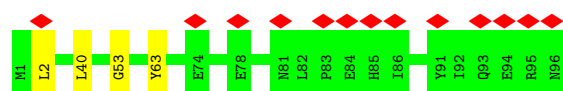
- Molecule 9: 40S ribosomal protein S8-A



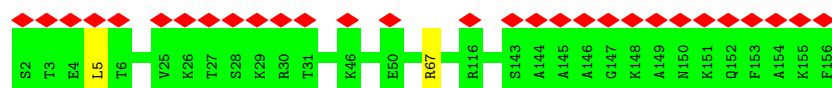
- Molecule 10: 40S ribosomal protein S9-A



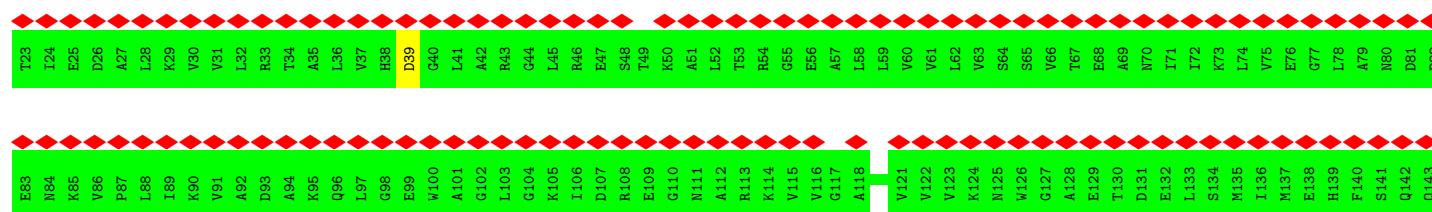
- Molecule 11: 40S ribosomal protein S10-A



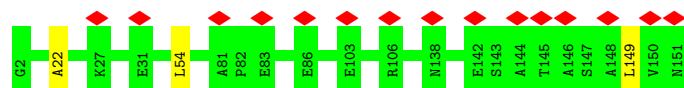
- Molecule 12: 40S ribosomal protein S11-A



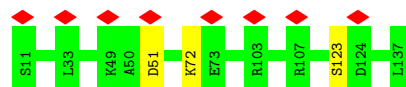
- Molecule 13: 40S ribosomal protein S12



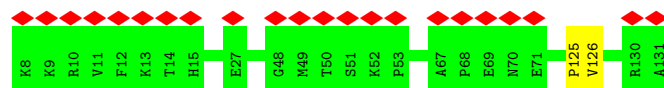
- Molecule 14: 40S ribosomal protein S13



- Molecule 15: 40S ribosomal protein S14-A

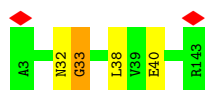


- Molecule 16: 40S ribosomal protein S15

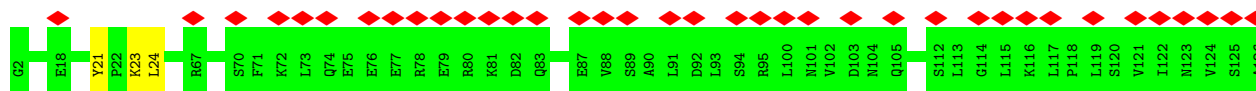


- Molecule 17: 40S ribosomal protein S16-A

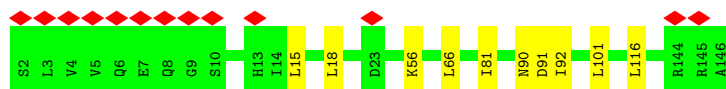




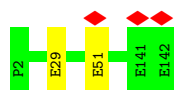
- Molecule 18: 40S ribosomal protein S17-A



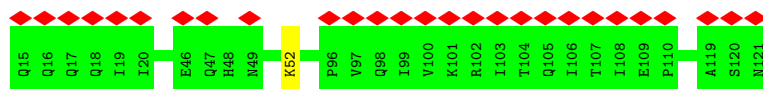
- Molecule 19: 40S ribosomal protein S18-A



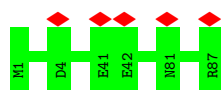
- Molecule 20: 40S ribosomal protein S19-A



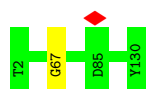
- Molecule 21: 40S ribosomal protein S20



- Molecule 22: 40S ribosomal protein S21-A

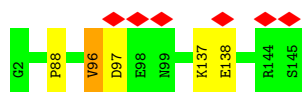


- Molecule 23: 40S ribosomal protein S22-A



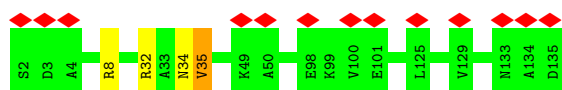
- Molecule 24: 40S ribosomal protein S23-A

Chain BX:  97% ..



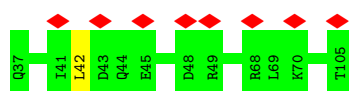
- Molecule 25: 40S ribosomal protein S24-A

Chain BY:  97% ..



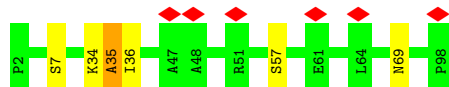
- Molecule 26: 40S ribosomal protein S25-A

Chain BZ:  99% .



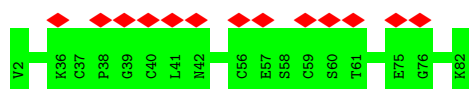
- Molecule 27: 40S ribosomal protein S26-A

Chain Ba:  94% 5% .



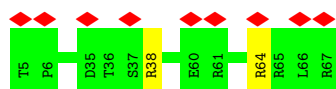
- Molecule 28: 40S ribosomal protein S27-A

Chain Bb:  100%



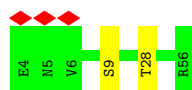
- Molecule 29: 40S ribosomal protein S28-A

Chain Bc:  97% .

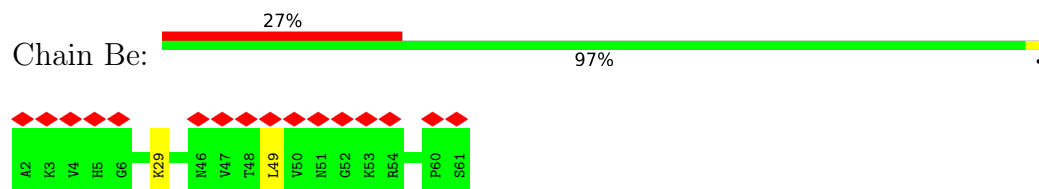


- Molecule 30: 40S ribosomal protein S29-A

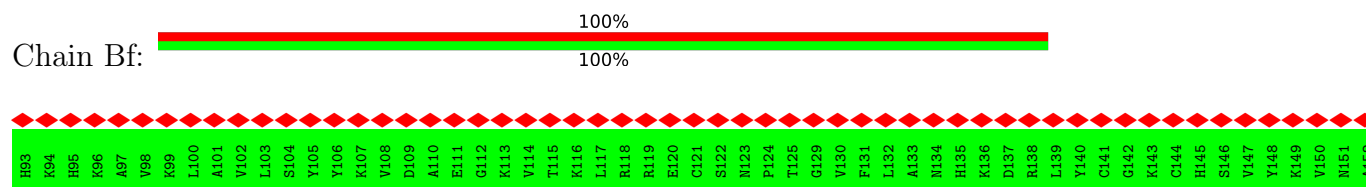
Chain Bd:  96% .



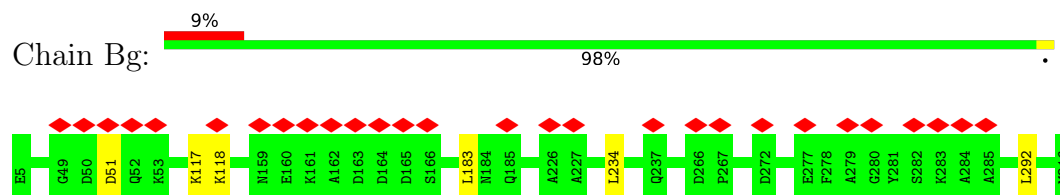
- Molecule 31: 40S ribosomal protein S30-A



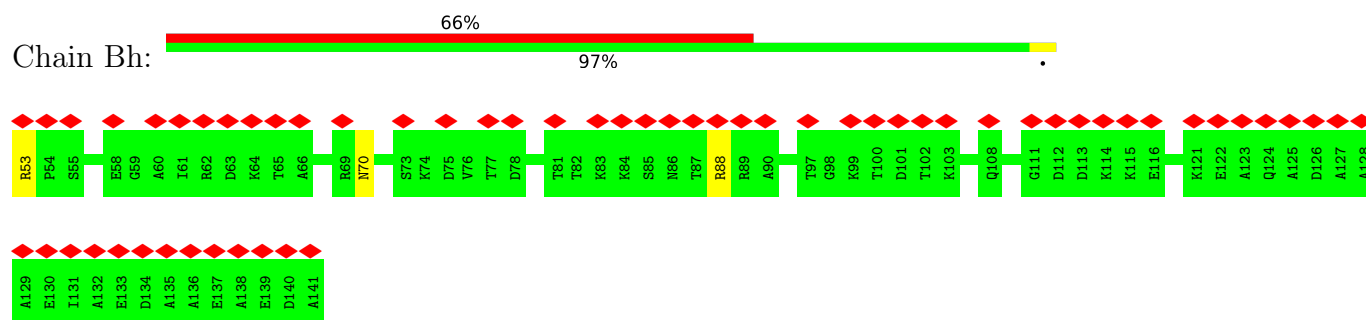
- Molecule 32: 40S ribosomal protein S31



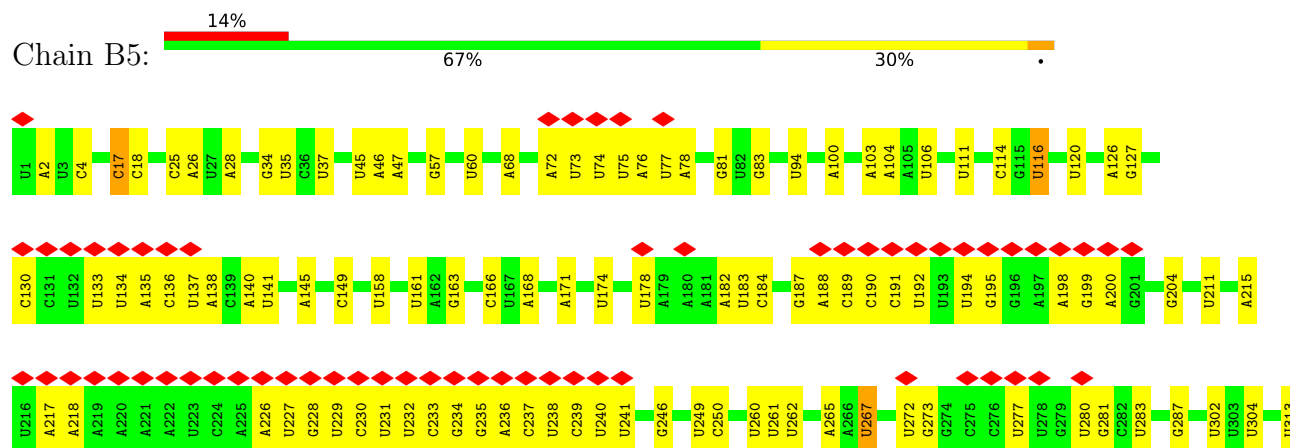
- Molecule 33: Guanine nucleotide-binding protein subunit beta-like protein

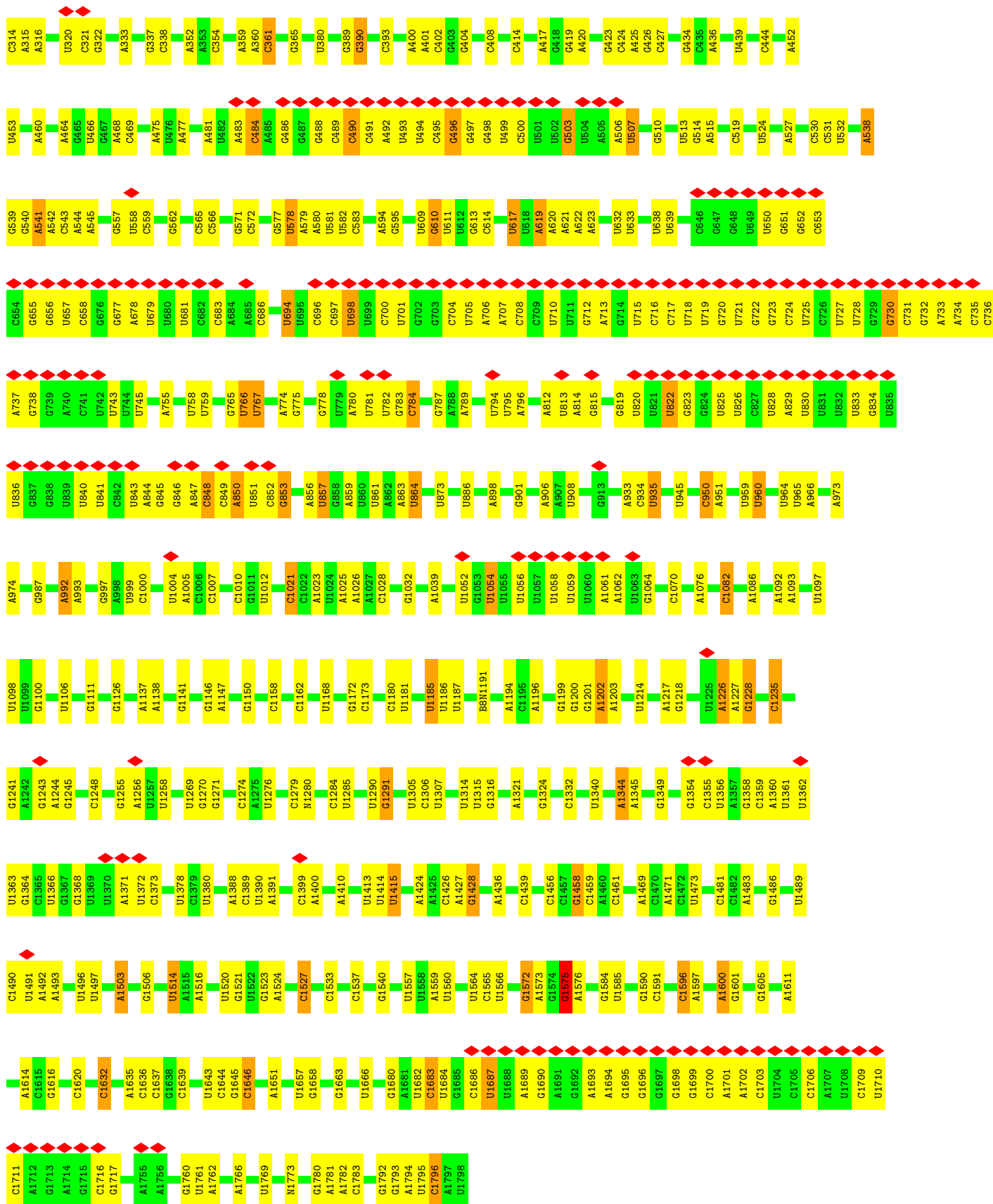


- Molecule 34: Suppressor protein STM1



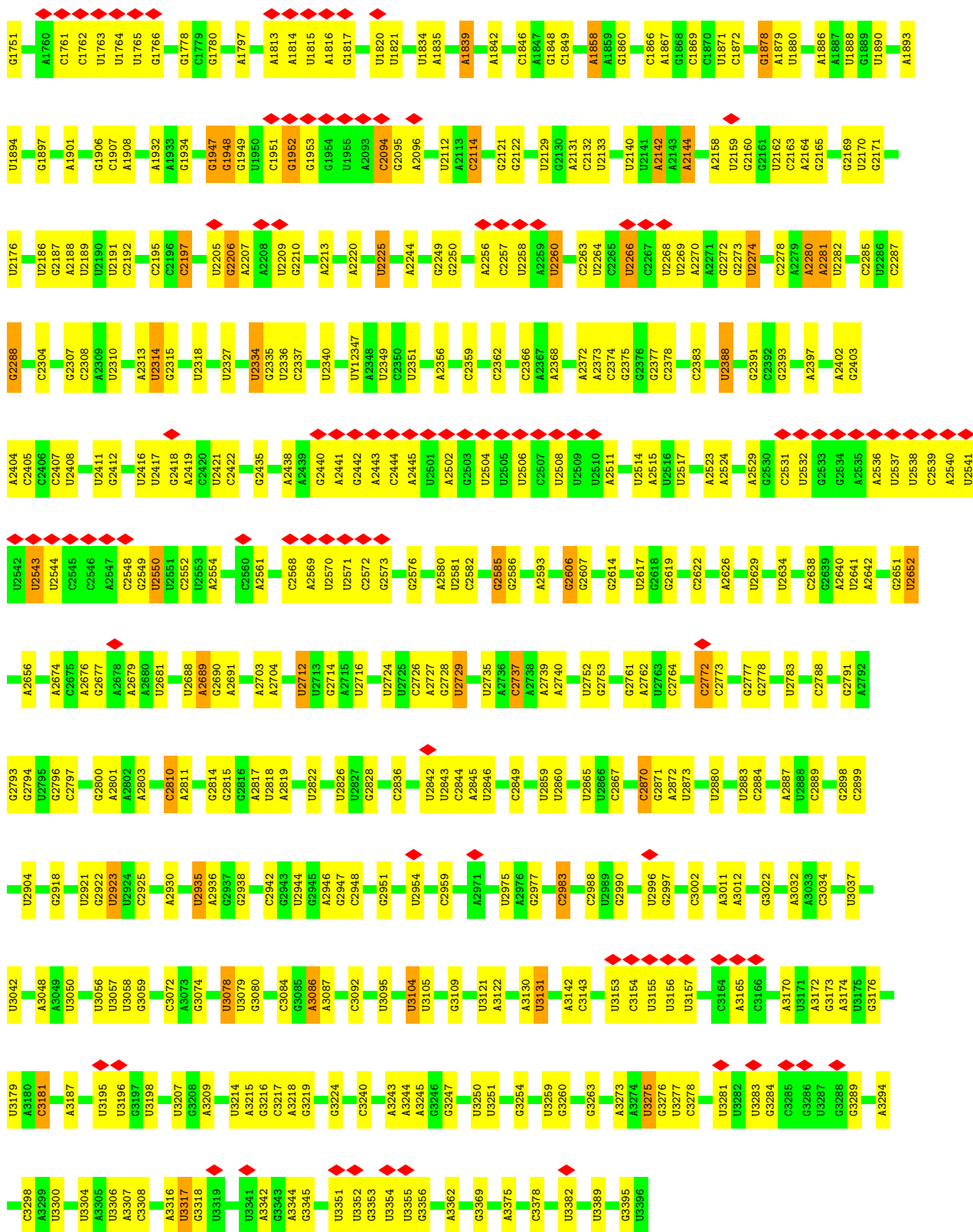
- Molecule 35: 18S rRNA

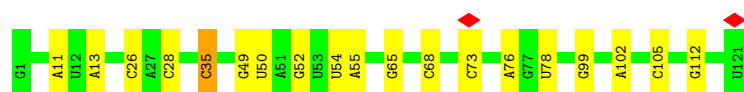




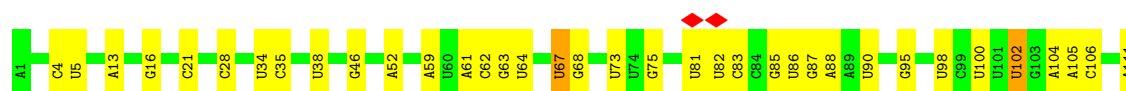
• Molecule 36: 25S rRNA



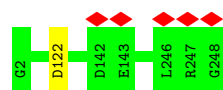




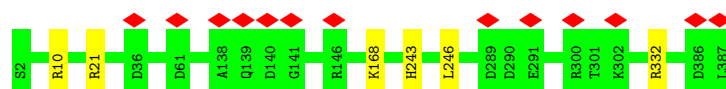
- Molecule 38: 5.8S rRNA



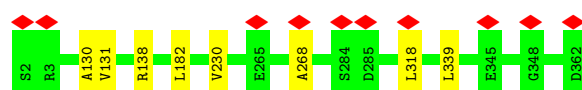
- Molecule 39: 60S ribosomal protein L2-A



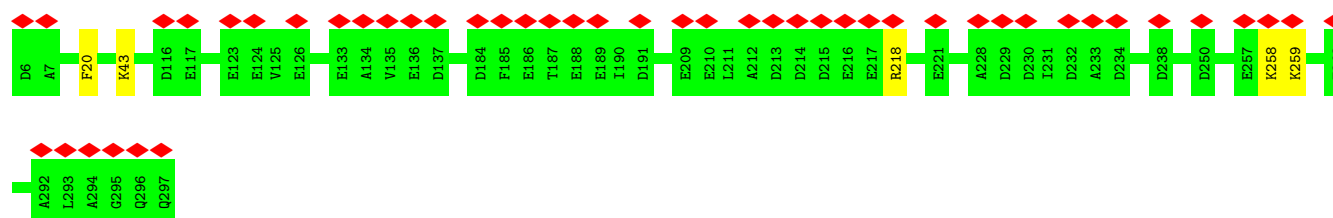
- Molecule 40: 60S ribosomal protein L3



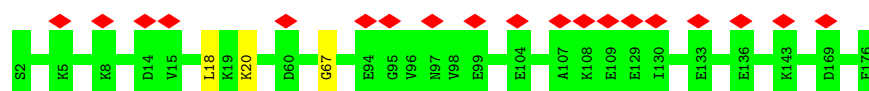
- Molecule 41: 60S ribosomal protein L4-A



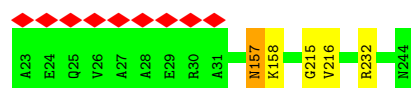
- Molecule 42: 60S ribosomal protein L5



- Molecule 43: 60S ribosomal protein L6-A



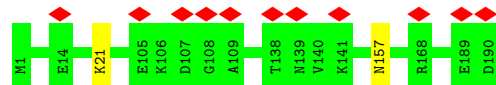
- Molecule 44: 60S ribosomal protein L7-A



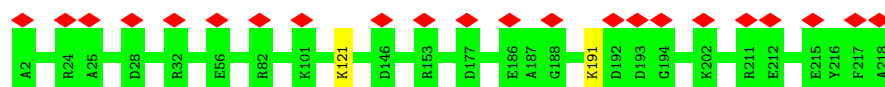
- Molecule 45: 60S ribosomal protein L8-A



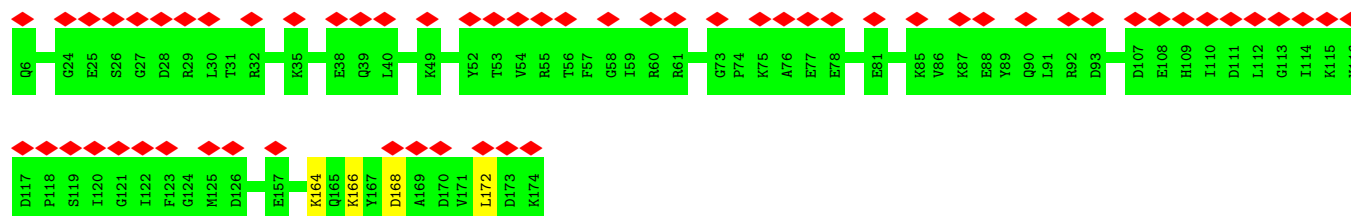
- Molecule 46: 60S ribosomal protein L9-A



- Molecule 47: 60S ribosomal protein L10

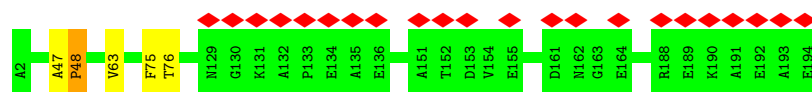


- Molecule 48: 60S ribosomal protein L11-A

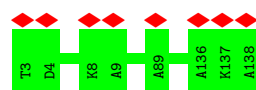


- Molecule 49: 60S ribosomal protein L13-A

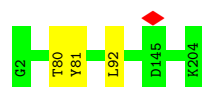




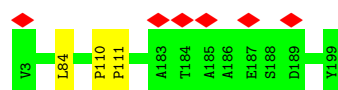
- Molecule 50: 60S ribosomal protein L14-A



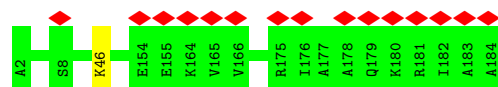
- Molecule 51: 60S ribosomal protein L15-A



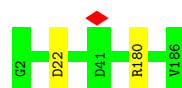
- Molecule 52: 60S ribosomal protein L16-A



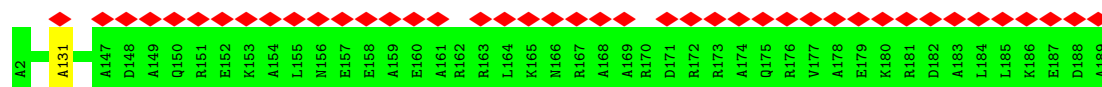
- Molecule 53: 60S ribosomal protein L17-A



- Molecule 54: 60S ribosomal protein L18-A



- Molecule 55: 60S ribosomal protein L19-A



- Molecule 56: 60S ribosomal protein L20-A

Chain AS:  99%



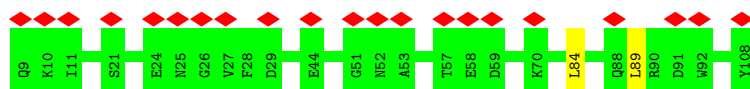
- Molecule 57: 60S ribosomal protein L21-A

Chain AT:  99%



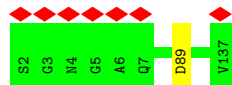
- Molecule 58: 60S ribosomal protein L22-A

Chain AU:  98%



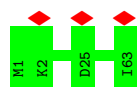
- Molecule 59: 60S ribosomal protein L23-A

Chain AV:  99%



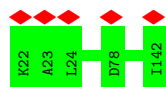
- Molecule 60: 60S ribosomal protein L24-A

Chain AW:  100%



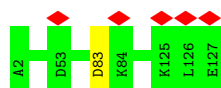
- Molecule 61: 60S ribosomal protein L25

Chain AX:  100%

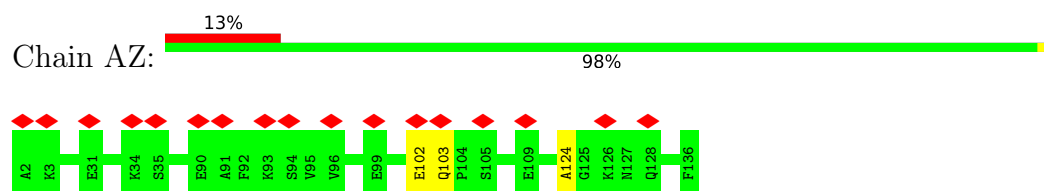


- Molecule 62: 60S ribosomal protein L26-A

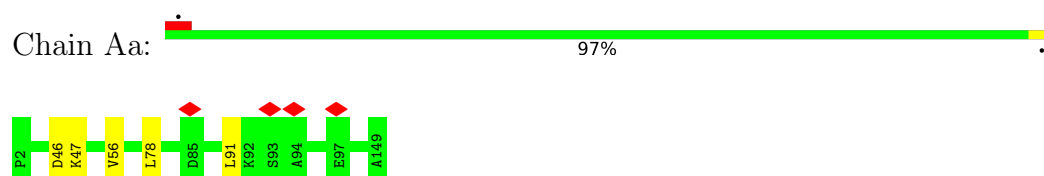
Chain AY:  99%



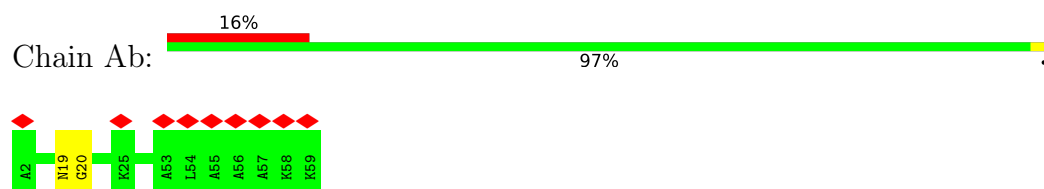
• Molecule 63: 60S ribosomal protein L27-A



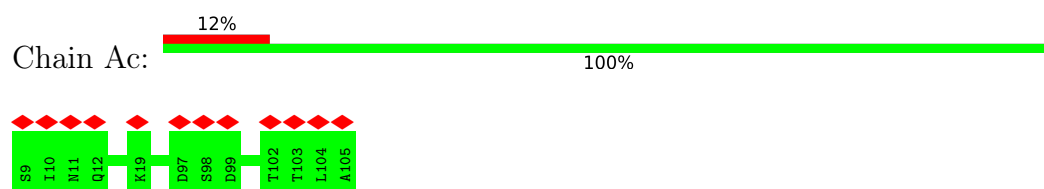
• Molecule 64: 60S ribosomal protein L28



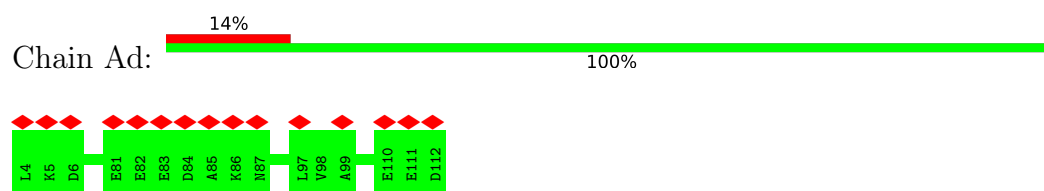
• Molecule 65: 60S ribosomal protein L29



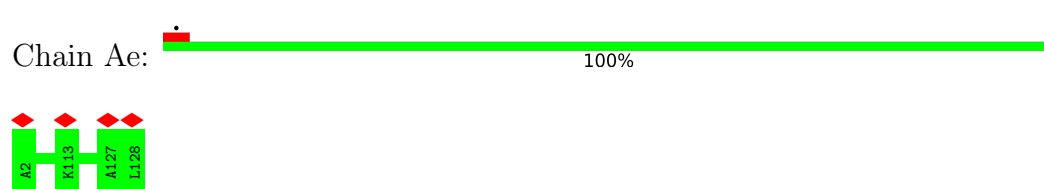
• Molecule 66: 60S ribosomal protein L30



• Molecule 67: 60S ribosomal protein L31-A

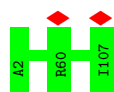


• Molecule 68: 60S ribosomal protein L32

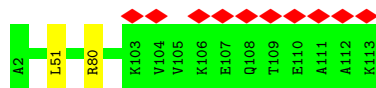


• Molecule 69: 60S ribosomal protein L33-A

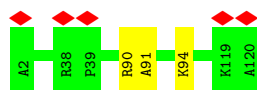




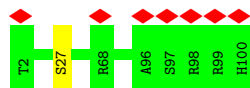
- Molecule 70: 60S ribosomal protein L34-A



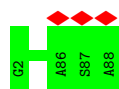
- Molecule 71: 60S ribosomal protein L35-A



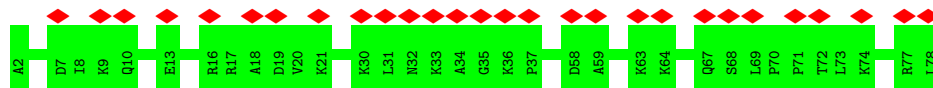
- Molecule 72: 60S ribosomal protein L36-A



- Molecule 73: 60S ribosomal protein L37-A



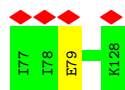
- Molecule 74: 60S ribosomal protein L38



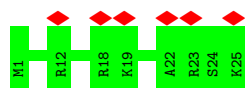
- Molecule 75: 60S ribosomal protein L39



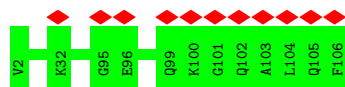
- Molecule 76: 60S ribosomal protein L40-A



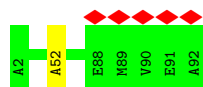
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	289345	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.428	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	463.968, 463.968, 463.968	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, OMC, ZN, MA6, G7M, 1MA, A2M, UY1, MG, UR3, OMU, PSU, HIC, 4AC, B8N, OMG

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	BA	0.38	0/1653	0.61	1/2261 (0.0%)
2	BB	0.35	0/1735	0.76	6/2335 (0.3%)
3	BC	0.40	0/1665	0.66	0/2263
4	BD	0.39	0/1759	0.68	1/2368 (0.0%)
5	BE	0.43	0/2109	0.68	2/2839 (0.1%)
6	BF	0.40	0/1629	0.68	0/2202
7	BG	0.34	0/1844	0.67	2/2464 (0.1%)
8	BH	0.37	0/1506	0.73	2/2028 (0.1%)
9	BI	0.42	0/1514	0.73	1/2021 (0.0%)
10	BJ	0.35	0/1519	0.65	0/2035
11	BK	0.45	0/837	0.77	1/1131 (0.1%)
12	BL	0.42	0/1272	0.58	0/1712
13	BM	0.30	0/921	0.70	1/1245 (0.1%)
14	BN	0.38	0/1215	0.66	3/1638 (0.2%)
15	BO	0.40	0/952	0.75	2/1279 (0.2%)
16	BP	0.42	0/1012	0.67	0/1356
17	BQ	0.42	0/1125	0.69	1/1510 (0.1%)
18	BR	0.45	1/984 (0.1%)	0.66	0/1318
19	BS	0.41	0/1211	0.78	4/1628 (0.2%)
20	BT	0.47	0/1113	0.71	1/1494 (0.1%)
21	BU	0.41	0/865	0.64	0/1169
22	BV	0.38	0/692	0.64	0/932
23	BW	0.44	0/1038	0.65	0/1395
24	BX	0.40	0/1139	0.72	0/1518
25	BY	0.42	0/1087	0.68	1/1449 (0.1%)
26	BZ	0.38	0/566	0.70	1/761 (0.1%)
27	Ba	0.41	0/782	0.70	0/1047
28	Bb	0.35	0/620	0.65	0/838
29	Bc	0.41	0/499	0.67	0/670
30	Bd	0.50	0/452	0.64	1/600 (0.2%)
31	Be	0.38	0/483	0.62	1/643 (0.2%)
32	Bf	0.31	0/462	0.62	0/617

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Bg	0.38	0/2454	0.71	4/3340 (0.1%)
34	Bh	0.31	0/678	0.56	0/905
35	B5	0.80	4/41414 (0.0%)	1.15	286/64521 (0.4%)
36	A1	0.89	0/73484	1.17	371/114569 (0.3%)
37	A3	0.74	0/2861	1.04	11/4457 (0.2%)
38	A4	0.87	0/3723	1.15	15/5794 (0.3%)
39	AA	0.45	0/1912	0.65	1/2569 (0.0%)
40	AB	0.46	0/3136	0.69	4/4213 (0.1%)
41	AC	0.43	1/2800 (0.0%)	0.66	1/3790 (0.0%)
42	AD	0.38	0/2390	0.63	1/3225 (0.0%)
43	AE	0.41	0/1260	0.60	1/1694 (0.1%)
44	AF	0.48	0/1821	0.66	0/2451
45	AG	0.39	0/1830	0.59	1/2469 (0.0%)
46	AH	0.40	0/1531	0.61	0/2062
47	AI	0.38	0/1708	0.61	0/2290
48	AJ	0.34	0/1374	0.71	2/1842 (0.1%)
49	AL	0.40	0/1568	0.66	1/2106 (0.0%)
50	AM	0.38	0/1068	0.56	0/1438
51	AN	0.49	0/1757	0.69	0/2354
52	AO	0.48	0/1585	0.65	1/2128 (0.0%)
53	AP	0.42	0/1410	0.60	0/1893
54	AQ	0.41	0/1465	0.64	2/1965 (0.1%)
55	AR	0.38	0/1538	0.56	0/2050
56	AS	0.47	0/1481	0.65	1/1990 (0.1%)
57	AT	0.44	0/1300	0.65	0/1743
58	AU	0.37	0/812	0.68	2/1099 (0.2%)
59	AV	0.45	0/1018	0.66	1/1369 (0.1%)
60	AW	0.41	0/533	0.63	0/707
61	AX	0.44	0/983	0.65	0/1325
62	AY	0.40	0/1004	0.64	1/1341 (0.1%)
63	AZ	0.37	0/1118	0.62	1/1497 (0.1%)
64	Aa	0.48	0/1204	0.73	3/1612 (0.2%)
65	Ab	0.34	0/473	0.59	0/629
66	Ac	0.39	0/751	0.67	0/1008
67	Ad	0.37	0/904	0.61	0/1213
68	Ae	0.45	0/1041	0.61	0/1394
69	Af	0.52	0/868	0.65	0/1168
70	Ag	0.44	0/890	0.68	1/1189 (0.1%)
71	Ah	0.41	0/978	0.63	0/1301
72	Ai	0.41	0/778	0.74	0/1034
73	Aj	0.48	0/696	0.64	0/923
74	Ak	0.36	0/618	0.59	0/826
75	Al	0.38	0/443	0.64	0/588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Am	0.41	0/423	0.61	1/562 (0.2%)
77	An	0.38	0/234	0.65	0/300
78	Ao	0.40	0/860	0.61	0/1136
79	Ap	0.41	0/701	0.68	0/934
All	All	0.70	6/211138 (0.0%)	1.00	745/309779 (0.2%)

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
2	BB	0	5
3	BC	0	2
5	BE	0	2
6	BF	0	2
7	BG	0	1
8	BH	0	3
9	BI	0	1
10	BJ	0	3
11	BK	0	3
12	BL	0	1
15	BO	0	1
17	BQ	0	3
19	BS	0	4
20	BT	0	1
24	BX	0	3
25	BY	0	1
27	Ba	0	4
35	B5	3	0
41	AC	0	2
42	AD	0	2
43	AE	0	1
44	AF	0	3
45	AG	0	5
46	AH	0	1
48	AJ	0	2
49	AL	0	2
51	AN	0	2
52	AO	0	1
55	AR	0	1
57	AT	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	AZ	0	1
64	Aa	0	1
65	Ab	0	2
70	Ag	0	1
71	Ah	0	1
72	Ai	0	1
All	All	3	70

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	BR	21	TYR	C-N	7.06	1.47	1.34
35	B5	1291	G	C2-N3	-6.61	1.27	1.32
35	B5	992	A	C2-N3	-5.98	1.28	1.33
35	B5	538	A	C2-N3	-5.74	1.28	1.33
41	AC	230	VAL	CB-CG1	-5.70	1.40	1.52
35	B5	1600	A	C2-N3	-5.57	1.28	1.33

All (745) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1948	G	O5'-P-OP1	-31.38	73.04	110.70
36	A1	266	A	O5'-P-OP1	-30.18	74.49	110.70
36	A1	266	A	OP1-P-OP2	-27.41	78.48	119.60
36	A1	1948	G	O5'-P-OP2	-23.68	82.28	110.70
36	A1	266	A	O5'-P-OP2	19.85	134.52	110.70
36	A1	115	A	O5'-P-OP1	14.65	128.28	110.70
36	A1	265	A	OP2-P-O3'	-13.75	74.95	105.20
36	A1	1948	G	OP1-P-OP2	13.10	139.25	119.60
40	AB	168	LYS	C-N-CA	13.06	154.35	121.70
35	B5	453	U	C2-N1-C1'	12.34	132.51	117.70
36	A1	1947	G	OP2-P-O3'	-12.33	78.07	105.20
36	A1	265	A	OP1-P-O3'	12.11	131.84	105.20
35	B5	453	U	N1-C2-O2	12.06	131.24	122.80
36	A1	2225	U	N3-C2-O2	-11.75	113.98	122.20
36	A1	406	G	O4'-C1'-N9	11.46	117.37	108.20
36	A1	1947	G	OP1-P-O3'	-10.91	81.19	105.20
38	A4	5	U	N3-C2-O2	-10.87	114.59	122.20
36	A1	922	U	C2-N1-C1'	10.67	130.50	117.70
35	B5	453	U	N3-C2-O2	-10.67	114.73	122.20
35	B5	1389	C	C2-N1-C1'	10.54	130.39	118.80
7	BG	68	LEU	CA-CB-CG	10.48	139.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1458	G	C2-N3-C4	10.10	116.95	111.90
35	B5	1560	U	N3-C2-O2	-10.06	115.16	122.20
36	A1	2263	C	N3-C2-O2	-9.82	115.02	121.90
36	A1	2263	C	N1-C2-O2	9.79	124.77	118.90
36	A1	2263	C	C2-N1-C1'	9.75	129.53	118.80
36	A1	1835	A	C6-N1-C2	9.70	124.42	118.60
36	A1	3034	C	C2-N1-C1'	9.64	129.41	118.80
35	B5	538	A	C8-N9-C4	-9.59	101.97	105.80
36	A1	1495	U	C4-C5-C6	9.59	125.45	119.70
36	A1	2225	U	N1-C2-O2	9.50	129.45	122.80
35	B5	1458	G	N3-C4-C5	-9.27	123.97	128.60
36	A1	3037	U	N3-C2-O2	-9.23	115.73	122.20
36	A1	922	U	N3-C2-O2	-9.20	115.76	122.20
36	A1	78	U	N3-C2-O2	-9.18	115.78	122.20
35	B5	1307	U	N1-C2-O2	9.03	129.12	122.80
36	A1	3034	C	N3-C2-O2	-8.90	115.67	121.90
35	B5	1389	C	C6-N1-C2	-8.88	116.75	120.30
35	B5	1082	C	C2-N1-C1'	8.87	128.56	118.80
36	A1	3181	C	N1-C2-O2	8.83	124.20	118.90
36	A1	954	U	N3-C2-O2	-8.79	116.04	122.20
36	A1	2225	U	C2-N1-C1'	8.71	128.16	117.70
36	A1	3057	U	N3-C2-O2	-8.71	116.10	122.20
35	B5	1389	C	C5-C6-N1	8.69	125.35	121.00
36	A1	2726	C	N1-C2-O2	8.69	124.12	118.90
35	B5	1514	U	N1-C2-O2	8.69	128.88	122.80
35	B5	1291	G	N3-C2-N2	-8.64	113.85	119.90
36	A1	922	U	N1-C2-O2	8.64	128.85	122.80
36	A1	3181	C	C2-N1-C1'	8.63	128.30	118.80
36	A1	2836	C	N3-C2-O2	-8.62	115.86	121.90
41	AC	182	LEU	CA-CB-CG	8.59	135.04	115.30
35	B5	1307	U	N3-C2-O2	-8.57	116.20	122.20
35	B5	1380	U	N3-C2-O2	-8.56	116.20	122.20
35	B5	795	U	C2-N1-C1'	8.53	127.93	117.70
36	A1	1871	U	N3-C2-O2	-8.50	116.25	122.20
36	A1	2726	C	C2-N1-C1'	8.50	128.15	118.80
36	A1	3306	U	N3-C2-O2	-8.49	116.26	122.20
36	A1	3034	C	N1-C2-O2	8.47	123.98	118.90
35	B5	1564	U	N3-C2-O2	-8.44	116.29	122.20
35	B5	453	U	C6-N1-C1'	-8.40	109.44	121.20
35	B5	1796	C	N1-C2-O2	8.39	123.94	118.90
35	B5	1596	C	N3-C2-O2	-8.38	116.03	121.90
35	B5	581	U	C2-N1-C1'	8.35	127.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	3037	U	C2-N1-C1'	8.29	127.65	117.70
36	A1	954	U	N1-C2-O2	8.28	128.60	122.80
36	A1	102	C	N3-C2-O2	-8.23	116.14	121.90
36	A1	2206	G	N3-C4-N9	8.23	130.94	126.00
36	A1	102	C	N1-C2-O2	8.21	123.83	118.90
36	A1	835	G	O4'-C1'-N9	8.19	114.75	108.20
36	A1	3306	U	C2-N1-C1'	8.17	127.51	117.70
36	A1	1694	U	N3-C2-O2	-8.16	116.49	122.20
35	B5	581	U	N3-C2-O2	-8.15	116.49	122.20
35	B5	1560	U	C2-N1-C1'	8.13	127.46	117.70
36	A1	3244	A	C4-C5-C6	-8.11	112.95	117.00
36	A1	1496	C	C2-N1-C1'	8.09	127.69	118.80
35	B5	1380	U	C2-N1-C1'	8.06	127.37	117.70
35	B5	1473	U	C2-N1-C1'	8.06	127.37	117.70
36	A1	2843	U	N1-C2-O2	8.05	128.44	122.80
35	B5	581	U	N1-C2-O2	8.05	128.44	122.80
58	AU	89	LEU	CA-CB-CG	8.05	133.81	115.30
35	B5	1307	U	C2-N1-C1'	8.04	127.34	117.70
36	A1	1597	C	C6-N1-C2	-7.99	117.11	120.30
36	A1	2846	U	C2-N1-C1'	7.96	127.25	117.70
25	BY	35	VAL	CG1-CB-CG2	-7.96	98.17	110.90
36	A1	3057	U	N1-C2-O2	7.96	128.37	122.80
35	B5	864	U	N3-C2-O2	-7.92	116.65	122.20
36	A1	1835	A	N1-C2-N3	-7.92	125.34	129.30
35	B5	1514	U	N3-C2-O2	-7.90	116.67	122.20
35	B5	1560	U	N1-C2-O2	7.89	128.33	122.80
52	AO	84[A]	LEU	CB-CG-CD1	-7.88	97.60	111.00
36	A1	269	G	C4-N9-C1'	7.88	136.74	126.50
36	A1	3037	U	N1-C2-O2	7.84	128.29	122.80
38	A4	64	U	N3-C2-O2	-7.84	116.71	122.20
36	A1	2983	C	C2-N1-C1'	7.83	127.41	118.80
36	A1	3214	U	C2-N1-C1'	7.81	127.07	117.70
35	B5	959	U	N1-C2-O2	7.80	128.26	122.80
36	A1	2836	C	N1-C2-O2	7.79	123.58	118.90
35	B5	1389	C	N1-C2-O2	7.78	123.57	118.90
35	B5	1456	C	N1-C2-O2	7.75	123.55	118.90
35	B5	1489	U	C2-N1-C1'	7.73	126.97	117.70
35	B5	583	C	C6-N1-C2	-7.72	117.21	120.30
35	B5	1596	C	N1-C2-O2	7.72	123.53	118.90
38	A4	5	U	C2-N1-C1'	7.72	126.96	117.70
36	A1	2836	C	C2-N1-C1'	7.67	127.23	118.80
36	A1	115	A	OP1-P-OP2	-7.66	108.11	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1456	C	C2-N1-C1'	7.63	127.19	118.80
36	A1	2206	G	C4-N9-C1'	7.61	136.39	126.50
35	B5	959	U	N3-C2-O2	-7.59	116.89	122.20
36	A1	2846	U	N1-C2-O2	7.57	128.10	122.80
36	A1	78	U	N1-C2-O2	7.57	128.10	122.80
35	B5	1600	A	C8-N9-C4	-7.54	102.78	105.80
36	A1	2843	U	N3-C2-O2	-7.54	116.92	122.20
35	B5	698	U	N1-C2-O2	7.53	128.07	122.80
36	A1	113	C	C2-N1-C1'	7.52	127.07	118.80
35	B5	1012	U	C5-C4-O4	-7.52	121.39	125.90
36	A1	2543	U	N1-C2-O2	7.51	128.06	122.80
36	A1	1645	U	N3-C2-O2	-7.46	116.97	122.20
35	B5	1012	U	N3-C4-O4	7.43	124.60	119.40
35	B5	1458	G	C4-N9-C1'	7.39	136.11	126.50
36	A1	3306	U	N1-C2-O2	7.39	127.97	122.80
59	AV	89	ASP	CB-CG-OD2	7.39	124.95	118.30
35	B5	1687	U	N1-C2-O2	7.38	127.96	122.80
36	A1	411	U	N3-C2-O2	-7.38	117.04	122.20
36	A1	2843	U	C2-N1-C1'	7.38	126.55	117.70
35	B5	767	U	N3-C2-O2	-7.37	117.04	122.20
35	B5	1082	C	N1-C2-O2	7.37	123.32	118.90
36	A1	1314	C	C6-N1-C2	-7.36	117.36	120.30
36	A1	2726	C	N3-C2-O2	-7.34	116.76	121.90
35	B5	1564	U	C2-N1-C1'	7.33	126.49	117.70
35	B5	538	A	N7-C8-N9	7.32	117.46	113.80
35	B5	864	U	N1-C2-O2	7.30	127.91	122.80
35	B5	1796	C	N3-C2-O2	-7.30	116.79	121.90
36	A1	2366	C	C2-N1-C1'	7.29	126.82	118.80
35	B5	1489	U	N3-C2-O2	-7.27	117.11	122.20
36	A1	2988	C	C6-N1-C2	-7.27	117.39	120.30
35	B5	864	U	C2-N1-C1'	7.25	126.40	117.70
35	B5	1473	U	N1-C2-O2	7.25	127.87	122.80
36	A1	269	G	N7-C8-N9	7.22	116.71	113.10
36	A1	2206	G	N3-C4-C5	-7.21	124.99	128.60
36	A1	2263	C	C6-N1-C2	-7.20	117.42	120.30
35	B5	1687	U	N3-C2-O2	-7.20	117.16	122.20
35	B5	507	U	N3-C2-O2	-7.20	117.16	122.20
35	B5	1000	C	C2-N1-C1'	7.15	126.67	118.80
36	A1	3034	C	C6-N1-C2	-7.15	117.44	120.30
36	A1	2407	C	C5-C6-N1	7.14	124.57	121.00
36	A1	2846	U	N3-C2-O2	-7.13	117.21	122.20
36	A1	2543	U	C2-N1-C1'	7.12	126.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1185	U	N1-C2-O2	7.10	127.77	122.80
35	B5	1226	A	O4'-C1'-N9	7.09	113.87	108.20
36	A1	3300	U	N3-C2-O2	-7.08	117.25	122.20
35	B5	116	U	N3-C2-O2	-7.08	117.25	122.20
36	A1	97	U	N3-C2-O2	-7.06	117.26	122.20
36	A1	1604	G	C4-N9-C1'	7.05	135.66	126.50
36	A1	2408	U	N3-C2-O2	-7.05	117.27	122.20
36	A1	2543	U	N3-C2-O2	-7.05	117.27	122.20
36	A1	1317	A	O4'-C1'-N9	7.03	113.82	108.20
36	A1	102	C	C6-N1-C2	-7.02	117.49	120.30
2	BB	61	LEU	CB-CG-CD2	-7.00	99.09	111.00
35	B5	1082	C	C6-N1-C2	-7.00	117.50	120.30
36	A1	2407	C	C6-N1-C2	-6.99	117.50	120.30
56	AS	109	ASP	CB-CG-OD1	6.98	124.59	118.30
35	B5	1456	C	N3-C2-O2	-6.98	117.01	121.90
35	B5	507	U	N1-C2-O2	6.98	127.68	122.80
35	B5	1291	G	N1-C2-N2	6.98	122.48	116.20
36	A1	2388	U	N3-C2-O2	-6.97	117.32	122.20
36	A1	2550	U	N3-C2-O2	-6.96	117.33	122.20
17	BQ	38	LEU	CA-CB-CG	6.95	131.28	115.30
35	B5	1796	C	C2-N1-C1'	6.94	126.43	118.80
36	A1	954	U	C2-N1-C1'	6.91	125.99	117.70
36	A1	3131	U	C2-N1-C1'	6.91	125.99	117.70
36	A1	2899	C	C6-N1-C2	-6.88	117.55	120.30
36	A1	299	G	O4'-C1'-N9	6.85	113.68	108.20
36	A1	1871	U	N1-C2-O2	6.84	127.59	122.80
35	B5	959	U	C2-N1-C1'	6.82	125.88	117.70
36	A1	1495	U	C5-C6-N1	-6.82	119.29	122.70
35	B5	361	C	C5-C6-N1	6.80	124.40	121.00
35	B5	1687	U	C2-N1-C1'	6.80	125.86	117.70
36	A1	3058	U	C2-N1-C1'	6.79	125.85	117.70
35	B5	861	U	C2-N1-C1'	6.79	125.84	117.70
35	B5	853	G	C4-N9-C1'	6.78	135.32	126.50
36	A1	288	C	C6-N1-C2	-6.77	117.59	120.30
36	A1	42	C	C6-N1-C2	-6.75	117.60	120.30
36	A1	315	C	C6-N1-C2	-6.74	117.60	120.30
36	A1	702	C	C6-N1-C2	-6.74	117.60	120.30
35	B5	795	U	N3-C2-O2	-6.74	117.48	122.20
36	A1	270	U	N1-C2-O2	6.74	127.52	122.80
35	B5	1458	G	N3-C4-N9	6.73	130.04	126.00
35	B5	1185	U	N3-C2-O2	-6.73	117.49	122.20
35	B5	1305	U	N3-C2-O2	-6.72	117.49	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1496	C	C6-N1-C2	-6.72	117.61	120.30
35	B5	686	C	C6-N1-C2	-6.70	117.62	120.30
36	A1	2638	C	N1-C2-O2	6.70	122.92	118.90
36	A1	3181	C	C6-N1-C1'	-6.69	112.77	120.80
36	A1	770	G	O4'-C1'-N9	6.69	113.55	108.20
35	B5	1489	U	N1-C2-O2	6.68	127.48	122.80
35	B5	530	C	N1-C2-O2	6.67	122.90	118.90
36	A1	2652	U	N3-C2-O2	-6.67	117.53	122.20
35	B5	543	C	N1-C2-O2	6.66	122.89	118.90
35	B5	1380	U	N1-C2-O2	6.65	127.45	122.80
35	B5	531	C	N3-C2-O2	-6.65	117.25	121.90
36	A1	850	U	N3-C2-O2	-6.64	117.55	122.20
35	B5	1458	G	C8-N9-C4	-6.64	103.75	106.40
36	A1	269	G	C6-C5-N7	-6.63	126.42	130.40
36	A1	3250	U	N1-C2-O2	6.63	127.44	122.80
35	B5	1389	C	C6-N1-C1'	-6.63	112.85	120.80
36	A1	269	G	C4-C5-N7	6.62	113.45	110.80
36	A1	2899	C	N3-C2-O2	-6.62	117.26	121.90
36	A1	1645	U	N1-C2-O2	6.62	127.43	122.80
36	A1	2189	U	N3-C2-O2	-6.61	117.57	122.20
36	A1	1597	C	C5-C6-N1	6.61	124.30	121.00
36	A1	42	C	C5-C6-N1	6.61	124.30	121.00
36	A1	2206	G	C8-N9-C1'	-6.60	118.41	127.00
36	A1	922	U	C6-N1-C1'	-6.58	111.99	121.20
19	BS	18	LEU	CA-CB-CG	6.57	130.40	115.30
36	A1	115	A	C5'-C4'-O4'	6.56	116.97	109.10
36	A1	2405	C	C6-N1-C2	-6.56	117.67	120.30
8	BH	64	VAL	CA-CB-CG1	6.56	120.74	110.90
35	B5	583	C	C2-N1-C1'	6.56	126.02	118.80
36	A1	3244	A	C6-C5-N7	6.55	136.89	132.30
35	B5	610	G	C4-N9-C1'	6.55	135.01	126.50
36	A1	113	C	C6-N1-C2	-6.54	117.68	120.30
35	B5	698	U	N3-C2-O2	-6.54	117.62	122.20
36	A1	2836	C	C6-N1-C2	-6.53	117.69	120.30
35	B5	1146	G	N1-C6-O6	-6.53	115.98	119.90
36	A1	3104	U	N1-C2-O2	6.53	127.37	122.80
35	B5	934	C	C2-N1-C1'	6.52	125.98	118.80
36	A1	1646	G	O4'-C1'-N9	6.52	113.42	108.20
35	B5	361	C	C6-N1-C2	-6.52	117.69	120.30
35	B5	1646	C	N1-C2-O2	6.51	122.81	118.90
35	B5	1596	C	C2-N1-C1'	6.51	125.96	118.80
36	A1	2263	C	C6-N1-C1'	-6.49	113.01	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1724	U	O4'-C1'-N1	6.47	113.38	108.20
36	A1	777	U	N3-C2-O2	-6.47	117.67	122.20
35	B5	1082	C	N3-C2-O2	-6.46	117.38	121.90
36	A1	2884	C	C6-N1-C2	-6.46	117.72	120.30
36	A1	3084	C	C6-N1-C2	-6.46	117.72	120.30
35	B5	543	C	N3-C2-O2	-6.45	117.38	121.90
36	A1	1878	G	C4-N9-C1'	6.44	134.87	126.50
35	B5	1473	U	C6-N1-C1'	-6.43	112.19	121.20
35	B5	507	U	C2-N1-C1'	6.43	125.42	117.70
36	A1	1333	C	C6-N1-C2	-6.43	117.73	120.30
36	A1	1425	U	N3-C2-O2	-6.42	117.71	122.20
36	A1	2366	C	C6-N1-C2	-6.41	117.74	120.30
36	A1	1695	U	O4'-C1'-N1	6.39	113.31	108.20
36	A1	2899	C	C2-N1-C1'	6.39	125.83	118.80
35	B5	1172	G	N7-C8-N9	6.39	116.29	113.10
38	A4	5	U	N1-C2-O2	6.38	127.27	122.80
36	A1	850	U	N1-C2-O2	6.38	127.27	122.80
35	B5	1683	C	O4'-C1'-N1	6.38	113.30	108.20
35	B5	698	U	C2-N1-C1'	6.37	125.35	117.70
36	A1	3034	C	C6-N1-C1'	-6.37	113.15	120.80
15	BO	72	LYS	C-N-CA	6.37	137.62	121.70
36	A1	2408	U	N1-C2-O2	6.37	127.26	122.80
36	A1	3058	U	N1-C2-O2	6.37	127.26	122.80
15	BO	51	ASP	CB-CG-OD1	6.36	124.03	118.30
35	B5	1291	G	N3-C4-N9	-6.36	122.19	126.00
35	B5	758	U	N1-C2-O2	6.36	127.25	122.80
35	B5	35	U	N3-C2-O2	-6.35	117.75	122.20
35	B5	694	U	N3-C2-O2	-6.35	117.76	122.20
35	B5	184	C	C2-N1-C1'	6.35	125.78	118.80
35	B5	758	U	N3-C2-O2	-6.34	117.76	122.20
36	A1	2617	U	N3-C2-O2	-6.34	117.76	122.20
35	B5	496	G	C4-N9-C1'	6.34	134.74	126.50
35	B5	822	U	C2-N1-C1'	6.33	125.30	117.70
35	B5	1473	U	N3-C2-O2	-6.33	117.77	122.20
35	B5	583	C	N1-C2-O2	6.32	122.69	118.90
31	Be	49	LEU	CA-CB-CG	6.31	129.82	115.30
35	B5	1258	U	N1-C2-O2	6.31	127.22	122.80
36	A1	269	G	C8-N9-C1'	-6.31	118.80	127.00
35	B5	965	U	C2-N1-C1'	6.31	125.27	117.70
35	B5	1533	C	N3-C2-O2	-6.30	117.49	121.90
39	AA	122	ASP	CB-CG-OD1	6.30	123.97	118.30
36	A1	439	C	P-O3'-C3'	6.29	127.25	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	531	C	C6-N1-C2	-6.28	117.79	120.30
35	B5	992	A	C8-N9-C4	-6.27	103.29	105.80
35	B5	901	G	O4'-C1'-N9	6.27	113.22	108.20
35	B5	730	G	N3-C4-C5	-6.26	125.47	128.60
36	A1	1878	G	N3-C4-N9	6.25	129.75	126.00
36	A1	3048	A	O4'-C1'-N9	6.25	113.20	108.20
36	A1	123	A	N1-C2-N3	-6.24	126.18	129.30
35	B5	1366	U	N1-C2-O2	6.23	127.16	122.80
36	A1	2726	C	C6-N1-C1'	-6.23	113.32	120.80
36	A1	3240	C	C6-N1-C2	-6.23	117.81	120.30
36	A1	713	U	N3-C2-O2	-6.23	117.84	122.20
38	A4	64	U	N1-C2-O2	6.22	127.15	122.80
36	A1	3050	U	N1-C2-O2	6.21	127.15	122.80
35	B5	1332	C	C2-N1-C1'	6.21	125.63	118.80
38	A4	5	U	C4-C5-C6	6.21	123.43	119.70
36	A1	873	C	P-O3'-C3'	6.20	127.14	119.70
48	AJ	172	LEU	CA-CB-CG	6.20	129.57	115.30
35	B5	1614	A	O4'-C1'-N9	6.18	113.15	108.20
36	A1	1333	C	C5-C6-N1	6.18	124.09	121.00
36	A1	2935	U	N1-C2-O2	6.18	127.13	122.80
35	B5	908	U	N1-C2-O2	6.18	127.12	122.80
35	B5	1185	U	C2-N1-C1'	6.17	125.11	117.70
54	AQ	22	ASP	CB-CG-OD1	6.17	123.86	118.30
36	A1	97	U	N1-C2-O2	6.17	127.12	122.80
36	A1	3244	A	N1-C6-N6	-6.17	114.90	118.60
35	B5	795	U	N1-C2-O2	6.16	127.11	122.80
36	A1	1146	C	C6-N1-C2	-6.16	117.83	120.30
35	B5	1600	A	OP1-P-O3'	6.16	118.75	105.20
2	BB	147	ALA	C-N-CA	6.14	137.06	121.70
36	A1	3181	C	O4'-C1'-N1	6.14	113.12	108.20
36	A1	2163	C	C6-N1-C2	-6.14	117.84	120.30
35	B5	1644	C	C6-N1-C2	-6.14	117.84	120.30
35	B5	149	C	C6-N1-C2	-6.13	117.85	120.30
35	B5	1106	U	N3-C2-O2	-6.13	117.91	122.20
36	A1	1495	U	N1-C2-N3	6.13	118.58	114.90
36	A1	922	U	C5-C6-N1	6.12	125.76	122.70
36	A1	315	C	C5-C6-N1	6.11	124.06	121.00
35	B5	1258	U	N3-C2-O2	-6.11	117.92	122.20
37	A3	105	C	N1-C2-O2	6.11	122.56	118.90
35	B5	453	U	C5-C6-N1	6.10	125.75	122.70
35	B5	1389	C	N3-C2-O2	-6.10	117.63	121.90
36	A1	1499	C	C6-N1-C2	-6.09	117.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2517	U	N3-C2-O2	-6.09	117.94	122.20
36	A1	1872	C	N1-C2-O2	6.09	122.55	118.90
36	A1	1314	C	C5-C6-N1	6.08	124.04	121.00
38	A4	100	U	C2-N1-C1'	6.08	125.00	117.70
35	B5	228	G	N3-C4-C5	-6.08	125.56	128.60
35	B5	283	U	N1-C2-O2	6.07	127.05	122.80
36	A1	3362	A	N7-C8-N9	6.07	116.84	113.80
35	B5	1481	C	N1-C2-O2	6.07	122.54	118.90
36	A1	418	A	C6-N1-C2	6.06	122.24	118.60
35	B5	530	C	N3-C2-O2	-6.05	117.66	121.90
35	B5	861	U	N3-C2-O2	-6.05	117.96	122.20
35	B5	1202	A	C2-N3-C4	6.04	113.62	110.60
36	A1	3181	C	N3-C2-O2	-6.04	117.67	121.90
36	A1	1425	U	N1-C2-O2	6.04	127.03	122.80
35	B5	1291	G	C8-N9-C4	-6.04	103.98	106.40
36	A1	354	U	N3-C2-O2	-6.02	117.98	122.20
35	B5	17	C	C6-N1-C2	-6.02	117.89	120.30
36	A1	1309	U	N1-C2-O2	6.02	127.01	122.80
36	A1	3250	U	N3-C2-O2	-6.02	117.99	122.20
35	B5	1173	C	C5-C6-N1	6.01	124.01	121.00
36	A1	995	U	N1-C2-O2	6.01	127.01	122.80
35	B5	901	G	C4-N9-C1'	6.01	134.31	126.50
36	A1	3078	U	C2-N1-C1'	6.01	124.91	117.70
35	B5	1596	C	C6-N1-C2	-6.01	117.90	120.30
35	B5	1000	C	N1-C2-O2	6.01	122.50	118.90
36	A1	1894	U	N3-C2-O2	-6.00	118.00	122.20
36	A1	3214	U	C6-N1-C1'	-5.99	112.81	121.20
36	A1	911	C	C6-N1-C2	-5.99	117.90	120.30
36	A1	3214	U	O4'-C1'-N1	5.98	112.99	108.20
35	B5	1332	C	C5-C6-N1	5.98	123.99	121.00
35	B5	1533	C	N1-C2-O2	5.98	122.49	118.90
36	A1	524	U	N3-C2-O2	-5.97	118.02	122.20
36	A1	3104	U	N3-C2-O2	-5.96	118.02	122.20
5	BE	180	LEU	CA-CB-CG	5.96	129.01	115.30
35	B5	1214	U	N3-C2-O2	-5.95	118.03	122.20
33	Bg	117	LYS	C-N-CA	5.95	136.57	121.70
35	B5	908	U	N3-C2-O2	-5.95	118.04	122.20
36	A1	2550	U	N1-C2-O2	5.95	126.96	122.80
36	A1	3244	A	C8-N9-C4	5.93	108.17	105.80
36	A1	1496	C	N1-C2-O2	5.93	122.46	118.90
35	B5	583	C	C5-C6-N1	5.92	123.96	121.00
36	A1	1858	A	O4'-C1'-N9	5.92	112.93	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2716	U	N3-C2-O2	-5.91	118.06	122.20
35	B5	1012	U	N1-C2-O2	5.91	126.94	122.80
35	B5	408	C	C5-C6-N1	5.90	123.95	121.00
36	A1	1115	G	C4-N9-C1'	5.89	134.16	126.50
36	A1	2189	U	N1-C2-O2	5.89	126.92	122.80
36	A1	2378	C	C6-N1-C2	-5.88	117.95	120.30
35	B5	1332	C	C6-N1-C2	-5.88	117.95	120.30
37	A3	35	C	N1-C2-O2	5.88	122.43	118.90
35	B5	935	U	N1-C2-O2	5.88	126.91	122.80
36	A1	2206	G	C2-N3-C4	5.88	114.84	111.90
36	A1	2983	C	C6-N1-C1'	-5.87	113.76	120.80
36	A1	2094	C	N3-C2-O2	-5.86	117.80	121.90
36	A1	2606	G	N3-C4-C5	-5.86	125.67	128.60
36	A1	1368	U	C2-N1-C1'	5.86	124.73	117.70
36	A1	2366	C	C5-C6-N1	5.85	123.93	121.00
35	B5	1783	C	C2-N1-C1'	5.85	125.23	118.80
35	B5	767	U	C2-N1-C1'	5.85	124.72	117.70
36	A1	411	U	N1-C2-O2	5.85	126.89	122.80
35	B5	496	G	N3-C4-N9	5.84	129.51	126.00
35	B5	484	C	N3-C2-O2	-5.84	117.81	121.90
36	A1	1292	C	C6-N1-C2	-5.84	117.97	120.30
36	A1	524	U	N1-C2-O2	5.83	126.88	122.80
36	A1	922	U	C6-N1-C2	-5.83	117.50	121.00
14	BN	22	ALA	C-N-CD	-5.82	107.79	120.60
36	A1	3244	A	C4-N9-C1'	-5.82	115.82	126.30
38	A4	102	U	N3-C2-O2	-5.82	118.13	122.20
36	A1	1540	U	N3-C2-O2	-5.81	118.13	122.20
36	A1	3300	U	N1-C2-O2	5.81	126.87	122.80
35	B5	1600	A	N7-C8-N9	5.81	116.70	113.80
35	B5	228	G	N3-C4-N9	5.81	129.49	126.00
36	A1	2773	C	C6-N1-C2	-5.81	117.98	120.30
36	A1	1604	G	N3-C4-C5	-5.80	125.70	128.60
36	A1	2617	U	N1-C2-O2	5.80	126.86	122.80
35	B5	1082	C	O4'-C1'-N1	5.80	112.84	108.20
35	B5	853	G	N3-C4-C5	-5.80	125.70	128.60
35	B5	496	G	N3-C4-C5	-5.80	125.70	128.60
35	B5	1276	U	N3-C2-O2	-5.80	118.14	122.20
36	A1	1878	G	C8-N9-C1'	-5.80	119.46	127.00
35	B5	610	G	C8-N9-C1'	-5.80	119.47	127.00
40	AB	246	LEU	CA-CB-CG	5.80	128.63	115.30
36	A1	1878	G	N3-C4-C5	-5.79	125.70	128.60
36	A1	1694	U	C4-C5-C6	5.79	123.17	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	610	G	N3-C4-N9	5.78	129.47	126.00
35	B5	1054	U	N3-C2-O2	-5.78	118.15	122.20
36	A1	269	G	C5-N7-C8	-5.78	101.41	104.30
35	B5	1082	C	C6-N1-C1'	-5.78	113.87	120.80
36	A1	890	C	N3-C2-O2	-5.77	117.86	121.90
36	A1	3344	A	N7-C8-N9	5.77	116.68	113.80
35	B5	767	U	N1-C2-O2	5.76	126.83	122.80
36	A1	2638	C	N3-C2-O2	-5.76	117.87	121.90
36	A1	880	G	O4'-C1'-N9	5.76	112.81	108.20
36	A1	2622	C	N3-C2-O2	-5.75	117.87	121.90
35	B5	730	G	C4-N9-C1'	5.74	133.97	126.50
35	B5	1643	U	N3-C2-O2	-5.74	118.18	122.20
64	Aa	47	LYS	C-N-CA	5.73	136.03	121.70
33	Bg	183	LEU	CA-CB-CG	5.73	128.48	115.30
35	B5	1235	C	N1-C2-O2	5.73	122.34	118.90
35	B5	1585	U	C2-N3-C4	5.73	130.44	127.00
36	A1	1872	C	N3-C2-O2	-5.73	117.89	121.90
35	B5	698	U	C5-C6-N1	5.72	125.56	122.70
30	Bd	9	SER	C-N-CA	5.72	136.00	121.70
35	B5	992	A	N1-C2-N3	5.72	132.16	129.30
36	A1	1049	C	C6-N1-C2	-5.71	118.01	120.30
35	B5	267	U	N3-C2-O2	-5.71	118.21	122.20
45	AG	189	LEU	CA-CB-CG	5.71	128.42	115.30
35	B5	1162	C	N1-C2-O2	5.70	122.32	118.90
35	B5	1564	U	N1-C2-O2	5.69	126.78	122.80
36	A1	2405	C	N3-C2-O2	-5.69	117.92	121.90
35	B5	1012	U	N3-C2-O2	-5.69	118.22	122.20
35	B5	686	C	C5-C6-N1	5.68	123.84	121.00
36	A1	1190	A	C4-N9-C1'	5.67	136.51	126.30
35	B5	1173	C	C6-N1-C2	-5.67	118.03	120.30
35	B5	850	A	C2-N3-C4	5.67	113.43	110.60
36	A1	178	U	C5-C4-O4	5.67	129.30	125.90
42	AD	218	ARG	NE-CZ-NH1	5.66	123.13	120.30
36	A1	2622	C	N1-C2-O2	5.66	122.30	118.90
36	A1	1561	G	O4'-C1'-N9	5.66	112.73	108.20
37	A3	78	U	N1-C2-O2	5.66	126.76	122.80
35	B5	617	U	C2-N1-C1'	5.65	124.48	117.70
35	B5	1391	A	C4-N9-C1'	5.65	136.47	126.30
36	A1	2225	U	C6-N1-C1'	-5.65	113.29	121.20
37	A3	78	U	N3-C2-O2	-5.65	118.25	122.20
35	B5	1414	U	N3-C2-O2	-5.65	118.25	122.20
36	A1	1596	C	C6-N1-C2	-5.64	118.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1490	C	C6-N1-C2	-5.64	118.04	120.30
36	A1	2737	C	C6-N1-C2	-5.64	118.04	120.30
36	A1	1433	A	O4'-C1'-N9	-5.64	103.69	108.20
36	A1	2094	C	C6-N1-C1'	5.64	127.56	120.80
35	B5	283	U	N3-C2-O2	-5.63	118.26	122.20
35	B5	853	G	N3-C4-N9	5.63	129.38	126.00
35	B5	174	U	N3-C2-O2	-5.63	118.26	122.20
38	A4	67	U	P-O3'-C3'	5.63	126.45	119.70
19	BS	116	LEU	CA-CB-CG	5.62	128.23	115.30
36	A1	3275	U	C2-N1-C1'	5.62	124.45	117.70
35	B5	694	U	N1-C2-O2	5.62	126.73	122.80
35	B5	1456	C	C6-N1-C1'	-5.62	114.06	120.80
36	A1	2362	C	C5-C6-N1	5.62	123.81	121.00
14	BN	149	LEU	CA-CB-CG	5.61	128.21	115.30
63	AZ	102	GLU	C-N-CA	5.61	135.72	121.70
36	A1	743	C	C6-N1-C2	-5.61	118.06	120.30
36	A1	2873	U	C2-N1-C1'	5.61	124.43	117.70
36	A1	2362	C	N1-C2-O2	5.61	122.26	118.90
36	A1	2327	U	N3-C2-O2	-5.60	118.28	122.20
36	A1	916	G	P-O3'-C3'	5.59	126.41	119.70
35	B5	1514	U	C2-N1-C1'	5.59	124.41	117.70
36	A1	2783	U	N3-C2-O2	-5.59	118.29	122.20
35	B5	1527	C	C5-C6-N1	5.59	123.79	121.00
36	A1	777	U	N1-C2-O2	5.58	126.71	122.80
35	B5	37	U	N3-C2-O2	-5.58	118.30	122.20
14	BN	54	LEU	CA-CB-CG	5.58	128.13	115.30
35	B5	1258	U	C2-N1-C1'	5.58	124.39	117.70
35	B5	1783	C	C5-C6-N1	5.57	123.78	121.00
36	A1	1604	G	C8-N9-C1'	-5.56	119.77	127.00
36	A1	944	C	C6-N1-C2	-5.56	118.08	120.30
35	B5	1761	U	C2-N1-C1'	5.55	124.36	117.70
35	B5	1611	A	O4'-C1'-N9	5.54	112.64	108.20
37	A3	68	C	C6-N1-C2	-5.54	118.08	120.30
35	B5	1324	G	N3-C2-N2	-5.54	116.02	119.90
36	A1	101	G	O4'-C1'-N9	5.54	112.64	108.20
35	B5	1235	C	C6-N1-C2	-5.54	118.08	120.30
35	B5	960	U	N3-C2-O2	-5.54	118.32	122.20
36	A1	169	U	C2-N1-C1'	5.54	124.35	117.70
36	A1	1376	C	C6-N1-C2	-5.54	118.09	120.30
35	B5	822	U	N1-C2-O2	5.53	126.67	122.80
36	A1	132	C	C6-N1-C2	-5.53	118.09	120.30
36	A1	3306	U	C6-N1-C1'	-5.53	113.46	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BB	132	ASP	CB-CG-OD1	5.53	123.28	118.30
36	A1	2378	C	C2-N1-C1'	5.53	124.88	118.80
36	A1	354	U	N1-C2-O2	5.53	126.67	122.80
36	A1	115	A	C8-N9-C4	5.52	108.01	105.80
36	A1	2652	U	N1-C2-O2	5.52	126.67	122.80
8	BH	27	LEU	CA-CB-CG	5.52	128.00	115.30
37	A3	105	C	N3-C2-O2	-5.51	118.04	121.90
36	A1	2114	C	C6-N1-C2	-5.51	118.10	120.30
35	B5	1380	U	C6-N1-C1'	-5.51	113.49	121.20
36	A1	1869	C	C6-N1-C2	-5.50	118.10	120.30
36	A1	3037	U	C6-N1-C1'	-5.50	113.49	121.20
36	A1	995	U	N3-C2-O2	-5.50	118.35	122.20
36	A1	1309	U	N3-C2-O2	-5.50	118.35	122.20
2	BB	73	LEU	CA-CB-CG	5.50	127.95	115.30
11	BK	40	LEU	CB-CG-CD1	-5.50	101.65	111.00
36	A1	3058	U	N3-C2-O2	-5.50	118.35	122.20
36	A1	3317	U	N3-C2-O2	-5.50	118.35	122.20
35	B5	853	G	C8-N9-C1'	-5.50	119.85	127.00
36	A1	2359	C	C5-C6-N1	5.50	123.75	121.00
19	BS	66	LEU	CA-CB-CG	5.49	127.92	115.30
35	B5	530	C	C6-N1-C2	-5.49	118.11	120.30
36	A1	1496	C	C5-C6-N1	5.49	123.74	121.00
35	B5	228	G	C4-N9-C1'	5.49	133.63	126.50
35	B5	850	A	C4-N9-C1'	5.49	136.18	126.30
48	AJ	168	ASP	CB-CG-OD1	5.49	123.24	118.30
35	B5	1497	U	N1-C2-O2	5.48	126.64	122.80
64	Aa	56	VAL	N-CA-C	-5.48	96.21	111.00
35	B5	1354	G	C4-N9-C1'	5.48	133.62	126.50
36	A1	2274	U	N1-C2-O2	5.48	126.63	122.80
36	A1	1368	U	N1-C2-O2	5.48	126.63	122.80
36	A1	3344	A	C5-N7-C8	-5.47	101.17	103.90
35	B5	18	C	C6-N1-C2	-5.47	118.11	120.30
35	B5	1344	A	P-O3'-C3'	5.47	126.26	119.70
35	B5	1173	C	C2-N1-C1'	5.46	124.81	118.80
20	BT	29	GLU	CA-CB-CG	5.46	125.40	113.40
35	B5	935	U	N3-C2-O2	-5.46	118.38	122.20
35	B5	1565	C	C6-N1-C2	-5.46	118.12	120.30
36	A1	2606	G	N3-C4-N9	5.46	129.27	126.00
35	B5	730	G	C2-N3-C4	5.45	114.63	111.90
36	A1	302	U	N3-C2-O2	-5.45	118.39	122.20
35	B5	1783	C	N1-C2-O2	5.44	122.17	118.90
36	A1	1307	G	O4'-C1'-N9	5.44	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1499	C	C5-C6-N1	5.44	123.72	121.00
35	B5	784	C	C5-C6-N1	5.44	123.72	121.00
36	A1	1513	G	N1-C6-O6	-5.44	116.64	119.90
36	A1	2550	U	C2-N1-C1'	5.44	124.23	117.70
35	B5	583	C	N3-C2-O2	-5.44	118.09	121.90
36	A1	1144	U	O5'-P-OP2	-5.44	100.81	105.70
36	A1	1172	G	N1-C6-O6	-5.43	116.64	119.90
36	A1	2716	U	N1-C2-O2	5.43	126.60	122.80
36	A1	2846	U	C6-N1-C1'	-5.43	113.60	121.20
36	A1	2368	A	C8-N9-C4	-5.43	103.63	105.80
35	B5	1106	U	N1-C2-O2	5.42	126.60	122.80
36	A1	3086	A	N7-C8-N9	5.42	116.51	113.80
33	Bg	234	LEU	CA-CB-CG	5.41	127.75	115.30
36	A1	3050	U	N3-C2-O2	-5.41	118.41	122.20
36	A1	3105	U	N3-C2-O2	-5.41	118.42	122.20
35	B5	822	U	N3-C2-O2	-5.40	118.42	122.20
36	A1	1907	C	N1-C2-O2	5.40	122.14	118.90
35	B5	1168	U	N3-C2-O2	-5.39	118.43	122.20
70	Ag	51	LEU	CA-CB-CG	5.39	127.70	115.30
36	A1	2772	C	N1-C2-O2	5.39	122.13	118.90
5	BE	182	TYR	CB-CG-CD1	-5.39	117.77	121.00
35	B5	1591	C	C6-N1-C2	-5.38	118.15	120.30
36	A1	123	A	C2-N3-C4	5.38	113.29	110.60
58	AU	84	LEU	CA-CB-CG	5.38	127.67	115.30
36	A1	2935	U	N3-C2-O2	-5.37	118.44	122.20
37	A3	78	U	C2-N1-C1'	5.37	124.15	117.70
36	A1	2811	A	N1-C6-N6	-5.37	115.38	118.60
35	B5	1274	C	C2-N1-C1'	5.37	124.70	118.80
36	A1	2585	G	N3-C4-C5	-5.37	125.92	128.60
36	A1	2356	A	N9-C4-C5	-5.36	103.66	105.80
36	A1	3078	U	N3-C2-O2	-5.36	118.45	122.20
35	B5	950	C	P-O3'-C3'	5.36	126.13	119.70
35	B5	934	C	C6-N1-C1'	-5.36	114.37	120.80
35	B5	1241	G	O4'-C1'-N9	5.36	112.49	108.20
36	A1	2543	U	C5-C6-N1	5.36	125.38	122.70
36	A1	362	U	N3-C2-O2	-5.36	118.45	122.20
35	B5	633	U	N3-C2-O2	-5.35	118.45	122.20
36	A1	1901	A	C2-N3-C4	5.35	113.28	110.60
4	BD	21	LEU	CA-CB-CG	5.35	127.61	115.30
43	AE	18	LEU	CA-CB-CG	5.35	127.61	115.30
35	B5	1248	C	N1-C2-O2	5.35	122.11	118.90
35	B5	1560	U	O4'-C1'-N1	5.35	112.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1527	C	C2-N1-C1'	5.35	124.68	118.80
38	A4	5	U	N1-C2-N3	5.34	118.11	114.90
35	B5	1214	U	N1-C2-O2	5.34	126.54	122.80
36	A1	3250	U	C2-N1-C1'	5.34	124.11	117.70
33	Bg	292	LEU	CA-CB-CG	5.34	127.58	115.30
35	B5	184	C	C5-C6-N1	5.34	123.67	121.00
35	B5	1228	G	C4-N9-C1'	5.34	133.44	126.50
35	B5	496	G	C8-N9-C1'	-5.34	120.06	127.00
36	A1	1525	G	C4-N9-C1'	5.34	133.44	126.50
38	A4	4	C	C6-N1-C2	-5.33	118.17	120.30
36	A1	2712	U	N1-C2-O2	5.33	126.53	122.80
35	B5	390	G	C2-N3-C4	5.33	114.56	111.90
36	A1	915	A	C4-N9-C1'	5.33	135.89	126.30
36	A1	3308	C	N1-C2-O2	5.32	122.09	118.90
36	A1	2388	U	N1-C2-O2	5.32	126.53	122.80
37	A3	78	U	C5-C6-N1	5.32	125.36	122.70
36	A1	1694	U	C2-N1-C1'	5.31	124.08	117.70
40	AB	10	ARG	CG-CD-NE	-5.31	100.64	111.80
35	B5	1366	U	C2-N1-C1'	5.30	124.07	117.70
35	B5	1503	A	O4'-C1'-N9	5.30	112.44	108.20
35	B5	184	C	C6-N1-C2	-5.30	118.18	120.30
35	B5	581	U	C5-C6-N1	5.30	125.35	122.70
36	A1	270	U	N3-C2-O2	-5.30	118.49	122.20
36	A1	915	A	C2-N3-C4	5.29	113.25	110.60
35	B5	1000	C	N3-C2-O2	-5.29	118.19	121.90
36	A1	2689	A	C2-N3-C4	5.29	113.25	110.60
36	A1	954	U	C6-N1-C1'	-5.29	113.80	121.20
36	A1	1540	U	N1-C2-O2	5.29	126.50	122.80
36	A1	1879	A	O4'-C1'-N9	5.28	112.42	108.20
36	A1	518	G	O4'-C1'-N9	5.28	112.42	108.20
36	A1	2788	C	C6-N1-C2	-5.28	118.19	120.30
35	B5	1054	U	N1-C2-O2	5.27	126.49	122.80
35	B5	1458	G	C8-N9-C1'	-5.27	120.14	127.00
36	A1	1907	C	N3-C2-O2	-5.27	118.21	121.90
35	B5	35	U	N1-C2-O2	5.27	126.49	122.80
36	A1	282	G	P-O3'-C3'	5.27	126.02	119.70
35	B5	354	C	C6-N1-C2	-5.26	118.20	120.30
35	B5	848	C	C6-N1-C1'	5.26	127.11	120.80
36	A1	3362	A	C5-N7-C8	-5.26	101.27	103.90
36	A1	1292	C	C2-N1-C1'	5.26	124.58	118.80
36	A1	3042	U	C5-C6-N1	5.26	125.33	122.70
36	A1	890	C	C6-N1-C2	-5.25	118.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	730	G	N3-C4-N9	5.25	129.15	126.00
35	B5	1439	C	C6-N1-C2	-5.25	118.20	120.30
36	A1	379	C	C6-N1-C2	-5.25	118.20	120.30
36	A1	2622	C	C6-N1-C2	-5.24	118.20	120.30
36	A1	1604	G	N3-C4-N9	5.24	129.15	126.00
35	B5	1228	G	N3-C4-C5	-5.24	125.98	128.60
36	A1	113	C	N1-C2-O2	5.24	122.04	118.90
36	A1	1688	U	N3-C2-O2	-5.24	118.53	122.20
36	A1	315	C	C2-N1-C1'	5.24	124.56	118.80
36	A1	2641	U	N3-C2-O2	-5.24	118.53	122.20
36	A1	2810	C	C6-N1-C2	-5.23	118.21	120.30
36	A1	2764	C	C6-N1-C2	-5.23	118.21	120.30
36	A1	283	G	C4-N9-C1'	5.23	133.30	126.50
36	A1	2904	U	C2-N1-C1'	5.22	123.97	117.70
36	A1	362	U	N1-C2-O2	5.22	126.45	122.80
40	AB	21	ARG	CG-CD-NE	5.22	122.75	111.80
38	A4	21	C	C6-N1-C2	-5.21	118.22	120.30
38	A4	102	U	N1-C2-O2	5.21	126.44	122.80
35	B5	354	C	C5-C6-N1	5.21	123.60	121.00
35	B5	1687	U	C5-C6-N1	5.21	125.30	122.70
35	B5	228	G	C2-N3-C4	5.20	114.50	111.90
36	A1	3298	C	C6-N1-C2	-5.20	118.22	120.30
36	A1	2582	C	C6-N1-C2	-5.20	118.22	120.30
36	A1	2186	U	N3-C2-O2	-5.20	118.56	122.20
36	A1	2582	C	C2-N1-C1'	5.20	124.52	118.80
36	A1	2681	U	C2-N1-C1'	5.20	123.94	117.70
35	B5	1566	U	N3-C2-O2	-5.19	118.57	122.20
35	B5	1082	C	C5-C6-N1	5.19	123.60	121.00
36	A1	615	U	N3-C2-O2	-5.19	118.57	122.20
36	A1	259	C	C2-N1-C1'	5.19	124.51	118.80
36	A1	1314	C	C2'-C3'-O3'	5.19	122.00	113.70
36	A1	1108	U	N3-C2-O2	-5.19	118.57	122.20
1	BA	201	LEU	CA-CB-CG	5.18	127.21	115.30
35	B5	610	G	N3-C4-C5	-5.18	126.01	128.60
35	B5	163	G	C4-N9-C1'	5.17	133.22	126.50
36	A1	2935	U	C2-N1-C1'	5.17	123.91	117.70
62	AY	83	ASP	CB-CG-OD1	5.17	122.95	118.30
7	BG	69	LEU	CA-CB-CG	5.17	127.19	115.30
36	A1	2094	C	C2-N1-C1'	-5.17	113.11	118.80
35	B5	484	C	N1-C2-O2	5.16	122.00	118.90
36	A1	880	G	C4-N9-C1'	-5.16	119.79	126.50
35	B5	18	C	C5-C6-N1	5.16	123.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1391	A	C8-N9-C1'	-5.16	118.42	127.70
35	B5	1228	G	N3-C4-N9	5.16	129.09	126.00
36	A1	1496	C	C6-N1-C1'	-5.16	114.61	120.80
36	A1	934	G	C4-C5-N7	5.15	112.86	110.80
36	A1	418	A	N1-C2-N3	-5.15	126.72	129.30
36	A1	2285	C	C5-C6-N1	5.15	123.58	121.00
35	B5	857	U	C5-C6-N1	5.15	125.28	122.70
36	A1	421	G	C4-N9-C1'	5.15	133.19	126.50
37	A3	35	C	N3-C2-O2	-5.15	118.30	121.90
36	A1	890	C	N1-C2-O2	5.14	121.98	118.90
37	A3	26	C	C6-N1-C2	-5.14	118.24	120.30
64	Aa	91	LEU	CA-CB-CG	5.14	127.11	115.30
35	B5	1360	A	C5-N7-C8	-5.13	101.33	103.90
36	A1	3095	U	C5-C6-N1	5.13	125.27	122.70
35	B5	614	C	C6-N1-C2	-5.13	118.25	120.30
36	A1	760	G	O4'-C1'-N9	5.13	112.30	108.20
36	A1	2132	C	C6-N1-C2	-5.12	118.25	120.30
36	A1	2925	C	C6-N1-C2	-5.12	118.25	120.30
36	A1	2819	A	C6-N1-C2	5.12	121.67	118.60
35	B5	992	A	N7-C8-N9	5.12	116.36	113.80
35	B5	149	C	C2-N1-C1'	5.12	124.43	118.80
36	A1	1839	A	N1-C2-N3	-5.12	126.74	129.30
38	A4	98	U	N3-C2-O2	-5.12	118.62	122.20
2	BB	120	LEU	CA-CB-CG	5.11	127.05	115.30
35	B5	1202	A	N3-C4-N9	5.11	131.49	127.40
36	A1	113	C	N3-C2-O2	-5.11	118.32	121.90
35	B5	490	C	C6-N1-C2	-5.11	118.26	120.30
36	A1	163	C	C2-N1-C1'	5.11	124.42	118.80
36	A1	1835	A	C5-C6-N1	-5.11	115.15	117.70
36	A1	2407	C	N1-C2-O2	5.11	121.97	118.90
26	BZ	42	LEU	CA-CB-CG	5.11	127.04	115.30
35	B5	1070	C	C2-N1-C1'	5.11	124.42	118.80
36	A1	2144	A	O4'-C1'-N9	5.11	112.28	108.20
13	BM	39	ASP	CB-CG-OD1	5.10	122.89	118.30
36	A1	946	U	C5-C6-N1	5.10	125.25	122.70
35	B5	1307	U	C6-N1-C1'	-5.10	114.06	121.20
36	A1	1275	C	N3-C2-O2	-5.10	118.33	121.90
35	B5	1540	G	N3-C4-C5	-5.09	126.05	128.60
36	A1	553	U	N3-C2-O2	-5.09	118.63	122.20
36	A1	1659	U	C5-C6-N1	5.09	125.25	122.70
36	A1	3002	C	C6-N1-C2	-5.09	118.26	120.30
35	B5	1646	C	C2-N1-C1'	5.09	124.40	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1314	C	P-O3'-C3'	5.09	125.81	119.70
36	A1	259	C	C6-N1-C2	-5.09	118.27	120.30
36	A1	2274	U	C2-N1-C1'	5.09	123.81	117.70
54	AQ	180	ARG	CA-CB-CG	5.09	124.59	113.40
36	A1	2285	C	C6-N1-C2	-5.08	118.27	120.30
36	A1	1952	G	N3-C4-N9	-5.08	122.95	126.00
35	B5	795	U	C6-N1-C1'	-5.08	114.09	121.20
35	B5	469	C	C6-N1-C2	-5.08	118.27	120.30
35	B5	1021	C	C2-N1-C1'	5.07	124.38	118.80
36	A1	3072	C	C6-N1-C2	-5.07	118.27	120.30
36	A1	1032	C	P-O3'-C3'	5.07	125.78	119.70
36	A1	2883	U	C5-C6-N1	5.07	125.23	122.70
49	AL	48	PRO	N-CA-C	5.06	125.27	112.10
38	A4	28	C	C5-C6-N1	5.06	123.53	121.00
35	B5	1214	U	C2-N1-C1'	5.06	123.77	117.70
36	A1	3057	U	C2-N1-C1'	5.06	123.77	117.70
36	A1	3362	A	O4'-C1'-N9	5.06	112.25	108.20
35	B5	283	U	C2-N1-C1'	5.06	123.77	117.70
36	A1	1688	U	N1-C2-O2	5.06	126.34	122.80
36	A1	1293	U	N3-C2-O2	-5.05	118.66	122.20
35	B5	1162	C	N3-C2-O2	-5.05	118.36	121.90
35	B5	532	U	N3-C2-O2	-5.05	118.67	122.20
35	B5	1000	C	C6-N1-C1'	-5.05	114.74	120.80
36	A1	1049	C	C5-C6-N1	5.05	123.52	121.00
36	A1	3176	G	O4'-C1'-N9	5.04	112.24	108.20
35	B5	1180	C	C6-N1-C2	-5.04	118.28	120.30
35	B5	1276	U	N1-C2-O2	5.04	126.33	122.80
35	B5	1279	C	C6-N1-C2	-5.04	118.28	120.30
35	B5	795	U	C6-N1-C2	-5.04	117.98	121.00
35	B5	1235	C	N3-C2-O2	-5.04	118.37	121.90
35	B5	513	U	C5-C4-O4	-5.04	122.88	125.90
2	BB	48	VAL	C-N-CA	5.04	134.29	121.70
19	BS	15	LEU	CA-CB-CG	5.03	126.87	115.30
36	A1	1368	U	C5-C6-N1	5.03	125.22	122.70
36	A1	2334	U	N3-C2-O2	-5.03	118.68	122.20
36	A1	2532	U	N1-C2-O2	5.03	126.32	122.80
35	B5	1796	C	C6-N1-C2	-5.02	118.29	120.30
36	A1	1273	A	C2-N3-C4	5.02	113.11	110.60
37	A3	28	C	C5-C6-N1	5.02	123.51	121.00
76	Am	79	GLU	CA-CB-CG	5.02	124.44	113.40
35	B5	795	U	C5-C6-N1	5.02	125.21	122.70
35	B5	945	U	N1-C2-O2	5.02	126.31	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1620	C	C6-N1-C2	-5.02	118.29	120.30
36	A1	3244	A	N7-C8-N9	-5.01	111.29	113.80
35	B5	1168	U	N1-C2-O2	5.01	126.31	122.80
36	A1	1457	U	N3-C2-O2	-5.01	118.69	122.20
9	BI	61	GLU	CA-CB-CG	5.01	124.42	113.40
36	A1	2356	A	C5-C6-N6	-5.01	119.69	123.70
36	A1	862	U	N3-C2-O2	-5.01	118.70	122.20
35	B5	861	U	N1-C2-O2	5.00	126.30	122.80
35	B5	503	G	C4-N9-C1'	5.00	133.00	126.50
35	B5	1632	C	C6-N1-C2	-5.00	118.30	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	B5	1575	G7M	C2',C3',C4'

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	AC	130	ALA	Peptide
41	AC	318	LEU	Peptide
42	AD	258	LYS	Peptide
42	AD	43	LYS	Peptide
43	AE	67	GLY	Peptide
44	AF	157	ASN	Peptide
44	AF	215	GLY	Peptide
44	AF	232	ARG	Peptide
45	AG	121	SER	Peptide
45	AG	123	GLN	Peptide
45	AG	30	THR	Peptide
45	AG	76	ALA	Peptide
45	AG	79	GLN	Peptide
46	AH	21	LYS	Peptide
48	AJ	164	LYS	Peptide
48	AJ	166	LYS	Peptide
49	AL	47	ALA	Peptide
49	AL	75	PHE	Peptide
51	AN	80	THR	Peptide
51	AN	92	LEU	Peptide
52	AO	110[A]	PRO	Peptide
55	AR	131	ALA	Peptide
57	AT	17	ARG	Peptide

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Mol	Chain	Res	Type	Group
63	AZ	124	ALA	Peptide
64	Aa	46	ASP	Peptide
65	Ab	19	ASN	Peptide
65	Ab	20	GLY	Peptide
70	Ag	80	ARG	Peptide
71	Ah	90	ARG	Peptide
72	Ai	27	SER	Peptide
2	BB	177	GLN	Peptide
2	BB	206	PRO	Peptide
2	BB	208	GLN	Peptide
2	BB	212	VAL	Peptide
2	BB	222	LYS	Peptide
3	BC	144	TRP	Peptide
3	BC	145	GLY	Peptide
5	BE	195	ILE	Peptide
5	BE	199	GLU	Peptide
6	BF	100	ASN	Peptide
6	BF	42	LEU	Peptide
7	BG	68	LEU	Peptide
8	BH	110	GLN	Peptide
8	BH	111	LYS	Peptide
8	BH	64	VAL	Peptide
9	BI	51	GLY	Peptide
10	BJ	117	GLY	Peptide
10	BJ	137	GLY	Peptide
10	BJ	163	PRO	Peptide
11	BK	2	LEU	Peptide
11	BK	53	GLY	Peptide
11	BK	63	TYR	Peptide
12	BL	5	LEU	Peptide
15	BO	123	SER	Peptide
17	BQ	32	ASN	Peptide
17	BQ	33	GLY	Peptide
17	BQ	40	GLU	Peptide
19	BS	101	LEU	Peptide
19	BS	56	LYS	Peptide
19	BS	81	ILE	Peptide
19	BS	90	ASN	Peptide
20	BT	51	GLU	Peptide
24	BX	138	GLU	Peptide
24	BX	88	PRO	Peptide
24	BX	96	VAL	Peptide

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Mol	Chain	Res	Type	Group
25	BY	34	ASN	Peptide
27	Ba	34	LYS	Peptide
27	Ba	35	ALA	Peptide
27	Ba	57	SER	Peptide
27	Ba	7	SER	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
1	BA	204/206 (99%)	184 (90%)	19 (9%)	1 (0%)	29	54
2	BB	212/214 (99%)	178 (84%)	32 (15%)	2 (1%)	17	40
3	BC	215/217 (99%)	196 (91%)	19 (9%)	0	100	100
4	BD	221/223 (99%)	208 (94%)	13 (6%)	0	100	100
5	BE	258/260 (99%)	236 (92%)	22 (8%)	0	100	100
6	BF	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
7	BG	224/226 (99%)	207 (92%)	13 (6%)	4 (2%)	8	21
8	BH	182/184 (99%)	165 (91%)	16 (9%)	1 (0%)	29	54
9	BI	184/188 (98%)	160 (87%)	24 (13%)	0	100	100
10	BJ	183/185 (99%)	166 (91%)	15 (8%)	2 (1%)	14	34
11	BK	94/96 (98%)	84 (89%)	10 (11%)	0	100	100
12	BL	153/155 (99%)	141 (92%)	12 (8%)	0	100	100
13	BM	119/121 (98%)	89 (75%)	30 (25%)	0	100	100
14	BN	148/150 (99%)	141 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	BO	125/127 (98%)	112 (90%)	13 (10%)	0	100	100
16	BP	122/124 (98%)	109 (89%)	11 (9%)	2 (2%)	9	24
17	BQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	22	46
18	BR	117/121 (97%)	107 (92%)	8 (7%)	2 (2%)	9	23
19	BS	143/145 (99%)	128 (90%)	13 (9%)	2 (1%)	11	28
20	BT	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
21	BU	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
22	BV	83/87 (95%)	75 (90%)	8 (10%)	0	100	100
23	BW	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	43
24	BX	142/144 (99%)	120 (84%)	19 (13%)	3 (2%)	7	18
25	BY	132/134 (98%)	124 (94%)	7 (5%)	1 (1%)	19	43
26	BZ	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
27	Ba	95/97 (98%)	78 (82%)	15 (16%)	2 (2%)	7	18
28	Bb	79/81 (98%)	66 (84%)	13 (16%)	0	100	100
29	Bc	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
30	Bd	51/53 (96%)	51 (100%)	0	0	100	100
31	Be	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
32	Bf	53/57 (93%)	39 (74%)	14 (26%)	0	100	100
33	Bg	310/312 (99%)	273 (88%)	36 (12%)	1 (0%)	41	66
34	Bh	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
39	AA	245/247 (99%)	233 (95%)	12 (5%)	0	100	100
40	AB	383/386 (99%)	364 (95%)	19 (5%)	0	100	100
41	AC	359/361 (99%)	329 (92%)	27 (8%)	3 (1%)	19	43
42	AD	290/292 (99%)	268 (92%)	20 (7%)	2 (1%)	22	46
43	AE	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
44	AF	220/222 (99%)	205 (93%)	13 (6%)	2 (1%)	17	40
45	AG	228/230 (99%)	214 (94%)	14 (6%)	0	100	100
46	AH	188/190 (99%)	177 (94%)	11 (6%)	0	100	100
47	AI	201/205 (98%)	193 (96%)	8 (4%)	0	100	100
48	AJ	167/169 (99%)	147 (88%)	20 (12%)	0	100	100
49	AL	191/193 (99%)	169 (88%)	19 (10%)	3 (2%)	9	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	AM	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
51	AN	201/203 (99%)	183 (91%)	17 (8%)	1 (0%)	29	54
52	AO	195/197 (99%)	191 (98%)	3 (2%)	1 (0%)	29	54
53	AP	171/175 (98%)	167 (98%)	4 (2%)	0	100	100
54	AQ	183/185 (99%)	175 (96%)	8 (4%)	0	100	100
55	AR	186/188 (99%)	179 (96%)	7 (4%)	0	100	100
56	AS	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
57	AT	157/159 (99%)	145 (92%)	12 (8%)	0	100	100
58	AU	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
59	AV	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
60	AW	61/63 (97%)	61 (100%)	0	0	100	100
61	AX	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
62	AY	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
63	AZ	133/135 (98%)	120 (90%)	12 (9%)	1 (1%)	19	43
64	Aa	146/148 (99%)	123 (84%)	22 (15%)	1 (1%)	22	46
65	Ab	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
66	Ac	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
67	Ad	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
68	Ae	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
69	Af	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
70	Ag	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
71	Ah	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	17	40
72	Ai	97/99 (98%)	87 (90%)	10 (10%)	0	100	100
73	Aj	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
74	Ak	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
75	Al	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
76	Am	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
77	An	23/25 (92%)	23 (100%)	0	0	100	100
78	Ao	103/105 (98%)	90 (87%)	13 (13%)	0	100	100
79	Ap	89/91 (98%)	83 (93%)	5 (6%)	1 (1%)	14	34
All	All	10956/11121 (98%)	10097 (92%)	818 (8%)	41 (0%)	38	60

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	AC	339	LEU
49	AL	48	PRO
49	AL	76	THR
51	AN	81	TYR
52	AO	111[A]	PRO
64	Aa	78	LEU
2	BB	206	PRO
2	BB	207	LEU
7	BG	173	PRO
8	BH	111	LYS
10	BJ	134	ILE
16	BP	125	PRO
19	BS	91	ASP
24	BX	97	ASP
42	AD	20	PHE
49	AL	63	VAL
1	BA	4	PRO
7	BG	68	LEU
10	BJ	133	HIS
27	Ba	35	ALA
27	Ba	36	ILE
42	AD	259	LYS
18	BR	23	LYS
18	BR	24	LEU
24	BX	137	LYS
41	AC	268	ALA
71	Ah	91	ALA
79	Ap	52	ALA
44	AF	158	LYS
17	BQ	33	GLY
24	BX	96	VAL
33	Bg	51	ASP
7	BG	69	LEU
19	BS	92	ILE
44	AF	216	VAL
16	BP	126	VAL
63	AZ	103	GLN
7	BG	67	VAL
41	AC	131	VAL
23	BW	67	GLY
25	BY	35	VAL

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	
1	BA	173/173 (100%)	173 (100%)	0	100	100
2	BB	191/191 (100%)	190 (100%)	1 (0%)	88	96
3	BC	176/176 (100%)	176 (100%)	0	100	100
4	BD	182/182 (100%)	180 (99%)	2 (1%)	73	90
5	BE	221/221 (100%)	220 (100%)	1 (0%)	88	96
6	BF	173/173 (100%)	173 (100%)	0	100	100
7	BG	193/193 (100%)	192 (100%)	1 (0%)	88	96
8	BH	165/165 (100%)	165 (100%)	0	100	100
9	BI	150/150 (100%)	150 (100%)	0	100	100
10	BJ	158/158 (100%)	158 (100%)	0	100	100
11	BK	89/89 (100%)	89 (100%)	0	100	100
12	BL	136/136 (100%)	135 (99%)	1 (1%)	84	94
13	BM	98/98 (100%)	98 (100%)	0	100	100
14	BN	127/127 (100%)	127 (100%)	0	100	100
15	BO	96/96 (100%)	96 (100%)	0	100	100
16	BP	104/104 (100%)	104 (100%)	0	100	100
17	BQ	117/117 (100%)	117 (100%)	0	100	100
18	BR	110/110 (100%)	110 (100%)	0	100	100
19	BS	128/128 (100%)	128 (100%)	0	100	100
20	BT	113/113 (100%)	113 (100%)	0	100	100
21	BU	100/100 (100%)	99 (99%)	1 (1%)	76	91
22	BV	74/74 (100%)	74 (100%)	0	100	100
23	BW	110/110 (100%)	110 (100%)	0	100	100
24	BX	119/119 (100%)	119 (100%)	0	100	100
25	BY	112/112 (100%)	110 (98%)	2 (2%)	59	83
26	BZ	61/61 (100%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	Ba	83/83 (100%)	82 (99%)	1 (1%)	71	88
28	Bb	70/70 (100%)	70 (100%)	0	100	100
29	Bc	56/56 (100%)	54 (96%)	2 (4%)	35	64
30	Bd	47/47 (100%)	46 (98%)	1 (2%)	53	80
31	Be	51/51 (100%)	50 (98%)	1 (2%)	55	81
32	Bf	49/49 (100%)	49 (100%)	0	100	100
33	Bg	256/257 (100%)	255 (100%)	1 (0%)	91	97
34	Bh	68/68 (100%)	65 (96%)	3 (4%)	28	56
39	AA	189/189 (100%)	189 (100%)	0	100	100
40	AB	319/321 (99%)	318 (100%)	1 (0%)	92	98
41	AC	288/288 (100%)	287 (100%)	1 (0%)	92	98
42	AD	241/241 (100%)	241 (100%)	0	100	100
43	AE	134/134 (100%)	133 (99%)	1 (1%)	84	94
44	AF	186/186 (100%)	185 (100%)	1 (0%)	88	96
45	AG	189/189 (100%)	189 (100%)	0	100	100
46	AH	170/170 (100%)	169 (99%)	1 (1%)	86	95
47	AI	176/176 (100%)	174 (99%)	2 (1%)	73	90
48	AJ	147/147 (100%)	147 (100%)	0	100	100
49	AL	154/154 (100%)	154 (100%)	0	100	100
50	AM	107/107 (100%)	107 (100%)	0	100	100
51	AN	175/175 (100%)	175 (100%)	0	100	100
52	AO	160/160 (100%)	160 (100%)	0	100	100
53	AP	141/141 (100%)	140 (99%)	1 (1%)	84	94
54	AQ	150/150 (100%)	150 (100%)	0	100	100
55	AR	153/153 (100%)	153 (100%)	0	100	100
56	AS	156/156 (100%)	156 (100%)	0	100	100
57	AT	136/136 (100%)	135 (99%)	1 (1%)	84	94
58	AU	87/87 (100%)	87 (100%)	0	100	100
59	AV	104/104 (100%)	104 (100%)	0	100	100
60	AW	55/55 (100%)	55 (100%)	0	100	100
61	AX	105/105 (100%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	AY	109/109 (100%)	109 (100%)	0	100	100
63	AZ	115/115 (100%)	115 (100%)	0	100	100
64	Aa	118/118 (100%)	118 (100%)	0	100	100
65	Ab	46/46 (100%)	46 (100%)	0	100	100
66	Ac	81/81 (100%)	81 (100%)	0	100	100
67	Ad	96/96 (100%)	96 (100%)	0	100	100
68	Ae	109/109 (100%)	109 (100%)	0	100	100
69	Af	90/90 (100%)	90 (100%)	0	100	100
70	Ag	95/95 (100%)	95 (100%)	0	100	100
71	Ah	104/104 (100%)	103 (99%)	1 (1%)	76	91
72	Ai	81/81 (100%)	81 (100%)	0	100	100
73	Aj	70/70 (100%)	70 (100%)	0	100	100
74	Ak	68/68 (100%)	68 (100%)	0	100	100
75	Al	45/45 (100%)	45 (100%)	0	100	100
76	Am	47/47 (100%)	47 (100%)	0	100	100
77	An	23/23 (100%)	23 (100%)	0	100	100
78	Ao	90/90 (100%)	90 (100%)	0	100	100
79	Ap	71/71 (100%)	71 (100%)	0	100	100
All	All	9336/9339 (100%)	9308 (100%)	28 (0%)	92	98

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BB	152	ARG
4	BD	51	ARG
4	BD	76	ARG
5	BE	258	GLN
7	BG	98	ARG
12	BL	67	ARG
21	BU	52	LYS
25	BY	8	ARG
25	BY	32	ARG
27	Ba	69	ASN
29	Bc	38	ARG
29	Bc	64	ARG
30	Bd	28	THR

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Mol	Chain	Res	Type
31	Be	29	LYS
33	Bg	118	LYS
34	Bh	53	ARG
34	Bh	70	ASN
34	Bh	88	ARG
40	AB	332	ARG
41	AC	138	ARG
43	AE	20	LYS
44	AF	157	ASN
46	AH	157	ASN
47	AI	121	LYS
47	AI	191	LYS
53	AP	46	LYS
57	AT	83	ARG
71	Ah	94	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	30	GLN
6	BF	66	GLN
34	Bh	71	ASN
41	AC	110	ASN
42	AD	151	GLN
48	AJ	95	ASN
59	AV	98	ASN
64	Aa	49	HIS
67	Ad	57	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	B5	1774/1781 (99%)	472 (26%)	12 (0%)
36	A1	3130/3137 (99%)	706 (22%)	17 (0%)
37	A3	120/121 (99%)	13 (10%)	0
38	A4	156/158 (98%)	37 (23%)	1 (0%)
All	All	5180/5197 (99%)	1228 (23%)	30 (0%)

All (1228) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	B5	2	A
35	B5	4	C
35	B5	17	C
35	B5	25	C
35	B5	26	A
35	B5	34	G
35	B5	45	U
35	B5	46	A
35	B5	47	A
35	B5	57	G
35	B5	60	U
35	B5	68	A
35	B5	72	A
35	B5	73	U
35	B5	74	U
35	B5	75	U
35	B5	76	A
35	B5	77	U
35	B5	78	A
35	B5	81	G
35	B5	83	G
35	B5	94	U
35	B5	103	A
35	B5	104	A
35	B5	111	U
35	B5	114	C
35	B5	116	U
35	B5	126	A
35	B5	127	G
35	B5	130	C
35	B5	133	U
35	B5	134	U
35	B5	135	A
35	B5	136	C
35	B5	137	U
35	B5	138	A
35	B5	140	A
35	B5	141	U
35	B5	145	A
35	B5	158	U
35	B5	161	U
35	B5	166	C
35	B5	168	A

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Mol	Chain	Res	Type
35	B5	171	A
35	B5	178	U
35	B5	182	A
35	B5	183	U
35	B5	188	A
35	B5	189	C
35	B5	190	C
35	B5	191	C
35	B5	192	U
35	B5	194	U
35	B5	195	G
35	B5	198	A
35	B5	199	G
35	B5	200	A
35	B5	204	G
35	B5	215	A
35	B5	217	A
35	B5	218	A
35	B5	226	A
35	B5	227	U
35	B5	229	U
35	B5	230	C
35	B5	231	U
35	B5	232	U
35	B5	233	C
35	B5	234	G
35	B5	235	G
35	B5	236	A
35	B5	237	C
35	B5	238	U
35	B5	239	C
35	B5	240	U
35	B5	241	U
35	B5	246	G
35	B5	249	U
35	B5	250	C
35	B5	260	U
35	B5	261	U
35	B5	262	U
35	B5	265	A
35	B5	267	U
35	B5	272	U

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Mol	Chain	Res	Type
35	B5	273	G
35	B5	277	U
35	B5	280	U
35	B5	281	G
35	B5	287	G
35	B5	304	U
35	B5	313	U
35	B5	314	C
35	B5	315	A
35	B5	316	A
35	B5	320	U
35	B5	321	C
35	B5	322	G
35	B5	333	A
35	B5	337	G
35	B5	338	C
35	B5	352	A
35	B5	359	A
35	B5	360	A
35	B5	361	C
35	B5	365	G
35	B5	380	U
35	B5	389	G
35	B5	390	G
35	B5	393	C
35	B5	400	A
35	B5	401	A
35	B5	402	C
35	B5	404	G
35	B5	417	A
35	B5	419	G
35	B5	423	G
35	B5	424	C
35	B5	425	A
35	B5	426	G
35	B5	427	C
35	B5	434	G
35	B5	439	U
35	B5	444	C
35	B5	452	A
35	B5	460	A
35	B5	464	A

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Mol	Chain	Res	Type
35	B5	468	A
35	B5	475	A
35	B5	477	A
35	B5	481	A
35	B5	483	A
35	B5	484	C
35	B5	486	G
35	B5	488	G
35	B5	489	C
35	B5	490	C
35	B5	491	C
35	B5	492	A
35	B5	493	U
35	B5	494	U
35	B5	495	C
35	B5	496	G
35	B5	497	G
35	B5	498	G
35	B5	499	U
35	B5	500	C
35	B5	503	G
35	B5	506	A
35	B5	507	U
35	B5	510	G
35	B5	514	G
35	B5	515	A
35	B5	519	C
35	B5	524	U
35	B5	527	A
35	B5	538	A
35	B5	539	G
35	B5	540	G
35	B5	541	A2M
35	B5	542	A
35	B5	544	A
35	B5	545	A
35	B5	557	G
35	B5	558	U
35	B5	559	C
35	B5	565	C
35	B5	566	C
35	B5	571	G

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Mol	Chain	Res	Type
35	B5	572	C
35	B5	577	G
35	B5	578	OMU
35	B5	579	A
35	B5	580	A
35	B5	582	U
35	B5	594	A
35	B5	595	G
35	B5	609	U
35	B5	610	G
35	B5	611	U
35	B5	613	G
35	B5	617	U
35	B5	619	A2M
35	B5	620	A
35	B5	621	A
35	B5	622	A
35	B5	623	A
35	B5	638	U
35	B5	639	U
35	B5	650	U
35	B5	651	G
35	B5	652	G
35	B5	653	C
35	B5	655	G
35	B5	656	G
35	B5	657	U
35	B5	658	C
35	B5	677	G
35	B5	678	A
35	B5	679	U
35	B5	681	U
35	B5	683	C
35	B5	694	U
35	B5	696	C
35	B5	697	C
35	B5	698	U
35	B5	700	C
35	B5	701	U
35	B5	704	C
35	B5	705	U
35	B5	706	A

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Mol	Chain	Res	Type
35	B5	707	A
35	B5	708	C
35	B5	710	U
35	B5	712	G
35	B5	713	A
35	B5	715	U
35	B5	716	C
35	B5	717	C
35	B5	718	U
35	B5	719	U
35	B5	720	G
35	B5	721	U
35	B5	722	G
35	B5	723	G
35	B5	724	C
35	B5	725	U
35	B5	727	U
35	B5	728	U
35	B5	730	G
35	B5	731	C
35	B5	732	G
35	B5	733	A
35	B5	734	A
35	B5	735	C
35	B5	736	C
35	B5	737	A
35	B5	738	G
35	B5	743	U
35	B5	745	U
35	B5	755	A
35	B5	765	G
35	B5	766	PSU
35	B5	767	U
35	B5	774	A
35	B5	775	G
35	B5	778	G
35	B5	780	A
35	B5	781	U
35	B5	782	U
35	B5	783	G
35	B5	784	C
35	B5	787	G

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Mol	Chain	Res	Type
35	B5	789	A
35	B5	794	U
35	B5	812	A
35	B5	813	U
35	B5	814	A
35	B5	815	G
35	B5	819	G
35	B5	820	U
35	B5	822	U
35	B5	823	G
35	B5	825	U
35	B5	826	U
35	B5	828	U
35	B5	829	A
35	B5	830	U
35	B5	833	U
35	B5	834	G
35	B5	836	U
35	B5	840	U
35	B5	841	U
35	B5	843	U
35	B5	844	A
35	B5	845	G
35	B5	846	G
35	B5	847	A
35	B5	848	C
35	B5	849	C
35	B5	850	A
35	B5	851	U
35	B5	852	C
35	B5	853	G
35	B5	856	A
35	B5	857	U
35	B5	859	A
35	B5	863	A
35	B5	864	U
35	B5	873	U
35	B5	886	U
35	B5	898	A
35	B5	906	A
35	B5	933	A
35	B5	935	U

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Mol	Chain	Res	Type
35	B5	951	A
35	B5	960	U
35	B5	964	U
35	B5	966	A
35	B5	973	A
35	B5	987	G
35	B5	992	A
35	B5	993	A
35	B5	997	G
35	B5	1004	U
35	B5	1005	A
35	B5	1010	C
35	B5	1021	C
35	B5	1023	A
35	B5	1025	A
35	B5	1026	A
35	B5	1028	C
35	B5	1032	G
35	B5	1039	A
35	B5	1052	U
35	B5	1054	U
35	B5	1056	U
35	B5	1058	U
35	B5	1059	U
35	B5	1061	A
35	B5	1062	A
35	B5	1064	G
35	B5	1076	A
35	B5	1082	C
35	B5	1086	A
35	B5	1092	A
35	B5	1093	A
35	B5	1097	U
35	B5	1098	U
35	B5	1100	G
35	B5	1111	G
35	B5	1137	A
35	B5	1138	A
35	B5	1141	G
35	B5	1147	A
35	B5	1150	G
35	B5	1158	C

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Mol	Chain	Res	Type
35	B5	1185	U
35	B5	1186	U
35	B5	1194	A
35	B5	1196	A
35	B5	1199	G
35	B5	1200	G
35	B5	1201	G
35	B5	1202	A
35	B5	1203	A
35	B5	1217	A
35	B5	1218	G
35	B5	1226	A
35	B5	1227	A
35	B5	1228	G
35	B5	1235	C
35	B5	1243	G
35	B5	1244	A
35	B5	1245	G
35	B5	1255	G
35	B5	1256	A
35	B5	1270	G
35	B5	1284	C
35	B5	1285	U
35	B5	1291	G
35	B5	1306	C
35	B5	1314	U
35	B5	1315	U
35	B5	1316	G
35	B5	1321	A
35	B5	1340	U
35	B5	1344	A
35	B5	1345	A
35	B5	1349	G
35	B5	1355	C
35	B5	1356	U
35	B5	1358	G
35	B5	1359	C
35	B5	1361	U
35	B5	1362	U
35	B5	1363	U
35	B5	1364	G
35	B5	1368	G

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Mol	Chain	Res	Type
35	B5	1371	A
35	B5	1372	U
35	B5	1373	C
35	B5	1378	U
35	B5	1388	A
35	B5	1390	U
35	B5	1399	C
35	B5	1400	A
35	B5	1410	A
35	B5	1413	U
35	B5	1415	PSU
35	B5	1424	A
35	B5	1426	C
35	B5	1427	A
35	B5	1428	OMG
35	B5	1436	A
35	B5	1459	C
35	B5	1461	C
35	B5	1469	A
35	B5	1471	A
35	B5	1483	A
35	B5	1486	G
35	B5	1491	U
35	B5	1492	A
35	B5	1493	A
35	B5	1496	U
35	B5	1503	A
35	B5	1506	G
35	B5	1514	U
35	B5	1516	A
35	B5	1520	U
35	B5	1521	G
35	B5	1523	G
35	B5	1524	A
35	B5	1527	C
35	B5	1537	C
35	B5	1557	U
35	B5	1559	A
35	B5	1573	A
35	B5	1575	G7M
35	B5	1576	A
35	B5	1584	G

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Mol	Chain	Res	Type
35	B5	1590	G
35	B5	1596	C
35	B5	1597	A
35	B5	1600	A
35	B5	1601	G
35	B5	1605	G
35	B5	1616	G
35	B5	1632	C
35	B5	1635	A
35	B5	1636	C
35	B5	1637	C
35	B5	1646	C
35	B5	1651	A
35	B5	1657	U
35	B5	1658	G
35	B5	1663	G
35	B5	1666	U
35	B5	1680	G
35	B5	1682	U
35	B5	1683	C
35	B5	1684	U
35	B5	1686	C
35	B5	1687	U
35	B5	1689	A
35	B5	1690	G
35	B5	1693	A
35	B5	1694	A
35	B5	1695	G
35	B5	1696	G
35	B5	1698	G
35	B5	1699	G
35	B5	1700	C
35	B5	1701	A
35	B5	1702	A
35	B5	1703	C
35	B5	1706	C
35	B5	1709	C
35	B5	1710	U
35	B5	1711	C
35	B5	1716	C
35	B5	1717	G
35	B5	1760	G

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Mol	Chain	Res	Type
35	B5	1762	A
35	B5	1766	A
35	B5	1769	U
35	B5	1780	G
35	B5	1792	G
35	B5	1793	G
35	B5	1794	A
35	B5	1795	U
35	B5	1796	C
36	A1	4	U
36	A1	11	A
36	A1	18	G
36	A1	26	A
36	A1	34	A
36	A1	40	A
36	A1	43	A
36	A1	49	A
36	A1	57	A
36	A1	59	G
36	A1	60	A
36	A1	65	A
36	A1	66	A
36	A1	68	C
36	A1	69	C
36	A1	75	G
36	A1	77	A
36	A1	83	U
36	A1	85	A
36	A1	92	G
36	A1	109	A
36	A1	110	G
36	A1	111	C
36	A1	115	A
36	A1	116	A
36	A1	117	U
36	A1	121	A
36	A1	122	A
36	A1	134	U
36	A1	135	C
36	A1	136	G
36	A1	143	G
36	A1	150	A

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Mol	Chain	Res	Type
36	A1	155	G
36	A1	156	G
36	A1	157	A
36	A1	163	C
36	A1	165	A
36	A1	166	C
36	A1	169	U
36	A1	173	G
36	A1	190	U
36	A1	191	U
36	A1	200	C
36	A1	210	U
36	A1	211	A
36	A1	216	G
36	A1	219	A
36	A1	220	G
36	A1	239	G
36	A1	240	U
36	A1	241	G
36	A1	242	C
36	A1	243	G
36	A1	249	U
36	A1	250	U
36	A1	252	U
36	A1	260	C
36	A1	266	A
36	A1	267	G
36	A1	268	A
36	A1	269	G
36	A1	283	G
36	A1	285	A
36	A1	286	U
36	A1	295	A
36	A1	298	U
36	A1	299	G
36	A1	300	G
36	A1	305	U
36	A1	315	C
36	A1	317	A
36	A1	326	U
36	A1	329	U
36	A1	334	A

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Mol	Chain	Res	Type
36	A1	337	G
36	A1	338	A
36	A1	339	C
36	A1	346	C
36	A1	349	A
36	A1	351	A
36	A1	352	A
36	A1	369	A
36	A1	370	U
36	A1	371	G
36	A1	372	A
36	A1	373	A
36	A1	374	A
36	A1	376	G
36	A1	385	A
36	A1	387	A
36	A1	398	A
36	A1	399	A
36	A1	400	G
36	A1	402	A
36	A1	403	C
36	A1	420	G
36	A1	421	G
36	A1	422	A
36	A1	438	A
36	A1	440	A
36	A1	495	G
36	A1	496	C
36	A1	510	G
36	A1	518	G
36	A1	521	A
36	A1	523	A
36	A1	532	A
36	A1	533	A
36	A1	535	G
36	A1	540	U
36	A1	542	G
36	A1	543	C
36	A1	545	U
36	A1	546	C
36	A1	547	G
36	A1	548	G

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Mol	Chain	Res	Type
36	A1	550	A
36	A1	552	G
36	A1	553	U
36	A1	555	U
36	A1	556	U
36	A1	557	A
36	A1	559	A
36	A1	569	A
36	A1	578	A
36	A1	579	G
36	A1	583	G
36	A1	591	G
36	A1	592	A
36	A1	602	A
36	A1	604	G
36	A1	608	A
36	A1	611	A
36	A1	612	U
36	A1	649	A2M
36	A1	660	A
36	A1	677	A
36	A1	681	U
36	A1	690	A
36	A1	691	A
36	A1	705	A
36	A1	715	A
36	A1	719	U
36	A1	725	G
36	A1	733	G
36	A1	735	A
36	A1	736	A
36	A1	737	G
36	A1	758	C
36	A1	764	U
36	A1	765	C
36	A1	766	U
36	A1	767	U
36	A1	771	A
36	A1	774	G
36	A1	776	PSU
36	A1	777	U
36	A1	780	A

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Mol	Chain	Res	Type
36	A1	781	G
36	A1	784	A
36	A1	785	G
36	A1	786	A
36	A1	799	G
36	A1	801	A
36	A1	806	A
36	A1	807	A2M
36	A1	808	A
36	A1	813	G
36	A1	817	A2M
36	A1	818	C
36	A1	830	A
36	A1	844	G
36	A1	848	A
36	A1	849	C
36	A1	857	G
36	A1	861	C
36	A1	862	U
36	A1	865	U
36	A1	874	U
36	A1	879	U
36	A1	881	C
36	A1	896	A
36	A1	897	U
36	A1	907	G
36	A1	908	OMG
36	A1	909	G
36	A1	914	A
36	A1	915	A
36	A1	916	G
36	A1	917	A
36	A1	920	A
36	A1	921	A
36	A1	923	C
36	A1	924	G
36	A1	925	A
36	A1	934	G
36	A1	937	G
36	A1	944	C
36	A1	959	C
36	A1	960	PSU

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Mol	Chain	Res	Type
36	A1	962	A
36	A1	963	G
36	A1	970	A
36	A1	979	U
36	A1	980	A
36	A1	981	U
36	A1	982	C
36	A1	984	G
36	A1	991	G
36	A1	995	U
36	A1	1002	A
36	A1	1006	A
36	A1	1010	G
36	A1	1016	C
36	A1	1017	C
36	A1	1018	G
36	A1	1019	G
36	A1	1022	U
36	A1	1023	C
36	A1	1031	C
36	A1	1032	C
36	A1	1033	U
36	A1	1034	U
36	A1	1035	G
36	A1	1041	U
36	A1	1045	C
36	A1	1047	A
36	A1	1049	C
36	A1	1063	G
36	A1	1064	A
36	A1	1066	G
36	A1	1068	C
36	A1	1072	G
36	A1	1074	U
36	A1	1081	U
36	A1	1087	G
36	A1	1094	U
36	A1	1097	G
36	A1	1098	A
36	A1	1099	A
36	A1	1103	A
36	A1	1104	G

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Mol	Chain	Res	Type
36	A1	1117	G
36	A1	1131	G
36	A1	1132	C
36	A1	1135	A
36	A1	1144	U
36	A1	1153	A
36	A1	1154	A
36	A1	1155	C
36	A1	1159	A
36	A1	1178	G
36	A1	1180	A
36	A1	1181	U
36	A1	1182	A
36	A1	1189	C
36	A1	1191	U
36	A1	1192	C
36	A1	1196	C
36	A1	1200	A
36	A1	1201	C
36	A1	1202	A
36	A1	1208	U
36	A1	1222	G
36	A1	1223	A
36	A1	1227	C
36	A1	1228	C
36	A1	1231	A
36	A1	1232	C
36	A1	1233	G
36	A1	1235	U
36	A1	1236	G
36	A1	1237	G
36	A1	1239	C
36	A1	1240	A
36	A1	1241	U
36	A1	1242	G
36	A1	1243	G
36	A1	1244	A
36	A1	1245	A
36	A1	1246	G
36	A1	1247	U
36	A1	1248	C
36	A1	1249	G

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Mol	Chain	Res	Type
36	A1	1250	G
36	A1	1251	A
36	A1	1252	A
36	A1	1263	A
36	A1	1268	G
36	A1	1270	A
36	A1	1271	A
36	A1	1272	C
36	A1	1273	A
36	A1	1277	C
36	A1	1281	G
36	A1	1282	G
36	A1	1283	C
36	A1	1286	A
36	A1	1287	A
36	A1	1292	C
36	A1	1305	U
36	A1	1307	G
36	A1	1309	U
36	A1	1315	U
36	A1	1317	A
36	A1	1318	A
36	A1	1332	A
36	A1	1348	U
36	A1	1349	G
36	A1	1350	A
36	A1	1351	U
36	A1	1352	A
36	A1	1353	U
36	A1	1354	G
36	A1	1355	A
36	A1	1356	U
36	A1	1357	G
36	A1	1386	A
36	A1	1392	G
36	A1	1399	A
36	A1	1400	G
36	A1	1408	G
36	A1	1417	G
36	A1	1418	A
36	A1	1419	A
36	A1	1434	G

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Mol	Chain	Res	Type
36	A1	1437	OMC
36	A1	1443	G
36	A1	1450	OMG
36	A1	1455	U
36	A1	1460	A
36	A1	1465	A
36	A1	1469	C
36	A1	1477	A
36	A1	1481	A
36	A1	1487	G
36	A1	1496	C
36	A1	1508	C
36	A1	1511	U
36	A1	1524	A
36	A1	1536	G
36	A1	1539	A
36	A1	1548	C
36	A1	1553	U
36	A1	1555	U
36	A1	1557	A
36	A1	1558	A
36	A1	1561	G
36	A1	1562	C
36	A1	1564	U
36	A1	1565	G
36	A1	1566	A
36	A1	1567	U
36	A1	1570	U
36	A1	1572	U
36	A1	1574	C
36	A1	1575	A
36	A1	1576	G
36	A1	1577	G
36	A1	1583	A
36	A1	1587	A
36	A1	1589	A
36	A1	1590	G
36	A1	1593	A
36	A1	1605	A
36	A1	1621	A
36	A1	1628	C
36	A1	1629	U

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Mol	Chain	Res	Type
36	A1	1630	U
36	A1	1641	U
36	A1	1642	A
36	A1	1643	A
36	A1	1645	U
36	A1	1657	C
36	A1	1664	G
36	A1	1714	A
36	A1	1724	U
36	A1	1730	G
36	A1	1736	G
36	A1	1741	A
36	A1	1742	U
36	A1	1750	A
36	A1	1751	G
36	A1	1761	C
36	A1	1762	C
36	A1	1763	U
36	A1	1764	U
36	A1	1765	U
36	A1	1766	G
36	A1	1778	G
36	A1	1780	G
36	A1	1797	A
36	A1	1813	A
36	A1	1814	A
36	A1	1815	U
36	A1	1816	A
36	A1	1817	G
36	A1	1820	U
36	A1	1821	U
36	A1	1834	U
36	A1	1839	A
36	A1	1842	A
36	A1	1846	C
36	A1	1848	G
36	A1	1849	C
36	A1	1858	A
36	A1	1860	G
36	A1	1866	C
36	A1	1867	A
36	A1	1878	G

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Mol	Chain	Res	Type
36	A1	1880	U
36	A1	1886	A
36	A1	1890	U
36	A1	1893	A
36	A1	1897	G
36	A1	1906	G
36	A1	1908	A
36	A1	1932	A
36	A1	1934	G
36	A1	1947	G
36	A1	1948	G
36	A1	1949	G
36	A1	1951	C
36	A1	1952	G
36	A1	1953	G
36	A1	2094	C
36	A1	2095	G
36	A1	2096	A
36	A1	2112	U
36	A1	2114	C
36	A1	2121	G
36	A1	2122	G
36	A1	2131	A
36	A1	2140	U
36	A1	2142	1MA
36	A1	2144	A
36	A1	2158	A
36	A1	2159	U
36	A1	2160	G
36	A1	2162	U
36	A1	2164	A
36	A1	2165	G
36	A1	2169	G
36	A1	2170	U
36	A1	2171	G
36	A1	2176	U
36	A1	2187	G
36	A1	2188	A
36	A1	2192	C
36	A1	2195	C
36	A1	2197	OMC
36	A1	2205	U

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Mol	Chain	Res	Type
36	A1	2206	G
36	A1	2207	A
36	A1	2209	U
36	A1	2210	G
36	A1	2213	A
36	A1	2225	U
36	A1	2244	A
36	A1	2249	G
36	A1	2250	G
36	A1	2256	A
36	A1	2257	C
36	A1	2258	U
36	A1	2260	PSU
36	A1	2266	PSU
36	A1	2268	U
36	A1	2269	U
36	A1	2270	A
36	A1	2272	G
36	A1	2273	G
36	A1	2274	U
36	A1	2280	A2M
36	A1	2281	A2M
36	A1	2282	U
36	A1	2287	C
36	A1	2288	OMG
36	A1	2304	C
36	A1	2307	G
36	A1	2308	C
36	A1	2310	U
36	A1	2313	A
36	A1	2314	PSU
36	A1	2315	G
36	A1	2318	U
36	A1	2334	U
36	A1	2335	G
36	A1	2336	U
36	A1	2372	A
36	A1	2373	A
36	A1	2374	C
36	A1	2375	G
36	A1	2377	G
36	A1	2383	C

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Mol	Chain	Res	Type
36	A1	2388	U
36	A1	2391	G
36	A1	2393	G
36	A1	2397	A
36	A1	2402	A
36	A1	2403	G
36	A1	2404	A
36	A1	2411	U
36	A1	2412	G
36	A1	2418	G
36	A1	2419	A
36	A1	2422	C
36	A1	2435	G
36	A1	2438	A
36	A1	2440	G
36	A1	2441	A
36	A1	2442	G
36	A1	2443	A
36	A1	2444	C
36	A1	2445	A
36	A1	2502	A
36	A1	2504	U
36	A1	2506	U
36	A1	2508	U
36	A1	2511	A
36	A1	2514	U
36	A1	2515	A
36	A1	2523	A
36	A1	2524	A
36	A1	2529	A
36	A1	2531	C
36	A1	2536	A
36	A1	2537	U
36	A1	2538	U
36	A1	2539	C
36	A1	2540	A
36	A1	2541	U
36	A1	2543	U
36	A1	2544	U
36	A1	2548	C
36	A1	2549	G
36	A1	2550	U

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Mol	Chain	Res	Type
36	A1	2552	C
36	A1	2554	A
36	A1	2561	A
36	A1	2568	C
36	A1	2569	A
36	A1	2570	U
36	A1	2571	U
36	A1	2572	C
36	A1	2573	G
36	A1	2576	G
36	A1	2580	A
36	A1	2581	U
36	A1	2585	G
36	A1	2586	G
36	A1	2593	A
36	A1	2606	G
36	A1	2607	G
36	A1	2614	G
36	A1	2626	A
36	A1	2629	U
36	A1	2642	A
36	A1	2651	G
36	A1	2652	U
36	A1	2656	A
36	A1	2674	A
36	A1	2676	A
36	A1	2677	G
36	A1	2679	A
36	A1	2688	U
36	A1	2689	A
36	A1	2690	G
36	A1	2691	A
36	A1	2703	A
36	A1	2704	A
36	A1	2712	U
36	A1	2714	G
36	A1	2727	A
36	A1	2728	G
36	A1	2729	OMU
36	A1	2737	C
36	A1	2739	A
36	A1	2740	A

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Mol	Chain	Res	Type
36	A1	2752	U
36	A1	2753	G
36	A1	2761	G
36	A1	2762	A
36	A1	2772	C
36	A1	2777	G
36	A1	2778	G
36	A1	2794	G
36	A1	2796	G
36	A1	2797	C
36	A1	2800	G
36	A1	2801	A
36	A1	2803	A
36	A1	2810	C
36	A1	2814	G
36	A1	2817	A
36	A1	2818	U
36	A1	2822	U
36	A1	2828	G
36	A1	2842	U
36	A1	2844	C
36	A1	2845	A
36	A1	2849	C
36	A1	2859	U
36	A1	2860	U
36	A1	2867	C
36	A1	2871	G
36	A1	2872	A
36	A1	2887	A
36	A1	2889	C
36	A1	2898	G
36	A1	2918	G
36	A1	2923	PSU
36	A1	2930	A
36	A1	2935	U
36	A1	2936	A
36	A1	2938	G
36	A1	2942	C
36	A1	2947	G
36	A1	2951	G
36	A1	2954	U
36	A1	2977	G

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Mol	Chain	Res	Type
36	A1	2983	C
36	A1	2990	G
36	A1	2996	U
36	A1	2997	G
36	A1	3011	A
36	A1	3012	A
36	A1	3022	G
36	A1	3032	A
36	A1	3056	U
36	A1	3059	G
36	A1	3074	G
36	A1	3078	U
36	A1	3079	U
36	A1	3080	G
36	A1	3086	A
36	A1	3087	A
36	A1	3092	C
36	A1	3104	U
36	A1	3109	G
36	A1	3122	A
36	A1	3130	A
36	A1	3131	U
36	A1	3142	A
36	A1	3143	C
36	A1	3153	U
36	A1	3154	C
36	A1	3155	U
36	A1	3156	U
36	A1	3157	U
36	A1	3165	A
36	A1	3170	A
36	A1	3172	A
36	A1	3173	G
36	A1	3174	A
36	A1	3179	U
36	A1	3181	C
36	A1	3187	A
36	A1	3195	U
36	A1	3196	U
36	A1	3198	U
36	A1	3207	U
36	A1	3209	A

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Mol	Chain	Res	Type
36	A1	3215	A
36	A1	3216	G
36	A1	3217	C
36	A1	3218	A
36	A1	3219	G
36	A1	3224	G
36	A1	3243	A
36	A1	3245	A
36	A1	3247	G
36	A1	3251	U
36	A1	3254	G
36	A1	3259	U
36	A1	3260	G
36	A1	3263	G
36	A1	3273	A
36	A1	3275	U
36	A1	3276	G
36	A1	3277	U
36	A1	3278	C
36	A1	3281	U
36	A1	3283	U
36	A1	3284	G
36	A1	3289	G
36	A1	3294	A
36	A1	3304	U
36	A1	3307	A
36	A1	3316	A
36	A1	3317	U
36	A1	3318	G
36	A1	3342	A
36	A1	3345	G
36	A1	3351	U
36	A1	3352	U
36	A1	3353	G
36	A1	3354	U
36	A1	3355	U
36	A1	3356	G
36	A1	3369	G
36	A1	3375	A
36	A1	3378	C
36	A1	3382	U
36	A1	3389	U

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Mol	Chain	Res	Type
36	A1	3395	G
37	A3	11	A
37	A3	13	A
37	A3	35	C
37	A3	49	G
37	A3	52	G
37	A3	54	U
37	A3	55	A
37	A3	65	G
37	A3	73	C
37	A3	76	A
37	A3	99	G
37	A3	102	A
37	A3	112	G
38	A4	13	A
38	A4	16	G
38	A4	34	U
38	A4	35	C
38	A4	38	U
38	A4	46	G
38	A4	52	A
38	A4	59	A
38	A4	61	A
38	A4	62	C
38	A4	63	G
38	A4	68	G
38	A4	75	G
38	A4	81	U
38	A4	82	U
38	A4	83	C
38	A4	85	G
38	A4	86	U
38	A4	87	G
38	A4	88	A
38	A4	90	U
38	A4	95	G
38	A4	102	U
38	A4	104	A
38	A4	105	A
38	A4	106	C
38	A4	111	A
38	A4	112	U

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Mol	Chain	Res	Type
38	A4	113	U
38	A4	116	G
38	A4	125	U
38	A4	126	A
38	A4	136	G
38	A4	148	G
38	A4	152	G
38	A4	157	U
38	A4	158	U

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	B5	187	G
35	B5	272	U
35	B5	488	G
35	B5	489	C
35	B5	847	A
35	B5	950	C
35	B5	1344	A
35	B5	1358	G
35	B5	1458	G
35	B5	1572	OMG
35	B5	1600	A
35	B5	1645	G
36	A1	115	A
36	A1	267	G
36	A1	282	G
36	A1	439	C
36	A1	588	G
36	A1	873	C
36	A1	916	G
36	A1	1032	C
36	A1	1280	C
36	A1	1314	C
36	A1	1354	G
36	A1	1575	A
36	A1	2372	A
36	A1	2585	G
36	A1	2801	A
36	A1	2870	5MC
36	A1	3121	U

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Mol	Chain	Res	Type
38	A4	67	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

110 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	4AC	B5	1773	35	21,24,25	1.11	3 (14%)	29,34,37	2.62	7 (24%)
35	PSU	B5	1187	35	18,21,22	1.50	4 (22%)	22,30,33	1.91	3 (13%)
35	PSU	B5	1181	35	18,21,22	1.54	4 (22%)	22,30,33	1.90	3 (13%)
35	OMC	B5	1639	35	19,22,23	0.84	0	26,31,34	0.78	1 (3%)
36	PSU	A1	2826	36,80	18,21,22	1.53	5 (27%)	22,30,33	2.17	5 (22%)
35	A2M	B5	796	35	18,25,26	0.99	1 (5%)	18,36,39	1.34	3 (16%)
36	PSU	A1	1110	36	18,21,22	1.51	4 (22%)	22,30,33	2.08	3 (13%)
36	OMG	A1	805	36	18,26,27	0.95	1 (5%)	19,38,41	1.28	3 (15%)
36	PSU	A1	2133	36	18,21,22	1.67	4 (22%)	22,30,33	2.14	4 (18%)
36	5MC	A1	2278	36,80	18,22,23	0.97	2 (11%)	26,32,35	1.36	3 (11%)
35	PSU	B5	466	35	18,21,22	1.51	4 (22%)	22,30,33	1.88	5 (22%)
36	OMG	A1	867	36	18,26,27	0.89	1 (5%)	19,38,41	1.15	2 (10%)
36	OMG	A1	2793	36	18,26,27	1.00	1 (5%)	19,38,41	1.10	3 (15%)
40	HIC	AB	243	40	8,11,12	1.42	1 (12%)	6,14,16	0.73	0
35	PSU	B5	120	35	18,21,22	1.45	4 (22%)	22,30,33	1.86	4 (18%)
36	PSU	A1	2340	36,80	18,21,22	1.62	4 (22%)	22,30,33	1.92	4 (18%)
35	MA6	B5	1781	35	19,26,27	0.90	1 (5%)	18,38,41	1.42	2 (11%)
36	A2M	A1	2220	36	18,25,26	0.94	1 (5%)	18,36,39	1.66	2 (11%)
36	PSU	A1	966	36,80	18,21,22	1.44	5 (27%)	22,30,33	1.93	4 (18%)
36	OMG	A1	2619	36,80	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
36	OMC	A1	2948	36,80	19,22,23	0.87	1 (5%)	26,31,34	1.26	3 (11%)
35	PSU	B5	1415	35	18,21,22	1.60	4 (22%)	22,30,33	1.97	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	PSU	A1	1042	36	18,21,22	1.45	3 (16%)	22,30,33	1.84	4 (18%)
36	UY1	A1	2347	36	19,22,23	2.59	3 (15%)	22,31,34	2.48	4 (18%)
35	OMG	B5	1572	35	18,26,27	0.98	1 (5%)	19,38,41	1.11	1 (5%)
36	1MA	A1	2142	36,80	16,25,26	1.38	2 (12%)	18,37,40	1.28	3 (16%)
36	PSU	A1	2416	36,80	18,21,22	1.55	5 (27%)	22,30,33	1.99	4 (18%)
36	A2M	A1	1133	36,80	18,25,26	0.96	1 (5%)	18,36,39	1.44	3 (16%)
36	PSU	A1	2351	36	18,21,22	1.53	4 (22%)	22,30,33	1.89	4 (18%)
36	OMC	A1	650	36,80	19,22,23	0.80	1 (5%)	26,31,34	0.88	1 (3%)
36	PSU	A1	986	36	18,21,22	1.55	4 (22%)	22,30,33	1.82	4 (18%)
35	OMG	B5	562	35	18,26,27	0.98	1 (5%)	19,38,41	1.14	2 (10%)
35	PSU	B5	759	35	18,21,22	1.49	4 (22%)	22,30,33	1.91	4 (18%)
36	PSU	A1	1124	36	18,21,22	1.54	4 (22%)	22,30,33	1.95	3 (13%)
36	PSU	A1	1052	36,80	18,21,22	1.46	4 (22%)	22,30,33	1.97	3 (13%)
36	OMU	A1	1888	36,80	19,22,23	1.27	3 (15%)	26,31,34	1.82	4 (15%)
36	OMG	A1	2815	36	18,26,27	1.04	1 (5%)	19,38,41	1.09	2 (10%)
35	A2M	B5	436	35	18,25,26	0.91	1 (5%)	18,36,39	1.30	2 (11%)
35	OMC	B5	414	35	19,22,23	0.82	0	26,31,34	0.80	1 (3%)
36	PSU	A1	2314	36	18,21,22	1.47	3 (16%)	22,30,33	1.85	3 (13%)
36	PSU	A1	2349	36,80	18,21,22	1.53	4 (22%)	22,30,33	1.85	4 (18%)
35	PSU	B5	1290	35	18,21,22	1.60	5 (27%)	22,30,33	2.09	3 (13%)
35	A2M	B5	541	35	18,25,26	0.97	1 (5%)	18,36,39	1.25	2 (11%)
35	PSU	B5	211	35	18,21,22	1.49	4 (22%)	22,30,33	1.95	3 (13%)
36	A2M	A1	817	36,80	18,25,26	0.91	0	18,36,39	1.42	2 (11%)
36	OMC	A1	2197	36,80	19,22,23	0.80	0	26,31,34	0.87	1 (3%)
36	OMU	A1	2724	36	19,22,23	1.26	3 (15%)	26,31,34	1.65	5 (19%)
36	OMU	A1	898	36	19,22,23	1.34	4 (21%)	26,31,34	1.77	5 (19%)
35	PSU	B5	999	35	18,21,22	1.39	3 (16%)	22,30,33	1.88	3 (13%)
36	OMG	A1	1450	36	18,26,27	1.08	1 (5%)	19,38,41	1.03	3 (15%)
36	PSU	A1	2865	36	18,21,22	1.45	5 (27%)	22,30,33	1.91	3 (13%)
36	A2M	A1	2640	36	18,25,26	0.95	0	18,36,39	1.16	2 (11%)
36	PSU	A1	2264	36	18,21,22	1.37	3 (16%)	22,30,33	1.95	4 (18%)
36	OMU	A1	2417	36	19,22,23	1.37	3 (15%)	26,31,34	1.75	4 (15%)
36	OMG	A1	2791	36	18,26,27	0.99	1 (5%)	19,38,41	1.10	2 (10%)
36	PSU	A1	2975	36	18,21,22	1.49	4 (22%)	22,30,33	2.01	4 (18%)
36	PSU	A1	776	36	18,21,22	1.54	4 (22%)	22,30,33	2.21	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	OMU	A1	2921	36,80	19,22,23	1.25	3 (15%)	26,31,34	1.77	5 (19%)
37	PSU	A3	50	37	18,21,22	1.44	3 (16%)	22,30,33	1.93	3 (13%)
35	A2M	B5	974	35	18,25,26	0.91	1 (5%)	18,36,39	1.20	2 (11%)
36	OMU	A1	2729	36	19,22,23	1.38	4 (21%)	26,31,34	1.62	7 (26%)
35	A2M	B5	100	80,35	18,25,26	0.95	1 (5%)	18,36,39	1.18	2 (11%)
35	OMG	B5	1271	35	18,26,27	0.95	1 (5%)	19,38,41	1.11	3 (15%)
35	OMG	B5	1428	80,35	18,26,27	1.00	1 (5%)	19,38,41	1.18	2 (10%)
36	PSU	A1	990	36	18,21,22	1.46	3 (16%)	22,30,33	1.97	3 (13%)
35	4AC	B5	1280	35	21,24,25	1.03	1 (4%)	29,34,37	2.45	8 (27%)
36	A2M	A1	876	36	18,25,26	0.91	0	18,36,39	1.30	2 (11%)
36	OMC	A1	2337	36	19,22,23	0.77	1 (5%)	26,31,34	0.94	1 (3%)
36	PSU	A1	2191	36	18,21,22	1.55	4 (22%)	22,30,33	2.14	4 (18%)
36	PSU	A1	960	36	18,21,22	1.48	3 (16%)	22,30,33	1.92	3 (13%)
35	A2M	B5	420	35	18,25,26	0.93	1 (5%)	18,36,39	1.32	3 (16%)
35	G7M	B5	1575	35	20,26,27	2.56	4 (20%)	17,39,42	1.15	1 (5%)
36	PSU	A1	2266	36	18,21,22	1.41	4 (22%)	22,30,33	1.98	5 (22%)
35	OMC	B5	1007	35	19,22,23	0.93	1 (5%)	26,31,34	1.35	3 (11%)
35	PSU	B5	766	35	18,21,22	1.49	5 (27%)	22,30,33	1.99	4 (18%)
36	OMC	A1	1437	36,80	19,22,23	0.86	1 (5%)	26,31,34	1.48	4 (15%)
36	OMC	A1	2959	36	19,22,23	0.82	0	26,31,34	0.96	1 (3%)
35	A2M	B5	619	80,35	18,25,26	0.94	0	18,36,39	1.44	2 (11%)
35	A2M	B5	28	80,35	18,25,26	0.95	1 (5%)	18,36,39	1.26	3 (16%)
36	1MA	A1	645	36,80	16,25,26	1.24	2 (12%)	18,37,40	1.10	2 (11%)
36	OMC	A1	663	36	19,22,23	0.85	1 (5%)	26,31,34	0.95	1 (3%)
36	A2M	A1	2280	36,80	18,25,26	0.93	1 (5%)	18,36,39	1.29	3 (16%)
36	A2M	A1	2946	36,80	18,25,26	0.98	1 (5%)	18,36,39	1.37	3 (16%)
38	PSU	A4	73	38	18,21,22	1.48	4 (22%)	22,30,33	1.97	4 (18%)
36	OMG	A1	908	36	18,26,27	1.00	1 (5%)	19,38,41	1.46	4 (21%)
36	OMU	A1	2421	36	19,22,23	1.31	3 (15%)	26,31,34	1.80	4 (15%)
35	MA6	B5	1782	80,35	19,26,27	0.82	1 (5%)	18,38,41	1.47	2 (11%)
36	OMG	A1	2922	36	18,26,27	0.92	1 (5%)	19,38,41	1.05	2 (10%)
35	OMU	B5	1269	80,35	19,22,23	1.31	4 (21%)	26,31,34	1.87	7 (26%)
36	A2M	A1	807	36	18,25,26	1.05	1 (5%)	18,36,39	1.60	3 (16%)
36	PSU	A1	2260	36	18,21,22	1.49	3 (16%)	22,30,33	1.84	4 (18%)
36	UR3	A1	2634	36,80	19,22,23	0.93	1 (5%)	26,32,35	1.45	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	OMG	B5	1126	35	18,26,27	0.94	1 (5%)	19,38,41	1.13	2 (10%)
36	PSU	A1	1004	36	18,21,22	1.44	4 (22%)	22,30,33	1.91	3 (13%)
36	PSU	A1	1056	36	18,21,22	1.57	4 (22%)	22,30,33	1.97	4 (18%)
36	PSU	A1	2880	36	18,21,22	1.53	5 (27%)	22,30,33	1.93	5 (22%)
36	A2M	A1	1449	36,80	18,25,26	0.94	1 (5%)	18,36,39	1.31	2 (11%)
35	B8N	B5	1191	35	24,29,30	0.96	1 (4%)	29,42,45	1.60	4 (13%)
36	PSU	A1	2735	36	18,21,22	1.48	5 (27%)	22,30,33	1.92	4 (18%)
35	OMU	B5	578	35	19,22,23	1.20	2 (10%)	26,31,34	1.76	5 (19%)
36	OMG	A1	2288	36	18,26,27	1.06	1 (5%)	19,38,41	1.02	2 (10%)
35	PSU	B5	106	35	18,21,22	1.50	4 (22%)	22,30,33	1.92	3 (13%)
35	PSU	B5	302	35	18,21,22	1.48	4 (22%)	22,30,33	2.00	4 (18%)
36	A2M	A1	649	36	18,25,26	0.90	1 (5%)	18,36,39	1.25	1 (5%)
35	PSU	B5	632	35	18,21,22	1.60	5 (27%)	22,30,33	1.94	4 (18%)
36	5MC	A1	2870	36,80	18,22,23	1.10	2 (11%)	26,32,35	1.52	5 (19%)
36	PSU	A1	2129	36	18,21,22	1.54	4 (22%)	22,30,33	2.01	4 (18%)
36	PSU	A1	2923	36	18,21,22	1.44	4 (22%)	22,30,33	1.92	3 (13%)
36	A2M	A1	2281	36,80	18,25,26	0.83	0	18,36,39	1.43	2 (11%)
36	PSU	A1	2944	36,80	18,21,22	1.53	5 (27%)	22,30,33	1.96	5 (22%)

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
35	4AC	B5	1773	35	-	4/11/29/30	0/2/2/2
35	PSU	B5	1187	35	-	0/7/25/26	0/2/2/2
35	PSU	B5	1181	35	-	0/7/25/26	0/2/2/2
35	OMC	B5	1639	35	-	1/9/27/28	0/2/2/2
36	PSU	A1	2826	36,80	-	0/7/25/26	0/2/2/2
35	A2M	B5	796	35	-	0/5/27/28	0/3/3/3
36	PSU	A1	1110	36	-	0/7/25/26	0/2/2/2
36	OMG	A1	805	36	-	0/5/27/28	0/3/3/3
36	PSU	A1	2133	36	-	0/7/25/26	0/2/2/2
36	5MC	A1	2278	36,80	-	0/7/25/26	0/2/2/2
35	PSU	B5	466	35	-	0/7/25/26	0/2/2/2
36	OMG	A1	867	36	-	0/5/27/28	0/3/3/3
36	OMG	A1	2793	36	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HIC	AB	243	40	-	1/5/6/8	0/1/1/1
35	PSU	B5	120	35	-	0/7/25/26	0/2/2/2
36	PSU	A1	2340	36,80	-	1/7/25/26	0/2/2/2
35	MA6	B5	1781	35	-	0/7/29/30	0/3/3/3
36	A2M	A1	2220	36	-	0/5/27/28	0/3/3/3
36	PSU	A1	966	36,80	-	0/7/25/26	0/2/2/2
36	OMG	A1	2619	36,80	-	1/5/27/28	0/3/3/3
36	OMC	A1	2948	36,80	-	0/9/27/28	0/2/2/2
35	PSU	B5	1415	35	-	1/7/25/26	0/2/2/2
36	PSU	A1	1042	36	-	0/7/25/26	0/2/2/2
36	UY1	A1	2347	36	-	2/9/27/28	0/2/2/2
35	OMG	B5	1572	35	-	0/5/27/28	0/3/3/3
36	1MA	A1	2142	36,80	-	2/3/25/26	0/3/3/3
36	PSU	A1	2416	36,80	-	0/7/25/26	0/2/2/2
36	A2M	A1	1133	36,80	-	0/5/27/28	0/3/3/3
36	PSU	A1	2351	36	-	0/7/25/26	0/2/2/2
36	OMC	A1	650	36,80	-	0/9/27/28	0/2/2/2
36	PSU	A1	986	36	-	0/7/25/26	0/2/2/2
35	OMG	B5	562	35	-	0/5/27/28	0/3/3/3
35	PSU	B5	759	35	-	0/7/25/26	0/2/2/2
36	PSU	A1	1124	36	-	2/7/25/26	0/2/2/2
36	PSU	A1	1052	36,80	-	2/7/25/26	0/2/2/2
36	OMU	A1	1888	36,80	-	0/9/27/28	0/2/2/2
36	OMG	A1	2815	36	-	0/5/27/28	0/3/3/3
35	A2M	B5	436	35	-	0/5/27/28	0/3/3/3
35	OMC	B5	414	35	-	0/9/27/28	0/2/2/2
36	PSU	A1	2314	36	-	3/7/25/26	0/2/2/2
36	PSU	A1	2349	36,80	-	0/7/25/26	0/2/2/2
35	PSU	B5	1290	35	-	0/7/25/26	0/2/2/2
35	A2M	B5	541	35	-	3/5/27/28	0/3/3/3
35	PSU	B5	211	35	-	0/7/25/26	0/2/2/2
36	A2M	A1	817	36,80	-	2/5/27/28	0/3/3/3
36	OMC	A1	2197	36,80	-	6/9/27/28	0/2/2/2
36	OMU	A1	2724	36	-	0/9/27/28	0/2/2/2
36	OMU	A1	898	36	-	0/9/27/28	0/2/2/2
35	PSU	B5	999	35	-	0/7/25/26	0/2/2/2
36	OMG	A1	1450	36	-	2/5/27/28	0/3/3/3
36	PSU	A1	2865	36	-	0/7/25/26	0/2/2/2
36	A2M	A1	2640	36	-	1/5/27/28	0/3/3/3
36	PSU	A1	2264	36	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	OMU	A1	2417	36	-	1/9/27/28	0/2/2/2
36	OMG	A1	2791	36	-	0/5/27/28	0/3/3/3
36	PSU	A1	2975	36	-	0/7/25/26	0/2/2/2
36	PSU	A1	776	36	-	4/7/25/26	0/2/2/2
36	OMU	A1	2921	36,80	-	0/9/27/28	0/2/2/2
37	PSU	A3	50	37	-	1/7/25/26	0/2/2/2
35	A2M	B5	974	35	-	0/5/27/28	0/3/3/3
36	OMU	A1	2729	36	-	3/9/27/28	0/2/2/2
35	A2M	B5	100	80,35	-	1/5/27/28	0/3/3/3
35	OMG	B5	1271	35	-	0/5/27/28	0/3/3/3
35	OMG	B5	1428	80,35	-	3/5/27/28	0/3/3/3
36	PSU	A1	990	36	-	0/7/25/26	0/2/2/2
35	4AC	B5	1280	35	-	3/11/29/30	0/2/2/2
36	A2M	A1	876	36	-	0/5/27/28	0/3/3/3
36	OMC	A1	2337	36	-	0/9/27/28	0/2/2/2
36	PSU	A1	2191	36	-	0/7/25/26	0/2/2/2
36	PSU	A1	960	36	-	1/7/25/26	0/2/2/2
35	A2M	B5	420	35	-	0/5/27/28	0/3/3/3
35	G7M	B5	1575	35	3/3/5/5	2/3/25/26	0/3/3/3
36	PSU	A1	2266	36	-	3/7/25/26	0/2/2/2
35	OMC	B5	1007	35	-	1/9/27/28	0/2/2/2
35	PSU	B5	766	35	-	1/7/25/26	0/2/2/2
36	OMC	A1	1437	36,80	-	4/9/27/28	0/2/2/2
36	OMC	A1	2959	36	-	0/9/27/28	0/2/2/2
35	A2M	B5	619	80,35	-	2/5/27/28	0/3/3/3
35	A2M	B5	28	80,35	-	0/5/27/28	0/3/3/3
36	1MA	A1	645	36,80	-	0/3/25/26	0/3/3/3
36	OMC	A1	663	36	-	0/9/27/28	0/2/2/2
36	A2M	A1	2280	36,80	-	2/5/27/28	0/3/3/3
36	A2M	A1	2946	36,80	-	1/5/27/28	0/3/3/3
38	PSU	A4	73	38	-	0/7/25/26	0/2/2/2
36	OMG	A1	908	36	-	3/5/27/28	0/3/3/3
36	OMU	A1	2421	36	-	0/9/27/28	0/2/2/2
35	MA6	B5	1782	80,35	-	3/7/29/30	0/3/3/3
36	OMG	A1	2922	36	-	1/5/27/28	0/3/3/3
35	OMU	B5	1269	80,35	-	2/9/27/28	0/2/2/2
36	A2M	A1	807	36	-	3/5/27/28	0/3/3/3
36	PSU	A1	2260	36	-	2/7/25/26	0/2/2/2
36	UR3	A1	2634	36,80	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	OMG	B5	1126	35	-	0/5/27/28	0/3/3/3
36	PSU	A1	1004	36	-	0/7/25/26	0/2/2/2
36	PSU	A1	1056	36	-	0/7/25/26	0/2/2/2
36	PSU	A1	2880	36	-	0/7/25/26	0/2/2/2
36	A2M	A1	1449	36,80	-	0/5/27/28	0/3/3/3
35	B8N	B5	1191	35	-	0/16/34/35	0/2/2/2
36	PSU	A1	2735	36	-	0/7/25/26	0/2/2/2
35	OMU	B5	578	35	-	0/9/27/28	0/2/2/2
36	OMG	A1	2288	36	-	2/5/27/28	0/3/3/3
35	PSU	B5	106	35	-	0/7/25/26	0/2/2/2
35	PSU	B5	302	35	-	1/7/25/26	0/2/2/2
36	A2M	A1	649	36	-	0/5/27/28	0/3/3/3
35	PSU	B5	632	35	-	0/7/25/26	0/2/2/2
36	5MC	A1	2870	36,80	-	4/7/25/26	0/2/2/2
36	PSU	A1	2129	36	-	0/7/25/26	0/2/2/2
36	PSU	A1	2923	36	-	5/7/25/26	0/2/2/2
36	A2M	A1	2281	36,80	-	2/5/27/28	0/3/3/3
36	PSU	A1	2944	36,80	-	0/7/25/26	0/2/2/2

All (266) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2347	UY1	C6-C5	9.58	1.46	1.35
35	B5	1575	G7M	C8-N9	7.98	1.47	1.33
35	B5	1575	G7M	C8-N7	5.66	1.43	1.33
35	B5	1575	G7M	C5-C4	4.27	1.47	1.39
36	A1	2142	1MA	C2-N3	4.25	1.34	1.29
36	A1	2133	PSU	C4-N3	-3.66	1.32	1.38
36	A1	1450	OMG	C6-N1	-3.62	1.32	1.37
36	A1	2191	PSU	C4-N3	-3.56	1.32	1.38
36	A1	776	PSU	C4-N3	-3.56	1.32	1.38
36	A1	2416	PSU	C4-N3	-3.55	1.32	1.38
36	A1	2417	OMU	C4-N3	-3.53	1.32	1.38
40	AB	243	HIC	CD2-NE2	-3.52	1.33	1.38
36	A1	1056	PSU	C6-C5	3.48	1.39	1.35
36	A1	2260	PSU	C6-C5	3.47	1.39	1.35
36	A1	2944	PSU	C4-N3	-3.47	1.32	1.38
37	A3	50	PSU	C6-C5	3.45	1.39	1.35
35	B5	632	PSU	C4-N3	-3.45	1.32	1.38
36	A1	2347	UY1	C4-N3	-3.43	1.32	1.38
36	A1	2288	OMG	C6-N1	-3.43	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2815	OMG	C6-N1	-3.39	1.32	1.37
36	A1	2880	PSU	C4-N3	-3.38	1.32	1.38
35	B5	466	PSU	C4-N3	-3.36	1.32	1.38
35	B5	1181	PSU	C4-N3	-3.36	1.32	1.38
36	A1	2351	PSU	C4-N3	-3.35	1.32	1.38
36	A1	2129	PSU	C4-N3	-3.34	1.32	1.38
36	A1	2314	PSU	C6-C5	3.34	1.39	1.35
35	B5	1187	PSU	C4-N3	-3.34	1.32	1.38
36	A1	2340	PSU	C4-N3	-3.33	1.32	1.38
36	A1	1124	PSU	C4-N3	-3.33	1.32	1.38
36	A1	986	PSU	C4-N3	-3.28	1.32	1.38
36	A1	2349	PSU	C4-N3	-3.26	1.32	1.38
35	B5	1290	PSU	C2-N1	-3.25	1.32	1.36
36	A1	960	PSU	C4-N3	-3.25	1.32	1.38
36	A1	2791	OMG	C6-N1	-3.24	1.33	1.37
35	B5	1290	PSU	C4-N3	-3.24	1.32	1.38
36	A1	1110	PSU	C4-N3	-3.24	1.32	1.38
35	B5	211	PSU	C4-N3	-3.22	1.32	1.38
36	A1	2975	PSU	C4-N3	-3.21	1.32	1.38
36	A1	898	OMU	C4-N3	-3.21	1.32	1.38
35	B5	1181	PSU	C6-C5	3.20	1.39	1.35
35	B5	1428	OMG	C6-N1	-3.18	1.33	1.37
36	A1	986	PSU	C6-C5	3.18	1.39	1.35
36	A1	1042	PSU	C4-N3	-3.18	1.32	1.38
36	A1	2826	PSU	C4-N3	-3.18	1.32	1.38
36	A1	645	1MA	C2-N3	3.17	1.32	1.29
35	B5	106	PSU	C4-N3	-3.16	1.33	1.38
36	A1	2264	PSU	C6-C5	3.16	1.39	1.35
36	A1	2735	PSU	C4-N3	-3.16	1.33	1.38
36	A1	1042	PSU	C6-C5	3.15	1.39	1.35
35	B5	1415	PSU	C6-C5	3.15	1.39	1.35
36	A1	1056	PSU	C4-N3	-3.15	1.33	1.38
36	A1	2340	PSU	C6-C5	3.14	1.39	1.35
36	A1	1052	PSU	C4-N3	-3.13	1.33	1.38
36	A1	2133	PSU	C6-C5	3.13	1.39	1.35
36	A1	2133	PSU	C2-N3	-3.13	1.32	1.37
35	B5	562	OMG	C6-N1	-3.12	1.33	1.37
36	A1	2421	OMU	C4-N3	-3.11	1.33	1.38
35	B5	1415	PSU	C4-N3	-3.10	1.33	1.38
36	A1	2191	PSU	C6-C5	3.07	1.38	1.35
36	A1	2266	PSU	C6-C5	3.05	1.38	1.35
36	A1	990	PSU	C4-N3	-3.05	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A4	73	PSU	C4-N3	-3.03	1.33	1.38
35	B5	766	PSU	C4-N3	-3.03	1.33	1.38
36	A1	776	PSU	C2-N3	-3.02	1.32	1.37
36	A1	2870	5MC	C6-C5	3.01	1.39	1.34
36	A1	990	PSU	C6-C5	3.01	1.38	1.35
36	A1	2729	OMU	C4-N3	-3.00	1.33	1.38
36	A1	2793	OMG	C6-N1	-3.00	1.33	1.37
36	A1	2923	PSU	C4-N3	-2.99	1.33	1.38
35	B5	1271	OMG	C6-N1	-2.99	1.33	1.37
36	A1	2865	PSU	C4-N3	-2.98	1.33	1.38
35	B5	759	PSU	C4-N3	-2.98	1.33	1.38
35	B5	120	PSU	C4-N3	-2.97	1.33	1.38
36	A1	805	OMG	C6-N1	-2.97	1.33	1.37
36	A1	1004	PSU	C4-N3	-2.95	1.33	1.38
35	B5	1269	OMU	C4-N3	-2.94	1.33	1.38
35	B5	302	PSU	C4-N3	-2.93	1.33	1.38
35	B5	466	PSU	C6-C5	2.93	1.38	1.35
36	A1	2619	OMG	C6-N1	-2.92	1.33	1.37
36	A1	2264	PSU	C4-N3	-2.90	1.33	1.38
35	B5	1126	OMG	C6-N1	-2.90	1.33	1.37
36	A1	776	PSU	C6-C5	2.90	1.38	1.35
35	B5	1572	OMG	C6-N1	-2.89	1.33	1.37
36	A1	2314	PSU	C4-N3	-2.89	1.33	1.38
38	A4	73	PSU	C6-C5	2.89	1.38	1.35
36	A1	1124	PSU	C6-C5	2.89	1.38	1.35
36	A1	2724	OMU	C4-N3	-2.88	1.33	1.38
35	B5	1191	B8N	C6-C5	2.88	1.39	1.34
36	A1	986	PSU	C2-N3	-2.88	1.32	1.37
36	A1	2975	PSU	C6-C5	2.87	1.38	1.35
36	A1	966	PSU	C4-N3	-2.87	1.33	1.38
35	B5	999	PSU	C4-N3	-2.87	1.33	1.38
36	A1	2129	PSU	C6-C5	2.87	1.38	1.35
36	A1	2340	PSU	C2-N3	-2.86	1.32	1.37
36	A1	2351	PSU	C6-C5	2.86	1.38	1.35
37	A3	50	PSU	C4-N3	-2.85	1.33	1.38
35	B5	999	PSU	C6-C5	2.85	1.38	1.35
36	A1	867	OMG	C6-N1	-2.84	1.33	1.37
36	A1	2260	PSU	C4-N3	-2.84	1.33	1.38
36	A1	2921	OMU	C4-N3	-2.83	1.33	1.38
36	A1	960	PSU	O4'-C1'	-2.83	1.39	1.43
36	A1	2880	PSU	C2-N3	-2.81	1.32	1.37
36	A1	2922	OMG	C6-N1	-2.80	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B5	211	PSU	C6-C5	2.80	1.38	1.35
36	A1	2351	PSU	C2-N3	-2.80	1.32	1.37
36	A1	1004	PSU	C6-C5	2.79	1.38	1.35
36	A1	2729	OMU	C2-N3	-2.78	1.33	1.38
36	A1	1052	PSU	C6-C5	2.77	1.38	1.35
36	A1	2729	OMU	C5-C4	-2.76	1.37	1.43
35	B5	120	PSU	C6-C5	2.76	1.38	1.35
36	A1	2347	UY1	C2-N3	-2.75	1.32	1.37
35	B5	632	PSU	C2-N1	-2.74	1.33	1.36
35	B5	1415	PSU	C2-N1	-2.74	1.33	1.36
36	A1	2826	PSU	C2-N1	-2.74	1.33	1.36
36	A1	2266	PSU	C4-N3	-2.73	1.33	1.38
36	A1	2421	OMU	C2-N3	-2.72	1.33	1.38
35	B5	1575	G7M	C6-N1	-2.72	1.33	1.37
36	A1	2417	OMU	C2-N3	-2.71	1.33	1.38
35	B5	302	PSU	C2-N3	-2.69	1.32	1.37
36	A1	2921	OMU	C2-N3	-2.69	1.33	1.38
35	B5	466	PSU	C2-N3	-2.69	1.32	1.37
36	A1	2340	PSU	C2-N1	-2.69	1.33	1.36
36	A1	908	OMG	C6-N1	-2.67	1.33	1.37
36	A1	645	1MA	C6-N6	2.66	1.34	1.27
36	A1	1052	PSU	C2-N3	-2.66	1.32	1.37
36	A1	966	PSU	C6-C5	2.66	1.38	1.35
36	A1	2278	5MC	C6-C5	2.65	1.38	1.34
36	A1	2349	PSU	C6-C5	2.65	1.38	1.35
36	A1	2944	PSU	C2-N3	-2.64	1.33	1.37
35	B5	632	PSU	C2-N3	-2.63	1.33	1.37
35	B5	759	PSU	C6-C5	2.63	1.38	1.35
35	B5	106	PSU	C6-C5	2.63	1.38	1.35
35	B5	766	PSU	C6-C5	2.62	1.38	1.35
36	A1	1888	OMU	C4-N3	-2.61	1.33	1.38
36	A1	2142	1MA	C6-N6	2.61	1.34	1.27
35	B5	1187	PSU	C6-C5	2.60	1.38	1.35
35	B5	1415	PSU	C2-N3	-2.59	1.33	1.37
36	A1	2735	PSU	C6-C5	2.58	1.38	1.35
35	B5	1290	PSU	C6-C5	2.57	1.38	1.35
36	A1	2975	PSU	C2-N3	-2.56	1.33	1.37
35	B5	302	PSU	C6-C5	2.55	1.38	1.35
35	B5	759	PSU	C2-N1	-2.55	1.33	1.36
36	A1	1110	PSU	C6-C5	2.54	1.38	1.35
36	A1	1056	PSU	C2-N3	-2.53	1.33	1.37
36	A1	2133	PSU	C2-N1	-2.53	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2944	PSU	C6-C5	2.53	1.38	1.35
35	B5	1187	PSU	C2-N3	-2.52	1.33	1.37
35	B5	211	PSU	C2-N3	-2.51	1.33	1.37
35	B5	578	OMU	C4-N3	-2.50	1.34	1.38
36	A1	2724	OMU	C5-C4	-2.50	1.38	1.43
36	A1	1888	OMU	C2-N3	-2.50	1.33	1.38
36	A1	2416	PSU	C2-N3	-2.50	1.33	1.37
36	A1	898	OMU	C2-N3	-2.50	1.33	1.38
36	A1	898	OMU	C5-C4	-2.48	1.38	1.43
36	A1	2417	OMU	C5-C4	-2.48	1.38	1.43
36	A1	2865	PSU	C6-C5	2.47	1.38	1.35
35	B5	578	OMU	C2-N3	-2.47	1.33	1.38
36	A1	2129	PSU	C2-N3	-2.47	1.33	1.37
38	A4	73	PSU	C2-N3	-2.46	1.33	1.37
35	B5	106	PSU	C2-N3	-2.46	1.33	1.37
35	B5	1773	4AC	C4-N4	-2.46	1.36	1.39
35	B5	1773	4AC	C7-N4	-2.45	1.32	1.37
35	B5	302	PSU	C2-N1	-2.45	1.33	1.36
35	B5	766	PSU	C2-N3	-2.44	1.33	1.37
36	A1	1124	PSU	C2-N3	-2.44	1.33	1.37
35	B5	1269	OMU	C2-N3	-2.44	1.33	1.38
38	A4	73	PSU	C2-N1	-2.44	1.33	1.36
35	B5	632	PSU	C6-C5	2.43	1.38	1.35
35	B5	759	PSU	C2-N3	-2.43	1.33	1.37
36	A1	2416	PSU	C2-N1	-2.43	1.33	1.36
36	A1	2129	PSU	C2-N1	-2.40	1.33	1.36
35	B5	120	PSU	C2-N3	-2.40	1.33	1.37
36	A1	2946	A2M	C5-C4	2.39	1.47	1.40
36	A1	2416	PSU	C6-C5	2.39	1.38	1.35
36	A1	1110	PSU	C2-N1	-2.39	1.33	1.36
36	A1	2880	PSU	C6-C5	2.38	1.38	1.35
36	A1	1110	PSU	C2-N3	-2.38	1.33	1.37
35	B5	106	PSU	C2-N1	-2.38	1.33	1.36
36	A1	1042	PSU	C2-N3	-2.37	1.33	1.37
35	B5	796	A2M	C5-C4	2.37	1.47	1.40
36	A1	2921	OMU	C5-C4	-2.37	1.38	1.43
36	A1	990	PSU	C2-N3	-2.37	1.33	1.37
36	A1	2349	PSU	C2-N3	-2.37	1.33	1.37
36	A1	1888	OMU	C5-C4	-2.36	1.38	1.43
35	B5	1280	4AC	C4-N4	-2.36	1.36	1.39
36	A1	2724	OMU	C2-N3	-2.35	1.33	1.38
36	A1	2870	5MC	C6-N1	-2.35	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2278	5MC	C6-N1	-2.34	1.34	1.38
36	A1	2826	PSU	C2-N3	-2.34	1.33	1.37
35	B5	1187	PSU	C2-N1	-2.33	1.33	1.36
36	A1	2865	PSU	C2-N1	-2.33	1.33	1.36
35	B5	1290	PSU	C2-N3	-2.33	1.33	1.37
35	B5	120	PSU	C2-N1	-2.32	1.33	1.36
36	A1	2280	A2M	C5-C4	2.32	1.47	1.40
36	A1	2349	PSU	C2-N1	-2.32	1.33	1.36
36	A1	2191	PSU	C2-N3	-2.31	1.33	1.37
35	B5	541	A2M	C5-C4	2.30	1.47	1.40
35	B5	1181	PSU	C2-N3	-2.30	1.33	1.37
36	A1	1056	PSU	C2-N1	-2.29	1.33	1.36
36	A1	650	OMC	C5-C4	-2.29	1.37	1.42
36	A1	966	PSU	C2-N1	-2.29	1.33	1.36
36	A1	2944	PSU	O4'-C1'	-2.29	1.40	1.43
35	B5	1007	OMC	C5-C4	-2.28	1.37	1.42
35	B5	1781	MA6	C5-C4	2.27	1.46	1.40
36	A1	2735	PSU	C2-N1	-2.27	1.33	1.36
36	A1	2880	PSU	C2-N1	-2.26	1.33	1.36
36	A1	1437	OMC	C5-C4	-2.26	1.37	1.42
35	B5	766	PSU	C2-N1	-2.26	1.33	1.36
36	A1	2735	PSU	C2-N3	-2.25	1.33	1.37
36	A1	2923	PSU	C6-C5	2.25	1.37	1.35
36	A1	663	OMC	C5-C4	-2.25	1.37	1.42
36	A1	2191	PSU	C2-N1	-2.25	1.33	1.36
36	A1	2826	PSU	C6-C5	2.24	1.37	1.35
36	A1	2220	A2M	C5-C4	2.24	1.46	1.40
36	A1	966	PSU	C2-N3	-2.24	1.33	1.37
36	A1	2260	PSU	C2-N3	-2.22	1.33	1.37
36	A1	1004	PSU	C2-N3	-2.21	1.33	1.37
35	B5	632	PSU	C6-N1	-2.21	1.32	1.36
35	B5	1782	MA6	C5-C4	2.19	1.46	1.40
36	A1	2944	PSU	C2-N1	-2.19	1.33	1.36
36	A1	2421	OMU	C5-C4	-2.18	1.38	1.43
36	A1	2923	PSU	C2-N1	-2.18	1.33	1.36
36	A1	1124	PSU	C2-N1	-2.17	1.33	1.36
35	B5	420	A2M	C5-C4	2.17	1.46	1.40
36	A1	776	PSU	O4'-C1'	-2.17	1.40	1.43
36	A1	1133	A2M	C5-C4	2.17	1.46	1.40
35	B5	1269	OMU	C2-N1	2.16	1.41	1.38
35	B5	100	A2M	C5-C4	2.16	1.46	1.40
36	A1	807	A2M	C5-C4	2.16	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B5	999	PSU	C2-N3	-2.15	1.33	1.37
35	B5	1290	PSU	C6-N1	-2.14	1.32	1.36
35	B5	28	A2M	C5-C4	2.13	1.46	1.40
36	A1	1004	PSU	C2-N1	-2.13	1.33	1.36
35	B5	974	A2M	C5-C4	2.13	1.46	1.40
35	B5	211	PSU	C2-N1	-2.12	1.33	1.36
36	A1	2729	OMU	C2-N1	2.12	1.41	1.38
36	A1	2416	PSU	C6-N1	-2.11	1.32	1.36
36	A1	2865	PSU	O4'-C1'	-2.11	1.40	1.43
36	A1	2264	PSU	C2-N3	-2.11	1.33	1.37
36	A1	966	PSU	C6-N1	-2.11	1.32	1.36
35	B5	766	PSU	O4'-C1'	-2.11	1.40	1.43
36	A1	2314	PSU	O4'-C1'	-2.10	1.40	1.43
35	B5	466	PSU	C2-N1	-2.10	1.33	1.36
36	A1	2634	UR3	C5-C4	-2.10	1.38	1.43
36	A1	2923	PSU	C2-N3	-2.10	1.33	1.37
36	A1	2266	PSU	C4-C5	2.09	1.50	1.44
36	A1	2865	PSU	C2-N3	-2.09	1.33	1.37
36	A1	2266	PSU	C2-N3	-2.09	1.33	1.37
36	A1	986	PSU	C2-N1	-2.09	1.33	1.36
36	A1	2880	PSU	O4'-C1'	-2.08	1.41	1.43
36	A1	649	A2M	C5-C4	2.08	1.46	1.40
36	A1	960	PSU	C2-N3	-2.07	1.34	1.37
35	B5	1181	PSU	C2-N1	-2.07	1.33	1.36
35	B5	1269	OMU	C5-C4	-2.06	1.39	1.43
36	A1	898	OMU	C2-N1	2.05	1.41	1.38
36	A1	1052	PSU	C2-N1	-2.05	1.33	1.36
36	A1	2337	OMC	C5-C4	-2.05	1.38	1.42
35	B5	1773	4AC	C6-N1	-2.05	1.33	1.38
36	A1	2948	OMC	C5-C4	-2.05	1.38	1.42
36	A1	2351	PSU	C2-N1	-2.05	1.34	1.36
36	A1	2735	PSU	C6-N1	-2.05	1.32	1.36
36	A1	2975	PSU	C2-N1	-2.05	1.34	1.36
36	A1	2826	PSU	C6-N1	-2.03	1.32	1.36
35	B5	436	A2M	C5-C4	2.03	1.46	1.40
36	A1	1449	A2M	C5-C4	2.02	1.46	1.40
37	A3	50	PSU	C2-N1	-2.00	1.34	1.36

All (352) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1773	4AC	N4-C4-N3	9.89	130.45	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1280	4AC	N4-C4-N3	8.81	128.63	113.85
36	A1	2133	PSU	N1-C2-N3	7.45	123.57	115.13
36	A1	2347	UY1	C6-C5-C4	-7.11	113.23	118.20
36	A1	2826	PSU	N1-C2-N3	6.98	123.04	115.13
35	B5	1773	4AC	C5-C4-N4	-6.91	110.91	122.92
36	A1	2191	PSU	N1-C2-N3	6.72	122.75	115.13
36	A1	1110	PSU	N1-C2-N3	6.68	122.70	115.13
36	A1	2347	UY1	N1-C2-N3	6.49	122.48	115.13
36	A1	1124	PSU	N1-C2-N3	6.42	122.41	115.13
36	A1	990	PSU	N1-C2-N3	6.36	122.33	115.13
36	A1	1052	PSU	N1-C2-N3	6.31	122.28	115.13
36	A1	2129	PSU	N1-C2-N3	6.28	122.24	115.13
36	A1	2975	PSU	N1-C2-N3	6.26	122.22	115.13
35	B5	1181	PSU	N1-C2-N3	6.25	122.22	115.13
35	B5	106	PSU	N1-C2-N3	6.21	122.17	115.13
35	B5	1290	PSU	N1-C2-N3	6.19	122.15	115.13
36	A1	2416	PSU	N1-C2-N3	6.19	122.14	115.13
37	A3	50	PSU	N1-C2-N3	6.19	122.14	115.13
35	B5	302	PSU	N1-C2-N3	6.16	122.11	115.13
36	A1	1056	PSU	N1-C2-N3	6.15	122.10	115.13
38	A4	73	PSU	N1-C2-N3	6.15	122.09	115.13
35	B5	1415	PSU	N1-C2-N3	6.13	122.07	115.13
35	B5	211	PSU	N1-C2-N3	6.12	122.07	115.13
36	A1	2865	PSU	N1-C2-N3	6.10	122.04	115.13
36	A1	2264	PSU	N1-C2-N3	6.10	122.04	115.13
36	A1	1042	PSU	N1-C2-N3	6.08	122.02	115.13
35	B5	632	PSU	N1-C2-N3	6.08	122.02	115.13
36	A1	2735	PSU	N1-C2-N3	6.07	122.00	115.13
35	B5	759	PSU	N1-C2-N3	6.06	122.00	115.13
36	A1	2266	PSU	N1-C2-N3	6.05	121.98	115.13
36	A1	2944	PSU	N1-C2-N3	6.04	121.97	115.13
36	A1	2314	PSU	N1-C2-N3	6.03	121.96	115.13
36	A1	960	PSU	N1-C2-N3	6.03	121.96	115.13
36	A1	2923	PSU	N1-C2-N3	6.02	121.95	115.13
35	B5	1187	PSU	N1-C2-N3	6.02	121.95	115.13
35	B5	766	PSU	N1-C2-N3	6.02	121.95	115.13
36	A1	1004	PSU	N1-C2-N3	5.97	121.89	115.13
35	B5	466	PSU	N1-C2-N3	5.96	121.88	115.13
36	A1	776	PSU	N1-C2-N3	5.95	121.87	115.13
35	B5	999	PSU	N1-C2-N3	5.93	121.85	115.13
36	A1	2634	UR3	C4-N3-C2	-5.89	119.02	124.56
35	B5	120	PSU	N1-C2-N3	5.87	121.78	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	986	PSU	N1-C2-N3	5.83	121.73	115.13
36	A1	2351	PSU	N1-C2-N3	5.80	121.70	115.13
36	A1	2880	PSU	N1-C2-N3	5.79	121.69	115.13
36	A1	2349	PSU	N1-C2-N3	5.75	121.64	115.13
35	B5	1191	B8N	C4-N3-C2	-5.71	118.23	125.46
36	A1	2340	PSU	N1-C2-N3	5.70	121.59	115.13
36	A1	966	PSU	N1-C2-N3	5.63	121.51	115.13
36	A1	2260	PSU	N1-C2-N3	5.54	121.40	115.13
35	B5	1280	4AC	C5-C4-N4	-5.50	113.38	122.92
36	A1	776	PSU	C4-N3-C2	-5.01	119.12	126.34
36	A1	2870	5MC	C5-C6-N1	-4.88	118.32	123.34
35	B5	1290	PSU	O2-C2-N1	-4.88	117.42	122.79
35	B5	578	OMU	C4-N3-C2	-4.79	120.27	126.58
36	A1	2421	OMU	C4-N3-C2	-4.77	120.29	126.58
36	A1	2191	PSU	C4-N3-C2	-4.72	119.54	126.34
36	A1	1888	OMU	C4-N3-C2	-4.66	120.43	126.58
36	A1	2417	OMU	C4-N3-C2	-4.46	120.70	126.58
35	B5	1280	4AC	CM7-C7-N4	4.41	122.92	115.29
36	A1	2826	PSU	C4-N3-C2	-4.40	120.00	126.34
36	A1	2921	OMU	C4-N3-C2	-4.39	120.79	126.58
36	A1	1110	PSU	C4-N3-C2	-4.36	120.06	126.34
36	A1	898	OMU	C4-N3-C2	-4.34	120.86	126.58
36	A1	2421	OMU	N3-C2-N1	4.32	120.63	114.89
36	A1	2826	PSU	O2-C2-N1	-4.31	118.04	122.79
36	A1	2417	OMU	C5-C4-N3	4.30	121.27	114.84
36	A1	2220	A2M	N3-C2-N1	-4.30	121.96	128.68
36	A1	2944	PSU	C4-N3-C2	-4.29	120.16	126.34
36	A1	2129	PSU	C4-N3-C2	-4.24	120.23	126.34
35	B5	1269	OMU	C4-N3-C2	-4.22	121.02	126.58
36	A1	2921	OMU	N3-C2-N1	4.21	120.48	114.89
36	A1	966	PSU	C4-N3-C2	-4.18	120.31	126.34
36	A1	1888	OMU	C5-C4-N3	4.15	121.05	114.84
35	B5	1290	PSU	C4-N3-C2	-4.12	120.41	126.34
36	A1	2880	PSU	C4-N3-C2	-4.09	120.44	126.34
36	A1	2417	OMU	N3-C2-N1	4.09	120.32	114.89
36	A1	960	PSU	C4-N3-C2	-4.08	120.47	126.34
35	B5	578	OMU	C5-C4-N3	4.07	120.93	114.84
35	B5	211	PSU	C4-N3-C2	-4.07	120.48	126.34
36	A1	2264	PSU	C4-N3-C2	-4.06	120.48	126.34
35	B5	766	PSU	C4-N3-C2	-4.05	120.50	126.34
36	A1	1888	OMU	N3-C2-N1	4.05	120.26	114.89
36	A1	898	OMU	N3-C2-N1	4.04	120.25	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2416	PSU	O2-C2-N1	-4.03	118.36	122.79
36	A1	2921	OMU	C5-C4-N3	4.01	120.84	114.84
36	A1	817	A2M	N3-C2-N1	-3.99	122.45	128.68
36	A1	1052	PSU	C4-N3-C2	-3.98	120.61	126.34
35	B5	1007	OMC	O2-C2-N3	-3.97	115.87	122.33
35	B5	302	PSU	C4-N3-C2	-3.95	120.64	126.34
36	A1	2340	PSU	O2-C2-N1	-3.95	118.44	122.79
36	A1	2416	PSU	C4-N3-C2	-3.95	120.65	126.34
35	B5	632	PSU	C4-N3-C2	-3.94	120.67	126.34
36	A1	2421	OMU	C5-C4-N3	3.93	120.72	114.84
36	A1	2975	PSU	C4-N3-C2	-3.93	120.68	126.34
36	A1	2266	PSU	C4-N3-C2	-3.92	120.69	126.34
36	A1	990	PSU	C4-N3-C2	-3.92	120.69	126.34
35	B5	999	PSU	C4-N3-C2	-3.92	120.69	126.34
36	A1	898	OMU	C5-C4-N3	3.91	120.69	114.84
36	A1	1437	OMC	O2-C2-N3	-3.90	115.98	122.33
36	A1	2948	OMC	O2-C2-N3	-3.90	115.98	122.33
35	B5	1269	OMU	N3-C2-N1	3.90	120.06	114.89
36	A1	2865	PSU	C4-N3-C2	-3.89	120.74	126.34
35	B5	1773	4AC	CM7-C7-N4	3.88	122.01	115.29
36	A1	2278	5MC	O2-C2-N3	-3.88	116.02	122.33
35	B5	578	OMU	N3-C2-N1	3.88	120.04	114.89
35	B5	1782	MA6	N3-C2-N1	-3.87	122.62	128.68
36	A1	1004	PSU	C4-N3-C2	-3.87	120.76	126.34
36	A1	2724	OMU	C4-N3-C2	-3.85	121.51	126.58
35	B5	1187	PSU	C4-N3-C2	-3.83	120.82	126.34
36	A1	2133	PSU	C4-N3-C2	-3.82	120.83	126.34
35	B5	766	PSU	O2-C2-N1	-3.82	118.59	122.79
36	A1	1056	PSU	C4-N3-C2	-3.82	120.84	126.34
36	A1	2735	PSU	O2-C2-N1	-3.81	118.59	122.79
37	A3	50	PSU	C4-N3-C2	-3.80	120.86	126.34
36	A1	1004	PSU	O2-C2-N1	-3.79	118.62	122.79
35	B5	1781	MA6	C4-C5-N7	-3.78	105.46	109.40
38	A4	73	PSU	C4-N3-C2	-3.78	120.90	126.34
35	B5	466	PSU	C4-N3-C2	-3.77	120.91	126.34
36	A1	2314	PSU	C4-N3-C2	-3.75	120.93	126.34
36	A1	1056	PSU	O2-C2-N1	-3.74	118.67	122.79
35	B5	1181	PSU	C4-N3-C2	-3.73	120.96	126.34
35	B5	302	PSU	O2-C2-N1	-3.72	118.69	122.79
36	A1	2975	PSU	O2-C2-N1	-3.72	118.70	122.79
35	B5	1415	PSU	O2-C2-N1	-3.70	118.72	122.79
35	B5	759	PSU	C4-N3-C2	-3.69	121.02	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2724	OMU	C5-C4-N3	3.69	120.35	114.84
35	B5	106	PSU	C4-N3-C2	-3.68	121.03	126.34
36	A1	2347	UY1	O2-C2-N1	-3.68	118.74	122.79
36	A1	2729	OMU	N3-C2-N1	3.67	119.76	114.89
36	A1	2735	PSU	C4-N3-C2	-3.65	121.08	126.34
35	B5	1269	OMU	C1'-N1-C2	3.65	124.18	117.57
36	A1	2923	PSU	C4-N3-C2	-3.65	121.08	126.34
36	A1	2129	PSU	O2-C2-N1	-3.64	118.78	122.79
35	B5	120	PSU	C4-N3-C2	-3.64	121.09	126.34
35	B5	1782	MA6	C4-C5-N7	-3.64	105.61	109.40
36	A1	2349	PSU	C4-N3-C2	-3.64	121.10	126.34
36	A1	2923	PSU	O2-C2-N1	-3.61	118.81	122.79
35	B5	1781	MA6	N3-C2-N1	-3.61	123.04	128.68
36	A1	1124	PSU	C4-N3-C2	-3.59	121.16	126.34
35	B5	1269	OMU	C5-C4-N3	3.59	120.21	114.84
36	A1	1042	PSU	C4-N3-C2	-3.59	121.17	126.34
36	A1	776	PSU	C5-C6-N1	-3.58	116.73	122.11
35	B5	420	A2M	N3-C2-N1	-3.55	123.13	128.68
36	A1	2349	PSU	O2-C2-N1	-3.54	118.90	122.79
36	A1	2220	A2M	C2-N1-C6	3.53	124.79	118.75
36	A1	2351	PSU	C4-N3-C2	-3.51	121.28	126.34
35	B5	759	PSU	O2-C2-N1	-3.49	118.95	122.79
36	A1	2351	PSU	O2-C2-N1	-3.49	118.95	122.79
36	A1	1449	A2M	N3-C2-N1	-3.48	123.25	128.68
35	B5	1415	PSU	C4-N3-C2	-3.48	121.33	126.34
36	A1	2865	PSU	O2-C2-N1	-3.46	118.98	122.79
38	A4	73	PSU	O2-C2-N1	-3.46	118.98	122.79
36	A1	649	A2M	N3-C2-N1	-3.45	123.29	128.68
36	A1	2921	OMU	O4-C4-C5	-3.44	119.11	125.16
36	A1	2724	OMU	N3-C2-N1	3.44	119.45	114.89
37	A3	50	PSU	O2-C2-N1	-3.44	119.01	122.79
36	A1	2729	OMU	C5-C4-N3	3.43	119.97	114.84
35	B5	106	PSU	O2-C2-N1	-3.43	119.02	122.79
36	A1	2281	A2M	N3-C2-N1	-3.42	123.33	128.68
36	A1	1110	PSU	O2-C2-N1	-3.42	119.02	122.79
35	B5	436	A2M	N3-C2-N1	-3.41	123.34	128.68
36	A1	2340	PSU	C4-N3-C2	-3.40	121.44	126.34
36	A1	2260	PSU	C6-C5-C4	-3.40	115.82	118.20
35	B5	974	A2M	N3-C2-N1	-3.40	123.37	128.68
36	A1	2191	PSU	O2-C2-N1	-3.39	119.06	122.79
35	B5	1280	4AC	C6-C5-C4	3.39	121.11	116.96
35	B5	1187	PSU	O2-C2-N1	-3.37	119.08	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2260	PSU	C4-N3-C2	-3.36	121.49	126.34
35	B5	632	PSU	O2-C2-N1	-3.36	119.09	122.79
35	B5	796	A2M	N3-C2-N1	-3.34	123.45	128.68
36	A1	807	A2M	C4-C5-N7	-3.34	105.92	109.40
35	B5	28	A2M	N3-C2-N1	-3.34	123.47	128.68
36	A1	898	OMU	O4-C4-C5	-3.32	119.33	125.16
36	A1	2264	PSU	O2-C2-N1	-3.31	119.14	122.79
35	B5	541	A2M	N3-C2-N1	-3.31	123.50	128.68
36	A1	2729	OMU	C4-N3-C2	-3.30	122.23	126.58
35	B5	1773	4AC	C6-C5-C4	3.29	120.98	116.96
36	A1	2640	A2M	N3-C2-N1	-3.28	123.55	128.68
36	A1	1888	OMU	O4-C4-C5	-3.25	119.44	125.16
35	B5	100	A2M	N3-C2-N1	-3.24	123.61	128.68
36	A1	807	A2M	O4'-C4'-C5'	3.24	120.04	109.37
36	A1	2347	UY1	C4-N3-C2	-3.22	121.71	126.34
36	A1	1437	OMC	CM2-O2'-C2'	3.21	122.95	114.52
36	A1	960	PSU	O2-C2-N1	-3.20	119.27	122.79
36	A1	876	A2M	C4-C5-N7	-3.19	106.07	109.40
35	B5	578	OMU	O4-C4-C5	-3.18	119.57	125.16
36	A1	876	A2M	N3-C2-N1	-3.18	123.71	128.68
35	B5	211	PSU	O2-C2-N1	-3.18	119.29	122.79
36	A1	2142	1MA	C5-C6-N1	3.17	118.63	113.90
36	A1	990	PSU	O2-C2-N1	-3.17	119.30	122.79
35	B5	619	A2M	N3-C2-N1	-3.15	123.75	128.68
35	B5	1575	G7M	CN7-N7-C8	-3.15	110.26	125.43
36	A1	908	OMG	CM2-O2'-C2'	3.14	122.77	114.52
36	A1	2421	OMU	O4-C4-C5	-3.14	119.64	125.16
36	A1	2142	1MA	N1-C2-N3	-3.11	122.40	126.02
36	A1	2133	PSU	O2-C2-N3	-3.10	115.96	121.82
35	B5	120	PSU	O2-C2-N1	-3.10	119.38	122.79
36	A1	2880	PSU	O2-C2-N1	-3.09	119.38	122.79
35	B5	999	PSU	O2-C2-N1	-3.09	119.39	122.79
36	A1	966	PSU	O2-C2-N1	-3.09	119.39	122.79
36	A1	1052	PSU	O2-C2-N1	-3.08	119.40	122.79
35	B5	1191	B8N	C31-N3-C2	3.08	122.28	117.67
36	A1	986	PSU	C4-N3-C2	-3.06	121.93	126.34
36	A1	908	OMG	O2'-C2'-C1'	3.06	115.16	109.09
36	A1	2724	OMU	O4-C4-C5	-3.06	119.78	125.16
36	A1	1437	OMC	C1'-N1-C2	3.05	125.22	118.42
35	B5	1181	PSU	O2-C2-N1	-3.04	119.45	122.79
36	A1	1133	A2M	C4-C5-N7	-3.01	106.26	109.40
36	A1	2266	PSU	O2-C2-N1	-3.01	119.48	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2959	OMC	O2-C2-N3	-2.99	117.47	122.33
36	A1	2278	5MC	C5-C6-N1	-2.99	120.26	123.34
35	B5	1269	OMU	O4-C4-C5	-2.98	119.92	125.16
36	A1	2417	OMU	O4-C4-C5	-2.95	119.97	125.16
36	A1	1124	PSU	O2-C2-N1	-2.95	119.54	122.79
36	A1	2870	5MC	O2-C2-N3	-2.95	117.54	122.33
36	A1	966	PSU	C6-C5-C4	-2.94	116.14	118.20
36	A1	2314	PSU	O2-C2-N1	-2.94	119.56	122.79
35	B5	1007	OMC	C1'-N1-C2	2.91	124.91	118.42
35	B5	1415	PSU	C6-C5-C4	-2.88	116.19	118.20
36	A1	986	PSU	C6-C5-C4	-2.87	116.19	118.20
35	B5	1280	4AC	C5-C4-N3	-2.86	117.99	122.59
36	A1	2340	PSU	C6-C5-C4	-2.85	116.21	118.20
36	A1	1133	A2M	N3-C2-N1	-2.84	124.23	128.68
36	A1	2351	PSU	C6-C5-C4	-2.84	116.21	118.20
36	A1	2948	OMC	C1'-N1-C2	2.84	124.75	118.42
36	A1	776	PSU	O2-C2-N1	-2.79	119.72	122.79
36	A1	2946	A2M	N3-C2-N1	-2.79	124.32	128.68
35	B5	1280	4AC	O7-C7-N4	-2.79	117.31	121.82
36	A1	776	PSU	O4-C4-C5	-2.77	116.81	124.05
36	A1	2944	PSU	O2-C2-N1	-2.76	119.75	122.79
36	A1	2278	5MC	C5-C4-N3	-2.76	118.70	121.67
36	A1	2280	A2M	N3-C2-N1	-2.75	124.38	128.68
35	B5	1007	OMC	O2-C2-N1	2.73	124.52	118.89
36	A1	2724	OMU	C1'-N1-C2	2.72	122.49	117.57
36	A1	2946	A2M	O2'-C2'-C1'	2.68	114.40	109.09
36	A1	2337	OMC	O2-C2-N3	-2.67	118.00	122.33
36	A1	2266	PSU	C6-C5-C4	-2.66	116.33	118.20
35	B5	1191	B8N	N3-C2-N1	2.66	120.52	116.76
35	B5	562	OMG	C5-C6-N1	2.66	118.65	113.95
35	B5	1773	4AC	O7-C7-N4	-2.65	117.53	121.82
35	B5	796	A2M	C4-C5-N7	-2.65	106.64	109.40
36	A1	2870	5MC	C5-C4-N3	-2.65	118.82	121.67
38	A4	73	PSU	C6-C5-C4	-2.64	116.35	118.20
36	A1	2729	OMU	C1'-N1-C2	2.64	122.35	117.57
36	A1	2288	OMG	C5-C6-N1	2.64	118.61	113.95
36	A1	2729	OMU	C6-N1-C2	-2.64	117.62	120.99
36	A1	2260	PSU	O2-C2-N1	-2.63	119.89	122.79
36	A1	1437	OMC	O2-C2-N1	2.63	124.33	118.89
36	A1	867	OMG	C8-N7-C5	2.62	107.99	102.99
35	B5	420	A2M	C4-C5-N7	-2.60	106.69	109.40
35	B5	302	PSU	C6-C5-C4	-2.59	116.39	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	807	A2M	N3-C2-N1	-2.59	124.64	128.68
35	B5	619	A2M	C4-C5-N7	-2.56	106.73	109.40
36	A1	2946	A2M	C4-C5-N7	-2.55	106.74	109.40
36	A1	805	OMG	C5-C6-N1	2.54	118.43	113.95
35	B5	541	A2M	C4-C5-N7	-2.53	106.76	109.40
36	A1	1042	PSU	O2-C2-N1	-2.52	120.01	122.79
36	A1	2791	OMG	C5-C6-N1	2.52	118.41	113.95
35	B5	28	A2M	C4-C5-N7	-2.52	106.77	109.40
36	A1	2815	OMG	C5-C6-N1	2.52	118.40	113.95
36	A1	986	PSU	O2-C2-N1	-2.52	120.02	122.79
36	A1	2191	PSU	C5-C6-N1	-2.48	118.39	122.11
36	A1	2280	A2M	C4-C5-N7	-2.48	106.81	109.40
35	B5	1773	4AC	C5-C4-N3	-2.48	118.61	122.59
35	B5	120	PSU	C6-C5-C4	-2.47	116.47	118.20
35	B5	974	A2M	C4-C5-N7	-2.47	106.83	109.40
36	A1	2870	5MC	C1'-N1-C6	2.46	125.22	121.12
36	A1	867	OMG	C5-C6-N1	2.45	118.29	113.95
35	B5	436	A2M	C4-C5-N7	-2.45	106.84	109.40
36	A1	805	OMG	C8-N7-C5	2.45	107.65	102.99
36	A1	2815	OMG	C8-N7-C5	2.45	107.65	102.99
35	B5	1572	OMG	C5-C6-N1	2.44	118.25	113.95
36	A1	2729	OMU	O2-C2-N3	-2.43	116.97	121.50
36	A1	2619	OMG	C8-N7-C5	2.43	107.61	102.99
36	A1	898	OMU	C1'-N1-C2	2.43	121.96	117.57
36	A1	2619	OMG	C5-C6-N1	2.42	118.22	113.95
35	B5	578	OMU	O2-C2-N1	-2.41	119.58	122.79
36	A1	645	1MA	C5-C6-N1	2.41	117.49	113.90
36	A1	2729	OMU	O4-C4-C5	-2.40	120.93	125.16
36	A1	2880	PSU	C6-C5-C4	-2.40	116.52	118.20
36	A1	2640	A2M	C4-C5-N7	-2.40	106.90	109.40
36	A1	2791	OMG	C8-N7-C5	2.40	107.55	102.99
36	A1	908	OMG	C5-C6-N1	2.39	118.17	113.95
35	B5	1773	4AC	C1'-N1-C2	2.39	123.75	118.42
36	A1	2922	OMG	C5-C6-N1	2.36	118.12	113.95
36	A1	2793	OMG	C8-N7-C5	2.35	107.46	102.99
35	B5	466	PSU	O2-C2-N1	-2.34	120.21	122.79
35	B5	1126	OMG	C8-N7-C5	2.32	107.41	102.99
36	A1	2266	PSU	O4'-C1'-C2'	2.31	108.41	105.14
35	B5	414	OMC	O2-C2-N3	-2.31	118.57	122.33
35	B5	562	OMG	C8-N7-C5	2.31	107.39	102.99
35	B5	100	A2M	C4-C5-N7	-2.31	106.99	109.40
35	B5	1280	4AC	O2-C2-N3	-2.30	118.59	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1269	OMU	O2-C2-N3	-2.28	117.26	121.50
36	A1	2281	A2M	C4-C5-N7	-2.26	107.04	109.40
36	A1	776	PSU	O4'-C1'-C2'	2.24	108.31	105.14
36	A1	645	1MA	N1-C2-N3	-2.23	123.42	126.02
36	A1	663	OMC	O2-C2-N3	-2.23	118.71	122.33
35	B5	1126	OMG	C5-C6-N1	2.22	117.88	113.95
35	B5	1639	OMC	O2-C2-N3	-2.21	118.73	122.33
36	A1	1133	A2M	C2-N1-C6	2.20	122.52	118.75
36	A1	2948	OMC	O2-C2-N1	2.20	123.43	118.89
36	A1	1056	PSU	C6-C5-C4	-2.19	116.66	118.20
35	B5	1271	OMG	C8-N7-C5	2.19	107.17	102.99
36	A1	2142	1MA	C8-N7-C5	2.19	107.16	102.99
36	A1	2349	PSU	C6-C5-C4	-2.18	116.67	118.20
35	B5	1191	B8N	O36-C34-O35	-2.18	119.14	124.09
35	B5	1271	OMG	C5-C6-N1	2.18	117.80	113.95
36	A1	1450	OMG	C8-N7-C5	2.17	107.13	102.99
36	A1	2880	PSU	O4'-C1'-C2'	2.17	108.20	105.14
36	A1	2870	5MC	N1-C2-N3	2.17	122.75	118.81
35	B5	1428	OMG	C5-C6-N1	2.16	117.77	113.95
36	A1	2197	OMC	O2-C2-N3	-2.16	118.82	122.33
35	B5	420	A2M	C2-N1-C6	2.16	122.44	118.75
36	A1	2922	OMG	C8-N7-C5	2.15	107.09	102.99
36	A1	817	A2M	C4-C5-N7	-2.15	107.16	109.40
36	A1	805	OMG	O6-C6-C5	-2.14	120.19	124.37
36	A1	2280	A2M	N6-C6-N1	2.14	123.02	118.57
36	A1	2634	UR3	C3U-N3-C4	2.14	120.94	117.89
36	A1	2921	OMU	O2-C2-N1	-2.13	119.95	122.79
35	B5	1428	OMG	C8-N7-C5	2.13	107.05	102.99
35	B5	1271	OMG	O6-C6-C5	-2.13	120.21	124.37
36	A1	2133	PSU	O2-C2-N1	-2.13	120.45	122.79
36	A1	2826	PSU	C5-C6-N1	-2.12	118.93	122.11
36	A1	908	OMG	C8-N7-C5	2.12	107.02	102.99
36	A1	2975	PSU	C6-C5-C4	-2.11	116.72	118.20
35	B5	1280	4AC	C1'-N1-C2	2.11	123.13	118.42
36	A1	1450	OMG	C5-C6-N1	2.11	117.68	113.95
35	B5	766	PSU	O4'-C1'-C2'	2.10	108.11	105.14
35	B5	759	PSU	C6-C5-C4	-2.10	116.73	118.20
36	A1	2288	OMG	C8-N7-C5	2.09	106.97	102.99
36	A1	2793	OMG	CM2-O2'-C2'	-2.08	109.05	114.52
35	B5	466	PSU	O2-C2-N3	-2.08	117.89	121.82
36	A1	2793	OMG	C5-C6-N1	2.07	117.60	113.95
36	A1	2944	PSU	O4'-C1'-C2'	2.07	108.06	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	632	PSU	C6-C5-C4	-2.06	116.76	118.20
36	A1	2264	PSU	C5-C6-N1	-2.05	119.03	122.11
36	A1	2129	PSU	C5-C6-N1	-2.05	119.03	122.11
35	B5	466	PSU	C6-C5-C4	-2.05	116.77	118.20
36	A1	1449	A2M	C2-N1-C6	2.05	122.26	118.75
36	A1	2826	PSU	O4'-C1'-C2'	2.04	108.03	105.14
36	A1	1042	PSU	O2-C2-N3	-2.04	117.96	121.82
36	A1	2944	PSU	C5-C6-N1	-2.04	119.05	122.11
35	B5	28	A2M	C2-N1-C6	2.03	122.22	118.75
35	B5	796	A2M	C2-N1-C6	2.03	122.22	118.75
36	A1	2416	PSU	C5-C6-N1	-2.02	119.08	122.11
36	A1	1450	OMG	O6-C6-C5	-2.02	120.43	124.37
36	A1	2735	PSU	C6-C5-C4	-2.02	116.79	118.20
35	B5	1269	OMU	C1'-N1-C6	-2.01	116.46	120.84
36	A1	650	OMC	N4-C4-N3	2.00	121.48	117.97

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	B5	1575	G7M	C2'
35	B5	1575	G7M	C3'
35	B5	1575	G7M	C4'

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	AB	243	HIC	CA-CB-CG-ND1
35	B5	619	A2M	O4'-C4'-C5'-O5'
35	B5	619	A2M	C3'-C4'-C5'-O5'
35	B5	1280	4AC	O7-C7-N4-C4
35	B5	1280	4AC	CM7-C7-N4-C4
35	B5	1428	OMG	O4'-C4'-C5'-O5'
35	B5	1575	G7M	C3'-C4'-C5'-O5'
35	B5	1773	4AC	N3-C4-N4-C7
36	A1	776	PSU	C2'-C1'-C5-C4
36	A1	776	PSU	C2'-C1'-C5-C6
36	A1	807	A2M	O4'-C4'-C5'-O5'
36	A1	807	A2M	C3'-C4'-C5'-O5'
36	A1	908	OMG	O4'-C4'-C5'-O5'
36	A1	908	OMG	C1'-C2'-O2'-CM2
36	A1	1437	OMC	C1'-C2'-O2'-CM2
36	A1	1450	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
36	A1	1450	OMG	C3'-C4'-C5'-O5'
36	A1	2197	OMC	C2'-C1'-N1-C2
36	A1	2197	OMC	C2'-C1'-N1-C6
36	A1	2260	PSU	O4'-C1'-C5-C4
36	A1	2260	PSU	O4'-C1'-C5-C6
36	A1	2266	PSU	O4'-C1'-C5-C4
36	A1	2266	PSU	O4'-C1'-C5-C6
36	A1	2288	OMG	O4'-C4'-C5'-O5'
36	A1	2417	OMU	C1'-C2'-O2'-CM2
36	A1	2619	OMG	C1'-C2'-O2'-CM2
36	A1	2640	A2M	C1'-C2'-O2'-CM'
36	A1	2729	OMU	C3'-C4'-C5'-O5'
36	A1	2729	OMU	O4'-C4'-C5'-O5'
36	A1	2923	PSU	O4'-C1'-C5-C4
36	A1	2923	PSU	O4'-C1'-C5-C6
36	A1	2946	A2M	C1'-C2'-O2'-CM'
35	B5	541	A2M	O4'-C4'-C5'-O5'
35	B5	541	A2M	C3'-C4'-C5'-O5'
35	B5	1782	MA6	O4'-C4'-C5'-O5'
36	A1	908	OMG	C3'-C4'-C5'-O5'
36	A1	2197	OMC	O4'-C4'-C5'-O5'
36	A1	2288	OMG	C3'-C4'-C5'-O5'
36	A1	2314	PSU	C3'-C4'-C5'-O5'
36	A1	2314	PSU	O4'-C4'-C5'-O5'
36	A1	2923	PSU	C3'-C4'-C5'-O5'
36	A1	2923	PSU	O4'-C4'-C5'-O5'
35	B5	1269	OMU	O4'-C1'-N1-C2
35	B5	1782	MA6	C3'-C4'-C5'-O5'
36	A1	1052	PSU	O4'-C4'-C5'-O5'
36	A1	2142	1MA	C3'-C4'-C5'-O5'
36	A1	2142	1MA	O4'-C4'-C5'-O5'
36	A1	2280	A2M	C3'-C4'-C5'-O5'
36	A1	817	A2M	C4'-C5'-O5'-P
36	A1	2314	PSU	C4'-C5'-O5'-P
36	A1	2197	OMC	C3'-C4'-C5'-O5'
36	A1	2280	A2M	O4'-C4'-C5'-O5'
36	A1	2870	5MC	C2'-C1'-N1-C6
35	B5	1782	MA6	C5-C6-N6-C9
36	A1	2347	UY1	C3'-C4'-C5'-O5'
35	B5	1269	OMU	O4'-C1'-N1-C6
35	B5	1773	4AC	O7-C7-N4-C4
35	B5	1773	4AC	CM7-C7-N4-C4

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Mol	Chain	Res	Type	Atoms
36	A1	2870	5MC	C2'-C1'-N1-C2
36	A1	2870	5MC	O4'-C1'-N1-C6
36	A1	2923	PSU	C4'-C5'-O5'-P
36	A1	2281	A2M	C3'-C2'-O2'-CM'
35	B5	1280	4AC	N3-C4-N4-C7
35	B5	541	A2M	C4'-C5'-O5'-P
35	B5	1575	G7M	O4'-C4'-C5'-O5'
36	A1	1124	PSU	C3'-C4'-C5'-O5'
36	A1	776	PSU	C4'-C5'-O5'-P
36	A1	2266	PSU	C4'-C5'-O5'-P
35	B5	100	A2M	O4'-C4'-C5'-O5'
36	A1	2870	5MC	O4'-C1'-N1-C2
36	A1	807	A2M	C4'-C5'-O5'-P
36	A1	2729	OMU	C4'-C5'-O5'-P
36	A1	2922	OMG	C3'-C2'-O2'-CM2
35	B5	1428	OMG	C4'-C5'-O5'-P
36	A1	2340	PSU	C4'-C5'-O5'-P
36	A1	1052	PSU	C3'-C4'-C5'-O5'
36	A1	2197	OMC	O4'-C1'-N1-C6
36	A1	1437	OMC	O4'-C4'-C5'-O5'
37	A3	50	PSU	C3'-C4'-C5'-O5'
36	A1	960	PSU	O4'-C1'-C5-C4
36	A1	1437	OMC	C3'-C2'-O2'-CM2
35	B5	766	PSU	C3'-C4'-C5'-O5'
35	B5	1415	PSU	C3'-C4'-C5'-O5'
35	B5	1428	OMG	C3'-C4'-C5'-O5'
36	A1	1124	PSU	O4'-C4'-C5'-O5'
36	A1	2347	UY1	O4'-C4'-C5'-O5'
35	B5	302	PSU	O4'-C4'-C5'-O5'
35	B5	1639	OMC	O4'-C4'-C5'-O5'
36	A1	776	PSU	O4'-C4'-C5'-O5'
36	A1	817	A2M	O4'-C4'-C5'-O5'
36	A1	2281	A2M	O4'-C4'-C5'-O5'
36	A1	2197	OMC	O4'-C1'-N1-C2
35	B5	1007	OMC	C2'-C1'-N1-C2
35	B5	1773	4AC	C5-C4-N4-C7
36	A1	1437	OMC	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 747 ligands modelled in this entry, 747 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
36	A1	5
53	AP	1
9	BI	1
35	B5	1
43	AE	1
47	AI	1
32	Bf	1
18	BR	1
22	BV	1
38	A4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	1955:U	O3'	2093:A	P	25.26
1	A1	1253:U	O3'	1260:A	P	24.88
1	AP	155:GLU	C	164:LYS	N	23.99

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BI	123:LYS	C	135:LYS	N	20.70
1	B5	658:C	O3'	676:G	P	18.22
1	A1	1023:C	O3'	1030:A	P	16.66
1	AE	109:GLU	C	129:GLU	N	14.66
1	A1	2445:A	O3'	2501:U	P	14.44
1	A1	440:A	O3'	494:G	P	10.21
1	AI	101:LYS	C	114:GLY	N	9.90
1	Bf	125:THR	C	129:GLY	N	7.22
1	BR	95:ARG	C	100:LEU	N	5.16
1	BV	11:LEU	C	12:TYR	N	4.99
1	A4	73:PSU	O3'	74:U	P	4.85

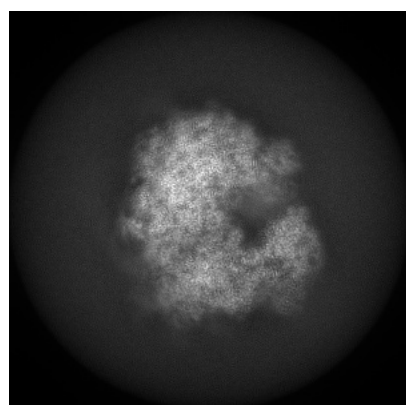
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23935. These allow visual inspection of the internal detail of the map and identification of artifacts.

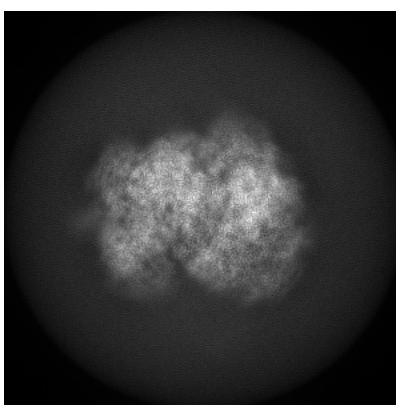
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

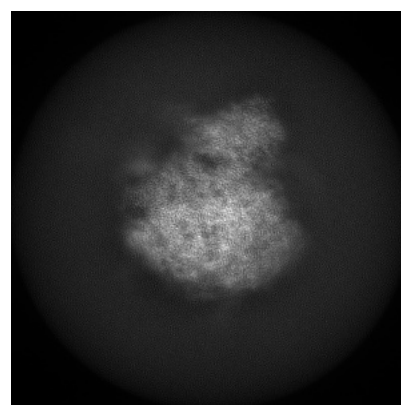
6.1.1 Primary map



X



Y

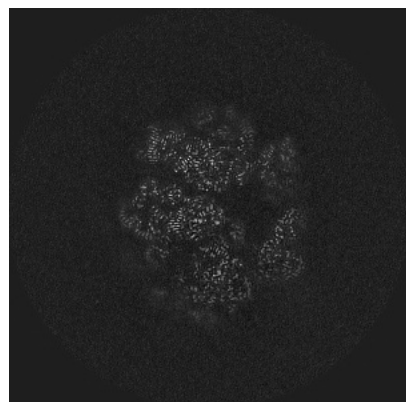


Z

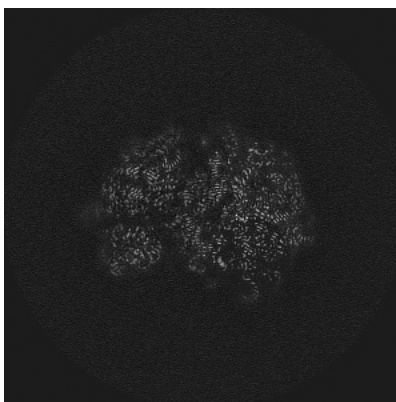
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

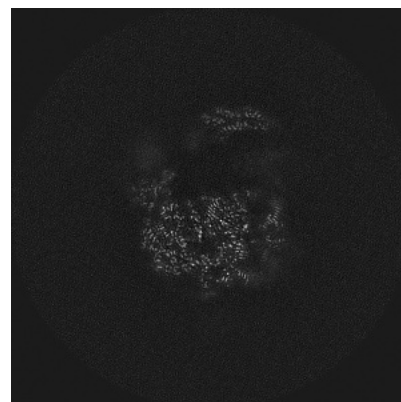
6.2.1 Primary map



X Index: 216



Y Index: 216

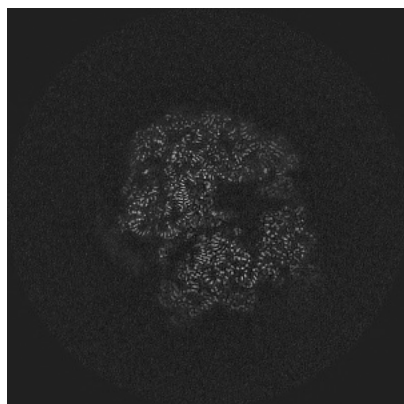


Z Index: 216

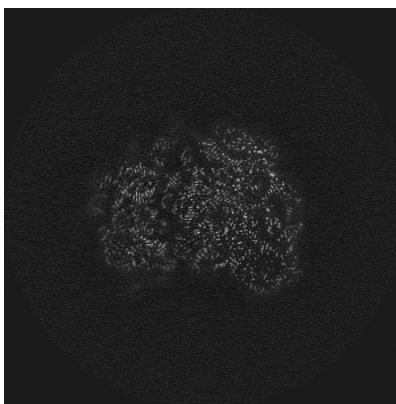
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

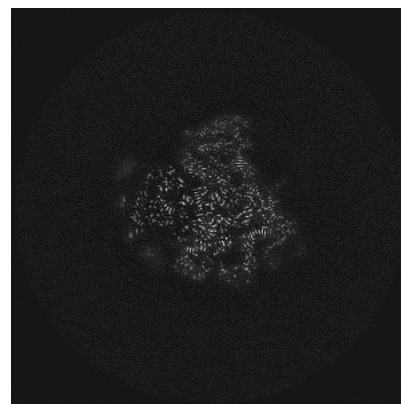
6.3.1 Primary map



X Index: 236



Y Index: 206

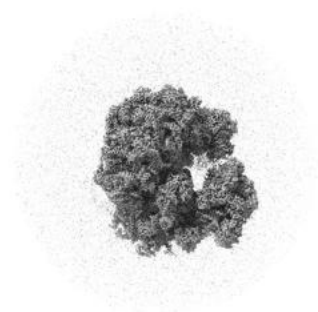


Z Index: 266

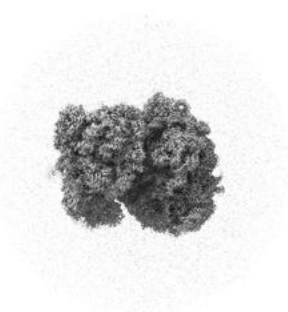
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

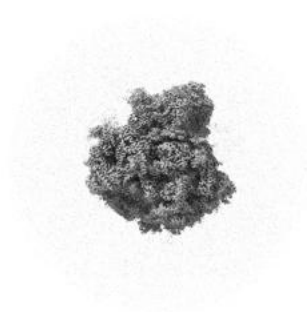
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

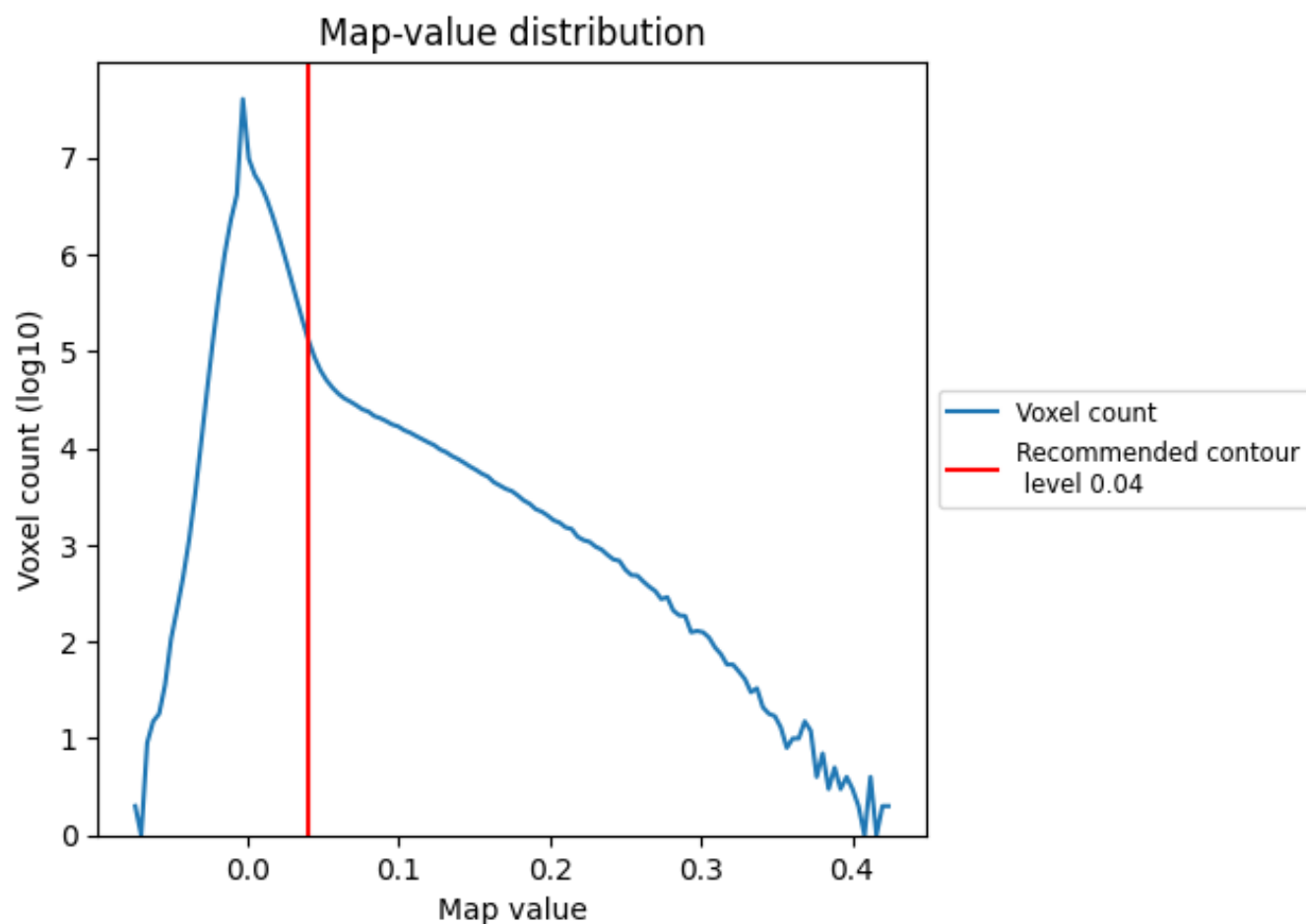
6.5 Mask visualisation

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

7 Map analysis [i](#)

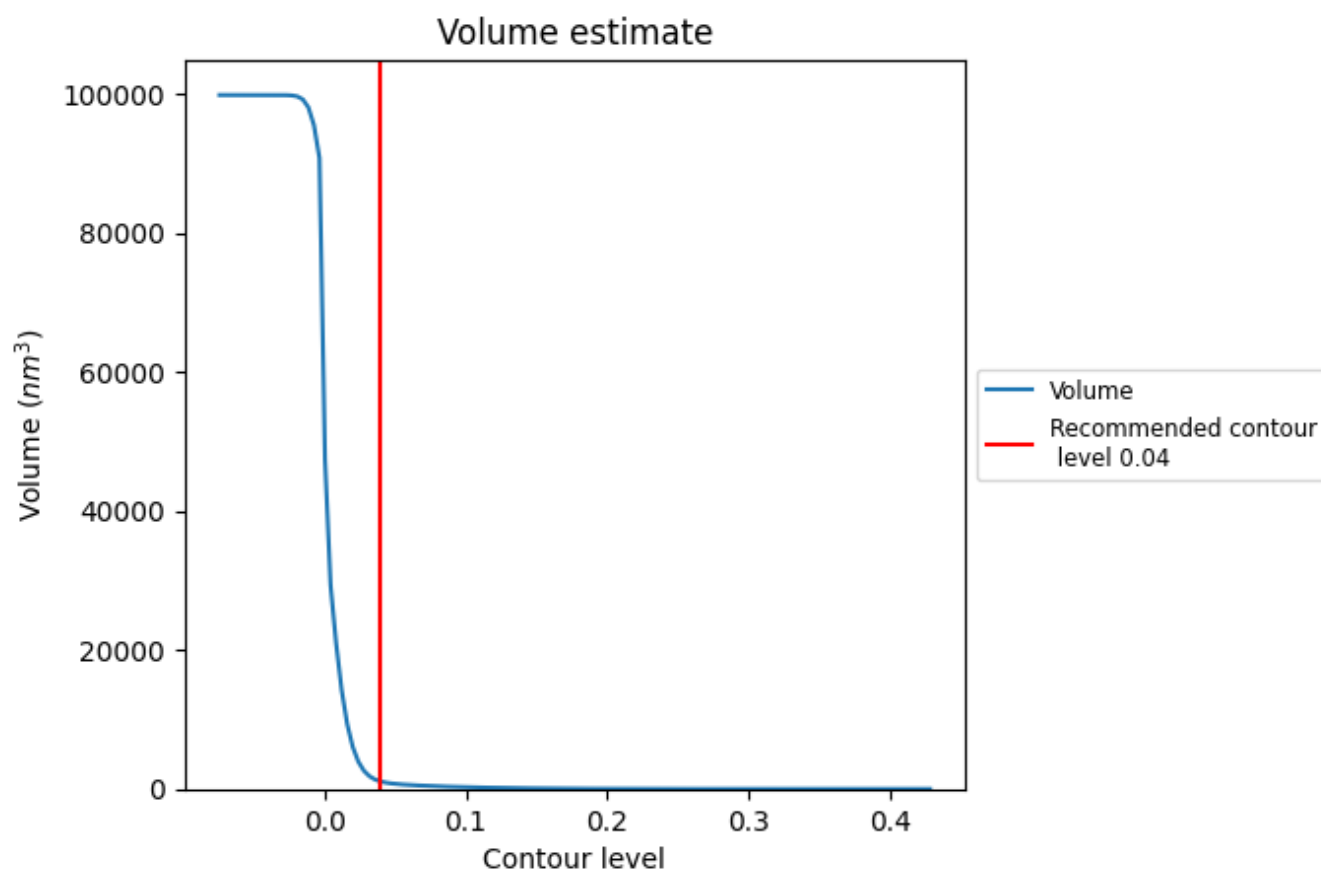
This section contains the results of statistical analysis of the map.

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.

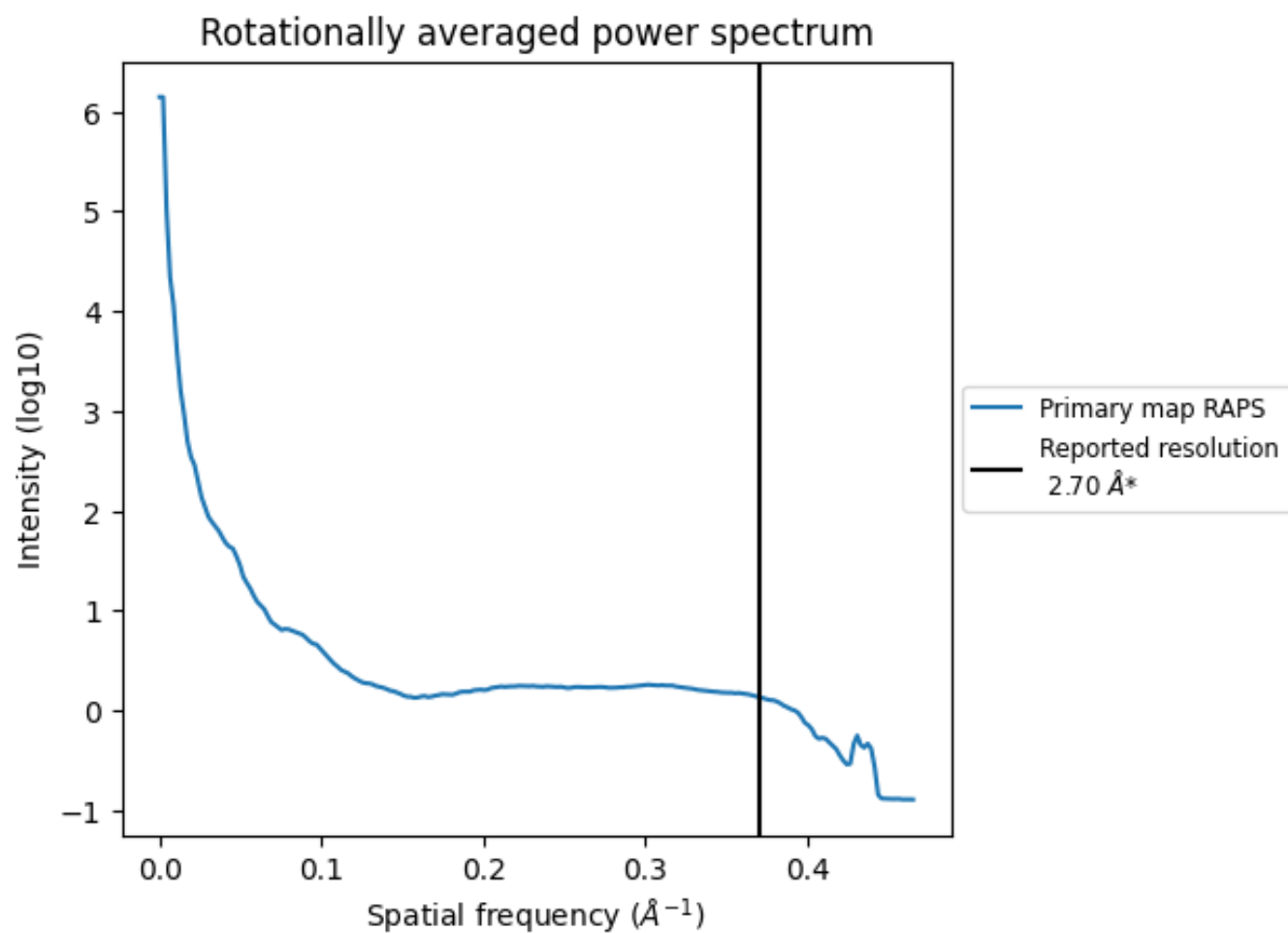
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1070 nm^3 ; this corresponds to an approximate mass of 967 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 0.370 Å⁻¹

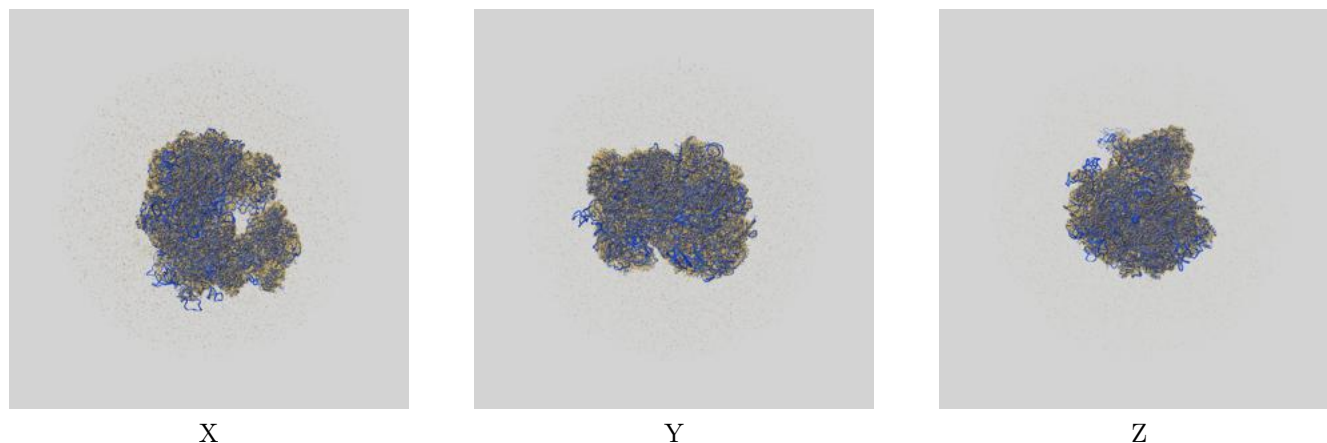
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

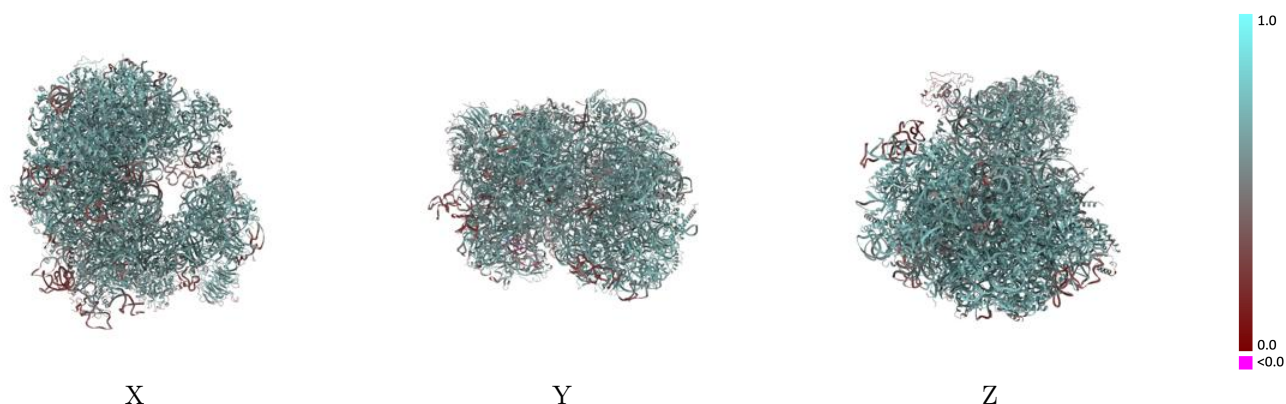
This section contains information regarding the fit between EMDB map EMD-23935 and PDB model 7MPJ. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



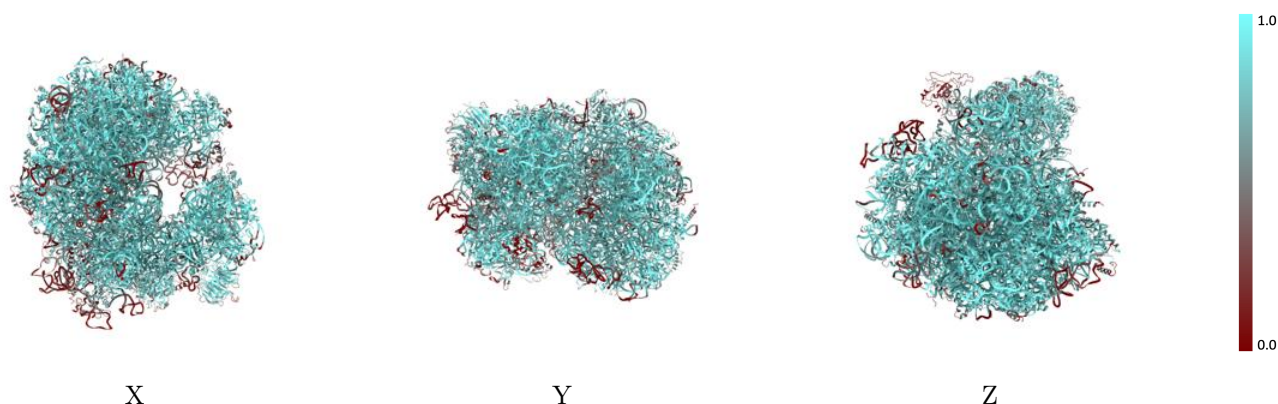
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



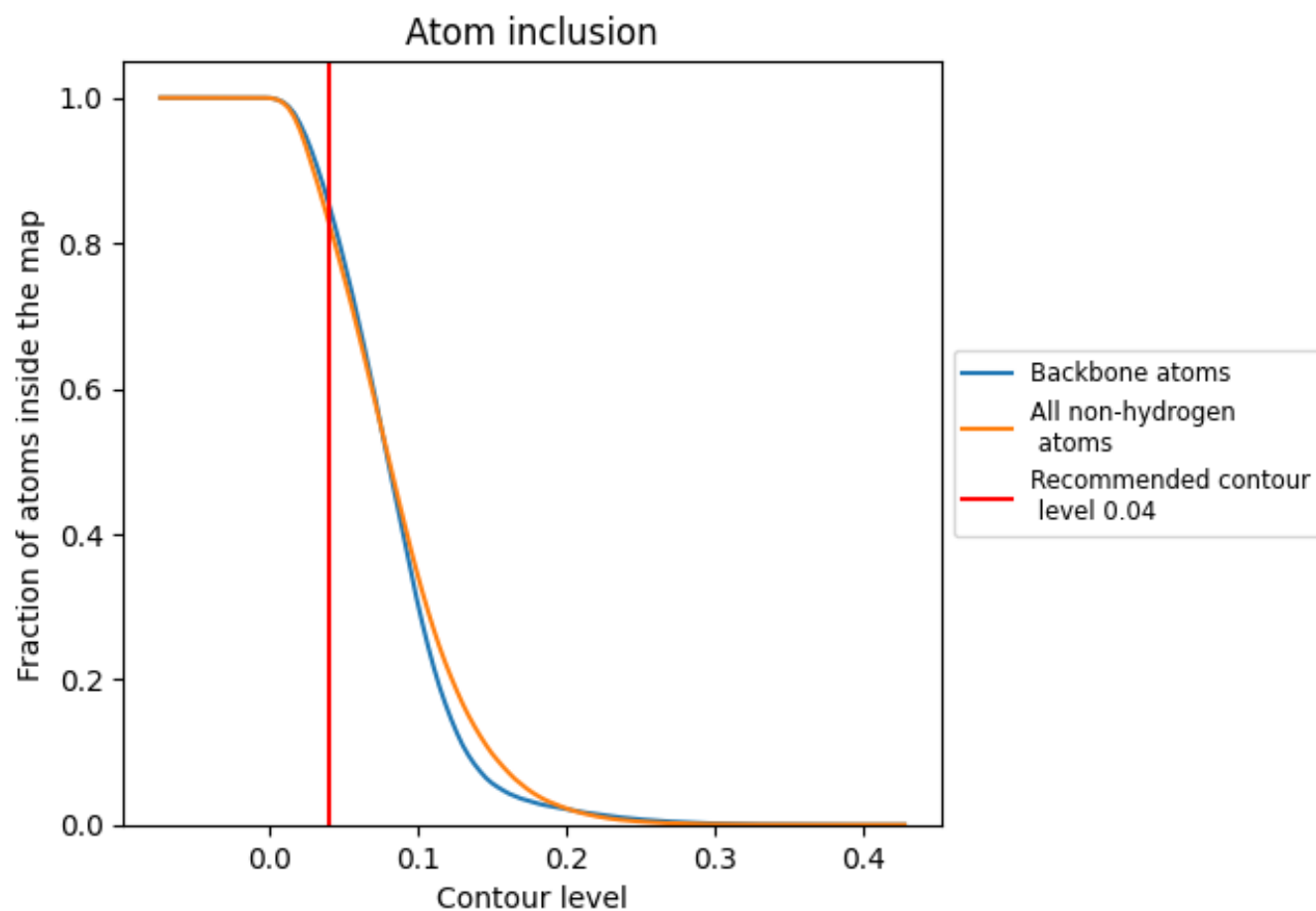
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8255	 0.6130
A1	 0.8730	 0.6280
A3	 0.9314	 0.6380
A4	 0.9267	 0.6530
AA	 0.9060	 0.6730
AB	 0.8893	 0.6730
AC	 0.8707	 0.6580
AD	 0.7287	 0.5920
AE	 0.7461	 0.6180
AF	 0.8778	 0.6680
AG	 0.7572	 0.6170
AH	 0.8043	 0.6440
AI	 0.7557	 0.6150
AJ	 0.5278	 0.5080
AL	 0.8334	 0.6550
AM	 0.8354	 0.6630
AN	 0.9519	 0.6790
AO	 0.9070	 0.6800
AP	 0.8482	 0.6560
AQ	 0.9077	 0.6730
AR	 0.7230	 0.5860
AS	 0.8754	 0.6700
AT	 0.8331	 0.6390
AU	 0.6381	 0.5700
AV	 0.8478	 0.6520
AW	 0.8436	 0.6570
AX	 0.8362	 0.6490
AY	 0.8459	 0.6490
AZ	 0.7367	 0.6050
Aa	 0.8978	 0.6630
Ab	 0.7412	 0.5910
Ac	 0.7196	 0.5870
Ad	 0.7945	 0.6310
Ae	 0.8816	 0.6690
Af	 0.9259	 0.6940









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Chain	Atom inclusion	Q-score
Ag	 0.8390	 0.6390
Ah	 0.8240	 0.6340
Ai	 0.7654	 0.6030
Aj	 0.9333	 0.6870
Ak	 0.5643	 0.5270
Al	 0.9036	 0.6620
Am	 0.8193	 0.6530
An	 0.6179	 0.5650
Ao	 0.7690	 0.6180
Ap	 0.8206	 0.6440
B5	 0.8244	 0.5850
BA	 0.7654	 0.5780
BB	 0.7099	 0.5630
BC	 0.8259	 0.6080
BD	 0.7584	 0.5820
BE	 0.8252	 0.6130
BF	 0.8141	 0.6000
BG	 0.6499	 0.5590
BH	 0.5358	 0.5090
BI	 0.7813	 0.5920
BJ	 0.8004	 0.5980
BK	 0.7113	 0.5390
BL	 0.7444	 0.5970
BM	 0.0467	 0.3070
BN	 0.7922	 0.6020
BO	 0.7849	 0.5780
BP	 0.7222	 0.5690
BQ	 0.8842	 0.6360
BR	 0.6378	 0.5330
BS	 0.7946	 0.5900
BT	 0.8817	 0.6260
BU	 0.6381	 0.5420
BV	 0.7997	 0.5950
BW	 0.8978	 0.6380
BX	 0.8364	 0.6150
BY	 0.7771	 0.5970
BZ	 0.7583	 0.5740
Ba	 0.8322	 0.5940
Bb	 0.7110	 0.5690
Bc	 0.7338	 0.5710
Bd	 0.9125	 0.6510
Be	 0.6500	 0.5650

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Chain	Atom inclusion	Q-score
Bf	 0.0878	 0.2970
Bg	 0.7719	 0.5850
Bh	 0.3308	 0.4820