Full wwPDB EM Validation Report (i)

Nov 23, 2022 – 01:02 AM EST

PDB ID	:	7N8B
EMDB ID	:	EMD-24235
Title	:	Cycloheximide bound vacant 80S structure isolated from cbf5-D95A
Authors	:	Rai, J.; Zhao, Y.; Li, H.
Deposited on	:	2021-06-14
Resolution	:	3.05 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 (i) 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 (i)) were used in the production of this report:

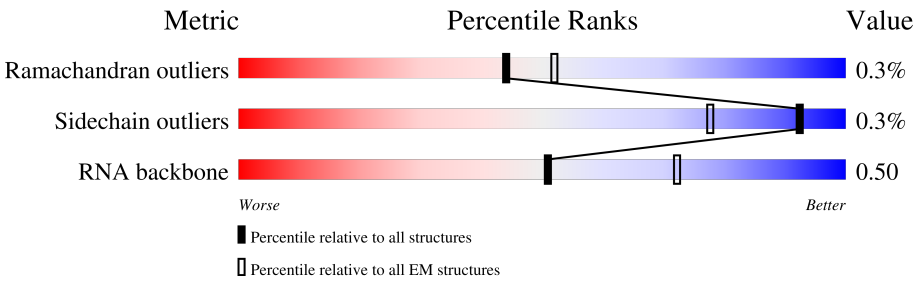
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.05 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	3156	72% 26%
2	A3	121	81% 19%
3	A4	158	72% 26%
4	AA	247	100%
5	AB	386	98%
6	AC	361	98%
7	AD	292	99%
8	AE	156	99%

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Mol	Chain	Length	Quality of chain
9	AF	222	97%
10	AG	230	97%
11	AH	190	100%
12	AI	205	100%
13	AJ	169	5% 98%
14	AL	193	96%
15	AM	136	99%
16	AN	203	99%
17	AO	197	98%
18	AP	175	99%
19	AQ	185	99%
20	AR	188	7% 99%
21	AS	172	99%
22	AT	159	99%
23	AU	100	99%
24	AV	136	100%
25	AW	63	98%
26	AX	121	100%
27	AY	126	99%
28	AZ	135	99%
29	Aa	148	98%
30	Ab	58	100%
31	Ac	97	100%
32	Ad	109	100%
33	Ae	127	100%

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Mol	Chain	Length	Quality of chain
34	Af	106	100%
35	Ag	112	99%
36	Ah	119	98%
37	Ai	99	98%
38	Aj	87	100%
39	Ak	77	100%
40	Al	50	98%
41	Am	52	98%
42	An	25	100%
43	Ao	105	100%
44	Ap	91	98%
45	BA	206	98%
46	BB	214	96%
47	BC	217	98%
48	BD	223	100%
49	BE	260	100%
50	BF	206	99%
51	BG	226	97%
52	BH	184	5% 98%
53	BI	188	98%
54	BJ	185	98%
55	BK	96	5% 100%
56	BL	155	12% 99%
57	BM	121	50% 99%
58	BN	150	100%

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Mol	Chain	Length	Quality of chain
59	BO	127	98%
60	BP	124	8%, 94%
61	BQ	141	97%
62	BR	121	5%, 97%
63	BS	145	96%
64	BT	141	100%
65	BU	107	9%, 98%
66	BV	87	100%
67	BW	129	98%
68	BX	144	95%
69	BY	134	99%
70	BZ	69	99%
71	Ba	97	95%
72	Bb	81	98%
73	Bc	63	5%, 100%
74	Bd	53	98%
75	Be	60	5%, 100%
76	Bf	57	42%, 98%
77	Bg	312	100%
78	Bh	89	33%, 97%
79	B5	1783	6%, 67%, 30%

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
79	3AU	B5	1191	X	-	-	-
79	G7M	B5	1575	X	-	-	-

2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 199900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A1	3156	67535	30189	12152	22038	3156	0	0

- Molecule 2 is a RNA chain called 5S.

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

- Molecule 3 is a RNA chain called 5.8S.

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

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

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

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AB	386	3079	1954	584	533	8	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 7 is a protein called 60S ribosomal protein L5.

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

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

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

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	?	-	LYS	deletion	UNP Q02326
AE	?	-	LEU	deletion	UNP Q02326
AE	?	-	THR	deletion	UNP Q02326
AE	?	-	LYS	deletion	UNP Q02326
AE	?	-	LYS	deletion	UNP Q02326
AE	?	-	GLU	deletion	UNP Q02326
AE	?	-	LYS	deletion	UNP Q02326
AE	?	-	LYS	deletion	UNP Q02326
AE	?	-	GLU	deletion	UNP Q02326
AE	?	-	ALA	deletion	UNP Q02326
AE	?	-	ASN	deletion	UNP Q02326
AE	?	-	LEU	deletion	UNP Q02326
AE	?	-	PHE	deletion	UNP Q02326
AE	?	-	PRO	deletion	UNP Q02326
AE	?	-	GLU	deletion	UNP Q02326
AE	?	-	GLN	deletion	UNP Q02326
AE	?	-	GLN	deletion	UNP Q02326
AE	?	-	ASN	deletion	UNP Q02326
AE	?	-	LYS	deletion	UNP Q02326

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 12 is a protein called 60S ribosomal protein L10.

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

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 13 is a protein called 60S ribosomal protein L11-A.

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

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

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

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 19 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

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

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

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

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

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

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L25.

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

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 29 is a protein called 60S ribosomal protein L28.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

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

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called 60S ribosomal protein L40-A.

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

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

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

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 45 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 46 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 47 is a protein called 40S ribosomal protein S2.

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

- Molecule 48 is a protein called 40S ribosomal protein S3.

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

- Molecule 49 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 50 is a protein called 40S ribosomal protein S5.

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

- Molecule 51 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 52 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 53 is a protein called 40S ribosomal protein S8-A.

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 54 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 55 is a protein called 40S ribosomal protein S10-A.

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

- Molecule 56 is a protein called 40S ribosomal protein S11-A.

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

- Molecule 57 is a protein called 40S ribosomal protein S12.

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

- Molecule 58 is a protein called 40S ribosomal protein S13.

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

- Molecule 59 is a protein called 40S ribosomal protein S14-A.

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

- Molecule 60 is a protein called 40S ribosomal protein S15.

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

- Molecule 61 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 62 is a protein called 40S ribosomal protein S17-A.

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

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 63 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 64 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 65 is a protein called 40S ribosomal protein S20.

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

- Molecule 66 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 67 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 69 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 70 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 71 is a protein called 40S ribosomal protein S26-B.

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

- Molecule 72 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 74 is a protein called 40S ribosomal protein S29-A.

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

- Molecule 75 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 76 is a protein called 40S ribosomal protein S31.

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

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

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

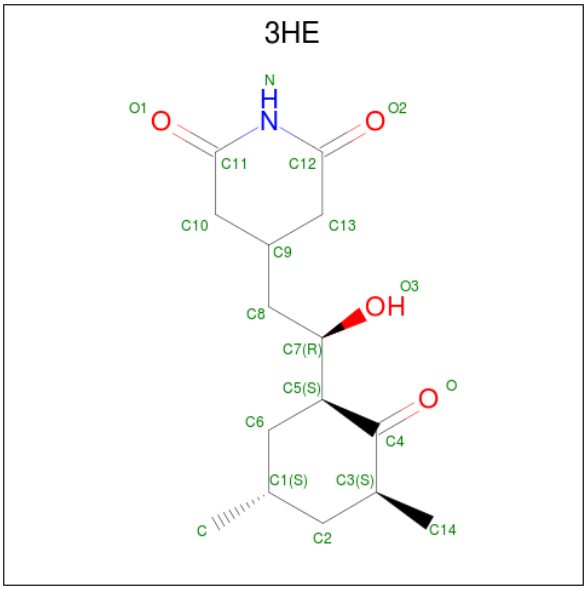
- Molecule 78 is a protein called Suppressor protein STM1.

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

- Molecule 79 is a RNA chain called 18S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
79	B5	1783	37891	16950	6664	12494	1783	1	0

- Molecule 80 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: $C_{15}H_{23}NO_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
80	A1	1	20	15	1	4	0

- Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
81	A1	247	247	247	0
81	A3	5	5	5	0
81	A4	9	9	9	0
81	AB	4	4	4	0
81	AC	1	1	1	0
81	AG	1	1	1	0
81	AL	3	3	3	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
81	AN	1	1	1	0
81	AO	1	1	1	0
81	AP	1	1	1	0
81	AR	1	1	1	0
81	AV	1	1	1	0
81	Aa	1	1	1	0
81	Ae	2	2	2	0
81	Af	1	1	1	0
81	Aj	1	1	1	0
81	BE	1	1	1	0
81	BG	1	1	1	0
81	BJ	1	1	1	0
81	Ba	1	1	1	0
81	B5	90	90	90	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

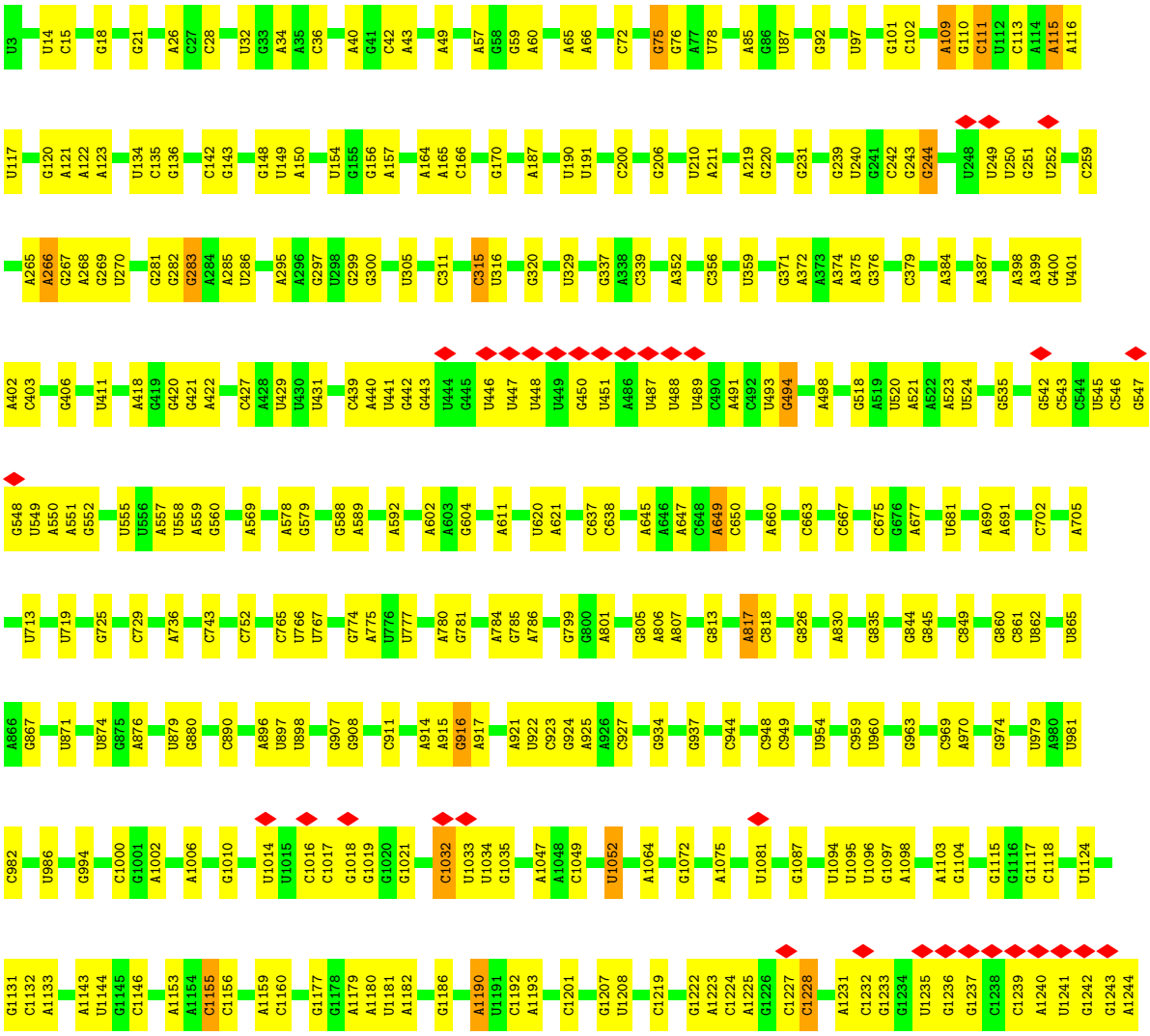
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
82	Ao	1	1	1	0
82	Bb	1	1	1	0

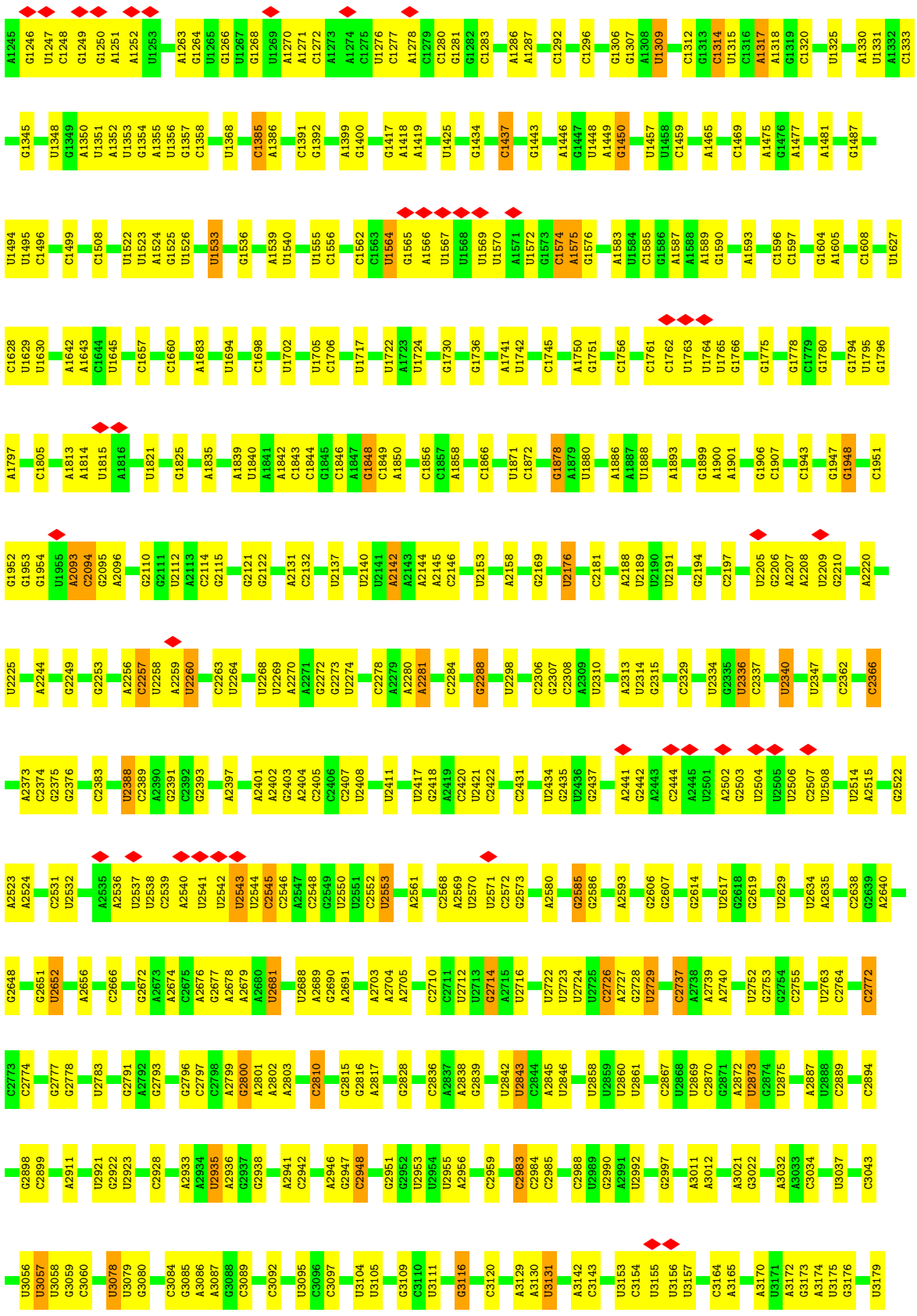
3 Residue-property plots (i)

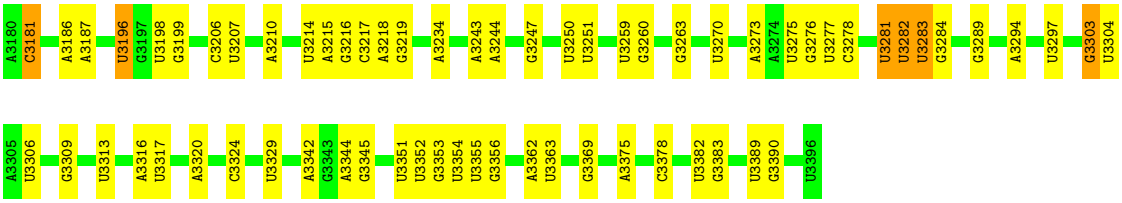
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 25S

Chain A1:

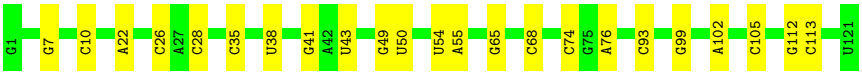



A1245 G1246 U1247 C1248 G1249 G1250 A1251 A1252 U1253 A1263 G1264 U1265 G1266 U1267 G1268 U1269 A1270 A1271 C1272 A1273 A1274 C1275 U1276 C1277 A1278 C1279 C1280 G1281 G1282 C1283 A1286 A1287 C1292 C1296 G1306 G1307 A1308 U1309 C1312 G1313 C1314 U1315 C1316 A1317 A1318 G1319 C1320 U1325 A1330 U1331 A1332 C1333
G1345 U1348 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 C1358 U1368 C1385 A1386 C1391 G1392 A1399 G1400 G1417 A1418 A1419 U1425 G1434 C1437 G1443 A1446 G1447 U1448 A1449 G1450 U1457 U1458 C1459 A1465 C1469 A1475 G1476 A1477 A1481 G1487
U1494 U1495 C1496 C1499 C1508 U1522 U1523 A1524 G1525 U1526 U1533 G1536 A1539 U1540 U1555 C1556 C1562 C1563 U1564 G1565 A1566 U1567 U1568 U1569 U1570 A1571 U1572 G1573 C1574 A1575 G1576 A1583 U1584 C1585 G1586 A1587 A1588 A1589 G1590 A1593 C1596 C1597 G1604 A1605 C1608 U1627
C1628 U1629 U1630 A1642 A1643 C1644 U1645 C1657 C1660 A1683 U1694 C1698 U1702 U1705 C1706 U1717 U1722 A1723 U1724 G1730 G1736 A1741 U1742 C1745 A1750 G1751 C1756 C1761 C1762 U1763 U1764 U1765 G1766 G1775 G1778 C1779 G1780 G1794 U1795 G1796
A1797 C1805 A1813 A1814 U1815 A1816 U1821 G1825 A1835 A1839 U1840 A1841 A1842 C1843 C1844 G1845 C1846 A1847 G1848 C1849 A1850 C1856 C1857 A1858 C1866 U1871 C1872 G1878 A1879 U1880 A1886 A1887 U1888 A1893 G1899 A1900 A1901 G1906 C1907 C1943 G1947 G1948 C1951
G1952 G1953 G1954 U1955 A2093 C2094 G2095 A2096 G2110 G2111 U2112 A2113 C2114 G2115 G2121 G2122 A2131 C2132 U2137 U2140 U2141 A2142 A2143 A2144 A2145 C2146 U2153 A2158 G2169 U2176 C2181 A2188 U2189 U2190 U2191 G2194 C2197 U2205 G2206 A2207 A2208 U2209 G2210 A2220
U2225 A2244 G2249 G2253 A2256 C2257 U2258 A2259 U2260 C2263 U2264 U2268 U2269 A2270 A2271 G2272 G2273 U2274 C2278 A2279 A2280 A2281 C2284 G2288 U2298 C2306 G2307 C2308 A2309 U2310 A2313 U2314 G2315 C2329 U2334 G2335 U2336 C2337 U2340 U2347 C2362 C2366
A2373 C2374 G2375 G2376 C2383 U2388 C2389 A2390 G2391 C2392 G2393 A2397 A2401 A2402 G2403 A2404 C2405 C2406 C2407 U2408 U2411 U2417 G2418 A2419 C2420 U2421 C2422 C2431 U2434 G2435 U2436 G2437 A2441 G2442 A2443 C2444 A2445 U2501 A2502 G2503 U2504 U2505 U2506 C2507 U2508 U2514 A2515 G2522
A2523 A2524 C2531 U2532 A2535 A2536 U2537 U2538 C2539 A2540 U2541 U2542 U2543 U2544 C2545 C2546 A2547 C2548 G2549 U2550 U2551 C2552 U2553 A2561 C2568 A2569 U2570 U2571 C2572 G2573 A2580 G2585 G2586 A2593 G2606 G2607 G2614 U2617 G2618 G2619 U2629 U2634 A2635 C2638 G2639 A2640
G2648 C2651 U2652 A2656 C2666 G2672 A2673 A2674 C2675 A2676 C2677 A2678 A2679 A2680 U2681 U2688 A2689 G2690 A2691 A2703 A2704 A2705 C2710 C2711 U2712 U2713 G2714 A2715 U2716 U2722 U2723 U2724 U2725 C2726 A2727 G2728 U2729 C2737 A2738 A2739 A2740 U2752 G2753 G2754 C2755 U2763 C2764 C2772
C2773 C2774 G2777 G2778 U2783 G2791 A2792 G2793 G2796 C2797 C2798 A2799 G2800 A2801 A2802 A2803 C2810 G2815 G2816 A2817 G2828 C2836 A2837 A2838 G2839 U2842 U2843 C2844 A2845 U2846 U2858 U2859 U2860 U2861 C2867 U2868 U2869 C2870 G2871 A2872 U2873 G2874 U2875 A2887 U2888 C2889 C2894
G2898 C2899 A2911 U2921 G2922 U2923 C2928 A2933 A2934 U2935 A2936 G2937 G2938 A2941 C2942 A2946 G2947 C2948 G2951 G2952 U2953 U2954 U2955 A2956 C2959 C2983 C2984 C2985 C2988 U2989 G2990 A2991 U2992 G2997 A3011 A3012 A3021 G3022 A3032 A3033 C3034 U3037 C3043
U3056 U3057 U3058 G3059 C3060 U3078 U3079 G3080 C3084 G3085 A3086 A3087 G3088 C3089 C3092 U3095 C3096 C3097 U3104 U3105 G3109 C3110 U3111 G3116 C3120 A3129 A3130 U3131 A3142 C3143 U3153 C3154 U3155 U3156 U3157 C3164 A3165 A3170 U3171 A3172 G3173 A3174 U3175 G3176 U3179



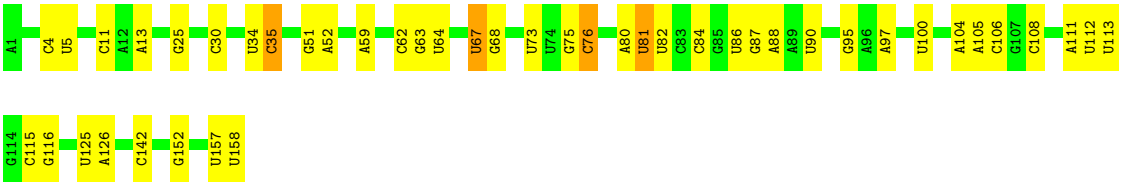
• Molecule 2: 5S

Chain A3:



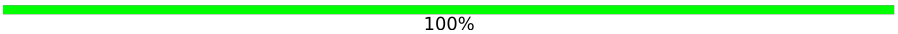
• Molecule 3: 5.8S

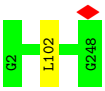
Chain A4:



• Molecule 4: 60S ribosomal protein L2-A

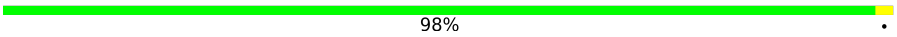
Chain AA:





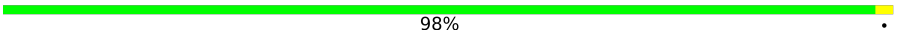
• Molecule 5: 60S ribosomal protein L3

Chain AB:



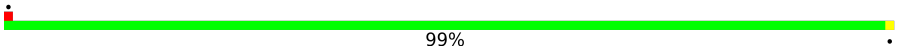
• Molecule 6: 60S ribosomal protein L4-A

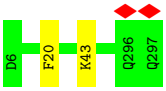
Chain AC:



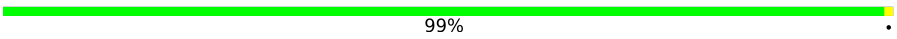
• Molecule 7: 60S ribosomal protein L5

Chain AD:

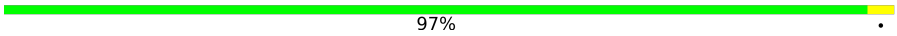




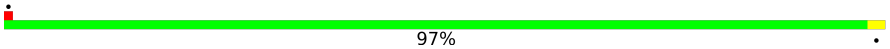
• Molecule 8: 60S ribosomal protein L6-A

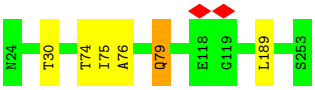
Chain AE: 

• Molecule 9: 60S ribosomal protein L7-A

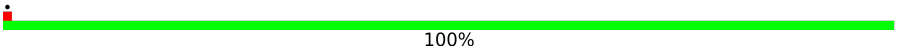
Chain AF: 

• Molecule 10: 60S ribosomal protein L8-A

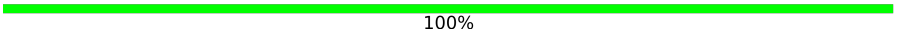
Chain AG: 

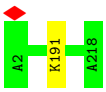


• Molecule 11: 60S ribosomal protein L9-A

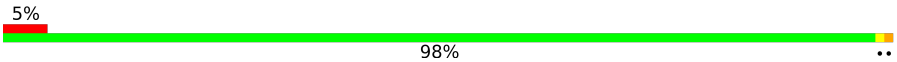
Chain AH: 

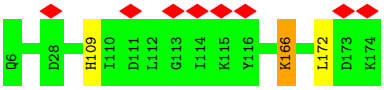
• Molecule 12: 60S ribosomal protein L10

Chain AI: 



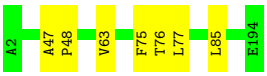
• Molecule 13: 60S ribosomal protein L11-A

Chain AJ: 



• Molecule 14: 60S ribosomal protein L13-A

Chain AL: 96%

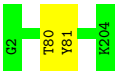


- Molecule 15: 60S ribosomal protein L14-A

Chain AM: 99%

- Molecule 16: 60S ribosomal protein L15-A

Chain AN: 99%

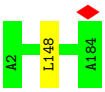


- Molecule 17: 60S ribosomal protein L16-A

Chain AO: 98%

- Molecule 18: 60S ribosomal protein L17-A

Chain AP: 99%

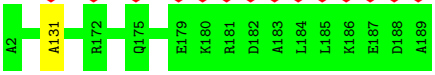


- Molecule 19: 60S ribosomal protein L18-A

Chain AQ: 99%

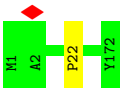
- Molecule 20: 60S ribosomal protein L19-A

Chain AR: 7% 99%



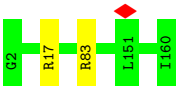
- Molecule 21: 60S ribosomal protein L20-A

Chain AS: 99%



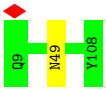
• Molecule 22: 60S ribosomal protein L21-A

Chain AT: 99%



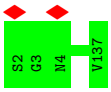
• Molecule 23: 60S ribosomal protein L22-A

Chain AU: 99%



• Molecule 24: 60S ribosomal protein L23-A

Chain AV: 100%



• Molecule 25: 60S ribosomal protein L24-A

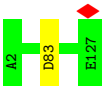
Chain AW: 98%

• Molecule 26: 60S ribosomal protein L25

Chain AX: 100%

• Molecule 27: 60S ribosomal protein L26-A

Chain AY: 99%

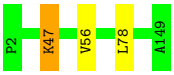


• Molecule 28: 60S ribosomal protein L27-A

Chain AZ: 99%

• Molecule 29: 60S ribosomal protein L28

Chain Aa: 98%



• Molecule 30: 60S ribosomal protein L29

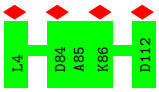
Chain Ab: 100%

• Molecule 31: 60S ribosomal protein L30

Chain Ac: 100%

• Molecule 32: 60S ribosomal protein L31-A

Chain Ad: 100%



• Molecule 33: 60S ribosomal protein L32

Chain Ae: 100%

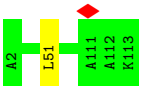
• Molecule 34: 60S ribosomal protein L33-A

Chain Af: 100%

There are no outlier residues recorded for this chain.

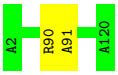
• Molecule 35: 60S ribosomal protein L34-A

Chain Ag: 99%



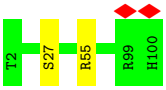
• Molecule 36: 60S ribosomal protein L35-A

Chain Ah: 98%



• Molecule 37: 60S ribosomal protein L36-A

Chain Ai: 98%



• Molecule 38: 60S ribosomal protein L37-A

Chain Aj: 100%

• Molecule 39: 60S ribosomal protein L38

Chain Ak: 100%

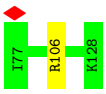
There are no outlier residues recorded for this chain.

• Molecule 40: 60S ribosomal protein L39

Chain Al: 98%

• Molecule 41: 60S ribosomal protein L40-A

Chain Am: 98%



• Molecule 42: 60S ribosomal protein L41-A

Chain An: 100%

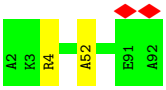
There are no outlier residues recorded for this chain.

• Molecule 43: 60S ribosomal protein L42-A

Chain Ao: 100%

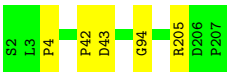
• Molecule 44: 60S ribosomal protein L43-A

Chain Ap: 98%



• Molecule 45: 40S ribosomal protein S0-A

Chain BA: 98%



• Molecule 46: 40S ribosomal protein S1-A

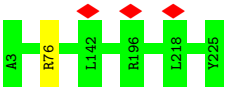
Chain BB: 96%

• Molecule 47: 40S ribosomal protein S2

Chain BC: 98%

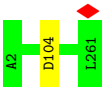
• Molecule 48: 40S ribosomal protein S3

Chain BD: 100%



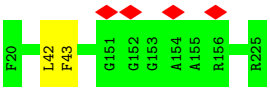
• Molecule 49: 40S ribosomal protein S4-A

Chain BE: 100%



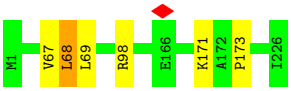
• Molecule 50: 40S ribosomal protein S5

Chain BF: 99%



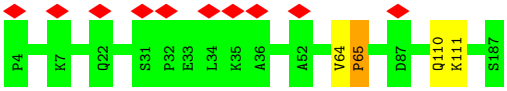
• Molecule 51: 40S ribosomal protein S6-A

Chain BG: 97%



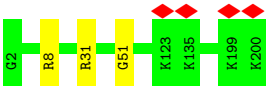
• Molecule 52: 40S ribosomal protein S7-A

Chain BH: 5% 98%



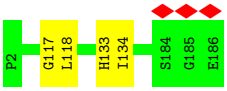
• Molecule 53: 40S ribosomal protein S8-A

Chain BI: 98%



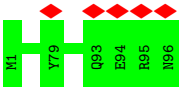
• Molecule 54: 40S ribosomal protein S9-A

Chain BJ: 98%



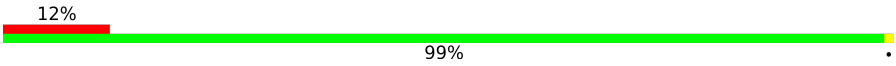
• Molecule 55: 40S ribosomal protein S10-A

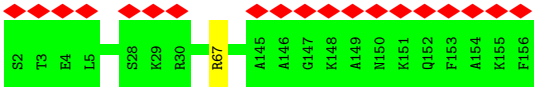
Chain BK: 5% 100%



• Molecule 56: 40S ribosomal protein S11-A

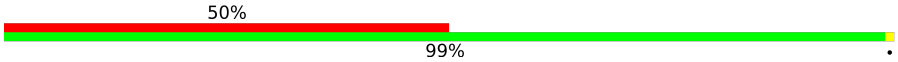
Chain BL:

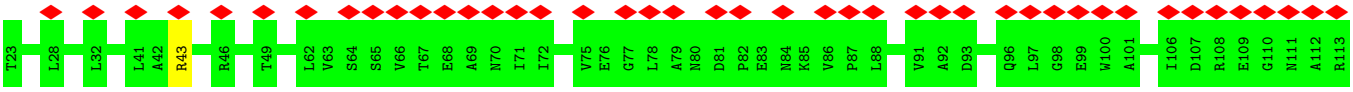


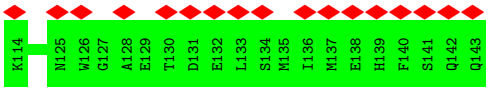


• Molecule 57: 40S ribosomal protein S12

Chain BM:

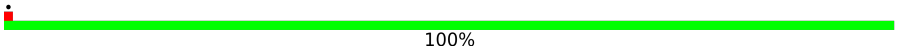






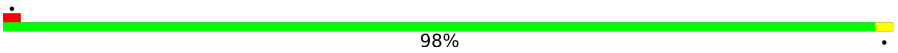
• Molecule 58: 40S ribosomal protein S13

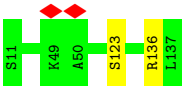
Chain BN:



• Molecule 59: 40S ribosomal protein S14-A

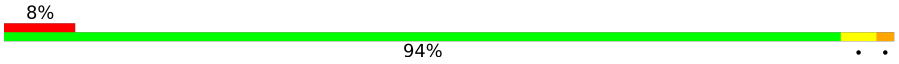
Chain BO:

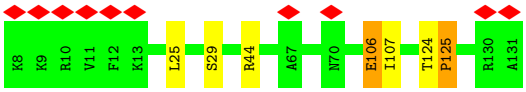




• Molecule 60: 40S ribosomal protein S15

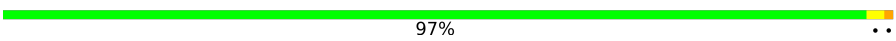
Chain BP:

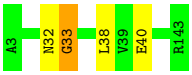




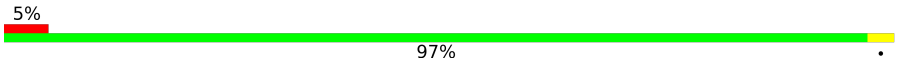
• Molecule 61: 40S ribosomal protein S16-A

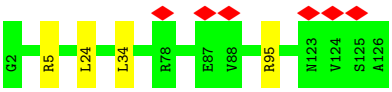
Chain BQ:



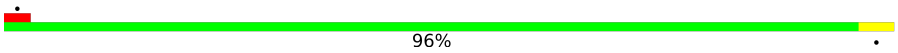


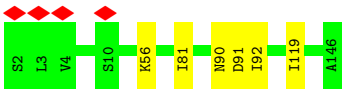
• Molecule 62: 40S ribosomal protein S17-A

Chain BR: 

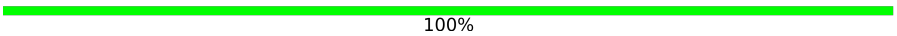


• Molecule 63: 40S ribosomal protein S18-A

Chain BS: 

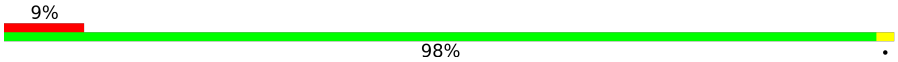


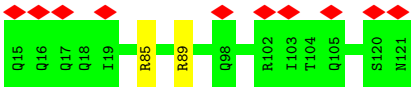
• Molecule 64: 40S ribosomal protein S19-A

Chain BT: 

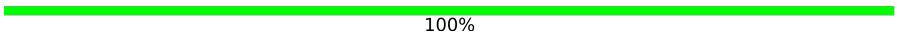
There are no outlier residues recorded for this chain.

• Molecule 65: 40S ribosomal protein S20

Chain BU: 

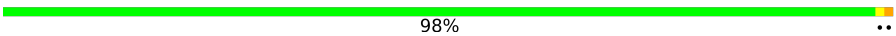


• Molecule 66: 40S ribosomal protein S21-A

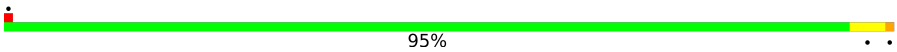
Chain BV: 

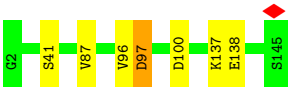
There are no outlier residues recorded for this chain.

• Molecule 67: 40S ribosomal protein S22-A

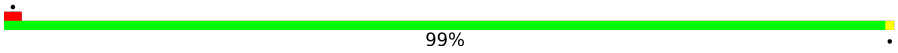
Chain BW: 

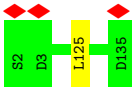
• Molecule 68: 40S ribosomal protein S23-A

Chain BX: 

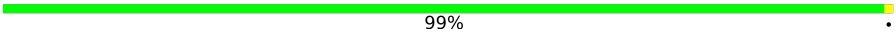


• Molecule 69: 40S ribosomal protein S24-A

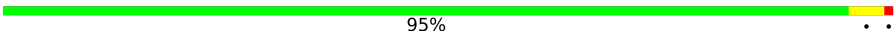
Chain BY: 

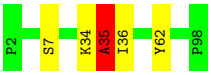


• Molecule 70: 40S ribosomal protein S25-A

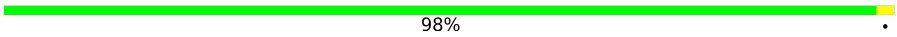
Chain BZ: 

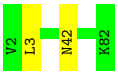
• Molecule 71: 40S ribosomal protein S26-B

Chain Ba: 

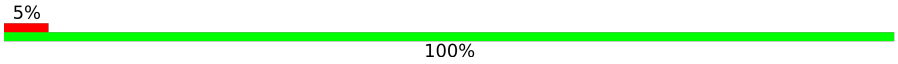


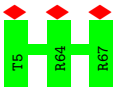
• Molecule 72: 40S ribosomal protein S27-A

Chain Bb: 

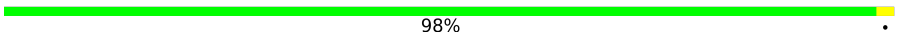


• Molecule 73: 40S ribosomal protein S28-A

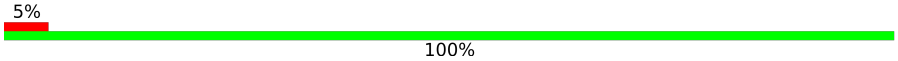
Chain Bc: 

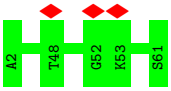


• Molecule 74: 40S ribosomal protein S29-A

Chain Bd: 

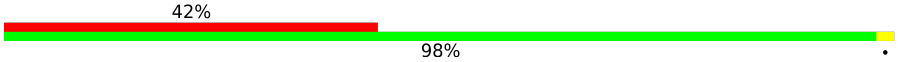
• Molecule 75: 40S ribosomal protein S30-A

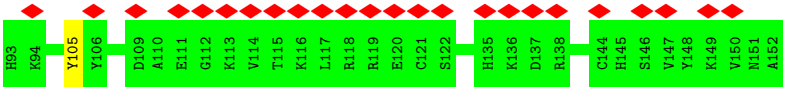
Chain Be: 



• Molecule 76: 40S ribosomal protein S31

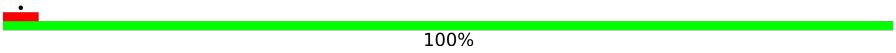
Chain Bf:

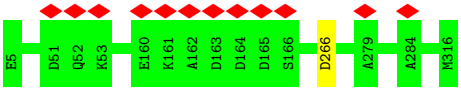




• Molecule 77: Guanine nucleotide-binding protein subunit beta-like protein

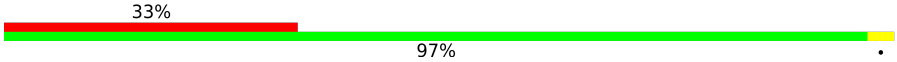
Chain Bg:

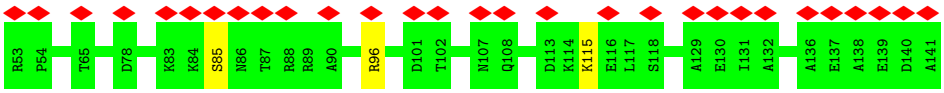




• Molecule 78: Suppressor protein STM1

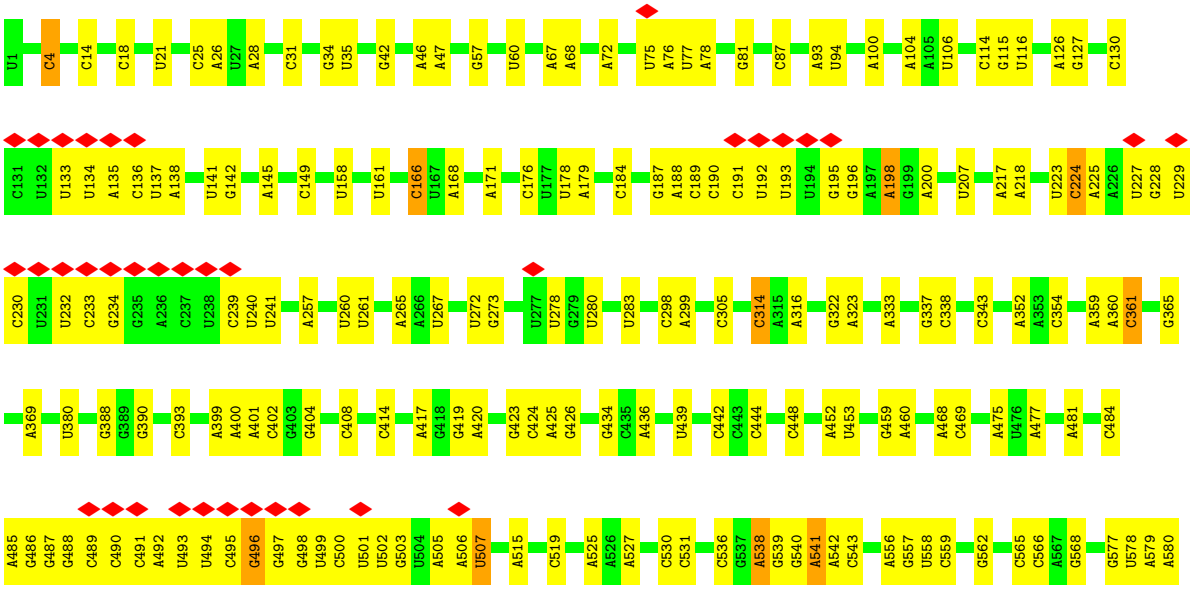
Chain Bh:

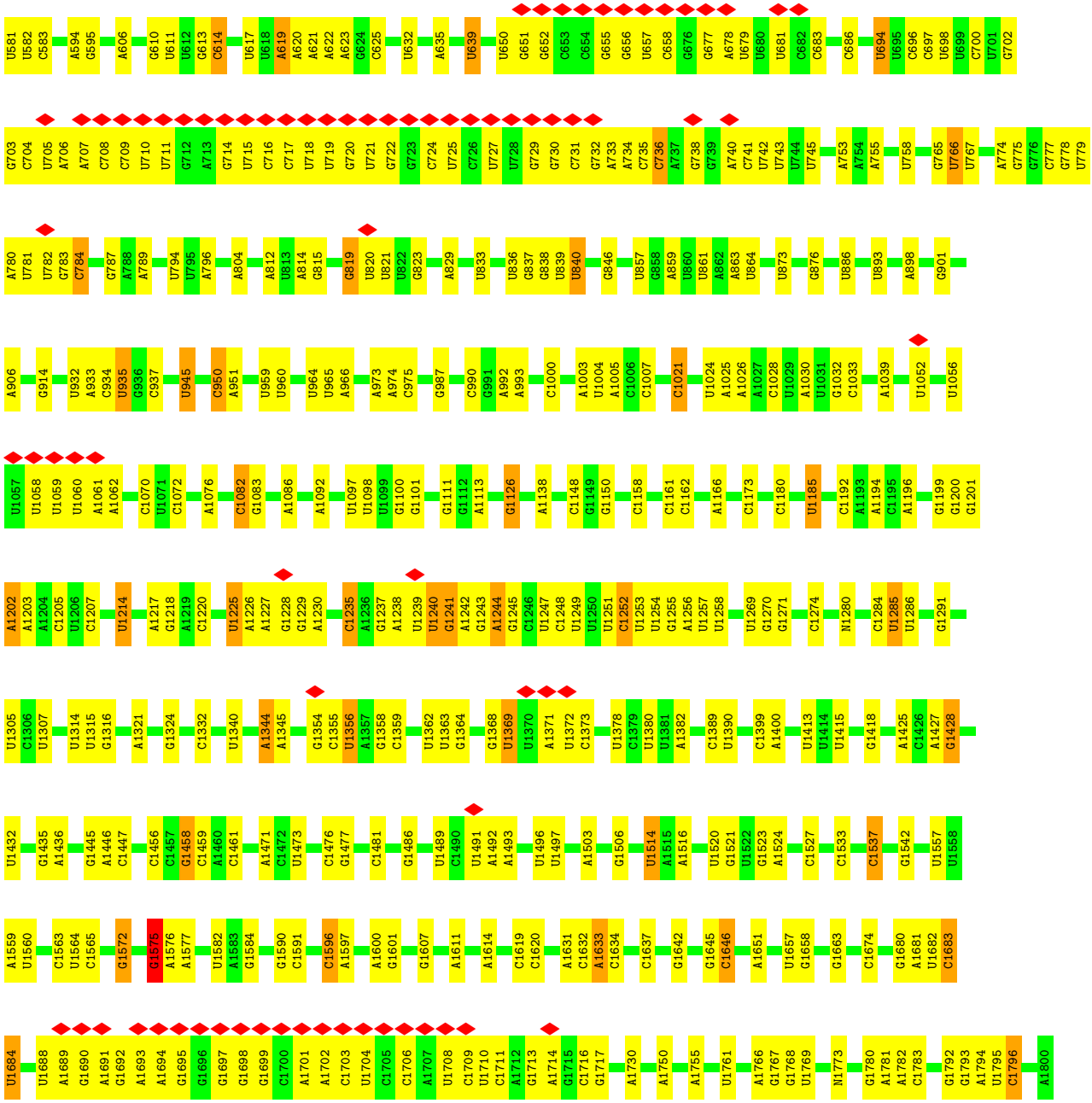




• Molecule 79: 18S RIBOSOMAL RNA

Chain B5:




U581 U582 C583 A594 G595 A606 G610 U611 U612 G613 C614 U617 U618 A619 A620 A621 A622 A623 G624 C625 U632 A635 U639 U650 G651 G652 C653 C654 G655 G656 U657 C658 G676 G677 A678 U679 U680 U681 C682 C683 C686 U694 U695 C696 C697 U698 U699 C700 U701 G702
G703 C704 U705 A706 A707 C708 C709 U710 U711 G712 A713 G714 U715 A716 C717 U718 U719 G720 U721 G722 G723 C724 U725 C726 U727 U728 G729 G730 C731 G732 A733 A734 C735 C736 A737 G738 G739 A740 C741 U742 U743 U744 U745 A753 A754 A755 U758 G765 U766 U767 A774 G775 G776 C777 G778 U779
A780 U781 U782 G783 C784 G787 A788 A789 U794 U795 A796 A804 A812 U813 A814 G815 G819 U820 U821 U822 G823 A829 U833 U836 G837 G838 U839 U840 G846 U857 G858 A859 U860 U861 A862 A863 U864 U873 G876 U886 U893 A898 G901
A906 G914 U932 A933 C934 U935 G936 C937 U945 G950 A951 U959 U960 U964 U965 A966 A973 A974 C975 G987 C990 G991 A992 A993 C1000 A1003 U1004 A1005 C1006 C1007 C1021 U1024 A1025 A1026 A1027 C1028 U1029 A1030 U1031 G1032 C1033 A1039 U1052 U1056
U1057 U1058 U1059 U1060 A1061 A1062 C1070 U1071 C1072 A1076 C1082 G1083 A1086 A1092 U1097 U1098 U1099 G1100 G1101 G1111 G1112 A1113 G1126 A1138 C1148 G1149 G1150 C1158 C1161 C1162 A1166 C1173 C1180 U1185 C1192 A1193 A1194 C1195 A1196 G1199 G1200 G1201
A1202 A1203 A1204 C1205 U1206 C1207 U1214 A1217 G1218 A1219 C1220 U1225 A1226 A1227 G1228 G1229 A1230 C1235 A1236 G1237 A1238 U1239 U1240 G1241 A1242 G1243 A1244 G1245 C1246 U1247 C1248 U1249 U1250 U1251 C1252 U1253 U1254 G1255 A1256 U1257 U1258 U1269 G1270 G1271 C1274 N1280 C1284 U1285 U1286 G1291
U1305 C1306 U1307 U1314 U1315 G1316 A1321 G1324 C1332 U1340 A1344 A1345 G1354 C1355 U1356 A1357 G1358 C1359 U1362 U1363 G1364 G1368 U1369 U1370 A1371 U1372 C1373 U1378 C1379 U1380 U1381 A1382 C1389 U1390 C1399 A1400 U1413 U1414 U1415 G1418 A1425 C1426 A1427 G1428
U1432 G1435 A1436 G1445 A1446 C1447 C1456 C1457 G1458 C1459 A1460 C1461 A1471 C1472 U1473 C1476 G1477 C1481 G1486 U1489 C1490 U1491 A1492 A1493 U1496 U1497 A1503 G1506 U1514 A1515 A1516 U1520 G1521 U1522 G1523 A1524 C1527 C1533 C1537 G1542 U1557 U1558
A1559 U1560 C1563 U1564 C1565 G1572 G1575 A1576 A1577 U1582 A1583 G1584 G1590 C1591 C1596 A1597 A1600 G1601 G1607 A1611 A1614 C1619 C1620 A1631 C1632 A1633 C1634 C1637 G1642 G1645 C1646 A1651 U1657 G1658 G1663 C1674 G1680 A1681 U1682 C1683
U1684 U1688 A1689 G1690 A1691 G1692 A1693 A1694 G1695 G1696 G1697 G1698 G1699 C1700 A1701 A1702 C1703 U1704 C1705 C1706 A1707 U1708 C1709 U1710 C1711 A1712 G1713 A1714 G1715 C1716 G1717 A1730 A1750 A1755 U1761 A1766 G1767 G1768 U1769 N1773 G1780 A1781 A1782 C1783 G1792 G1793 A1794 U1795 C1796 A1800

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	178990	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 ($e^-/Å^2$)	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	0.233	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	455.75998, 455.75998, 455.75998	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 3HE, OMU, MG, 1MA, ZN, OMC, A2M, 3AU, OMG, 4AC, HIC, UR3, 5MC, G7M

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A1	1.02	2/74562 (0.0%)	1.14	436/116239 (0.4%)
2	A3	0.86	0/2883	1.06	13/4491 (0.3%)
3	A4	1.09	0/3745	1.14	25/5828 (0.4%)
4	AA	0.55	0/1912	0.65	1/2569 (0.0%)
5	AB	0.59	0/3137	0.66	4/4215 (0.1%)
6	AC	0.54	1/2800 (0.0%)	0.66	1/3790 (0.0%)
7	AD	0.44	0/2390	0.58	0/3225
8	AE	0.51	0/1260	0.59	0/1694
9	AF	0.54	0/1821	0.64	2/2451 (0.1%)
10	AG	0.50	0/1830	0.62	3/2469 (0.1%)
11	AH	0.52	0/1531	0.62	0/2062
12	AI	0.42	0/1708	0.57	0/2290
13	AJ	0.36	0/1374	0.63	1/1842 (0.1%)
14	AL	0.54	0/1568	0.63	1/2106 (0.0%)
15	AM	0.55	0/1068	0.62	1/1438 (0.1%)
16	AN	0.62	0/1757	0.68	0/2354
17	AO	0.56	0/1585	0.58	1/2128 (0.0%)
18	AP	0.53	0/1410	0.56	1/1893 (0.1%)
19	AQ	0.50	0/1465	0.61	1/1965 (0.1%)
20	AR	0.46	0/1538	0.54	0/2050
21	AS	0.60	0/1481	0.65	0/1990
22	AT	0.52	0/1300	0.63	0/1743
23	AU	0.48	0/812	0.64	0/1099
24	AV	0.52	0/1018	0.62	0/1369
25	AW	0.53	0/533	0.62	1/707 (0.1%)
26	AX	0.56	0/983	0.61	0/1325
27	AY	0.55	0/1004	0.70	1/1341 (0.1%)
28	AZ	0.51	0/1118	0.65	0/1497
29	Aa	0.54	0/1204	0.71	2/1612 (0.1%)
30	Ab	0.39	0/473	0.53	0/629
31	Ac	0.49	0/751	0.56	0/1008
32	Ad	0.56	0/904	0.58	0/1213

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ae	0.53	0/1041	0.55	0/1394
34	Af	0.61	0/868	0.56	0/1168
35	Ag	0.56	0/890	0.66	2/1189 (0.2%)
36	Ah	0.49	0/978	0.56	0/1301
37	Ai	0.47	0/778	0.66	0/1034
38	Aj	0.60	0/696	0.63	0/923
39	Ak	0.51	0/618	0.65	0/826
40	Al	0.55	0/443	0.73	1/588 (0.2%)
41	Am	0.53	0/423	0.56	0/562
42	An	0.33	0/234	0.51	0/300
43	Ao	0.45	0/860	0.62	0/1136
44	Ap	0.52	0/701	0.67	0/934
45	BA	0.42	0/1653	0.60	2/2261 (0.1%)
46	BB	0.43	0/1735	0.71	2/2335 (0.1%)
47	BC	0.47	1/1665 (0.1%)	0.66	1/2263 (0.0%)
48	BD	0.42	0/1759	0.64	0/2368
49	BE	0.48	0/2109	0.67	1/2839 (0.0%)
50	BF	0.42	0/1629	0.62	0/2202
51	BG	0.42	0/1844	0.63	3/2464 (0.1%)
52	BH	0.40	0/1506	0.71	0/2028
53	BI	0.46	1/1514 (0.1%)	0.63	0/2021
54	BJ	0.43	0/1519	0.65	1/2035 (0.0%)
55	BK	0.45	0/837	0.71	0/1131
56	BL	0.47	0/1272	0.55	0/1712
57	BM	0.31	0/921	0.67	0/1245
58	BN	0.46	0/1215	0.63	0/1638
59	BO	0.43	0/952	0.67	0/1279
60	BP	0.47	0/1012	0.71	2/1356 (0.1%)
61	BQ	0.44	0/1125	0.67	1/1510 (0.1%)
62	BR	0.36	0/984	0.64	1/1318 (0.1%)
63	BS	0.45	0/1211	0.67	1/1628 (0.1%)
64	BT	0.48	0/1113	0.71	0/1494
65	BU	0.42	0/865	0.66	2/1169 (0.2%)
66	BV	0.48	0/692	0.61	0/932
67	BW	0.52	0/1038	0.66	1/1395 (0.1%)
68	BX	0.48	0/1139	0.74	1/1518 (0.1%)
69	BY	0.48	0/1087	0.66	1/1449 (0.1%)
70	BZ	0.39	0/566	0.70	1/761 (0.1%)
71	Ba	0.46	0/782	0.73	1/1047 (0.1%)
72	Bb	0.41	0/620	0.66	1/838 (0.1%)
73	Bc	0.39	0/499	0.71	0/670
74	Bd	0.48	0/452	0.64	0/600
75	Be	0.40	0/483	0.53	0/643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Bf	0.33	0/462	0.69	0/617
77	Bg	0.39	0/2454	0.65	1/3340 (0.0%)
78	Bh	0.28	0/678	0.54	0/905
79	B5	0.81	0/41746	1.15	315/65032 (0.5%)
All	All	0.79	5/212593 (0.0%)	0.98	837/312030 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	AC	0	2
7	AD	0	1
8	AE	0	1
9	AF	0	3
10	AG	0	4
13	AJ	0	2
14	AL	0	2
16	AN	0	1
17	AO	0	1
20	AR	0	1
21	AS	0	1
22	AT	0	1
28	AZ	0	1
36	Ah	0	1
37	Ai	0	1
45	BA	0	1
46	BB	0	4
47	BC	0	1
50	BF	0	2
51	BG	0	1
52	BH	0	3
53	BI	0	2
54	BJ	0	2
59	BO	0	1
60	BP	0	4
61	BQ	0	3
63	BS	0	3
67	BW	0	1
68	BX	0	5
71	Ba	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
76	Bf	0	1
78	Bh	0	1
79	B5	4	0
All	All	4	61

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	BC	111	VAL	CB-CG1	-5.29	1.41	1.52
53	BI	31	ARG	C-N	-5.22	1.22	1.34
1	A1	300	G	N9-C8	-5.16	1.34	1.37
1	A1	1835	A	C6-N1	-5.16	1.31	1.35
6	AC	230	VAL	CB-CG1	-5.13	1.42	1.52

All (837) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	266	A	O5'-P-OP1	-29.63	75.14	110.70
1	A1	266	A	OP1-P-OP2	-28.49	76.86	119.60
1	A1	266	A	O5'-P-OP2	18.43	132.82	110.70
79	B5	1537	C	N1-C2-O2	13.61	127.07	118.90
1	A1	1948	G	OP1-P-OP2	13.40	139.70	119.60
1	A1	265	A	OP2-P-O3'	-13.16	76.24	105.20
79	B5	1537	C	C2-N1-C1'	13.13	133.24	118.80
1	A1	265	A	OP1-P-O3'	13.03	133.87	105.20
79	B5	453	U	N1-C2-O2	12.65	131.66	122.80
79	B5	453	U	N3-C2-O2	-12.48	113.46	122.20
79	B5	453	U	C2-N1-C1'	12.16	132.30	117.70
1	A1	1947	G	OP2-P-O3'	-11.88	79.06	105.20
79	B5	224	C	N1-C2-O2	11.44	125.77	118.90
1	A1	1385	C	C6-N1-C2	-10.83	115.97	120.30
1	A1	2225	U	N3-C2-O2	-10.74	114.68	122.20
1	A1	3057	U	N3-C2-O2	-10.55	114.82	122.20
79	B5	581	U	C2-N1-C1'	10.13	129.85	117.70
79	B5	1537	C	N3-C2-O2	-10.09	114.84	121.90
1	A1	300	G	N7-C8-N9	10.07	118.13	113.10
79	B5	1389	C	C2-N1-C1'	10.03	129.83	118.80
1	A1	1597	C	C5-C6-N1	10.02	126.01	121.00
1	A1	3034	C	C2-N1-C1'	10.01	129.81	118.80
1	A1	922	U	C2-N1-C1'	9.94	129.62	117.70
79	B5	224	C	N3-C2-O2	-9.78	115.05	121.90
79	B5	1254	U	N3-C2-O2	-9.73	115.39	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	1314	C	C6-N1-C2	-9.71	116.42	120.30
79	B5	581	U	N1-C2-O2	9.70	129.59	122.80
1	A1	2550	U	N3-C2-O2	-9.55	115.52	122.20
1	A1	3034	C	N3-C2-O2	-9.53	115.23	121.90
1	A1	406	G	O4'-C1'-N9	9.38	115.71	108.20
1	A1	3306	U	N3-C2-O2	-9.32	115.67	122.20
79	B5	224	C	C2-N1-C1'	9.29	129.03	118.80
1	A1	1385	C	C5-C6-N1	9.29	125.65	121.00
3	A4	5	U	N3-C2-O2	-9.29	115.70	122.20
79	B5	1537	C	C6-N1-C1'	-9.23	109.72	120.80
79	B5	1564	U	N3-C2-O2	-9.17	115.78	122.20
1	A1	2836	C	C2-N1-C1'	9.03	128.73	118.80
79	B5	767	U	N3-C2-O2	-8.99	115.90	122.20
1	A1	78	U	N3-C2-O2	-8.96	115.92	122.20
79	B5	581	U	N3-C2-O2	-8.96	115.93	122.20
1	A1	3181	C	N1-C2-O2	8.94	124.26	118.90
1	A1	2550	U	N1-C2-O2	8.87	129.01	122.80
1	A1	3057	U	N1-C2-O2	8.87	129.01	122.80
79	B5	1380	U	N3-C2-O2	-8.81	116.03	122.20
3	A4	5	U	C2-N1-C1'	8.78	128.24	117.70
1	A1	1496	C	C2-N1-C1'	8.78	128.46	118.80
1	A1	2983	C	C2-N1-C1'	8.73	128.41	118.80
1	A1	2836	C	N3-C2-O2	-8.70	115.81	121.90
1	A1	1694	U	N3-C2-O2	-8.68	116.12	122.20
79	B5	784	C	C5-C6-N1	8.67	125.33	121.00
79	B5	959	U	N3-C2-O2	-8.64	116.15	122.20
1	A1	42	C	C5-C6-N1	8.62	125.31	121.00
1	A1	1835	A	C6-N1-C2	8.61	123.77	118.60
79	B5	959	U	N1-C2-O2	8.52	128.77	122.80
79	B5	1560	U	C2-N1-C1'	8.50	127.90	117.70
79	B5	538	A	N7-C8-N9	8.49	118.05	113.80
1	A1	3058	U	C2-N1-C1'	8.48	127.87	117.70
1	A1	3058	U	N1-C2-O2	8.41	128.69	122.80
1	A1	922	U	N1-C2-O2	8.41	128.69	122.80
79	B5	1254	U	N1-C2-O2	8.40	128.68	122.80
1	A1	1496	C	C6-N1-C2	-8.35	116.96	120.30
1	A1	2225	U	C2-N1-C1'	8.34	127.70	117.70
1	A1	2263	C	C2-N1-C1'	8.31	127.94	118.80
1	A1	3034	C	N1-C2-O2	8.31	123.89	118.90
79	B5	1560	U	N3-C2-O2	-8.29	116.40	122.20
3	A4	64	U	N3-C2-O2	-8.28	116.41	122.20
79	B5	1380	U	C2-N1-C1'	8.27	127.63	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	B5	1254	U	C2-N1-C1'	8.24	127.59	117.70
3	A4	73	U	N3-C2-O2	-8.22	116.45	122.20
1	A1	3034	C	C6-N1-C2	-8.21	117.02	120.30
1	A1	2225	U	N1-C2-O2	8.21	128.54	122.80
1	A1	3181	C	C2-N1-C1'	8.18	127.80	118.80
79	B5	116	U	N3-C2-O2	-8.18	116.47	122.20
79	B5	1537	C	C6-N1-C2	-8.18	117.03	120.30
1	A1	2836	C	N1-C2-O2	8.17	123.80	118.90
79	B5	1646	C	N1-C2-O2	8.15	123.79	118.90
1	A1	969	C	C6-N1-C2	-8.13	117.05	120.30
79	B5	1241	G	O4'-C1'-N9	8.13	114.71	108.20
79	B5	531	C	C6-N1-C2	-8.13	117.05	120.30
1	A1	2550	U	C2-N1-C1'	8.12	127.44	117.70
79	B5	224	C	C6-N1-C2	-8.11	117.06	120.30
61	BQ	38	LEU	CA-CB-CG	8.09	133.91	115.30
79	B5	864	U	C2-N1-C1'	8.09	127.41	117.70
3	A4	73	U	C2-N1-C1'	8.08	127.40	117.70
6	AC	182	LEU	CA-CB-CG	8.07	133.87	115.30
1	A1	1314	C	C5-C6-N1	8.00	125.00	121.00
79	B5	1489	U	C2-N1-C1'	8.00	127.30	117.70
79	B5	864	U	N3-C2-O2	-7.99	116.61	122.20
1	A1	2800	G	O5'-P-OP2	-7.96	98.53	105.70
79	B5	1173	C	C5-C6-N1	7.96	124.98	121.00
79	B5	934	C	C2-N1-C1'	7.95	127.54	118.80
79	B5	1082	C	C2-N1-C1'	7.94	127.54	118.80
79	B5	1537	C	C5-C6-N1	7.94	124.97	121.00
1	A1	2652	U	N3-C2-O2	-7.89	116.67	122.20
79	B5	1307	U	N1-C2-O2	7.89	128.32	122.80
79	B5	496	G	C4-N9-C1'	7.89	136.76	126.50
1	A1	3181	C	N3-C2-O2	-7.87	116.39	121.90
79	B5	1458	G	C4-N9-C1'	7.87	136.72	126.50
1	A1	1947	G	OP1-P-O3'	-7.86	87.90	105.20
79	B5	861	U	C2-N1-C1'	7.86	127.13	117.70
1	A1	1872	C	N1-C2-O2	7.83	123.60	118.90
40	Al	45	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A1	3037	U	N3-C2-O2	-7.82	116.72	122.20
79	B5	767	U	C2-N1-C1'	7.82	127.09	117.70
1	A1	1496	C	C5-C6-N1	7.82	124.91	121.00
79	B5	1489	U	N1-C2-O2	7.81	128.27	122.80
1	A1	102	C	N3-C2-O2	-7.80	116.44	121.90
1	A1	2846	U	N3-C2-O2	-7.80	116.74	122.20
1	A1	3131	U	C2-N1-C1'	7.79	127.05	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	B5	453	U	C6-N1-C1'	-7.79	110.30	121.20
1	A1	2264	U	N3-C2-O2	-7.74	116.78	122.20
1	A1	3317	U	N3-C2-O2	-7.73	116.79	122.20
79	B5	864	U	N1-C2-O2	7.73	128.21	122.80
79	B5	1489	U	N3-C2-O2	-7.72	116.79	122.20
79	B5	1307	U	N3-C2-O2	-7.72	116.80	122.20
1	A1	1495	U	C4-C5-C6	7.71	124.33	119.70
1	A1	3037	U	C2-N1-C1'	7.71	126.95	117.70
1	A1	102	C	C6-N1-C2	-7.70	117.22	120.30
1	A1	2846	U	C2-N1-C1'	7.68	126.92	117.70
79	B5	767	U	N1-C2-O2	7.67	128.17	122.80
79	B5	18	C	C5-C6-N1	7.66	124.83	121.00
2	A3	105	C	N1-C2-O2	7.65	123.49	118.90
79	B5	507	U	N3-C2-O2	-7.64	116.85	122.20
1	A1	3306	U	C2-N1-C1'	7.57	126.79	117.70
1	A1	922	U	N3-C2-O2	-7.54	116.92	122.20
1	A1	2407	C	C5-C6-N1	7.51	124.76	121.00
1	A1	954	U	C2-N1-C1'	7.50	126.70	117.70
79	B5	959	U	C2-N1-C1'	7.50	126.70	117.70
1	A1	3196	U	C2-N1-C1'	7.50	126.70	117.70
79	B5	1591	C	C6-N1-C2	-7.49	117.31	120.30
79	B5	1533	C	N1-C2-O2	7.47	123.38	118.90
79	B5	1173	C	C6-N1-C2	-7.47	117.31	120.30
79	B5	840	U	N3-C2-O2	-7.45	116.98	122.20
79	B5	1307	U	C2-N1-C1'	7.44	126.63	117.70
1	A1	3057	U	C2-N1-C1'	7.43	126.62	117.70
1	A1	3214	U	N3-C2-O2	-7.41	117.01	122.20
1	A1	2206	G	N3-C4-C5	-7.40	124.90	128.60
79	B5	583	C	N1-C2-O2	7.40	123.34	118.90
79	B5	1564	U	C2-N1-C1'	7.40	126.58	117.70
79	B5	1473	U	N1-C2-O2	7.38	127.96	122.80
15	AM	40	ASP	CB-CG-OD2	7.37	124.94	118.30
79	B5	1162	C	N1-C2-O2	7.37	123.32	118.90
1	A1	3317	U	N1-C2-O2	7.34	127.94	122.80
1	A1	2264	U	N1-C2-O2	7.34	127.94	122.80
1	A1	3058	U	N3-C2-O2	-7.33	117.07	122.20
1	A1	300	G	C8-N9-C4	-7.32	103.47	106.40
51	BG	171	LYS	C-N-CA	7.31	139.97	121.70
79	B5	538	A	C8-N9-C4	-7.30	102.88	105.80
1	A1	3084	C	C6-N1-C2	-7.28	117.39	120.30
79	B5	1560	U	N1-C2-O2	7.25	127.88	122.80
79	B5	1389	C	C5-C6-N1	7.25	124.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	B5	507	U	N1-C2-O2	7.21	127.85	122.80
1	A1	2899	C	C2-N1-C1'	7.21	126.73	118.80
79	B5	1389	C	N1-C2-O2	7.21	123.22	118.90
1	A1	102	C	N1-C2-O2	7.18	123.21	118.90
3	A4	73	U	N1-C2-O2	7.16	127.81	122.80
79	B5	1389	C	C6-N1-C2	-7.16	117.44	120.30
79	B5	965	U	C2-N1-C1'	7.13	126.26	117.70
3	A4	64	U	N1-C2-O2	7.11	127.78	122.80
79	B5	840	U	N1-C2-O2	7.08	127.76	122.80
79	B5	1473	U	C2-N1-C1'	7.07	126.19	117.70
1	A1	2983	C	N3-C2-O2	-7.07	116.95	121.90
79	B5	1148	C	C6-N1-C2	-7.06	117.48	120.30
1	A1	78	U	N1-C2-O2	7.06	127.74	122.80
79	B5	1291	G	N3-C2-N2	-7.06	114.96	119.90
1	A1	42	C	C6-N1-C2	-7.05	117.48	120.30
79	B5	1000	C	C2-N1-C1'	7.05	126.56	118.80
79	B5	1514	U	N1-C2-O2	7.05	127.73	122.80
79	B5	1458	G	C8-N9-C1'	-7.05	117.84	127.00
79	B5	839	U	N1-C2-O2	7.04	127.73	122.80
1	A1	2716	U	N3-C2-O2	-7.04	117.27	122.20
1	A1	3306	U	N1-C2-O2	7.04	127.73	122.80
79	B5	1683	C	O4'-C1'-N1	7.01	113.81	108.20
1	A1	702	C	C6-N1-C2	-7.01	117.50	120.30
79	B5	1285	U	P-O3'-C3'	7.00	128.10	119.70
1	A1	2206	G	C4-N9-C1'	7.00	135.60	126.50
1	A1	1604	G	C4-N9-C1'	6.99	135.58	126.50
1	A1	1115	G	C4-N9-C1'	6.98	135.57	126.50
1	A1	1645	U	N3-C2-O2	-6.97	117.32	122.20
79	B5	1796	C	C6-N1-C2	-6.96	117.52	120.30
79	B5	1021	C	C6-N1-C2	-6.96	117.52	120.30
1	A1	3037	U	N1-C2-O2	6.95	127.66	122.80
79	B5	583	C	C6-N1-C2	-6.95	117.52	120.30
1	A1	1574	C	N1-C2-O2	6.94	123.07	118.90
79	B5	1796	C	C2-N1-C1'	6.90	126.39	118.80
79	B5	1082	C	N1-C2-O2	6.90	123.04	118.90
79	B5	839	U	N3-C2-O2	-6.89	117.37	122.20
2	A3	50	U	N1-C2-O2	6.88	127.61	122.80
79	B5	1646	C	C6-N1-C2	-6.87	117.55	120.30
1	A1	2263	C	N1-C2-O2	6.86	123.02	118.90
1	A1	300	G	C4-N9-C1'	6.85	135.41	126.50
1	A1	2737	C	N1-C2-O2	6.85	123.01	118.90
1	A1	2652	U	N1-C2-O2	6.85	127.59	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	B5	1514	U	N3-C2-O2	-6.85	117.41	122.20
49	BE	104	ASP	CB-CG-OD2	6.83	124.45	118.30
79	B5	1082	C	C6-N1-C2	-6.83	117.57	120.30
1	A1	2846	U	N1-C2-O2	6.83	127.58	122.80
1	A1	2405	C	C6-N1-C2	-6.82	117.57	120.30
1	A1	969	C	N1-C2-O2	6.81	122.99	118.90
2	A3	50	U	C2-N1-C1'	6.81	125.87	117.70
79	B5	610	G	C4-N9-C1'	6.81	135.35	126.50
45	BA	43	ASP	CB-CG-OD1	6.80	124.42	118.30
79	B5	736	C	N3-C2-O2	-6.80	117.14	121.90
1	A1	835	G	O4'-C1'-N9	6.80	113.64	108.20
1	A1	2366	C	C2-N1-C1'	6.80	126.28	118.80
1	A1	2726	C	C2-N1-C1'	6.79	126.27	118.80
79	B5	581	U	C6-N1-C1'	-6.78	111.70	121.20
1	A1	2146	C	C6-N1-C2	-6.77	117.59	120.30
79	B5	14	C	C6-N1-C2	-6.76	117.60	120.30
79	B5	758	U	N1-C2-O2	6.75	127.53	122.80
79	B5	784	C	C6-N1-C2	-6.75	117.60	120.30
1	A1	3317	U	C2-N1-C1'	6.75	125.80	117.70
79	B5	1533	C	N3-C2-O2	-6.74	117.18	121.90
1	A1	922	U	C6-N1-C1'	-6.74	111.77	121.20
1	A1	1597	C	C6-N1-C2	-6.74	117.61	120.30
1	A1	3362	A	N7-C8-N9	6.74	117.17	113.80
79	B5	1389	C	C6-N1-C1'	-6.73	112.72	120.80
79	B5	496	G	C8-N9-C1'	-6.73	118.25	127.00
79	B5	1456	C	C2-N1-C1'	6.73	126.20	118.80
1	A1	1118	C	C6-N1-C2	-6.73	117.61	120.30
79	B5	935	U	N1-C2-O2	6.72	127.50	122.80
79	B5	1646	C	N3-C2-O2	-6.72	117.19	121.90
1	A1	880	G	O4'-C1'-N9	6.72	113.58	108.20
3	A4	5	U	N1-C2-O2	6.70	127.49	122.80
1	A1	1368	U	C5-C6-N1	6.70	126.05	122.70
79	B5	224	C	C5-C6-N1	6.70	124.35	121.00
1	A1	3131	U	C5-C6-N1	6.68	126.04	122.70
1	A1	3214	U	C2-N1-C1'	6.68	125.72	117.70
1	A1	2714	G	N3-C4-C5	6.68	131.94	128.60
1	A1	411	U	N3-C2-O2	-6.67	117.53	122.20
79	B5	543	C	C2-N1-C1'	6.67	126.13	118.80
1	A1	1698	C	C6-N1-C2	-6.65	117.64	120.30
1	A1	954	U	N3-C2-O2	-6.64	117.55	122.20
3	A4	100	U	C5-C6-N1	6.64	126.02	122.70
79	B5	839	U	C2-N1-C1'	6.63	125.65	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	B5	840	U	C2-N1-C1'	6.62	125.65	117.70
1	A1	2553	U	C2-N1-C1'	6.62	125.64	117.70
79	B5	935	U	N3-C2-O2	-6.62	117.57	122.20
1	A1	2405	C	N1-C2-O2	6.61	122.87	118.90
1	A1	1495	U	N1-C2-N3	6.61	118.86	114.90
1	A1	3362	A	O4'-C1'-N9	6.59	113.47	108.20
1	A1	2405	C	C2-N1-C1'	6.59	126.05	118.80
2	A3	50	U	N3-C2-O2	-6.58	117.59	122.20
1	A1	2132	C	C6-N1-C2	-6.58	117.67	120.30
25	AW	6	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A1	2362	C	C5-C6-N1	6.57	124.28	121.00
79	B5	1024	U	N3-C2-O2	-6.56	117.61	122.20
79	B5	21	U	N3-C2-O2	-6.55	117.61	122.20
79	B5	758	U	N3-C2-O2	-6.55	117.61	122.20
79	B5	496	G	N3-C4-N9	6.55	129.93	126.00
1	A1	1496	C	N1-C2-O2	6.54	122.83	118.90
1	A1	1368	U	C2-N1-C1'	6.54	125.55	117.70
79	B5	1796	C	N3-C2-O2	-6.54	117.32	121.90
1	A1	2274	U	N1-C2-O2	6.54	127.38	122.80
1	A1	113	C	C2-N1-C1'	6.53	125.98	118.80
79	B5	934	C	N1-C2-O2	6.52	122.81	118.90
79	B5	1646	C	C2-N1-C1'	6.51	125.96	118.80
1	A1	2189	U	N3-C2-O2	-6.51	117.64	122.20
3	A4	35	C	C6-N1-C2	-6.50	117.70	120.30
79	B5	18	C	C6-N1-C2	-6.50	117.70	120.30
79	B5	1380	U	N1-C2-O2	6.50	127.35	122.80
79	B5	583	C	N3-C2-O2	-6.49	117.36	121.90
1	A1	1320	C	C6-N1-C2	-6.49	117.71	120.30
1	A1	1425	U	N3-C2-O2	-6.48	117.66	122.20
1	A1	1385	C	P-O3'-C3'	6.47	127.46	119.70
79	B5	1620	C	N1-C2-O2	6.45	122.77	118.90
1	A1	675	C	C6-N1-C2	-6.45	117.72	120.30
79	B5	1564	U	N1-C2-O2	6.44	127.31	122.80
1	A1	818	C	C6-N1-C2	-6.44	117.72	120.30
1	A1	2191	U	N3-C2-O2	-6.43	117.70	122.20
1	A1	524	U	N1-C2-O2	6.43	127.30	122.80
1	A1	986	U	N3-C2-O2	-6.42	117.71	122.20
79	B5	496	G	N3-C4-C5	-6.42	125.39	128.60
79	B5	1596	C	N3-C2-O2	-6.42	117.41	121.90
1	A1	2094	C	N3-C2-O2	-6.41	117.41	121.90
1	A1	2836	C	C6-N1-C1'	-6.41	113.11	120.80
1	A1	1844	C	C6-N1-C2	-6.40	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	2638	C	N1-C2-O2	6.40	122.74	118.90
1	A1	3250	U	N1-C2-O2	6.40	127.28	122.80
79	B5	1596	C	C2-N1-C1'	6.39	125.83	118.80
79	B5	184	C	C2-N1-C1'	6.39	125.83	118.80
1	A1	969	C	N3-C2-O2	-6.38	117.43	121.90
1	A1	2716	U	N1-C2-O2	6.38	127.27	122.80
1	A1	982	C	C2-N1-C1'	6.38	125.82	118.80
79	B5	1000	C	N1-C2-O2	6.38	122.73	118.90
1	A1	1155	C	N1-C2-O2	6.37	122.72	118.90
1	A1	915	A	N7-C8-N9	6.37	116.98	113.80
3	A4	100	U	C2-N1-C1'	6.36	125.33	117.70
1	A1	2206	G	N3-C4-N9	6.36	129.82	126.00
1	A1	3034	C	C6-N1-C1'	-6.36	113.17	120.80
1	A1	1872	C	N3-C2-O2	-6.34	117.46	121.90
68	BX	100	ASP	CB-CG-OD2	6.34	124.01	118.30
3	A4	5	U	C6-N1-C1'	-6.33	112.33	121.20
1	A1	1604	G	C8-N9-C1'	-6.33	118.77	127.00
1	A1	1604	G	N3-C4-N9	6.33	129.79	126.00
27	AY	83	ASP	CB-CG-OD1	6.32	123.98	118.30
1	A1	418	A	C6-N1-C2	6.31	122.39	118.60
1	A1	1608	C	C5-C6-N1	6.30	124.15	121.00
79	B5	1162	C	N3-C2-O2	-6.29	117.50	121.90
1	A1	818	C	C5-C6-N1	6.29	124.14	121.00
1	A1	2146	C	C5-C6-N1	6.28	124.14	121.00
3	A4	81	U	P-O3'-C3'	6.27	127.23	119.70
10	AG	75	ILE	CG1-CB-CG2	-6.27	97.61	111.40
4	AA	102	LEU	CA-CB-CG	6.24	129.66	115.30
1	A1	2366	C	C5-C6-N1	6.24	124.12	121.00
1	A1	2843	U	C2-N1-C1'	6.24	125.19	117.70
79	B5	502	U	N1-C2-O2	6.24	127.17	122.80
1	A1	2726	C	N3-C2-O2	-6.23	117.54	121.90
1	A1	1115	G	C8-N9-C1'	-6.22	118.91	127.00
79	B5	1244	A	C8-N9-C4	-6.22	103.31	105.80
1	A1	2843	U	N1-C2-O2	6.21	127.15	122.80
79	B5	267	U	N3-C2-O2	-6.21	117.85	122.20
3	A4	4	C	C5-C6-N1	6.21	124.10	121.00
79	B5	354	C	C5-C6-N1	6.21	124.10	121.00
1	A1	1309	U	N1-C2-O2	6.20	127.14	122.80
1	A1	2093	A	P-O3'-C3'	6.19	127.13	119.70
79	B5	1258	U	N1-C2-O2	6.18	127.13	122.80
1	A1	1694	U	C6-N1-C2	-6.18	117.29	121.00
1	A1	2983	C	C6-N1-C1'	-6.18	113.39	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	Bb	3	LEU	CB-CG-CD1	-6.18	100.50	111.00
79	B5	354	C	N1-C2-O2	6.17	122.60	118.90
1	A1	2953	U	N3-C2-O2	-6.17	117.88	122.20
1	A1	3111	U	C5-C6-N1	6.16	125.78	122.70
1	A1	2405	C	N3-C2-O2	-6.16	117.59	121.90
79	B5	1021	C	C2-N1-C1'	6.16	125.57	118.80
1	A1	15	C	C6-N1-C2	-6.15	117.84	120.30
1	A1	3058	U	C6-N1-C1'	-6.14	112.60	121.20
79	B5	934	C	C6-N1-C1'	-6.14	113.43	120.80
79	B5	1527	C	C5-C6-N1	6.14	124.07	121.00
1	A1	113	C	C6-N1-C2	-6.14	117.84	120.30
79	B5	1220	C	C5-C6-N1	6.13	124.07	121.00
1	A1	2726	C	N1-C2-O2	6.12	122.57	118.90
1	A1	2189	U	N1-C2-O2	6.12	127.08	122.80
79	B5	1235	C	N1-C2-O2	6.12	122.57	118.90
1	A1	1694	U	N1-C2-N3	6.11	118.57	114.90
1	A1	2264	U	C2-N1-C1'	6.11	125.03	117.70
79	B5	1180	C	C5-C6-N1	6.10	124.05	121.00
79	B5	1258	U	N3-C2-O2	-6.10	117.93	122.20
1	A1	1901	A	C8-N9-C4	-6.10	103.36	105.80
5	AB	289	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A1	1585	C	C6-N1-C2	-6.09	117.86	120.30
1	A1	2274	U	N3-C2-O2	-6.09	117.94	122.20
1	A1	2191	U	C2-N1-C1'	6.09	125.00	117.70
79	B5	1220	C	C6-N1-C2	-6.08	117.87	120.30
1	A1	283	G	N3-C4-N9	6.08	129.65	126.00
1	A1	2260	U	N3-C2-O2	-6.08	117.94	122.20
1	A1	3250	U	N3-C2-O2	-6.08	117.95	122.20
1	A1	2810	C	C6-N1-C2	-6.06	117.88	120.30
79	B5	530	C	N1-C2-O2	6.06	122.54	118.90
79	B5	610	G	C8-N9-C1'	-6.05	119.13	127.00
79	B5	453	U	C6-N1-C2	-6.05	117.37	121.00
79	B5	1591	C	C5-C6-N1	6.04	124.02	121.00
1	A1	3283	U	C2-N1-C1'	6.04	124.94	117.70
9	AF	33	ARG	NE-CZ-NH1	6.04	123.32	120.30
79	B5	583	C	C2-N1-C1'	6.04	125.44	118.80
1	A1	87	U	N1-C2-O2	6.03	127.02	122.80
79	B5	1161	C	C5-C6-N1	6.03	124.02	121.00
79	B5	530	C	N3-C2-O2	-6.03	117.68	121.90
79	B5	1162	C	C2-N1-C1'	6.01	125.42	118.80
1	A1	1320	C	C5-C6-N1	6.01	124.01	121.00
1	A1	2206	G	C2-N3-C4	6.01	114.90	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	2522	G	N3-C4-N9	6.01	129.60	126.00
1	A1	2737	C	N3-C2-O2	-6.00	117.70	121.90
1	A1	713	U	N3-C2-O2	-6.00	118.00	122.20
79	B5	361	C	C5-C6-N1	5.99	124.00	121.00
1	A1	2407	C	C6-N1-C2	-5.99	117.91	120.30
1	A1	915	A	C4-N9-C1'	5.97	137.05	126.30
79	B5	639	U	N3-C2-O2	-5.97	118.02	122.20
1	A1	1292	C	C6-N1-C2	-5.96	117.92	120.30
60	BP	25	LEU	CA-CB-CG	5.95	128.98	115.30
1	A1	954	U	N1-C2-O2	5.95	126.96	122.80
1	A1	149	U	N3-C2-O2	-5.94	118.04	122.20
1	A1	2263	C	C6-N1-C1'	-5.94	113.67	120.80
1	A1	969	C	C5-C6-N1	5.94	123.97	121.00
1	A1	3250	U	C2-N1-C1'	5.94	124.83	117.70
1	A1	3283	U	N1-C2-O2	5.93	126.95	122.80
1	A1	36	C	N1-C2-O2	5.93	122.46	118.90
1	A1	2260	U	C2-N1-C1'	5.93	124.82	117.70
1	A1	916	G	P-O3'-C3'	5.93	126.81	119.70
1	A1	3196	U	N1-C2-O2	5.93	126.95	122.80
79	B5	1291	G	N1-C2-N2	5.93	121.53	116.20
79	B5	1600	A	C8-N9-C4	-5.92	103.43	105.80
79	B5	583	C	C5-C6-N1	5.92	123.96	121.00
1	A1	356	C	C6-N1-C2	-5.92	117.93	120.30
79	B5	1021	C	C5-C6-N1	5.91	123.96	121.00
1	A1	494	G	C8-N9-C4	-5.91	104.04	106.40
1	A1	1296	C	C6-N1-C2	-5.91	117.94	120.30
1	A1	97	U	N3-C2-O2	-5.91	118.06	122.20
1	A1	1835	A	N1-C2-N3	-5.91	126.35	129.30
1	A1	2681	U	N3-C2-O2	-5.90	118.07	122.20
79	B5	950	C	C6-N1-C2	-5.90	117.94	120.30
1	A1	2543	U	C2-N1-C1'	5.90	124.78	117.70
79	B5	4	C	C6-N1-C2	-5.90	117.94	120.30
79	B5	1473	U	N3-C2-O2	-5.90	118.07	122.20
1	A1	2953	U	N1-C2-O2	5.90	126.93	122.80
1	A1	283	G	C4-N9-C1'	5.89	134.16	126.50
1	A1	2983	C	N1-C2-O2	5.89	122.44	118.90
1	A1	2617	U	N3-C2-O2	-5.88	118.08	122.20
1	A1	75	G	C8-N9-C1'	-5.88	119.36	127.00
1	A1	87	U	N3-C2-O2	-5.88	118.08	122.20
1	A1	2843	U	N3-C2-O2	-5.88	118.08	122.20
79	B5	1180	C	C6-N1-C2	-5.88	117.95	120.30
62	BR	34	LEU	CA-CB-CG	5.88	128.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	259	C	C2-N1-C1'	5.87	125.26	118.80
79	B5	536	C	C6-N1-C2	-5.87	117.95	120.30
1	A1	115	A	O5'-P-OP1	5.87	117.74	110.70
77	Bg	266	ASP	CB-CG-OD1	5.87	123.58	118.30
79	B5	538	A	C4-N9-C1'	5.87	136.86	126.30
1	A1	300	G	C5-N7-C8	-5.86	101.37	104.30
1	A1	2546	C	N3-C2-O2	-5.86	117.80	121.90
79	B5	543	C	N1-C2-O2	5.86	122.42	118.90
1	A1	1495	U	N3-C2-O2	-5.86	118.10	122.20
65	BU	89	ARG	NE-CZ-NH2	5.85	123.23	120.30
79	B5	223	U	N1-C2-O2	5.85	126.90	122.80
79	B5	1024	U	N1-C2-O2	5.85	126.89	122.80
1	A1	2366	C	C6-N1-C2	-5.84	117.96	120.30
3	A4	11	C	C6-N1-C2	-5.83	117.97	120.30
1	A1	123	A	N1-C2-N3	-5.83	126.38	129.30
79	B5	1332	C	C2-N1-C1'	5.83	125.21	118.80
79	B5	314	C	C6-N1-C2	-5.82	117.97	120.30
51	BG	67	VAL	C-N-CA	5.81	136.24	121.70
79	B5	31	C	C6-N1-C2	-5.81	117.97	120.30
1	A1	2585	G	N3-C4-C5	-5.81	125.69	128.60
1	A1	729	C	C6-N1-C2	-5.80	117.98	120.30
79	B5	4	C	C2-N1-C1'	5.80	125.18	118.80
79	B5	1646	C	C5-C6-N1	5.80	123.90	121.00
1	A1	549	U	C2-N1-C1'	5.80	124.66	117.70
79	B5	965	U	N1-C2-O2	5.80	126.86	122.80
2	A3	68	C	C6-N1-C2	-5.79	117.98	120.30
1	A1	36	C	N3-C2-O2	-5.79	117.84	121.90
79	B5	1258	U	C2-N1-C1'	5.79	124.65	117.70
79	B5	1082	C	C5-C6-N1	5.79	123.89	121.00
1	A1	2988	C	C5-C6-N1	5.79	123.89	121.00
9	AF	157	ASN	C-N-CA	5.78	136.15	121.70
1	A1	1900	A	N1-C6-N6	-5.78	115.13	118.60
1	A1	1448	U	N3-C2-O2	-5.78	118.16	122.20
1	A1	2263	C	N3-C2-O2	-5.78	117.86	121.90
79	B5	1633	A	P-O3'-C3'	5.78	126.63	119.70
1	A1	1146	C	C6-N1-C2	-5.77	117.99	120.30
1	A1	315	C	C6-N1-C2	-5.77	117.99	120.30
1	A1	729	C	C5-C6-N1	5.76	123.88	121.00
1	A1	1052	U	C2-N1-C1'	5.76	124.62	117.70
1	A1	1146	C	C2-N1-C1'	5.76	125.14	118.80
1	A1	2257	C	O4'-C1'-N1	5.76	112.81	108.20
1	A1	3214	U	N1-C2-O2	5.76	126.83	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	B5	224	C	C6-N1-C1'	-5.76	113.89	120.80
1	A1	3362	A	C5-N7-C8	-5.75	101.02	103.90
79	B5	1368	G	N1-C6-O6	-5.75	116.45	119.90
1	A1	1660	C	C5-C6-N1	5.75	123.87	121.00
35	Ag	51	LEU	CB-CG-CD2	-5.74	101.23	111.00
51	BG	69	LEU	CA-CB-CG	5.74	128.50	115.30
1	A1	2984	C	C6-N1-C2	-5.74	118.00	120.30
79	B5	1332	C	C5-C6-N1	5.74	123.87	121.00
1	A1	2783	U	N3-C2-O2	-5.73	118.19	122.20
5	AB	16	PHE	C-N-CA	5.73	136.03	121.70
1	A1	1878	G	C4-N9-C1'	5.73	133.94	126.50
1	A1	1190	A	C4-N9-C1'	5.72	136.61	126.30
1	A1	3089	C	C6-N1-C2	-5.72	118.01	120.30
1	A1	2225	U	C6-N1-C1'	-5.71	113.20	121.20
79	B5	1458	G	N3-C4-N9	5.71	129.43	126.00
1	A1	927	C	C6-N1-C2	-5.71	118.02	120.30
79	B5	639	U	C2-N1-C1'	5.71	124.55	117.70
79	B5	777	C	C6-N1-C2	-5.70	118.02	120.30
79	B5	1497	U	N1-C2-O2	5.70	126.79	122.80
79	B5	1354	G	C4-N9-C1'	5.70	133.91	126.50
1	A1	752	C	C6-N1-C2	-5.69	118.02	120.30
79	B5	354	C	C2-N3-C4	5.69	122.75	119.90
79	B5	1456	C	N3-C2-O2	-5.69	117.92	121.90
79	B5	1072	C	C6-N1-C2	-5.69	118.02	120.30
79	B5	1332	C	C6-N1-C2	-5.69	118.03	120.30
1	A1	1907	C	N1-C2-O2	5.69	122.31	118.90
1	A1	1499	C	C6-N1-C2	-5.68	118.03	120.30
79	B5	1082	C	N3-C2-O2	-5.68	117.92	121.90
1	A1	3181	C	C6-N1-C1'	-5.68	113.98	120.80
79	B5	1070	C	C6-N1-C2	-5.68	118.03	120.30
10	AG	189	LEU	CA-CB-CG	5.68	128.36	115.30
79	B5	1783	C	C2-N1-C1'	5.68	125.04	118.80
79	B5	408	C	C5-C6-N1	5.67	123.83	121.00
1	A1	2336	U	N3-C2-O2	-5.67	118.23	122.20
1	A1	75	G	C4-N9-C1'	5.67	133.87	126.50
2	A3	105	C	N3-C2-O2	-5.66	117.94	121.90
79	B5	314	C	N3-C2-O2	-5.66	117.94	121.90
1	A1	2550	U	C6-N1-C1'	-5.66	113.28	121.20
79	B5	819	G	P-O3'-C3'	5.66	126.49	119.70
79	B5	861	U	C6-N1-C1'	-5.66	113.28	121.20
2	A3	28	C	C6-N1-C2	-5.66	118.04	120.30
79	B5	543	C	C6-N1-C1'	-5.65	114.02	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	B5	116	U	N1-C2-O2	5.65	126.75	122.80
1	A1	3097	C	C6-N1-C2	-5.64	118.04	120.30
1	A1	922	U	C5-C6-N1	5.64	125.52	122.70
79	B5	538	A	C5-N7-C8	-5.63	101.08	103.90
79	B5	1324	G	N3-C4-N9	-5.63	122.62	126.00
1	A1	315	C	C5-C6-N1	5.63	123.82	121.00
1	A1	1155	C	C2-N1-C1'	5.63	124.99	118.80
1	A1	2543	U	N1-C2-O2	5.63	126.74	122.80
29	Aa	47	LYS	C-N-CA	5.63	135.78	121.70
79	B5	1000	C	N3-C2-O2	-5.62	117.97	121.90
67	BW	115	GLU	CA-CB-CG	5.62	125.77	113.40
1	A1	1425	U	N1-C2-O2	5.61	126.73	122.80
1	A1	2263	C	O4'-C1'-N1	5.61	112.69	108.20
1	A1	2985	C	C6-N1-C2	-5.61	118.06	120.30
1	A1	87	U	C2-N1-C1'	5.60	124.42	117.70
1	A1	97	U	N1-C2-O2	5.60	126.72	122.80
1	A1	865	U	N3-C2-O2	-5.59	118.29	122.20
79	B5	1202	A	C2-N3-C4	5.58	113.39	110.60
1	A1	1190	A	C2-N3-C4	5.58	113.39	110.60
1	A1	2206	G	C8-N9-C1'	-5.58	119.75	127.00
1	A1	3104	U	N3-C2-O2	-5.58	118.29	122.20
1	A1	986	U	N1-C2-O2	5.58	126.70	122.80
1	A1	2522	G	C4-N9-C1'	5.57	133.75	126.50
1	A1	1604	G	N3-C4-C5	-5.57	125.81	128.60
1	A1	3057	U	C6-N1-C2	-5.57	117.66	121.00
1	A1	2408	U	N3-C2-O2	-5.57	118.30	122.20
1	A1	890	C	N3-C2-O2	-5.57	118.00	121.90
5	AB	46	PHE	CB-CG-CD1	-5.57	116.91	120.80
79	B5	1481	C	N1-C2-O2	5.56	122.24	118.90
1	A1	1115	G	N3-C4-C5	-5.56	125.82	128.60
1	A1	2522	G	N3-C4-C5	-5.56	125.82	128.60
1	A1	1574	C	N3-C2-O2	-5.56	118.01	121.90
1	A1	2764	C	C6-N1-C2	-5.56	118.08	120.30
1	A1	2836	C	C6-N1-C2	-5.56	118.08	120.30
79	B5	1560	U	O4'-C1'-N1	5.56	112.64	108.20
1	A1	2274	U	C2-N1-C1'	5.55	124.37	117.70
3	A4	76	C	C5-C6-N1	5.55	123.78	121.00
79	B5	1560	U	C6-N1-C1'	-5.55	113.42	121.20
79	B5	1614	A	O4'-C1'-N9	5.54	112.64	108.20
1	A1	2153	U	N3-C2-O2	-5.54	118.32	122.20
1	A1	2260	U	N1-C2-O2	5.54	126.68	122.80
79	B5	223	U	N3-C2-O2	-5.54	118.33	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	2783	U	N1-C2-O2	5.53	126.67	122.80
1	A1	1309	U	N3-C2-O2	-5.53	118.33	122.20
17	AO	84[A]	LEU	CB-CG-CD1	-5.53	101.61	111.00
79	B5	1600	A	OP1-P-O3'	5.52	117.35	105.20
79	B5	1456	C	N1-C2-O2	5.52	122.21	118.90
79	B5	614	C	C6-N1-C2	-5.52	118.09	120.30
79	B5	730	G	C4-N9-C1'	5.52	133.67	126.50
1	A1	123	A	C2-N3-C4	5.51	113.36	110.60
79	B5	35	U	N3-C2-O2	-5.51	118.34	122.20
79	B5	223	U	C2-N1-C1'	5.51	124.31	117.70
79	B5	1354	G	N3-C4-N9	5.50	129.30	126.00
1	A1	1124	U	N1-C2-O2	5.50	126.65	122.80
1	A1	1317	A	O4'-C1'-N9	5.50	112.60	108.20
1	A1	1495	U	C5-C6-N1	-5.49	119.95	122.70
79	B5	694	U	N3-C2-O2	-5.49	118.36	122.20
1	A1	3329	U	C5-C6-N1	5.49	125.44	122.70
79	B5	1596	C	N1-C2-O2	5.49	122.19	118.90
1	A1	2836	C	O4'-C1'-N1	5.48	112.59	108.20
79	B5	1356	U	C2-N1-C1'	5.48	124.28	117.70
1	A1	3283	U	N3-C2-O2	-5.48	118.36	122.20
3	A4	76	C	C6-N1-C2	-5.48	118.11	120.30
79	B5	323	A	O5'-P-OP2	-5.48	100.77	105.70
79	B5	305	C	C6-N1-C2	-5.46	118.11	120.30
79	B5	1173	C	C2-N1-C1'	5.46	124.81	118.80
79	B5	166	C	N1-C2-O2	5.46	122.18	118.90
79	B5	1252	C	C5-C6-N1	5.46	123.73	121.00
79	B5	1380	U	C6-N1-C1'	-5.46	113.56	121.20
79	B5	531	C	N3-C2-O2	-5.45	118.08	121.90
1	A1	494	G	N7-C8-N9	5.45	115.83	113.10
35	Ag	51	LEU	CA-CB-CG	5.45	127.84	115.30
1	A1	431	U	C5-C6-N1	5.45	125.42	122.70
79	B5	343	C	C2-N1-C1'	5.45	124.80	118.80
79	B5	965	U	C6-N1-C1'	-5.45	113.57	121.20
79	B5	625	C	C6-N1-C2	-5.44	118.12	120.30
1	A1	638	C	C5-C6-N1	5.44	123.72	121.00
1	A1	948	C	C5-C6-N1	5.44	123.72	121.00
79	B5	1344	A	C3'-C2'-C1'	5.44	105.85	101.50
10	AG	79	GLN	CA-CB-CG	5.44	125.36	113.40
1	A1	865	U	N1-C2-O2	5.43	126.60	122.80
5	AB	46	PHE	CB-CG-CD2	5.43	124.60	120.80
79	B5	1674	C	C5-C6-N1	5.43	123.72	121.00
1	A1	2726	C	C6-N1-C2	-5.43	118.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	1333	C	C6-N1-C2	-5.43	118.13	120.30
1	A1	1385	C	C2'-C3'-O3'	5.43	122.39	113.70
1	A1	890	C	C6-N1-C2	-5.42	118.13	120.30
1	A1	2388	U	N3-C2-O2	-5.42	118.40	122.20
79	B5	990	C	C5-C6-N1	5.42	123.71	121.00
70	BZ	69	LEU	CA-CB-CG	5.42	127.77	115.30
1	A1	2722	U	N3-C2-O2	-5.42	118.41	122.20
1	A1	743	C	N3-C2-O2	-5.42	118.11	121.90
79	B5	1070	C	C5-C6-N1	5.42	123.71	121.00
1	A1	1540	U	N3-C2-O2	-5.42	118.41	122.20
1	A1	1694	U	C2-N1-C1'	5.42	124.20	117.70
79	B5	1291	G	C8-N9-C4	-5.42	104.23	106.40
1	A1	3104	U	N1-C2-O2	5.41	126.59	122.80
3	A4	35	C	C5-C6-N1	5.41	123.70	121.00
79	B5	1252	C	C6-N1-C2	-5.41	118.14	120.30
3	A4	4	C	C6-N1-C2	-5.41	118.14	120.30
79	B5	1684	U	N3-C2-O2	-5.41	118.42	122.20
1	A1	743	C	N1-C2-O2	5.40	122.14	118.90
79	B5	1620	C	N3-C2-O2	-5.40	118.12	121.90
79	B5	1611	A	O4'-C1'-N9	5.40	112.52	108.20
1	A1	283	G	C8-N9-C1'	-5.39	119.99	127.00
69	BY	125	LEU	CA-CB-CG	5.39	127.69	115.30
79	B5	1344	A	P-O3'-C3'	5.39	126.17	119.70
1	A1	2710	C	C5-C6-N1	5.38	123.69	121.00
1	A1	2710	C	C6-N1-C2	-5.38	118.15	120.30
19	AQ	180	ARG	CA-CB-CG	5.38	125.24	113.40
1	A1	3344	A	C5-N7-C8	-5.38	101.21	103.90
71	Ba	35	ALA	C-N-CA	5.38	135.15	121.70
1	A1	2772	C	C2-N1-C1'	5.38	124.72	118.80
1	A1	2869	U	O5'-P-OP2	5.38	117.15	110.70
1	A1	3324	C	C6-N1-C2	-5.38	118.15	120.30
79	B5	283	U	N1-C2-O2	5.38	126.56	122.80
79	B5	343	C	C6-N1-C2	-5.38	118.15	120.30
79	B5	469	C	C6-N1-C2	-5.38	118.15	120.30
1	A1	311	C	C6-N1-C2	-5.38	118.15	120.30
79	B5	507	U	C2-N1-C1'	5.37	124.14	117.70
1	A1	15	C	C5-C6-N1	5.37	123.68	121.00
1	A1	1052	U	N1-C2-O2	5.37	126.56	122.80
1	A1	3181	C	C6-N1-C2	-5.37	118.15	120.30
79	B5	176	C	C6-N1-C2	-5.37	118.15	120.30
1	A1	1358	C	C5-C6-N1	5.36	123.68	121.00
1	A1	1499	C	C5-C6-N1	5.36	123.68	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	1533	U	N3-C2-O2	-5.36	118.44	122.20
1	A1	1805	C	C6-N1-C2	-5.36	118.16	120.30
1	A1	982	C	C6-N1-C2	-5.36	118.16	120.30
79	B5	166	C	C6-N1-C2	-5.36	118.16	120.30
79	B5	323	A	N7-C8-N9	5.36	116.48	113.80
79	B5	106	U	N3-C2-O2	-5.35	118.45	122.20
29	Aa	56	VAL	N-CA-C	-5.35	96.55	111.00
79	B5	453	U	C5-C6-N1	5.35	125.38	122.70
1	A1	36	C	C6-N1-C2	-5.35	118.16	120.30
79	B5	1632	C	C6-N1-C2	-5.35	118.16	120.30
1	A1	1627	U	N3-C2-O2	-5.35	118.46	122.20
79	B5	1356	U	C5-C6-N1	5.34	125.37	122.70
79	B5	632	U	N3-C2-O2	-5.34	118.46	122.20
79	B5	1796	C	N1-C2-O2	5.34	122.11	118.90
1	A1	954	U	C6-N1-C1'	-5.34	113.72	121.20
79	B5	502	U	N3-C2-O2	-5.34	118.46	122.20
79	B5	1235	C	N3-C2-O2	-5.33	118.17	121.90
79	B5	1356	U	N1-C2-O2	5.33	126.53	122.80
79	B5	864	U	C6-N1-C1'	-5.33	113.74	121.20
1	A1	1496	C	C6-N1-C1'	-5.33	114.41	120.80
46	BB	73	LEU	CA-CB-CG	5.33	127.55	115.30
79	B5	1214	U	N1-C2-O2	5.32	126.53	122.80
1	A1	2340	U	N3-C2-O2	-5.32	118.48	122.20
79	B5	1565	C	C5-C6-N1	5.32	123.66	121.00
1	A1	1228	C	N1-C2-O2	5.32	122.09	118.90
1	A1	2420	C	C6-N1-C2	-5.31	118.17	120.30
1	A1	32	U	C5-C6-N1	5.31	125.35	122.70
79	B5	614	C	C5-C6-N1	5.31	123.66	121.00
79	B5	990	C	C6-N1-C2	-5.31	118.18	120.30
1	A1	1604	G	C2-N3-C4	5.30	114.55	111.90
1	A1	2191	U	N1-C2-O2	5.30	126.51	122.80
1	A1	1312	C	C6-N1-C2	-5.30	118.18	120.30
79	B5	694	U	C2-N1-C1'	5.30	124.06	117.70
79	B5	1527	C	C2-N1-C1'	5.30	124.63	118.80
60	BP	106	GLU	CA-CB-CG	5.30	125.06	113.40
1	A1	1052	U	N3-C2-O2	-5.30	118.49	122.20
1	A1	111	C	C6-N1-C2	-5.29	118.18	120.30
1	A1	860	G	C2-N3-C4	5.29	114.55	111.90
1	A1	1702	U	N3-C2-O2	-5.29	118.49	122.20
79	B5	1033	C	C6-N1-C2	-5.29	118.19	120.30
79	B5	975	C	C6-N1-C2	-5.29	118.19	120.30
79	B5	1274	C	N1-C2-O2	5.28	122.07	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	B5	198	A	C2-N3-C4	5.28	113.24	110.60
79	B5	937	C	C6-N1-C2	-5.28	118.19	120.30
79	B5	1473	U	C6-N1-C1'	-5.28	113.81	121.20
1	A1	2928	C	C6-N1-C2	-5.28	118.19	120.30
79	B5	945	U	C5-C6-N1	5.27	125.34	122.70
65	BU	85	ARG	NE-CZ-NH1	5.27	122.93	120.30
79	B5	543	C	N3-C2-O2	-5.27	118.21	121.90
79	B5	1082	C	O4'-C1'-N1	5.27	112.42	108.20
79	B5	87	C	C6-N1-C2	-5.27	118.19	120.30
79	B5	1489	U	C6-N1-C1'	-5.27	113.83	121.20
79	B5	176	C	C5-C6-N1	5.26	123.63	121.00
1	A1	2983	C	C6-N1-C2	-5.26	118.19	120.30
46	BB	147	ALA	C-N-CA	5.26	134.86	121.70
1	A1	2714	G	N3-C4-N9	-5.26	122.84	126.00
1	A1	2985	C	C5-C6-N1	5.26	123.63	121.00
1	A1	1645	U	N1-C2-O2	5.26	126.48	122.80
1	A1	2284	C	N1-C2-O2	5.26	122.05	118.90
1	A1	3196	U	C6-N1-C1'	-5.26	113.84	121.20
1	A1	1564	U	N3-C2-O2	-5.25	118.52	122.20
3	A4	73	U	C6-N1-C2	-5.25	117.85	121.00
79	B5	1225	U	N1-C2-O2	5.25	126.48	122.80
1	A1	927	C	C5-C6-N1	5.25	123.62	121.00
1	A1	1032	C	P-O3'-C3'	5.24	125.99	119.70
1	A1	2137	U	O4'-C1'-N1	5.24	112.39	108.20
2	A3	26	C	C6-N1-C2	-5.24	118.20	120.30
79	B5	1274	C	C2-N1-C1'	5.24	124.56	118.80
1	A1	982	C	C5-C6-N1	5.23	123.62	121.00
1	A1	1496	C	C2-N3-C4	5.23	122.52	119.90
79	B5	1185	U	C2-N1-C1'	5.23	123.98	117.70
1	A1	777	U	N3-C2-O2	-5.23	118.54	122.20
79	B5	149	C	C6-N1-C2	-5.23	118.21	120.30
1	A1	3105	U	N3-C2-O2	-5.23	118.54	122.20
79	B5	1369	U	C5-C6-N1	5.23	125.31	122.70
1	A1	2389	C	C5-C6-N1	5.23	123.61	121.00
79	B5	530	C	C6-N1-C2	-5.23	118.21	120.30
79	B5	901	G	C4-N9-C1'	5.23	133.29	126.50
1	A1	1843	C	C6-N1-C2	-5.22	118.21	120.30
1	A1	3281	U	N1-C2-O2	5.22	126.46	122.80
79	B5	184	C	C6-N1-C2	-5.22	118.21	120.30
2	A3	28	C	N1-C2-O2	5.22	122.03	118.90
1	A1	743	C	C6-N1-C2	-5.22	118.21	120.30
79	B5	901	G	O4'-C1'-N9	5.22	112.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	1694	U	C4-C5-C6	5.21	122.83	119.70
1	A1	379	C	C5-C6-N1	5.21	123.61	121.00
1	A1	2681	U	C2-N1-C1'	5.21	123.95	117.70
1	A1	244	G	C4-N9-C1'	-5.21	119.73	126.50
79	B5	142	G	C4-N9-C1'	5.21	133.28	126.50
1	A1	2652	U	C2-N1-C1'	5.20	123.94	117.70
1	A1	2894	C	C6-N1-C2	-5.20	118.22	120.30
1	A1	1124	U	N3-C2-O2	-5.20	118.56	122.20
1	A1	915	A	C2-N3-C4	5.20	113.20	110.60
1	A1	1155	C	C5-C6-N1	5.19	123.60	121.00
79	B5	1354	G	C8-N9-C1'	-5.19	120.25	127.00
1	A1	3344	A	N7-C8-N9	5.19	116.39	113.80
1	A1	2434	U	N3-C2-O2	-5.18	118.57	122.20
79	B5	777	C	C5-C6-N1	5.18	123.59	121.00
13	AJ	172	LEU	CA-CB-CG	5.18	127.21	115.30
79	B5	1240	U	N3-C2-O2	-5.18	118.58	122.20
79	B5	21	U	N1-C2-O2	5.18	126.42	122.80
1	A1	518	G	O4'-C1'-N9	5.18	112.34	108.20
1	A1	1224	C	C2-N1-C1'	5.18	124.49	118.80
1	A1	3037	U	C6-N1-C1'	-5.18	113.95	121.20
3	A4	142	C	C6-N1-C2	-5.17	118.23	120.30
79	B5	804	A	C2-N3-C4	5.17	113.19	110.60
79	B5	935	U	C2-N1-C1'	5.17	123.91	117.70
1	A1	1574	C	C2-N1-C1'	5.17	124.49	118.80
2	A3	28	C	N3-C2-O2	-5.17	118.28	121.90
1	A1	1856	C	C5-C6-N1	5.17	123.58	121.00
1	A1	3043	C	C6-N1-C2	-5.17	118.23	120.30
1	A1	109	A	OP1-P-O3'	5.17	116.56	105.20
1	A1	1448	U	C5-C6-N1	5.17	125.28	122.70
79	B5	730	G	N3-C4-C5	-5.17	126.02	128.60
79	B5	1389	C	N3-C2-O2	-5.17	118.28	121.90
1	A1	2763	U	N3-C2-O2	-5.16	118.59	122.20
79	B5	1684	U	N1-C2-O2	5.16	126.42	122.80
79	B5	1254	U	C6-N1-C1'	-5.16	113.97	121.20
1	A1	777	U	N1-C2-O2	5.16	126.41	122.80
1	A1	3297	U	N3-C2-O2	-5.16	118.59	122.20
2	A3	113	C	C5-C6-N1	5.16	123.58	121.00
1	A1	2681	U	N1-C2-O2	5.16	126.41	122.80
1	A1	1333	C	C5-C6-N1	5.16	123.58	121.00
1	A1	667	C	C5-C6-N1	5.16	123.58	121.00
1	A1	2585	G	C2-N3-C4	5.15	114.48	111.90
1	A1	2181	C	C6-N1-C2	-5.15	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	1901	A	C4-N9-C1'	5.15	135.57	126.30
1	A1	2431	C	C6-N1-C2	-5.15	118.24	120.30
1	A1	3281	U	N3-C2-O2	-5.15	118.59	122.20
79	B5	581	U	C5-C6-N1	5.15	125.28	122.70
1	A1	2263	C	C6-N1-C2	-5.15	118.24	120.30
79	B5	766	U	C2-N1-C1'	5.15	123.88	117.70
79	B5	686	C	C5-C6-N1	5.14	123.57	121.00
1	A1	524	U	N3-C2-O2	-5.14	118.60	122.20
1	A1	2899	C	O4'-C1'-N1	5.14	112.31	108.20
79	B5	1537	C	C2-N3-C4	5.14	122.47	119.90
1	A1	1457	U	N3-C2-O2	-5.13	118.61	122.20
1	A1	1872	C	C6-N1-C2	-5.13	118.25	120.30
1	A1	28	C	C6-N1-C2	-5.13	118.25	120.30
14	AL	85	LEU	CA-CB-CG	5.13	127.10	115.30
1	A1	379	C	C6-N1-C2	-5.13	118.25	120.30
1	A1	2543	U	N3-C2-O2	-5.12	118.61	122.20
79	B5	1305	U	N3-C2-O2	-5.12	118.61	122.20
3	A4	108	C	C6-N1-C2	-5.12	118.25	120.30
79	B5	93	A	OP2-P-O3'	5.12	116.46	105.20
2	A3	93	C	C6-N1-C2	-5.12	118.25	120.30
79	B5	442	C	C5-C6-N1	5.12	123.56	121.00
1	A1	320	G	N3-C2-N2	-5.11	116.32	119.90
79	B5	1244	A	N7-C8-N9	5.11	116.36	113.80
1	A1	1745	C	C6-N1-C2	-5.11	118.25	120.30
1	A1	2176	U	N3-C2-O2	-5.11	118.62	122.20
1	A1	427	C	C5-C6-N1	5.11	123.56	121.00
1	A1	1575	A	P-O3'-C3'	5.11	125.83	119.70
79	B5	469	C	C5-C6-N1	5.11	123.56	121.00
1	A1	3303	G	O4'-C1'-N9	5.11	112.29	108.20
3	A4	67	U	P-O3'-C3'	5.11	125.83	119.70
79	B5	1476	C	C6-N1-C2	-5.11	118.26	120.30
1	A1	2935	U	N1-C2-O2	5.10	126.37	122.80
79	B5	1214	U	C2-N1-C1'	5.10	123.82	117.70
1	A1	101	G	O4'-C1'-N9	5.10	112.28	108.20
1	A1	1224	C	C6-N1-C2	-5.10	118.26	120.30
79	B5	298	C	C6-N1-C2	-5.09	118.26	120.30
1	A1	1706	C	N1-C2-O2	5.09	121.95	118.90
1	A1	2899	C	C6-N1-C2	-5.09	118.27	120.30
1	A1	2284	C	C2-N1-C1'	5.08	124.39	118.80
1	A1	2774	C	C6-N1-C2	-5.08	118.27	120.30
79	B5	354	C	C6-N1-C2	-5.08	118.27	120.30
1	A1	969	C	C2-N1-C1'	5.08	124.38	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	BS	119	ILE	CG1-CB-CG2	-5.08	100.23	111.40
1	A1	1459	C	C5-C6-N1	5.07	123.53	121.00
79	B5	442	C	C6-N1-C2	-5.07	118.27	120.30
79	B5	1600	A	N7-C8-N9	5.06	116.33	113.80
1	A1	3085	G	C4-C5-N7	5.06	112.83	110.80
79	B5	142	G	C8-N9-C1'	-5.06	120.42	127.00
79	B5	1755	A	C2-N3-C4	5.06	113.13	110.60
18	AP	148	LEU	CA-CB-CG	5.06	126.94	115.30
79	B5	224	C	P-O3'-C3'	5.06	125.77	119.70
79	B5	1202	A	C4-N9-C1'	5.06	135.40	126.30
1	A1	1848	G	O4'-C1'-N9	-5.05	104.16	108.20
1	A1	3196	U	N3-C2-O2	-5.05	118.66	122.20
79	B5	1632	C	N1-C2-O2	5.05	121.93	118.90
1	A1	949	C	C6-N1-C2	-5.05	118.28	120.30
79	B5	1253	U	C5-C6-N1	5.05	125.22	122.70
79	B5	149	C	C2-N1-C1'	5.05	124.35	118.80
1	A1	1597	C	C2-N3-C4	5.04	122.42	119.90
1	A1	1901	A	N1-C6-N6	-5.04	115.58	118.60
54	BJ	118	LEU	CA-CB-CG	5.04	126.90	115.30
1	A1	3250	U	C5-C6-N1	5.04	125.22	122.70
1	A1	2873	U	N3-C2-O2	-5.04	118.67	122.20
79	B5	1761	U	C2-N1-C1'	5.04	123.75	117.70
1	A1	2329	C	C6-N1-C2	-5.04	118.29	120.30
1	A1	3120	C	N1-C2-O2	5.03	121.92	118.90
1	A1	356	C	C5-C6-N1	5.03	123.51	121.00
1	A1	3085	G	N9-C4-C5	-5.03	103.39	105.40
1	A1	3282	U	C2-N1-C1'	5.03	123.73	117.70
45	BA	42	PRO	C-N-CA	5.03	134.27	121.70
79	B5	1632	C	C5-C6-N1	5.03	123.51	121.00
79	B5	1527	C	C6-N1-C2	-5.03	118.29	120.30
1	A1	911	C	C6-N1-C2	-5.02	118.29	120.30
1	A1	2553	U	C6-N1-C1'	-5.02	114.17	121.20
1	A1	3116	G	N1-C6-O6	-5.02	116.89	119.90
3	A4	115	C	C5-C6-N1	5.02	123.51	121.00
1	A1	2259	A	C2-N3-C4	5.02	113.11	110.60
1	A1	1190	A	C8-N9-C1'	-5.02	118.67	127.70
1	A1	1292	C	C5-C6-N1	5.02	123.51	121.00
1	A1	2984	C	C2-N1-C1'	5.02	124.32	118.80
3	A4	30	C	C6-N1-C2	-5.02	118.29	120.30
79	B5	819	G	OP2-P-O3'	5.02	116.24	105.20
79	B5	1205	C	C6-N1-C2	-5.02	118.29	120.30
79	B5	893	U	N3-C2-O2	-5.01	118.69	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	142	C	C6-N1-C2	-5.01	118.30	120.30
2	A3	35	C	N1-C2-O2	5.01	121.91	118.90
79	B5	639	U	N1-C2-O2	5.01	126.31	122.80
1	A1	270	U	N3-C2-O2	-5.01	118.69	122.20
1	A1	1705	U	N3-C2-O2	-5.01	118.69	122.20
1	A1	1115	G	N3-C4-N9	5.00	129.00	126.00
1	A1	2764	C	N1-C2-O2	5.00	121.90	118.90
1	A1	2545	C	N3-C2-O2	-5.00	118.40	121.90
1	A1	2546	C	N1-C2-O2	5.00	121.90	118.90
79	B5	1082	C	C6-N1-C1'	-5.00	114.80	120.80
1	A1	1878	G	N3-C4-C5	-5.00	126.10	128.60
1	A1	3060	C	C6-N1-C2	-5.00	118.30	120.30
1	A1	3078	U	C2-N1-C1'	5.00	123.70	117.70
47	BC	145	GLY	C-N-CA	5.00	134.21	121.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
79	B5	1191	3AU	C12
79	B5	1575	G7M	C4',C2',C3'

All (61) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	AC	131	VAL	Peptide
6	AC	318	LEU	Peptide
7	AD	43	LYS	Peptide
8	AE	67	GLY	Peptide
9	AF	158	LYS	Peptide
9	AF	215	GLY	Peptide
9	AF	232	ARG	Peptide
10	AG	30	THR	Peptide
10	AG	74	THR	Peptide
10	AG	76	ALA	Peptide
10	AG	79	GLN	Peptide
13	AJ	109	HIS	Peptide
13	AJ	166	LYS	Peptide
14	AL	47	ALA	Peptide
14	AL	75	PHE	Peptide
16	AN	80	THR	Peptide
17	AO	110[A]	PRO	Peptide
20	AR	131	ALA	Peptide

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Mol	Chain	Res	Type	Group
21	AS	22	PRO	Peptide
22	AT	17	ARG	Peptide
28	AZ	123	GLN	Peptide
36	Ah	90	ARG	Peptide
37	Ai	27	SER	Peptide
45	BA	94	GLY	Peptide
46	BB	177	GLN	Peptide
46	BB	205	PHE	Peptide
46	BB	206	PRO	Peptide
46	BB	208	GLN	Peptide
47	BC	148	LEU	Peptide
50	BF	42	LEU	Peptide
50	BF	43	PHE	Peptide
51	BG	68	LEU	Peptide
52	BH	110	GLN	Peptide
52	BH	64	VAL	Peptide
52	BH	65	PRO	Peptide
53	BI	51	GLY	Peptide
53	BI	8	ARG	Peptide
54	BJ	117	GLY	Peptide
54	BJ	133	HIS	Peptide
59	BO	123	SER	Peptide
60	BP	106	GLU	Peptide
60	BP	124	THR	Peptide
60	BP	125	PRO	Peptide
60	BP	29	SER	Peptide
61	BQ	32	ASN	Peptide
61	BQ	33	GLY	Peptide
61	BQ	40	GLU	Peptide
63	BS	56	LYS	Peptide
63	BS	81	ILE	Peptide
63	BS	90	ASN	Peptide
67	BW	115	GLU	Peptide
68	BX	137	LYS	Peptide
68	BX	138	GLU	Peptide
68	BX	41	SER	Peptide
68	BX	87	VAL	Peptide
68	BX	97	ASP	Peptide
71	Ba	34	LYS	Peptide
71	Ba	35	ALA	Peptide
71	Ba	7	SER	Peptide
76	Bf	105	TYR	Peptide

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Mol	Chain	Res	Type	Group
78	Bh	85	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	
4	AA	245/247 (99%)	232 (95%)	13 (5%)	0	100	100
5	AB	383/386 (99%)	363 (95%)	20 (5%)	0	100	100
6	AC	359/361 (99%)	326 (91%)	31 (9%)	2 (1%)	25	55
7	AD	290/292 (99%)	272 (94%)	17 (6%)	1 (0%)	41	70
8	AE	152/156 (97%)	139 (91%)	13 (9%)	0	100	100
9	AF	220/222 (99%)	207 (94%)	11 (5%)	2 (1%)	17	47
10	AG	228/230 (99%)	216 (95%)	12 (5%)	0	100	100
11	AH	188/190 (99%)	171 (91%)	17 (9%)	0	100	100
12	AI	201/205 (98%)	187 (93%)	14 (7%)	0	100	100
13	AJ	167/169 (99%)	147 (88%)	20 (12%)	0	100	100
14	AL	191/193 (99%)	165 (86%)	22 (12%)	4 (2%)	7	26
15	AM	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
16	AN	201/203 (99%)	186 (92%)	14 (7%)	1 (0%)	29	60
17	AO	195/197 (99%)	191 (98%)	2 (1%)	2 (1%)	15	45
18	AP	171/175 (98%)	163 (95%)	8 (5%)	0	100	100
19	AQ	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
20	AR	186/188 (99%)	176 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	AS	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
22	AT	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
23	AU	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
24	AV	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
25	AW	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
26	AX	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
27	AY	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
28	AZ	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	19	50
29	Aa	146/148 (99%)	126 (86%)	18 (12%)	2 (1%)	11	36
30	Ab	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
31	Ac	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
32	Ad	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
33	Ae	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
34	Af	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
35	Ag	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
36	Ah	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	17	47
37	Ai	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
38	Aj	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
39	Ak	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
40	Al	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
41	Am	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
42	An	23/25 (92%)	23 (100%)	0	0	100	100
43	Ao	103/105 (98%)	93 (90%)	10 (10%)	0	100	100
44	Ap	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	14	42
45	BA	204/206 (99%)	185 (91%)	18 (9%)	1 (0%)	29	60
46	BB	212/214 (99%)	186 (88%)	24 (11%)	2 (1%)	17	47
47	BC	215/217 (99%)	197 (92%)	17 (8%)	1 (0%)	29	60
48	BD	221/223 (99%)	207 (94%)	14 (6%)	0	100	100
49	BE	258/260 (99%)	240 (93%)	18 (7%)	0	100	100
50	BF	204/206 (99%)	185 (91%)	19 (9%)	0	100	100
51	BG	224/226 (99%)	209 (93%)	13 (6%)	2 (1%)	17	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	BH	182/184 (99%)	166 (91%)	14 (8%)	2 (1%)	14	42
53	BI	184/188 (98%)	156 (85%)	28 (15%)	0	100	100
54	BJ	183/185 (99%)	168 (92%)	14 (8%)	1 (0%)	29	60
55	BK	94/96 (98%)	77 (82%)	17 (18%)	0	100	100
56	BL	153/155 (99%)	145 (95%)	8 (5%)	0	100	100
57	BM	119/121 (98%)	93 (78%)	26 (22%)	0	100	100
58	BN	148/150 (99%)	140 (95%)	8 (5%)	0	100	100
59	BO	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
60	BP	122/124 (98%)	101 (83%)	19 (16%)	2 (2%)	9	33
61	BQ	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	52
62	BR	117/121 (97%)	106 (91%)	10 (8%)	1 (1%)	17	47
63	BS	143/145 (99%)	128 (90%)	13 (9%)	2 (1%)	11	36
64	BT	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
65	BU	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
66	BV	83/87 (95%)	78 (94%)	5 (6%)	0	100	100
67	BW	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	50
68	BX	142/144 (99%)	120 (84%)	20 (14%)	2 (1%)	11	36
69	BY	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
70	BZ	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
71	Ba	95/97 (98%)	76 (80%)	16 (17%)	3 (3%)	4	18
72	Bb	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
73	Bc	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
74	Bd	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
75	Be	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
76	Bf	53/57 (93%)	39 (74%)	14 (26%)	0	100	100
77	Bg	310/312 (99%)	275 (89%)	35 (11%)	0	100	100
78	Bh	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
All	All	10956/11121 (98%)	10091 (92%)	827 (8%)	38 (0%)	44	70

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	AC	339	LEU

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Mol	Chain	Res	Type
9	AF	159	GLN
14	AL	48	PRO
14	AL	63	VAL
16	AN	81	TYR
17	AO	111[A]	PRO
29	Aa	78	LEU
51	BG	68	LEU
68	BX	97	ASP
46	BB	206	PRO
46	BB	207	LEU
47	BC	40	LYS
51	BG	173	PRO
52	BH	111	LYS
54	BJ	134	ILE
63	BS	91	ASP
71	Ba	36	ILE
7	AD	20	PHE
14	AL	76	THR
14	AL	77	LEU
45	BA	4	PRO
60	BP	125	PRO
62	BR	24	LEU
71	Ba	35	ALA
71	Ba	62	TYR
36	Ah	91	ALA
44	Ap	52	ALA
6	AC	268	ALA
68	BX	96	VAL
28	AZ	17	ARG
29	Aa	47	LYS
61	BQ	33	GLY
60	BP	107	ILE
9	AF	216	VAL
63	BS	92	ILE
52	BH	65	PRO
17	AO	110[A]	PRO
67	BW	67	GLY

5.3.2 Protein sidechains (i)

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	
4	AA	189/189 (100%)	189 (100%)	0	100	100
5	AB	321/321 (100%)	319 (99%)	2 (1%)	86	93
6	AC	288/288 (100%)	287 (100%)	1 (0%)	92	96
7	AD	241/241 (100%)	241 (100%)	0	100	100
8	AE	134/134 (100%)	134 (100%)	0	100	100
9	AF	186/186 (100%)	186 (100%)	0	100	100
10	AG	189/189 (100%)	189 (100%)	0	100	100
11	AH	170/170 (100%)	170 (100%)	0	100	100
12	AI	176/176 (100%)	175 (99%)	1 (1%)	86	93
13	AJ	147/147 (100%)	146 (99%)	1 (1%)	84	92
14	AL	154/154 (100%)	154 (100%)	0	100	100
15	AM	107/107 (100%)	107 (100%)	0	100	100
16	AN	175/175 (100%)	175 (100%)	0	100	100
17	AO	160/160 (100%)	160 (100%)	0	100	100
18	AP	141/141 (100%)	141 (100%)	0	100	100
19	AQ	150/150 (100%)	150 (100%)	0	100	100
20	AR	153/153 (100%)	153 (100%)	0	100	100
21	AS	156/156 (100%)	156 (100%)	0	100	100
22	AT	136/136 (100%)	135 (99%)	1 (1%)	84	92
23	AU	87/87 (100%)	86 (99%)	1 (1%)	73	88
24	AV	104/104 (100%)	104 (100%)	0	100	100
25	AW	55/55 (100%)	55 (100%)	0	100	100
26	AX	105/105 (100%)	105 (100%)	0	100	100
27	AY	109/109 (100%)	109 (100%)	0	100	100
28	AZ	115/115 (100%)	115 (100%)	0	100	100
29	Aa	118/118 (100%)	118 (100%)	0	100	100
30	Ab	46/46 (100%)	46 (100%)	0	100	100
31	Ac	81/81 (100%)	81 (100%)	0	100	100
32	Ad	96/96 (100%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	Ae	109/109 (100%)	109 (100%)	0	100	100
34	Af	90/90 (100%)	90 (100%)	0	100	100
35	Ag	95/95 (100%)	95 (100%)	0	100	100
36	Ah	104/104 (100%)	104 (100%)	0	100	100
37	Ai	81/81 (100%)	80 (99%)	1 (1%)	71	87
38	Aj	70/70 (100%)	70 (100%)	0	100	100
39	Ak	68/68 (100%)	68 (100%)	0	100	100
40	Al	45/45 (100%)	45 (100%)	0	100	100
41	Am	47/47 (100%)	46 (98%)	1 (2%)	53	77
42	An	23/23 (100%)	23 (100%)	0	100	100
43	Ao	90/90 (100%)	90 (100%)	0	100	100
44	Ap	71/71 (100%)	70 (99%)	1 (1%)	67	84
45	BA	173/173 (100%)	172 (99%)	1 (1%)	86	93
46	BB	191/191 (100%)	190 (100%)	1 (0%)	88	94
47	BC	176/176 (100%)	176 (100%)	0	100	100
48	BD	182/182 (100%)	181 (100%)	1 (0%)	88	94
49	BE	221/221 (100%)	221 (100%)	0	100	100
50	BF	173/173 (100%)	173 (100%)	0	100	100
51	BG	193/193 (100%)	192 (100%)	1 (0%)	88	94
52	BH	165/165 (100%)	165 (100%)	0	100	100
53	BI	150/150 (100%)	150 (100%)	0	100	100
54	BJ	158/158 (100%)	158 (100%)	0	100	100
55	BK	89/89 (100%)	89 (100%)	0	100	100
56	BL	136/136 (100%)	135 (99%)	1 (1%)	84	92
57	BM	98/98 (100%)	97 (99%)	1 (1%)	76	89
58	BN	127/127 (100%)	127 (100%)	0	100	100
59	BO	96/96 (100%)	95 (99%)	1 (1%)	76	89
60	BP	104/104 (100%)	103 (99%)	1 (1%)	76	89
61	BQ	117/117 (100%)	117 (100%)	0	100	100
62	BR	110/110 (100%)	108 (98%)	2 (2%)	59	80
63	BS	128/128 (100%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	BT	113/113 (100%)	113 (100%)	0	100	100
65	BU	100/100 (100%)	100 (100%)	0	100	100
66	BV	74/74 (100%)	74 (100%)	0	100	100
67	BW	110/110 (100%)	110 (100%)	0	100	100
68	BX	119/119 (100%)	119 (100%)	0	100	100
69	BY	112/112 (100%)	112 (100%)	0	100	100
70	BZ	61/61 (100%)	61 (100%)	0	100	100
71	Ba	83/83 (100%)	83 (100%)	0	100	100
72	Bb	70/70 (100%)	69 (99%)	1 (1%)	67	84
73	Bc	56/56 (100%)	56 (100%)	0	100	100
74	Bd	47/47 (100%)	46 (98%)	1 (2%)	53	77
75	Be	51/51 (100%)	51 (100%)	0	100	100
76	Bf	49/49 (100%)	49 (100%)	0	100	100
77	Bg	256/257 (100%)	256 (100%)	0	100	100
78	Bh	68/68 (100%)	66 (97%)	2 (3%)	42	70
All	All	9338/9339 (100%)	9314 (100%)	24 (0%)	92	96

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	AB	10	ARG
5	AB	332	ARG
6	AC	138	ARG
12	AI	191	LYS
13	AJ	166	LYS
22	AT	83	ARG
23	AU	49	ASN
37	Ai	55	ARG
41	Am	106	ARG
44	Ap	4	ARG
45	BA	205	ARG
46	BB	146	GLN
48	BD	76	ARG
51	BG	98	ARG
56	BL	67	ARG
57	BM	43	ARG
59	BO	136	ARG

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Mol	Chain	Res	Type
60	BP	44	ARG
62	BR	5	ARG
62	BR	95	ARG
72	Bb	42	ASN
74	Bd	28	THR
78	Bh	96	ARG
78	Bh	115	LYS

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

Mol	Chain	Res	Type
6	AC	320	ASN
23	AU	49	ASN
46	BB	146	GLN
50	BF	63	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	3150/3156 (99%)	694 (22%)	13 (0%)
2	A3	120/121 (99%)	15 (12%)	0
3	A4	156/158 (98%)	34 (21%)	2 (1%)
79	B5	1775/1783 (99%)	458 (25%)	14 (0%)
All	All	5201/5218 (99%)	1201 (23%)	29 (0%)

All (1201) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	14	U
1	A1	18	G
1	A1	21	G
1	A1	26	A
1	A1	34	A
1	A1	40	A
1	A1	43	A
1	A1	49	A
1	A1	57	A
1	A1	59	G
1	A1	60	A
1	A1	65	A

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Mol	Chain	Res	Type
1	A1	66	A
1	A1	72	C
1	A1	75	G
1	A1	76	G
1	A1	85	A
1	A1	92	G
1	A1	109	A
1	A1	110	G
1	A1	111	C
1	A1	115	A
1	A1	116	A
1	A1	117	U
1	A1	120	G
1	A1	121	A
1	A1	122	A
1	A1	134	U
1	A1	135	C
1	A1	136	G
1	A1	143	G
1	A1	148	G
1	A1	150	A
1	A1	154	U
1	A1	156	G
1	A1	157	A
1	A1	164	A
1	A1	165	A
1	A1	166	C
1	A1	170	G
1	A1	187	A
1	A1	190	U
1	A1	191	U
1	A1	200	C
1	A1	206	G
1	A1	210	U
1	A1	211	A
1	A1	219	A
1	A1	220	G
1	A1	231	G
1	A1	239	G
1	A1	240	U
1	A1	242	C
1	A1	243	G

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Mol	Chain	Res	Type
1	A1	244	G
1	A1	249	U
1	A1	250	U
1	A1	251	G
1	A1	252	U
1	A1	266	A
1	A1	267	G
1	A1	268	A
1	A1	269	G
1	A1	281	G
1	A1	283	G
1	A1	285	A
1	A1	286	U
1	A1	295	A
1	A1	297	G
1	A1	299	G
1	A1	305	U
1	A1	315	C
1	A1	316	U
1	A1	329	U
1	A1	337	G
1	A1	339	C
1	A1	352	A
1	A1	359	U
1	A1	371	G
1	A1	372	A
1	A1	374	A
1	A1	375	A
1	A1	376	G
1	A1	384	A
1	A1	387	A
1	A1	398	A
1	A1	399	A
1	A1	400	G
1	A1	401	U
1	A1	402	A
1	A1	403	C
1	A1	420	G
1	A1	421	G
1	A1	422	A
1	A1	429	U
1	A1	439	C

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Mol	Chain	Res	Type
1	A1	440	A
1	A1	441	U
1	A1	442	G
1	A1	443	G
1	A1	446	U
1	A1	447	U
1	A1	448	U
1	A1	450	G
1	A1	451	U
1	A1	487	U
1	A1	488	U
1	A1	489	U
1	A1	491	A
1	A1	493	U
1	A1	494	G
1	A1	498	A
1	A1	520	U
1	A1	521	A
1	A1	523	A
1	A1	535	G
1	A1	542	G
1	A1	543	C
1	A1	545	U
1	A1	546	C
1	A1	547	G
1	A1	548	G
1	A1	550	A
1	A1	551	A
1	A1	552	G
1	A1	555	U
1	A1	557	A
1	A1	558	U
1	A1	559	A
1	A1	560	G
1	A1	569	A
1	A1	578	A
1	A1	579	G
1	A1	589	A
1	A1	592	A
1	A1	602	A
1	A1	604	G
1	A1	611	A

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Mol	Chain	Res	Type
1	A1	620	U
1	A1	621	A
1	A1	637	C
1	A1	647	A
1	A1	649	A2M
1	A1	660	A
1	A1	677	A
1	A1	681	U
1	A1	690	A
1	A1	691	A
1	A1	705	A
1	A1	719	U
1	A1	725	G
1	A1	736	A
1	A1	765	C
1	A1	766	U
1	A1	767	U
1	A1	774	G
1	A1	775	A
1	A1	780	A
1	A1	781	G
1	A1	784	A
1	A1	785	G
1	A1	786	A
1	A1	799	G
1	A1	801	A
1	A1	806	A
1	A1	813	G
1	A1	817	A2M
1	A1	826	G
1	A1	830	A
1	A1	844	G
1	A1	845	G
1	A1	849	C
1	A1	861	C
1	A1	862	U
1	A1	871	U
1	A1	874	U
1	A1	879	U
1	A1	896	A
1	A1	897	U
1	A1	907	G

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Mol	Chain	Res	Type
1	A1	914	A
1	A1	916	G
1	A1	917	A
1	A1	921	A
1	A1	923	C
1	A1	924	G
1	A1	925	A
1	A1	934	G
1	A1	937	G
1	A1	944	C
1	A1	959	C
1	A1	960	U
1	A1	963	G
1	A1	970	A
1	A1	974	G
1	A1	979	U
1	A1	981	U
1	A1	994	G
1	A1	1000	C
1	A1	1002	A
1	A1	1006	A
1	A1	1010	G
1	A1	1014	U
1	A1	1016	C
1	A1	1017	C
1	A1	1018	G
1	A1	1019	G
1	A1	1021	G
1	A1	1032	C
1	A1	1033	U
1	A1	1034	U
1	A1	1035	G
1	A1	1047	A
1	A1	1049	C
1	A1	1052	U
1	A1	1064	A
1	A1	1072	G
1	A1	1075	A
1	A1	1081	U
1	A1	1087	G
1	A1	1094	U
1	A1	1095	U

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Mol	Chain	Res	Type
1	A1	1096	U
1	A1	1097	G
1	A1	1098	A
1	A1	1103	A
1	A1	1104	G
1	A1	1117	G
1	A1	1131	G
1	A1	1132	C
1	A1	1143	A
1	A1	1144	U
1	A1	1153	A
1	A1	1155	C
1	A1	1156	C
1	A1	1159	A
1	A1	1160	C
1	A1	1177	G
1	A1	1179	A
1	A1	1180	A
1	A1	1181	U
1	A1	1182	A
1	A1	1186	G
1	A1	1190	A
1	A1	1192	C
1	A1	1193	A
1	A1	1201	C
1	A1	1207	G
1	A1	1208	U
1	A1	1219	C
1	A1	1222	G
1	A1	1223	A
1	A1	1225	A
1	A1	1227	C
1	A1	1228	C
1	A1	1231	A
1	A1	1232	C
1	A1	1233	G
1	A1	1235	U
1	A1	1236	G
1	A1	1237	G
1	A1	1239	C
1	A1	1240	A
1	A1	1241	U

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Mol	Chain	Res	Type
1	A1	1242	G
1	A1	1243	G
1	A1	1244	A
1	A1	1246	G
1	A1	1247	U
1	A1	1248	C
1	A1	1249	G
1	A1	1250	G
1	A1	1251	A
1	A1	1252	A
1	A1	1263	A
1	A1	1264	G
1	A1	1266	G
1	A1	1268	G
1	A1	1270	A
1	A1	1271	A
1	A1	1272	C
1	A1	1276	U
1	A1	1277	C
1	A1	1278	A
1	A1	1281	G
1	A1	1283	C
1	A1	1286	A
1	A1	1287	A
1	A1	1306	G
1	A1	1307	G
1	A1	1309	U
1	A1	1315	U
1	A1	1317	A
1	A1	1318	A
1	A1	1325	U
1	A1	1330	A
1	A1	1331	U
1	A1	1345	G
1	A1	1348	U
1	A1	1350	A
1	A1	1351	U
1	A1	1352	A
1	A1	1353	U
1	A1	1354	G
1	A1	1355	A
1	A1	1356	U

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Mol	Chain	Res	Type
1	A1	1357	G
1	A1	1386	A
1	A1	1391	C
1	A1	1392	G
1	A1	1399	A
1	A1	1400	G
1	A1	1417	G
1	A1	1418	A
1	A1	1419	A
1	A1	1434	G
1	A1	1437	OMC
1	A1	1443	G
1	A1	1446	A
1	A1	1450	OMG
1	A1	1465	A
1	A1	1469	C
1	A1	1475	A
1	A1	1477	A
1	A1	1481	A
1	A1	1487	G
1	A1	1494	U
1	A1	1508	C
1	A1	1522	U
1	A1	1523	U
1	A1	1524	A
1	A1	1525	G
1	A1	1526	U
1	A1	1533	U
1	A1	1536	G
1	A1	1539	A
1	A1	1555	U
1	A1	1556	C
1	A1	1562	C
1	A1	1564	U
1	A1	1565	G
1	A1	1566	A
1	A1	1567	U
1	A1	1569	U
1	A1	1570	U
1	A1	1572	U
1	A1	1574	C
1	A1	1576	G

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Mol	Chain	Res	Type
1	A1	1583	A
1	A1	1587	A
1	A1	1589	A
1	A1	1590	G
1	A1	1593	A
1	A1	1596	C
1	A1	1605	A
1	A1	1628	C
1	A1	1629	U
1	A1	1630	U
1	A1	1642	A
1	A1	1643	A
1	A1	1657	C
1	A1	1683	A
1	A1	1717	U
1	A1	1722	U
1	A1	1724	U
1	A1	1730	G
1	A1	1736	G
1	A1	1741	A
1	A1	1742	U
1	A1	1750	A
1	A1	1751	G
1	A1	1756	C
1	A1	1761	C
1	A1	1762	C
1	A1	1763	U
1	A1	1764	U
1	A1	1765	U
1	A1	1766	G
1	A1	1775	G
1	A1	1778	G
1	A1	1780	G
1	A1	1794	G
1	A1	1795	U
1	A1	1796	G
1	A1	1797	A
1	A1	1813	A
1	A1	1814	A
1	A1	1815	U
1	A1	1821	U
1	A1	1825	G

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Mol	Chain	Res	Type
1	A1	1839	A
1	A1	1840	U
1	A1	1842	A
1	A1	1846	C
1	A1	1848	G
1	A1	1849	C
1	A1	1850	A
1	A1	1858	A
1	A1	1866	C
1	A1	1871	U
1	A1	1878	G
1	A1	1880	U
1	A1	1886	A
1	A1	1893	A
1	A1	1899	G
1	A1	1906	G
1	A1	1943	C
1	A1	1948	G
1	A1	1951	C
1	A1	1952	G
1	A1	1953	G
1	A1	1954	G
1	A1	2094	C
1	A1	2095	G
1	A1	2096	A
1	A1	2110	G
1	A1	2112	U
1	A1	2114	C
1	A1	2115	G
1	A1	2121	G
1	A1	2122	G
1	A1	2131	A
1	A1	2140	U
1	A1	2142	1MA
1	A1	2144	A
1	A1	2145	A
1	A1	2158	A
1	A1	2169	G
1	A1	2176	U
1	A1	2188	A
1	A1	2194	G
1	A1	2197	OMC

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Mol	Chain	Res	Type
1	A1	2205	U
1	A1	2207	A
1	A1	2208	A
1	A1	2209	U
1	A1	2210	G
1	A1	2244	A
1	A1	2249	G
1	A1	2253	G
1	A1	2256	A
1	A1	2257	C
1	A1	2258	U
1	A1	2260	U
1	A1	2268	U
1	A1	2269	U
1	A1	2270	A
1	A1	2272	G
1	A1	2273	G
1	A1	2281	A2M
1	A1	2288	OMG
1	A1	2298	U
1	A1	2306	C
1	A1	2307	G
1	A1	2308	C
1	A1	2310	U
1	A1	2313	A
1	A1	2314	U
1	A1	2315	G
1	A1	2334	U
1	A1	2336	U
1	A1	2340	U
1	A1	2366	C
1	A1	2373	A
1	A1	2374	C
1	A1	2375	G
1	A1	2376	G
1	A1	2383	C
1	A1	2388	U
1	A1	2391	G
1	A1	2393	G
1	A1	2397	A
1	A1	2401	A
1	A1	2402	A

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Mol	Chain	Res	Type
1	A1	2403	G
1	A1	2404	A
1	A1	2411	U
1	A1	2418	G
1	A1	2422	C
1	A1	2435	G
1	A1	2437	G
1	A1	2441	A
1	A1	2442	G
1	A1	2444	C
1	A1	2502	A
1	A1	2503	G
1	A1	2504	U
1	A1	2506	U
1	A1	2507	C
1	A1	2508	U
1	A1	2514	U
1	A1	2515	A
1	A1	2523	A
1	A1	2524	A
1	A1	2531	C
1	A1	2532	U
1	A1	2536	A
1	A1	2537	U
1	A1	2538	U
1	A1	2539	C
1	A1	2540	A
1	A1	2541	U
1	A1	2542	U
1	A1	2543	U
1	A1	2544	U
1	A1	2545	C
1	A1	2548	C
1	A1	2552	C
1	A1	2553	U
1	A1	2561	A
1	A1	2568	C
1	A1	2569	A
1	A1	2570	U
1	A1	2571	U
1	A1	2572	C
1	A1	2573	G

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Mol	Chain	Res	Type
1	A1	2580	A
1	A1	2585	G
1	A1	2586	G
1	A1	2593	A
1	A1	2606	G
1	A1	2607	G
1	A1	2614	G
1	A1	2629	U
1	A1	2635	A
1	A1	2648	G
1	A1	2651	G
1	A1	2652	U
1	A1	2656	A
1	A1	2666	C
1	A1	2672	G
1	A1	2674	A
1	A1	2676	A
1	A1	2677	G
1	A1	2678	A
1	A1	2679	A
1	A1	2681	U
1	A1	2688	U
1	A1	2689	A
1	A1	2690	G
1	A1	2691	A
1	A1	2703	A
1	A1	2704	A
1	A1	2705	A
1	A1	2712	U
1	A1	2714	G
1	A1	2723	U
1	A1	2726	C
1	A1	2727	A
1	A1	2728	G
1	A1	2729	OMU
1	A1	2737	C
1	A1	2739	A
1	A1	2740	A
1	A1	2752	U
1	A1	2753	G
1	A1	2755	C
1	A1	2772	C

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Mol	Chain	Res	Type
1	A1	2777	G
1	A1	2778	G
1	A1	2796	G
1	A1	2797	C
1	A1	2799	A
1	A1	2800	G
1	A1	2801	A
1	A1	2802	A
1	A1	2803	A
1	A1	2810	C
1	A1	2816	G
1	A1	2817	A
1	A1	2828	G
1	A1	2838	A
1	A1	2839	G
1	A1	2842	U
1	A1	2843	U
1	A1	2845	A
1	A1	2858	U
1	A1	2860	U
1	A1	2861	U
1	A1	2867	C
1	A1	2872	A
1	A1	2873	U
1	A1	2875	U
1	A1	2887	A
1	A1	2889	C
1	A1	2898	G
1	A1	2911	A
1	A1	2923	U
1	A1	2933	A
1	A1	2935	U
1	A1	2936	A
1	A1	2938	G
1	A1	2941	A
1	A1	2942	C
1	A1	2947	G
1	A1	2948	OMC
1	A1	2951	G
1	A1	2955	U
1	A1	2956	A
1	A1	2983	C

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Mol	Chain	Res	Type
1	A1	2990	G
1	A1	2992	U
1	A1	2997	G
1	A1	3011	A
1	A1	3012	A
1	A1	3021	A
1	A1	3022	G
1	A1	3032	A
1	A1	3056	U
1	A1	3057	U
1	A1	3059	G
1	A1	3078	U
1	A1	3079	U
1	A1	3080	G
1	A1	3086	A
1	A1	3087	A
1	A1	3092	C
1	A1	3095	U
1	A1	3109	G
1	A1	3116	G
1	A1	3129	A
1	A1	3130	A
1	A1	3131	U
1	A1	3142	A
1	A1	3143	C
1	A1	3153	U
1	A1	3154	C
1	A1	3155	U
1	A1	3156	U
1	A1	3157	U
1	A1	3165	A
1	A1	3170	A
1	A1	3172	A
1	A1	3173	G
1	A1	3174	A
1	A1	3175	U
1	A1	3176	G
1	A1	3179	U
1	A1	3181	C
1	A1	3186	A
1	A1	3187	A
1	A1	3196	U

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Mol	Chain	Res	Type
1	A1	3198	U
1	A1	3199	G
1	A1	3206	C
1	A1	3207	U
1	A1	3210	A
1	A1	3215	A
1	A1	3216	G
1	A1	3217	C
1	A1	3218	A
1	A1	3219	G
1	A1	3234	A
1	A1	3243	A
1	A1	3244	A
1	A1	3247	G
1	A1	3251	U
1	A1	3259	U
1	A1	3260	G
1	A1	3263	G
1	A1	3270	U
1	A1	3273	A
1	A1	3275	U
1	A1	3276	G
1	A1	3277	U
1	A1	3278	C
1	A1	3281	U
1	A1	3282	U
1	A1	3283	U
1	A1	3284	G
1	A1	3289	G
1	A1	3294	A
1	A1	3303	G
1	A1	3304	U
1	A1	3309	G
1	A1	3313	U
1	A1	3316	A
1	A1	3320	A
1	A1	3342	A
1	A1	3345	G
1	A1	3351	U
1	A1	3352	U
1	A1	3353	G
1	A1	3354	U

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Mol	Chain	Res	Type
1	A1	3355	U
1	A1	3356	G
1	A1	3363	U
1	A1	3369	G
1	A1	3375	A
1	A1	3378	C
1	A1	3382	U
1	A1	3383	G
1	A1	3389	U
1	A1	3390	G
2	A3	7	G
2	A3	10	C
2	A3	22	A
2	A3	38	U
2	A3	41	G
2	A3	43	U
2	A3	49	G
2	A3	54	U
2	A3	55	A
2	A3	65	G
2	A3	74	C
2	A3	76	A
2	A3	99	G
2	A3	102	A
2	A3	112	G
3	A4	13	A
3	A4	25	G
3	A4	34	U
3	A4	35	C
3	A4	51	G
3	A4	52	A
3	A4	59	A
3	A4	62	C
3	A4	63	G
3	A4	68	G
3	A4	75	G
3	A4	76	C
3	A4	80	A
3	A4	81	U
3	A4	82	U
3	A4	84	C
3	A4	86	U

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Mol	Chain	Res	Type
3	A4	87	G
3	A4	88	A
3	A4	90	U
3	A4	95	G
3	A4	97	A
3	A4	104	A
3	A4	105	A
3	A4	106	C
3	A4	111	A
3	A4	112	U
3	A4	113	U
3	A4	116	G
3	A4	125	U
3	A4	126	A
3	A4	152	G
3	A4	157	U
3	A4	158	U
79	B5	4	C
79	B5	25	C
79	B5	26	A
79	B5	34	G
79	B5	42	G
79	B5	46	A
79	B5	47	A
79	B5	57	G
79	B5	60	U
79	B5	67	A
79	B5	68	A
79	B5	72	A
79	B5	75	U
79	B5	76	A
79	B5	77	U
79	B5	78	A
79	B5	81	G
79	B5	94	U
79	B5	104	A
79	B5	114	C
79	B5	115	G
79	B5	126	A
79	B5	127	G
79	B5	130	C
79	B5	133	U

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Mol	Chain	Res	Type
79	B5	134	U
79	B5	135	A
79	B5	136	C
79	B5	137	U
79	B5	138	A
79	B5	141	U
79	B5	145	A
79	B5	158	U
79	B5	161	U
79	B5	166	C
79	B5	168	A
79	B5	171	A
79	B5	178	U
79	B5	179	A
79	B5	188	A
79	B5	189	C
79	B5	190	C
79	B5	191	C
79	B5	192	U
79	B5	193	U
79	B5	195	G
79	B5	196	G
79	B5	198	A
79	B5	200	A
79	B5	207	U
79	B5	217	A
79	B5	218	A
79	B5	224	C
79	B5	225	A
79	B5	227	U
79	B5	228	G
79	B5	229	U
79	B5	230	C
79	B5	232	U
79	B5	233	C
79	B5	234	G
79	B5	239	C
79	B5	240	U
79	B5	241	U
79	B5	257	A
79	B5	260	U
79	B5	261	U

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Mol	Chain	Res	Type
79	B5	265	A
79	B5	273	G
79	B5	278	U
79	B5	280	U
79	B5	299	A
79	B5	314	C
79	B5	316	A
79	B5	322	G
79	B5	333	A
79	B5	337	G
79	B5	338	C
79	B5	352	A
79	B5	359	A
79	B5	360	A
79	B5	361	C
79	B5	365	G
79	B5	369	A
79	B5	380	U
79	B5	388	G
79	B5	390	G
79	B5	393	C
79	B5	399	A
79	B5	400	A
79	B5	401	A
79	B5	402	C
79	B5	404	G
79	B5	417	A
79	B5	419	G
79	B5	423	G
79	B5	424	C
79	B5	425	A
79	B5	426	G
79	B5	434	G
79	B5	439	U
79	B5	444	C
79	B5	448	C
79	B5	452	A
79	B5	459	G
79	B5	460	A
79	B5	468	A
79	B5	475	A
79	B5	477	A

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Mol	Chain	Res	Type
79	B5	481	A
79	B5	484	C
79	B5	485	A
79	B5	486	G
79	B5	487	G
79	B5	489	C
79	B5	490	C
79	B5	491	C
79	B5	492	A
79	B5	493	U
79	B5	494	U
79	B5	495	C
79	B5	496	G
79	B5	497	G
79	B5	498	G
79	B5	499	U
79	B5	500	C
79	B5	501	U
79	B5	503	G
79	B5	505	A
79	B5	506	A
79	B5	507	U
79	B5	515	A
79	B5	519	C
79	B5	525	A
79	B5	527	A
79	B5	538	A
79	B5	539	G
79	B5	540	G
79	B5	541	A2M
79	B5	542	A
79	B5	556	A
79	B5	557	G
79	B5	558	U
79	B5	559	C
79	B5	565	C
79	B5	566	C
79	B5	568	G
79	B5	577	G
79	B5	579	A
79	B5	580	A
79	B5	582	U

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Mol	Chain	Res	Type
79	B5	594	A
79	B5	595	G
79	B5	606	A
79	B5	611	U
79	B5	613	G
79	B5	614	C
79	B5	617	U
79	B5	619	A2M
79	B5	620	A
79	B5	621	A
79	B5	622	A
79	B5	623	A
79	B5	635	A
79	B5	639	U
79	B5	650	U
79	B5	651	G
79	B5	652	G
79	B5	655	G
79	B5	656	G
79	B5	657	U
79	B5	658	C
79	B5	677	G
79	B5	678	A
79	B5	679	U
79	B5	681	U
79	B5	683	C
79	B5	694	U
79	B5	696	C
79	B5	697	C
79	B5	698	U
79	B5	700	C
79	B5	702	G
79	B5	703	G
79	B5	704	C
79	B5	705	U
79	B5	706	A
79	B5	707	A
79	B5	708	C
79	B5	709	C
79	B5	710	U
79	B5	711	U
79	B5	714	G

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Mol	Chain	Res	Type
79	B5	715	U
79	B5	716	C
79	B5	717	C
79	B5	718	U
79	B5	719	U
79	B5	720	G
79	B5	721	U
79	B5	722	G
79	B5	724	C
79	B5	725	U
79	B5	727	U
79	B5	729	G
79	B5	731	C
79	B5	732	G
79	B5	733	A
79	B5	734	A
79	B5	735	C
79	B5	736	C
79	B5	738	G
79	B5	740	A
79	B5	741	C
79	B5	742	U
79	B5	743	U
79	B5	745	U
79	B5	753	A
79	B5	755	A
79	B5	765	G
79	B5	766	U
79	B5	774	A
79	B5	775	G
79	B5	778	G
79	B5	779	U
79	B5	780	A
79	B5	781	U
79	B5	782	U
79	B5	783	G
79	B5	784	C
79	B5	787	G
79	B5	789	A
79	B5	794	U
79	B5	812	A
79	B5	814	A

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Mol	Chain	Res	Type
79	B5	815	G
79	B5	820	U
79	B5	821	U
79	B5	823	G
79	B5	829	A
79	B5	833	U
79	B5	836	U
79	B5	837	G
79	B5	838	G
79	B5	840	U
79	B5	846	G
79	B5	857	U
79	B5	859	A
79	B5	863	A
79	B5	873	U
79	B5	876	G
79	B5	886	U
79	B5	898	A
79	B5	906	A
79	B5	914	G
79	B5	932	U
79	B5	933	A
79	B5	935	U
79	B5	945	U
79	B5	951	A
79	B5	960	U
79	B5	964	U
79	B5	966	A
79	B5	973	A
79	B5	987	G
79	B5	992	A
79	B5	993	A
79	B5	1003	A
79	B5	1004	U
79	B5	1005	A
79	B5	1021	C
79	B5	1025	A
79	B5	1026	A
79	B5	1028	C
79	B5	1030	A
79	B5	1032	G
79	B5	1039	A

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Mol	Chain	Res	Type
79	B5	1052	U
79	B5	1056	U
79	B5	1058	U
79	B5	1060	U
79	B5	1061	A
79	B5	1062	A
79	B5	1076	A
79	B5	1082	C
79	B5	1083	G
79	B5	1086	A
79	B5	1092	A
79	B5	1097	U
79	B5	1098	U
79	B5	1100	G
79	B5	1101	G
79	B5	1111	G
79	B5	1113	A
79	B5	1126	OMG
79	B5	1138	A
79	B5	1150	G
79	B5	1158	C
79	B5	1166	A
79	B5	1185	U
79	B5	1192	C
79	B5	1194	A
79	B5	1196	A
79	B5	1199	G
79	B5	1200	G
79	B5	1201	G
79	B5	1202	A
79	B5	1203	A
79	B5	1207	C
79	B5	1214	U
79	B5	1217	A
79	B5	1218	G
79	B5	1225	U
79	B5	1226	A
79	B5	1227	A
79	B5	1228	G
79	B5	1229	G
79	B5	1230	A
79	B5	1235	C

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Mol	Chain	Res	Type
79	B5	1237	G
79	B5	1238	A
79	B5	1239	U
79	B5	1240	U
79	B5	1241	G
79	B5	1242	A
79	B5	1243	G
79	B5	1244	A
79	B5	1245	G
79	B5	1247	U
79	B5	1248	C
79	B5	1249	U
79	B5	1251	U
79	B5	1252	C
79	B5	1255	G
79	B5	1256	A
79	B5	1257	U
79	B5	1270	G
79	B5	1284	C
79	B5	1285	U
79	B5	1286	U
79	B5	1314	U
79	B5	1315	U
79	B5	1316	G
79	B5	1321	A
79	B5	1340	U
79	B5	1344	A
79	B5	1345	A
79	B5	1355	C
79	B5	1356	U
79	B5	1359	C
79	B5	1362	U
79	B5	1363	U
79	B5	1364	G
79	B5	1369	U
79	B5	1371	A
79	B5	1372	U
79	B5	1373	C
79	B5	1378	U
79	B5	1382	A
79	B5	1390	U
79	B5	1399	C

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Mol	Chain	Res	Type
79	B5	1400	A
79	B5	1413	U
79	B5	1415	U
79	B5	1418	G
79	B5	1425	A
79	B5	1427	A
79	B5	1428	OMG
79	B5	1432	U
79	B5	1435	G
79	B5	1436	A
79	B5	1445	G
79	B5	1446	A
79	B5	1447	C
79	B5	1458	G
79	B5	1459	C
79	B5	1461	C
79	B5	1471	A
79	B5	1477	G
79	B5	1486	G
79	B5	1491	U
79	B5	1492	A
79	B5	1493	A
79	B5	1496	U
79	B5	1503	A
79	B5	1506	G
79	B5	1514	U
79	B5	1516	A
79	B5	1520	U
79	B5	1521	G
79	B5	1523	G
79	B5	1524	A
79	B5	1537	C
79	B5	1542	G
79	B5	1557	U
79	B5	1559	A
79	B5	1563	C
79	B5	1575	G7M
79	B5	1576	A
79	B5	1577	A
79	B5	1582	U
79	B5	1584	G
79	B5	1590	G

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Mol	Chain	Res	Type
79	B5	1596	C
79	B5	1597	A
79	B5	1601	G
79	B5	1607	G
79	B5	1619	C
79	B5	1631	A
79	B5	1634	C
79	B5	1637	C
79	B5	1642	G
79	B5	1646	C
79	B5	1651	A
79	B5	1657	U
79	B5	1658	G
79	B5	1663	G
79	B5	1680	G
79	B5	1681	A
79	B5	1682	U
79	B5	1683	C
79	B5	1684	U
79	B5	1688	U
79	B5	1689	A
79	B5	1690	G
79	B5	1691	A
79	B5	1692	G
79	B5	1693	A
79	B5	1694	A
79	B5	1695	G
79	B5	1697	G
79	B5	1698	G
79	B5	1699	G
79	B5	1701	A
79	B5	1702	A
79	B5	1703	C
79	B5	1704	U
79	B5	1706	C
79	B5	1708	U
79	B5	1709	C
79	B5	1710	U
79	B5	1711	C
79	B5	1713	G
79	B5	1714	A
79	B5	1716	C

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Mol	Chain	Res	Type
79	B5	1717	G
79	B5	1730	A
79	B5	1750	A
79	B5	1766	A
79	B5	1767	G
79	B5	1768	G
79	B5	1769	U
79	B5	1780	G
79	B5	1792	G
79	B5	1793	G
79	B5	1794	A
79	B5	1795	U
79	B5	1796	C

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A1	267	G
1	A1	282	G
1	A1	588	G
1	A1	916	G
1	A1	1032	C
1	A1	1280	C
1	A1	1314	C
1	A1	1385	C
1	A1	1575	A
1	A1	2093	A
1	A1	2401	A
1	A1	2585	G
1	A1	3164	C
3	A4	67	U
3	A4	81	U
79	B5	187	G
79	B5	224	C
79	B5	272	U
79	B5	488	G
79	B5	489	C
79	B5	819	G
79	B5	950	C
79	B5	1059	U
79	B5	1285	U
79	B5	1344	A

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Mol	Chain	Res	Type
79	B5	1358	G
79	B5	1572	OMG
79	B5	1633	A
79	B5	1645	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMC	A1	1437	81,1	19,22,23	0.94	1 (5%)	26,31,34	1.44	4 (15%)
79	OMC	B5	414	79	19,22,23	0.84	1 (5%)	26,31,34	0.86	1 (3%)
1	OMC	A1	663	1	19,22,23	0.92	2 (10%)	26,31,34	0.83	0
1	OMC	A1	2197	1	19,22,23	0.83	0	26,31,34	0.78	0
1	OMC	A1	650	1	19,22,23	0.89	1 (5%)	26,31,34	0.86	1 (3%)
1	A2M	A1	1133	1	18,25,26	0.95	1 (5%)	18,36,39	1.37	2 (11%)
79	OMU	B5	1269	81,79	19,22,23	1.37	4 (21%)	26,31,34	1.85	6 (23%)
79	A2M	B5	436	79	18,25,26	0.93	1 (5%)	18,36,39	1.17	2 (11%)
79	A2M	B5	541	79	18,25,26	0.95	1 (5%)	18,36,39	1.25	2 (11%)
79	A2M	B5	619	81,79	18,25,26	0.94	0	18,36,39	1.49	2 (11%)
1	A2M	A1	649	1	18,25,26	0.85	0	18,36,39	1.38	3 (16%)
1	OMG	A1	1450	1	18,26,27	0.98	1 (5%)	19,38,41	1.18	3 (15%)
1	UR3	A1	2634	81,1	19,22,23	0.95	2 (10%)	26,32,35	1.60	3 (11%)
79	A2M	B5	974	79	18,25,26	0.93	1 (5%)	18,36,39	1.25	3 (16%)
79	4AC	B5	1773	79	21,24,25	1.03	2 (9%)	29,34,37	1.33	5 (17%)
1	OMG	A1	908	81,1	18,26,27	0.95	1 (5%)	19,38,41	1.40	4 (21%)
1	1MA	A1	645	81,1	16,25,26	1.37	2 (12%)	18,37,40	1.15	3 (16%)
1	1MA	A1	2142	81,1	16,25,26	1.34	2 (12%)	18,37,40	1.17	3 (16%)
79	OMU	B5	578	79	19,22,23	1.21	3 (15%)	26,31,34	1.75	6 (23%)
1	OMG	A1	2793	1	18,26,27	0.95	1 (5%)	19,38,41	1.15	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	OMC	A1	2948	1	19,22,23	0.94	2 (10%)	26,31,34	0.98	2 (7%)
1	OMU	A1	2724	1	19,22,23	1.32	3 (15%)	26,31,34	1.74	5 (19%)
1	OMC	A1	2337	1	19,22,23	0.97	1 (5%)	26,31,34	1.00	1 (3%)
1	OMU	A1	898	1	19,22,23	1.39	4 (21%)	26,31,34	1.67	4 (15%)
5	HIC	AB	243	5	8,11,12	1.43	1 (12%)	6,14,16	0.67	0
79	A2M	B5	420	79	18,25,26	0.94	1 (5%)	18,36,39	1.33	2 (11%)
79	OMC	B5	1639	79	19,22,23	0.85	0	26,31,34	0.77	0
79	OMG	B5	1126	79	18,26,27	1.00	1 (5%)	19,38,41	1.07	2 (10%)
1	OMG	A1	2922	1	18,26,27	0.96	1 (5%)	19,38,41	1.07	2 (10%)
1	A2M	A1	2640	1	18,25,26	0.94	1 (5%)	18,36,39	1.11	2 (11%)
79	G7M	B5	1575	79	20,26,27	2.67	4 (20%)	17,39,42	1.06	1 (5%)
1	OMU	A1	1888	1	19,22,23	1.38	4 (21%)	26,31,34	1.87	4 (15%)
1	OMG	A1	805	1	18,26,27	1.01	1 (5%)	19,38,41	1.09	2 (10%)
1	OMG	A1	2288	1	18,26,27	1.00	1 (5%)	19,38,41	1.10	2 (10%)
1	A2M	A1	2946	81,1	18,25,26	0.94	0	18,36,39	1.53	3 (16%)
79	A2M	B5	100	81,79	18,25,26	0.92	0	18,36,39	1.22	2 (11%)
79	MA6	B5	1781	79	19,26,27	0.98	1 (5%)	18,38,41	1.45	2 (11%)
79	OMG	B5	1271	79	18,26,27	1.00	1 (5%)	19,38,41	1.07	2 (10%)
1	A2M	A1	876	1	18,25,26	0.98	0	18,36,39	1.23	2 (11%)
1	A2M	A1	2280	1	18,25,26	0.99	1 (5%)	18,36,39	1.29	2 (11%)
1	OMG	A1	2791	1	18,26,27	0.97	1 (5%)	19,38,41	1.20	2 (10%)
1	OMU	A1	2729	1	19,22,23	1.38	3 (15%)	26,31,34	1.63	6 (23%)
1	OMU	A1	2921	1	19,22,23	1.32	3 (15%)	26,31,34	1.76	5 (19%)
1	A2M	A1	2281	1	18,25,26	0.88	0	18,36,39	1.38	2 (11%)
1	OMG	A1	2815	1	18,26,27	1.01	1 (5%)	19,38,41	1.30	3 (15%)
79	OMC	B5	1007	79	19,22,23	0.85	1 (5%)	26,31,34	0.95	1 (3%)
1	OMU	A1	2347	1	19,22,23	1.43	4 (21%)	26,31,34	1.83	7 (26%)
79	A2M	B5	28	81,79	18,25,26	0.97	0	18,36,39	1.22	2 (11%)
1	5MC	A1	2278	81,1	18,22,23	0.99	2 (11%)	26,32,35	1.29	4 (15%)
79	OMG	B5	1572	79	18,26,27	0.99	1 (5%)	19,38,41	1.09	1 (5%)
79	OMG	B5	562	79	18,26,27	0.97	1 (5%)	19,38,41	1.16	2 (10%)
1	OMU	A1	2421	1	19,22,23	1.32	3 (15%)	26,31,34	1.76	4 (15%)
1	A2M	A1	1449	81,1	18,25,26	0.93	0	18,36,39	1.12	2 (11%)
1	OMU	A1	2417	1	19,22,23	1.31	3 (15%)	26,31,34	1.67	5 (19%)
79	OMG	B5	1428	81,79	18,26,27	0.96	1 (5%)	19,38,41	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	A2M	A1	817	81,1	18,25,26	0.90	0	18,36,39	1.35	2 (11%)
1	A2M	A1	2220	1	18,25,26	0.90	1 (5%)	18,36,39	1.61	3 (16%)
79	4AC	B5	1280	79	21,24,25	1.19	3 (14%)	29,34,37	1.64	3 (10%)
1	OMG	A1	2619	1	18,26,27	0.92	1 (5%)	19,38,41	1.04	2 (10%)
79	A2M	B5	796	79	18,25,26	0.94	0	18,36,39	1.24	2 (11%)
1	5MC	A1	2870	81,1	18,22,23	0.88	2 (11%)	26,32,35	1.28	3 (11%)
1	A2M	A1	807	1	18,25,26	0.99	1 (5%)	18,36,39	1.24	2 (11%)
1	OMC	A1	2959	1	19,22,23	0.92	1 (5%)	26,31,34	0.97	1 (3%)
79	MA6	B5	1782	79	19,26,27	0.89	1 (5%)	18,38,41	1.42	2 (11%)
79	3AU	B5	1191	79	24,28,29	0.50	0	33,40,43	0.72	0
1	OMG	A1	867	81,1	18,26,27	0.95	1 (5%)	19,38,41	1.19	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	A1	1437	81,1	-	3/9/27/28	0/2/2/2
79	OMC	B5	414	79	-	0/9/27/28	0/2/2/2
1	OMC	A1	663	1	-	0/9/27/28	0/2/2/2
1	OMC	A1	2197	1	-	6/9/27/28	0/2/2/2
1	OMC	A1	650	1	-	0/9/27/28	0/2/2/2
1	A2M	A1	1133	1	-	0/5/27/28	0/3/3/3
79	OMU	B5	1269	81,79	-	2/9/27/28	0/2/2/2
79	A2M	B5	436	79	-	0/5/27/28	0/3/3/3
79	A2M	B5	541	79	-	2/5/27/28	0/3/3/3
79	A2M	B5	619	81,79	-	2/5/27/28	0/3/3/3
1	A2M	A1	649	1	-	1/5/27/28	0/3/3/3
1	OMG	A1	1450	1	-	2/5/27/28	0/3/3/3
1	UR3	A1	2634	81,1	-	0/7/25/26	0/2/2/2
79	A2M	B5	974	79	-	0/5/27/28	0/3/3/3
79	4AC	B5	1773	79	-	2/11/29/30	0/2/2/2
1	OMG	A1	908	81,1	-	3/5/27/28	0/3/3/3
1	1MA	A1	645	81,1	-	0/3/25/26	0/3/3/3
1	1MA	A1	2142	81,1	-	2/3/25/26	0/3/3/3
79	OMU	B5	578	79	-	0/9/27/28	0/2/2/2
1	OMG	A1	2793	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	A1	2948	1	-	0/9/27/28	0/2/2/2
1	OMU	A1	2724	1	-	0/9/27/28	0/2/2/2
1	OMC	A1	2337	1	-	1/9/27/28	0/2/2/2
1	OMU	A1	898	1	-	0/9/27/28	0/2/2/2
5	HIC	AB	243	5	-	1/5/6/8	0/1/1/1
79	A2M	B5	420	79	-	0/5/27/28	0/3/3/3
79	OMC	B5	1639	79	-	0/9/27/28	0/2/2/2
79	OMG	B5	1126	79	-	2/5/27/28	0/3/3/3
79	G7M	B5	1575	79	3/3/5/5	2/3/25/26	0/3/3/3
1	A2M	A1	2640	1	-	0/5/27/28	0/3/3/3
1	OMG	A1	2922	1	-	0/5/27/28	0/3/3/3
1	OMU	A1	1888	1	-	0/9/27/28	0/2/2/2
1	OMG	A1	805	1	-	0/5/27/28	0/3/3/3
1	OMG	A1	2288	1	-	2/5/27/28	0/3/3/3
1	A2M	A1	2946	81,1	-	0/5/27/28	0/3/3/3
79	A2M	B5	100	81,79	-	1/5/27/28	0/3/3/3
79	MA6	B5	1781	79	-	0/7/29/30	0/3/3/3
79	OMG	B5	1271	79	-	1/5/27/28	0/3/3/3
1	A2M	A1	876	1	-	0/5/27/28	0/3/3/3
1	A2M	A1	2280	1	-	0/5/27/28	0/3/3/3
1	OMG	A1	2791	1	-	0/5/27/28	0/3/3/3
1	OMU	A1	2729	1	-	2/9/27/28	0/2/2/2
1	OMU	A1	2921	1	-	0/9/27/28	0/2/2/2
1	A2M	A1	2281	1	-	4/5/27/28	0/3/3/3
1	OMG	A1	2815	1	-	0/5/27/28	0/3/3/3
79	OMC	B5	1007	79	-	0/9/27/28	0/2/2/2
1	OMU	A1	2347	1	-	2/9/27/28	0/2/2/2
79	A2M	B5	28	81,79	-	0/5/27/28	0/3/3/3
1	5MC	A1	2278	81,1	-	0/7/25/26	0/2/2/2
79	OMG	B5	1572	79	-	0/5/27/28	0/3/3/3
79	OMG	B5	562	79	-	0/5/27/28	0/3/3/3
1	OMU	A1	2421	1	-	0/9/27/28	0/2/2/2
1	A2M	A1	1449	81,1	-	0/5/27/28	0/3/3/3
1	OMU	A1	2417	1	-	2/9/27/28	0/2/2/2
79	OMG	B5	1428	81,79	-	3/5/27/28	0/3/3/3
1	A2M	A1	817	81,1	-	2/5/27/28	0/3/3/3
1	A2M	A1	2220	1	-	0/5/27/28	0/3/3/3
79	4AC	B5	1280	79	-	4/11/29/30	0/2/2/2
1	OMG	A1	2619	1	-	1/5/27/28	0/3/3/3
79	A2M	B5	796	79	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A1	2870	81,1	-	6/7/25/26	0/2/2/2
1	A2M	A1	807	1	-	1/5/27/28	0/3/3/3
1	OMC	A1	2959	1	-	0/9/27/28	0/2/2/2
79	MA6	B5	1782	79	-	5/7/29/30	0/3/3/3
79	3AU	B5	1191	79	1/1/7/7	3/16/34/35	0/2/2/2
1	OMG	A1	867	81,1	-	0/5/27/28	0/3/3/3

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	B5	1575	G7M	C8-N9	8.06	1.47	1.33
79	B5	1575	G7M	C8-N7	6.44	1.44	1.33
79	B5	1575	G7M	C5-C4	4.28	1.47	1.39
1	A1	2142	1MA	C2-N3	4.00	1.33	1.29
5	AB	243	HIC	CD2-NE2	-3.63	1.32	1.38
1	A1	645	1MA	C2-N3	3.55	1.33	1.29
1	A1	2815	OMG	C6-N1	-3.30	1.33	1.37
1	A1	898	OMU	C4-N3	-3.27	1.32	1.38
1	A1	2347	OMU	C4-N3	-3.24	1.32	1.38
1	A1	805	OMG	C6-N1	-3.24	1.33	1.37
79	B5	1126	OMG	C6-N1	-3.15	1.33	1.37
79	B5	1269	OMU	C4-N3	-3.14	1.32	1.38
1	A1	1888	OMU	C4-N3	-3.10	1.33	1.38
1	A1	2921	OMU	C4-N3	-3.09	1.33	1.38
1	A1	2288	OMG	C6-N1	-3.09	1.33	1.37
1	A1	2729	OMU	C4-N3	-3.08	1.33	1.38
1	A1	2791	OMG	C6-N1	-3.06	1.33	1.37
1	A1	2421	OMU	C4-N3	-3.02	1.33	1.38
79	B5	1271	OMG	C6-N1	-3.00	1.33	1.37
79	B5	1280	4AC	C4-N4	-3.00	1.35	1.39
1	A1	2347	OMU	C2-N3	-2.99	1.32	1.38
79	B5	562	OMG	C6-N1	-2.97	1.33	1.37
1	A1	2417	OMU	C4-N3	-2.96	1.33	1.38
1	A1	867	OMG	C6-N1	-2.95	1.33	1.37
1	A1	2793	OMG	C6-N1	-2.94	1.33	1.37
1	A1	2729	OMU	C5-C4	-2.90	1.37	1.43
1	A1	2278	5MC	C6-N1	-2.89	1.33	1.38
1	A1	2922	OMG	C6-N1	-2.89	1.33	1.37
79	B5	1572	OMG	C6-N1	-2.88	1.33	1.37
1	A1	1450	OMG	C6-N1	-2.87	1.33	1.37
1	A1	2724	OMU	C4-N3	-2.87	1.33	1.38
79	B5	1575	G7M	C6-N1	-2.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	2724	OMU	C2-N3	-2.77	1.33	1.38
1	A1	645	1MA	C6-N6	2.76	1.34	1.27
1	A1	2921	OMU	C2-N3	-2.74	1.33	1.38
1	A1	898	OMU	C5-C4	-2.74	1.37	1.43
1	A1	898	OMU	C2-N3	-2.72	1.33	1.38
1	A1	2421	OMU	C2-N3	-2.70	1.33	1.38
79	B5	1269	OMU	C2-N3	-2.69	1.33	1.38
79	B5	1428	OMG	C6-N1	-2.67	1.33	1.37
1	A1	2724	OMU	C5-C4	-2.67	1.37	1.43
1	A1	2417	OMU	C2-N3	-2.65	1.33	1.38
1	A1	2948	OMC	C5-C4	-2.63	1.36	1.42
1	A1	2347	OMU	C5-C4	-2.62	1.37	1.43
1	A1	908	OMG	C6-N1	-2.62	1.34	1.37
1	A1	2729	OMU	C2-N3	-2.61	1.33	1.38
79	B5	1781	MA6	C5-C4	2.60	1.47	1.40
1	A1	1437	OMC	C5-C4	-2.60	1.37	1.42
1	A1	1888	OMU	C2-N3	-2.60	1.33	1.38
79	B5	1773	4AC	C4-N4	-2.58	1.36	1.39
1	A1	1888	OMU	C5-C4	-2.56	1.38	1.43
79	B5	578	OMU	C4-N3	-2.56	1.34	1.38
1	A1	2619	OMG	C6-N1	-2.55	1.34	1.37
79	B5	1280	4AC	C7-N4	-2.54	1.32	1.37
1	A1	2421	OMU	C5-C4	-2.49	1.38	1.43
1	A1	2959	OMC	C5-C4	-2.47	1.37	1.42
1	A1	663	OMC	C5-C4	-2.47	1.37	1.42
1	A1	650	OMC	C5-C4	-2.46	1.37	1.42
1	A1	2142	1MA	C6-N6	2.44	1.33	1.27
1	A1	2417	OMU	C5-C4	-2.41	1.38	1.43
1	A1	2337	OMC	C5-C4	-2.40	1.37	1.42
1	A1	2870	5MC	C6-C5	2.39	1.38	1.34
79	B5	578	OMU	C2-N3	-2.34	1.33	1.38
79	B5	1782	MA6	C5-C4	2.28	1.47	1.40
1	A1	2921	OMU	C5-C4	-2.23	1.38	1.43
79	B5	541	A2M	C5-C4	2.23	1.46	1.40
79	B5	1269	OMU	C2-N1	2.23	1.42	1.38
1	A1	2948	OMC	C6-N1	-2.20	1.32	1.38
79	B5	578	OMU	C5-C4	-2.19	1.38	1.43
1	A1	1888	OMU	C6-N1	-2.16	1.32	1.38
1	A1	807	A2M	C5-C4	2.15	1.46	1.40
79	B5	1007	OMC	C5-C4	-2.14	1.38	1.42
1	A1	2280	A2M	C5-C4	2.13	1.46	1.40
1	A1	2870	5MC	C6-N1	-2.12	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	2278	5MC	C6-C5	2.12	1.38	1.34
1	A1	2634	UR3	C6-N1	-2.12	1.32	1.38
1	A1	2634	UR3	C5-C4	-2.10	1.38	1.43
1	A1	2640	A2M	C5-C4	2.10	1.46	1.40
79	B5	1280	4AC	C6-N1	-2.10	1.32	1.38
79	B5	1269	OMU	C5-C4	-2.09	1.39	1.43
79	B5	974	A2M	C5-C4	2.09	1.46	1.40
1	A1	898	OMU	C6-N1	-2.08	1.33	1.38
1	A1	2220	A2M	C5-C4	2.06	1.46	1.40
1	A1	1133	A2M	C5-C4	2.03	1.46	1.40
79	B5	420	A2M	C5-C4	2.03	1.46	1.40
79	B5	414	OMC	C5-C4	-2.03	1.38	1.42
1	A1	2347	OMU	C6-N1	-2.02	1.33	1.38
79	B5	436	A2M	C5-C4	2.01	1.46	1.40
79	B5	1773	4AC	C7-N4	-2.01	1.33	1.37
1	A1	663	OMC	C6-N1	-2.00	1.33	1.38

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	2634	UR3	C4-N3-C2	-6.46	118.48	124.56
79	B5	1280	4AC	N4-C4-N3	6.29	124.41	113.85
1	A1	1888	OMU	C4-N3-C2	-4.69	120.39	126.58
1	A1	2921	OMU	N3-C2-N1	4.60	120.99	114.89
79	B5	578	OMU	C4-N3-C2	-4.54	120.60	126.58
1	A1	2921	OMU	C4-N3-C2	-4.50	120.65	126.58
1	A1	2724	OMU	C4-N3-C2	-4.39	120.79	126.58
1	A1	2421	OMU	C4-N3-C2	-4.37	120.82	126.58
1	A1	2421	OMU	N3-C2-N1	4.26	120.55	114.89
1	A1	2220	A2M	N3-C2-N1	-4.23	122.06	128.68
1	A1	2417	OMU	C4-N3-C2	-4.23	121.01	126.58
1	A1	1888	OMU	N3-C2-N1	4.20	120.47	114.89
1	A1	2347	OMU	N3-C2-N1	4.18	120.44	114.89
79	B5	1269	OMU	N3-C2-N1	4.14	120.39	114.89
1	A1	898	OMU	C4-N3-C2	-4.14	121.12	126.58
79	B5	1269	OMU	C4-N3-C2	-4.09	121.19	126.58
1	A1	2347	OMU	C4-N3-C2	-4.06	121.22	126.58
1	A1	1437	OMC	O2-C2-N3	-4.02	115.79	122.33
1	A1	898	OMU	N3-C2-N1	4.02	120.22	114.89
1	A1	2724	OMU	C5-C4-N3	4.01	120.83	114.84
79	B5	1781	MA6	C4-C5-N7	-3.91	105.33	109.40
1	A1	1888	OMU	C5-C4-N3	3.89	120.66	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	2417	OMU	N3-C2-N1	3.87	120.03	114.89
1	A1	2724	OMU	N3-C2-N1	3.86	120.01	114.89
79	B5	578	OMU	N3-C2-N1	3.83	119.97	114.89
1	A1	2421	OMU	C5-C4-N3	3.77	120.48	114.84
1	A1	2417	OMU	C5-C4-N3	3.74	120.44	114.84
79	B5	1280	4AC	C5-C4-N4	-3.71	116.48	122.92
1	A1	2347	OMU	C1'-N1-C2	3.69	124.26	117.57
1	A1	649	A2M	N3-C2-N1	-3.69	122.91	128.68
79	B5	578	OMU	C5-C4-N3	3.66	120.32	114.84
1	A1	2347	OMU	C5-C4-N3	3.64	120.29	114.84
1	A1	898	OMU	C5-C4-N3	3.63	120.27	114.84
1	A1	2946	A2M	N3-C2-N1	-3.60	123.05	128.68
1	A1	2921	OMU	C5-C4-N3	3.59	120.21	114.84
1	A1	2729	OMU	N3-C2-N1	3.58	119.65	114.89
79	B5	1269	OMU	C5-C4-N3	3.52	120.10	114.84
79	B5	1781	MA6	N3-C2-N1	-3.52	123.18	128.68
79	B5	1269	OMU	C1'-N1-C2	3.49	123.89	117.57
1	A1	2729	OMU	C4-N3-C2	-3.47	122.01	126.58
1	A1	2220	A2M	C2-N1-C6	3.46	124.67	118.75
79	B5	1782	MA6	C4-C5-N7	-3.42	105.84	109.40
1	A1	817	A2M	N3-C2-N1	-3.41	123.34	128.68
1	A1	2870	5MC	C5-C6-N1	-3.41	119.83	123.34
79	B5	28	A2M	N3-C2-N1	-3.38	123.40	128.68
1	A1	2729	OMU	C5-C4-N3	3.36	119.86	114.84
1	A1	1133	A2M	N3-C2-N1	-3.34	123.46	128.68
79	B5	541	A2M	N3-C2-N1	-3.33	123.47	128.68
79	B5	974	A2M	N3-C2-N1	-3.32	123.48	128.68
79	B5	420	A2M	N3-C2-N1	-3.32	123.49	128.68
1	A1	2421	OMU	O4-C4-C5	-3.32	119.33	125.16
1	A1	2724	OMU	O4-C4-C5	-3.30	119.36	125.16
79	B5	1782	MA6	N3-C2-N1	-3.29	123.53	128.68
1	A1	2280	A2M	N3-C2-N1	-3.28	123.55	128.68
1	A1	2870	5MC	O2-C2-N3	-3.27	117.01	122.33
1	A1	2281	A2M	N3-C2-N1	-3.26	123.59	128.68
1	A1	1437	OMC	C1'-N1-C2	3.21	125.59	118.42
79	B5	578	OMU	O4-C4-C5	-3.21	119.52	125.16
1	A1	876	A2M	N3-C2-N1	-3.19	123.70	128.68
79	B5	1773	4AC	O2-C2-N3	-3.17	117.17	122.33
79	B5	796	A2M	N3-C2-N1	-3.15	123.76	128.68
1	A1	2278	5MC	O2-C2-N3	-3.14	117.22	122.33
79	B5	100	A2M	N3-C2-N1	-3.12	123.80	128.68
1	A1	898	OMU	O4-C4-C5	-3.09	119.72	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	1888	OMU	O4-C4-C5	-3.08	119.73	125.16
1	A1	1449	A2M	N3-C2-N1	-3.08	123.87	128.68
1	A1	2417	OMU	O4-C4-C5	-3.07	119.76	125.16
1	A1	2729	OMU	O4-C4-C5	-3.03	119.83	125.16
1	A1	2142	1MA	C5-C6-N1	3.00	118.37	113.90
1	A1	2640	A2M	N3-C2-N1	-2.97	124.04	128.68
1	A1	2278	5MC	C5-C4-N3	-2.96	118.48	121.67
1	A1	908	OMG	O2'-C2'-C1'	2.95	114.95	109.09
79	B5	436	A2M	N3-C2-N1	-2.94	124.08	128.68
1	A1	2815	OMG	CM2-O2'-C2'	-2.93	106.83	114.52
1	A1	908	OMG	CM2-O2'-C2'	2.90	122.14	114.52
1	A1	2347	OMU	O4-C4-C5	-2.85	120.15	125.16
1	A1	645	1MA	N1-C2-N3	-2.85	122.70	126.02
1	A1	807	A2M	C4-C5-N7	-2.83	106.45	109.40
79	B5	1575	G7M	CN7-N7-C8	-2.83	111.82	125.43
79	B5	619	A2M	C4-C5-N7	-2.82	106.46	109.40
1	A1	2280	A2M	C4-C5-N7	-2.79	106.49	109.40
1	A1	2337	OMC	O2-C2-N3	-2.78	117.81	122.33
1	A1	2921	OMU	O4-C4-C5	-2.76	120.30	125.16
79	B5	28	A2M	C4-C5-N7	-2.74	106.54	109.40
1	A1	2948	OMC	O2-C2-N3	-2.74	117.87	122.33
1	A1	2870	5MC	C5-C4-N3	-2.72	118.73	121.67
79	B5	1007	OMC	O2-C2-N3	-2.68	117.97	122.33
1	A1	807	A2M	N3-C2-N1	-2.67	124.51	128.68
1	A1	1437	OMC	O2-C2-N1	2.66	124.39	118.89
79	B5	619	A2M	N3-C2-N1	-2.65	124.53	128.68
79	B5	1269	OMU	O2-C2-N3	-2.64	116.59	121.50
79	B5	1773	4AC	O7-C7-N4	2.61	126.05	121.82
79	B5	420	A2M	C4-C5-N7	-2.61	106.68	109.40
1	A1	867	OMG	C5-C6-N1	2.60	118.55	113.95
79	B5	796	A2M	C4-C5-N7	-2.60	106.69	109.40
79	B5	100	A2M	C4-C5-N7	-2.60	106.69	109.40
1	A1	2142	1MA	N1-C2-N3	-2.59	123.00	126.02
79	B5	1269	OMU	O4-C4-C5	-2.58	120.62	125.16
79	B5	436	A2M	C4-C5-N7	-2.58	106.71	109.40
1	A1	2815	OMG	C5-C6-N1	2.56	118.47	113.95
1	A1	2791	OMG	C8-N7-C5	2.55	107.84	102.99
79	B5	1271	OMG	C5-C6-N1	2.53	118.42	113.95
79	B5	1773	4AC	C6-C5-C4	2.53	120.05	116.96
1	A1	2959	OMC	O2-C2-N3	-2.53	118.22	122.33
1	A1	2729	OMU	C1'-N1-C2	2.52	122.14	117.57
79	B5	541	A2M	C4-C5-N7	-2.51	106.78	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	2288	OMG	C5-C6-N1	2.50	118.36	113.95
1	A1	1450	OMG	C5-C6-N1	2.49	118.36	113.95
1	A1	876	A2M	C4-C5-N7	-2.46	106.83	109.40
1	A1	2791	OMG	C5-C6-N1	2.45	118.27	113.95
1	A1	2640	A2M	C4-C5-N7	-2.43	106.87	109.40
1	A1	649	A2M	C4-C5-N7	-2.43	106.87	109.40
1	A1	2724	OMU	O2-C2-N1	-2.41	119.59	122.79
79	B5	1271	OMG	C8-N7-C5	2.40	107.56	102.99
79	B5	1773	4AC	C5-C4-N3	-2.40	118.73	122.59
1	A1	2921	OMU	O2-C2-N1	-2.38	119.62	122.79
1	A1	2347	OMU	O2-C2-N3	-2.38	117.07	121.50
79	B5	974	A2M	C4-C5-N7	-2.37	106.92	109.40
1	A1	2922	OMG	C5-C6-N1	2.37	118.14	113.95
1	A1	1437	OMC	CM2-O2'-C2'	2.37	120.73	114.52
79	B5	1572	OMG	C5-C6-N1	2.36	118.12	113.95
79	B5	562	OMG	C5-C6-N1	2.34	118.08	113.95
1	A1	2815	OMG	C8-N7-C5	2.32	107.41	102.99
79	B5	562	OMG	C8-N7-C5	2.31	107.40	102.99
1	A1	2793	OMG	C8-N7-C5	2.31	107.40	102.99
1	A1	645	1MA	C5-C6-N1	2.31	117.35	113.90
1	A1	2619	OMG	C5-C6-N1	2.29	118.00	113.95
1	A1	1133	A2M	C4-C5-N7	-2.29	107.01	109.40
1	A1	2946	A2M	C4-C5-N7	-2.29	107.02	109.40
1	A1	867	OMG	C8-N7-C5	2.28	107.33	102.99
1	A1	2278	5MC	C5-C6-N1	-2.27	121.01	123.34
1	A1	2729	OMU	C6-N1-C2	-2.24	118.13	120.99
79	B5	1126	OMG	C5-C6-N1	2.23	117.90	113.95
1	A1	2793	OMG	C5-C6-N1	2.23	117.89	113.95
79	B5	1126	OMG	C8-N7-C5	2.23	107.23	102.99
79	B5	1773	4AC	N4-C4-N3	2.22	117.58	113.85
79	B5	578	OMU	O2-C2-N1	-2.22	119.84	122.79
79	B5	414	OMC	O2-C2-N3	-2.21	118.74	122.33
1	A1	2619	OMG	C8-N7-C5	2.20	107.19	102.99
1	A1	908	OMG	C5-C6-N1	2.20	117.83	113.95
1	A1	2946	A2M	O4'-C4'-C3'	-2.19	100.78	105.11
1	A1	2634	UR3	C1'-N1-C2	2.19	120.68	116.99
1	A1	805	OMG	C5-C6-N1	2.18	117.80	113.95
79	B5	1280	4AC	C5-C4-N3	-2.17	119.09	122.59
1	A1	2417	OMU	C1'-N1-C2	2.15	121.45	117.57
1	A1	2288	OMG	C8-N7-C5	2.14	107.08	102.99
1	A1	867	OMG	O6-C6-C5	-2.14	120.19	124.37
1	A1	2948	OMC	C1'-N1-C2	2.14	123.19	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	2922	OMG	C8-N7-C5	2.13	107.05	102.99
1	A1	2347	OMU	C6-N1-C2	-2.11	118.29	120.99
1	A1	2634	UR3	C3U-N3-C4	2.10	120.89	117.89
1	A1	2220	A2M	C4-C5-N7	-2.10	107.21	109.40
1	A1	650	OMC	CM2-O2'-C2'	-2.10	109.02	114.52
1	A1	1450	OMG	C8-N7-C5	2.09	106.97	102.99
1	A1	649	A2M	C2-N1-C6	2.09	122.32	118.75
1	A1	2278	5MC	C1'-N1-C6	-2.09	117.65	121.12
79	B5	974	A2M	C2-N1-C6	2.07	122.30	118.75
79	B5	578	OMU	C1'-N1-C2	2.07	121.32	117.57
1	A1	645	1MA	C8-N7-C5	2.07	106.93	102.99
1	A1	817	A2M	O3'-C3'-C4'	-2.05	105.12	111.05
1	A1	1449	A2M	C4-C5-N7	-2.05	107.26	109.40
1	A1	1450	OMG	O6-C6-C5	-2.05	120.37	124.37
1	A1	805	OMG	C8-N7-C5	2.03	106.85	102.99
1	A1	908	OMG	C8-N7-C5	2.02	106.85	102.99
1	A1	2281	A2M	C4-C5-N7	-2.01	107.31	109.40
79	B5	1428	OMG	C8-N7-C5	2.01	106.81	102.99
1	A1	2142	1MA	C8-N7-C5	2.00	106.80	102.99

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
79	B5	1191	3AU	C12
79	B5	1575	G7M	C4'
79	B5	1575	G7M	C2'
79	B5	1575	G7M	C3'

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AB	243	HIC	CA-CB-CG-ND1
1	A1	908	OMG	C1'-C2'-O2'-CM2
1	A1	1437	OMC	C1'-C2'-O2'-CM2
1	A1	1450	OMG	O4'-C4'-C5'-O5'
1	A1	2197	OMC	C2'-C1'-N1-C6
1	A1	2197	OMC	O4'-C4'-C5'-O5'
1	A1	2288	OMG	O4'-C4'-C5'-O5'
1	A1	2288	OMG	C3'-C4'-C5'-O5'
1	A1	2417	OMU	C1'-C2'-O2'-CM2
1	A1	2619	OMG	C1'-C2'-O2'-CM2
1	A1	2729	OMU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A1	2870	5MC	C2'-C1'-N1-C2
1	A1	2870	5MC	C2'-C1'-N1-C6
79	B5	619	A2M	C3'-C4'-C5'-O5'
79	B5	1191	3AU	N3-C10-C11-C12
79	B5	1191	3AU	N40-C12-C13-O30
79	B5	1280	4AC	N3-C4-N4-C7
79	B5	1280	4AC	C5-C4-N4-C7
79	B5	1280	4AC	O7-C7-N4-C4
79	B5	1280	4AC	CM7-C7-N4-C4
79	B5	1575	G7M	C3'-C4'-C5'-O5'
79	B5	1773	4AC	N3-C4-N4-C7
79	B5	1782	MA6	O4'-C4'-C5'-O5'
79	B5	1782	MA6	C5-C6-N6-C9
79	B5	1782	MA6	C5-C6-N6-C10
1	A1	2197	OMC	C2'-C1'-N1-C2
1	A1	908	OMG	O4'-C4'-C5'-O5'
1	A1	1450	OMG	C3'-C4'-C5'-O5'
1	A1	2197	OMC	C3'-C4'-C5'-O5'
1	A1	2729	OMU	O4'-C4'-C5'-O5'
79	B5	541	A2M	O4'-C4'-C5'-O5'
79	B5	541	A2M	C3'-C4'-C5'-O5'
79	B5	1428	OMG	O4'-C4'-C5'-O5'
79	B5	1782	MA6	C3'-C4'-C5'-O5'
79	B5	1269	OMU	O4'-C1'-N1-C2
1	A1	908	OMG	C3'-C4'-C5'-O5'
1	A1	2142	1MA	O4'-C4'-C5'-O5'
1	A1	2142	1MA	C3'-C4'-C5'-O5'
79	B5	619	A2M	O4'-C4'-C5'-O5'
79	B5	1782	MA6	N1-C6-N6-C9
79	B5	1191	3AU	N40-C12-C13-O31
1	A1	2347	OMU	C3'-C4'-C5'-O5'
79	B5	1575	G7M	O4'-C4'-C5'-O5'
1	A1	2870	5MC	O4'-C4'-C5'-O5'
1	A1	2870	5MC	C3'-C4'-C5'-O5'
1	A1	2347	OMU	O4'-C4'-C5'-O5'
79	B5	1269	OMU	O4'-C1'-N1-C6
79	B5	1271	OMG	C1'-C2'-O2'-CM2
1	A1	2870	5MC	O4'-C1'-N1-C6
1	A1	2281	A2M	C3'-C2'-O2'-CM'
79	B5	1773	4AC	C5-C4-N4-C7
1	A1	817	A2M	C4'-C5'-O5'-P
79	B5	1126	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
79	B5	1428	OMG	C3'-C4'-C5'-O5'
1	A1	2197	OMC	O4'-C1'-N1-C6
1	A1	2197	OMC	O4'-C1'-N1-C2
1	A1	2870	5MC	O4'-C1'-N1-C2
1	A1	649	A2M	C4'-C5'-O5'-P
79	B5	1428	OMG	C4'-C5'-O5'-P
1	A1	2281	A2M	O4'-C4'-C5'-O5'
79	B5	100	A2M	O4'-C4'-C5'-O5'
1	A1	817	A2M	O4'-C4'-C5'-O5'
1	A1	2417	OMU	O4'-C4'-C5'-O5'
1	A1	2281	A2M	C1'-C2'-O2'-CM'
1	A1	807	A2M	C3'-C2'-O2'-CM'
1	A1	1437	OMC	C2'-C1'-N1-C2
1	A1	1437	OMC	O4'-C4'-C5'-O5'
1	A1	2337	OMC	O4'-C4'-C5'-O5'
79	B5	1126	OMG	C3'-C4'-C5'-O5'
1	A1	2281	A2M	C3'-C4'-C5'-O5'

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 377 ligands modelled in this entry, 376 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
80	3HE	A1	3401	-	21,21,21	0.43	0	19,30,30	0.59	0

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
80	3HE	A1	3401	-	-	0/8/36/36	0/2/2/2

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
1	A1	6
79	B5	2
18	AP	1
53	BI	1
8	AE	1
12	AI	1
62	BR	1
76	Bf	1
3	A4	1
66	BV	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	1253:U	O3'	1260:A	P	26.34
1	AP	155:GLU	C	164:LYS	N	24.32
1	BI	123:LYS	C	135:LYS	N	18.64

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	1955:U	O3'	2093:A	P	18.09
1	B5	658:C	O3'	676:G	P	17.61
1	A1	1023:C	O3'	1030:A	P	17.20
1	AE	109:GLU	C	129:GLU	N	14.45
1	A1	2445:A	O3'	2501:U	P	13.63
1	AI	101:LYS	C	114:GLY	N	10.06
1	A1	451:U	O3'	486:A	P	9.84
1	BR	95:ARG	C	100:LEU	N	6.89
1	Bf	125:THR	C	129:GLY	N	6.42
1	A4	73:U	O3'	74:U	P	5.20
1	BV	11:LEU	C	12:TYR	N	5.14
1	A1	444:U	O3'	445:G	P	3.94
1	B5	1798:U	O3'	1799:U	P	3.20

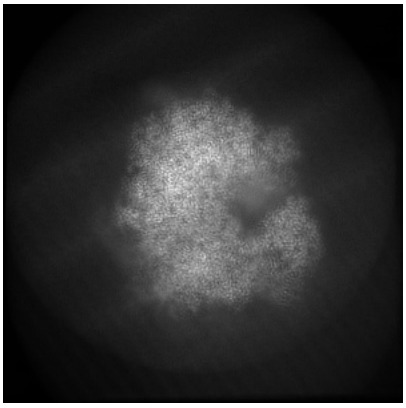
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24235. These allow visual inspection of the internal detail of the map and identification of artifacts.

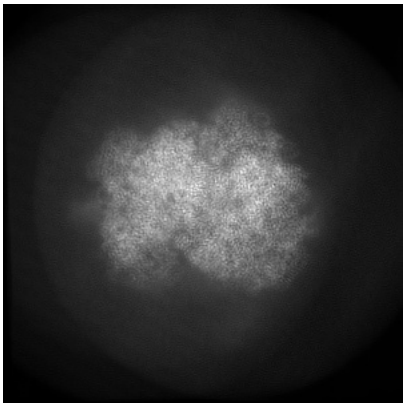
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

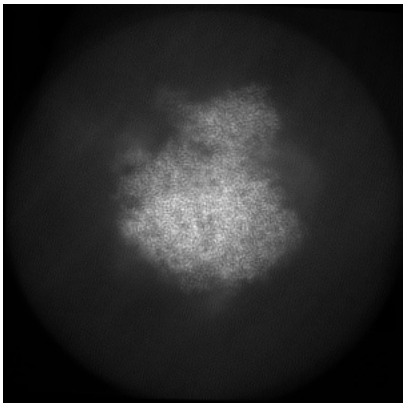
6.1.1 Primary map



X



Y

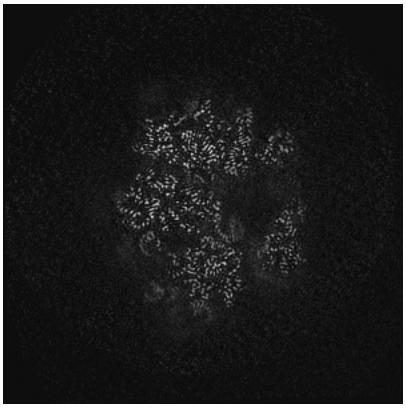


Z

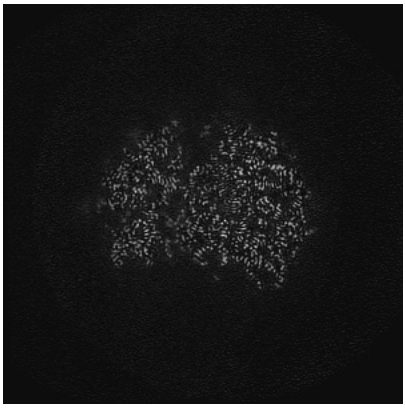
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

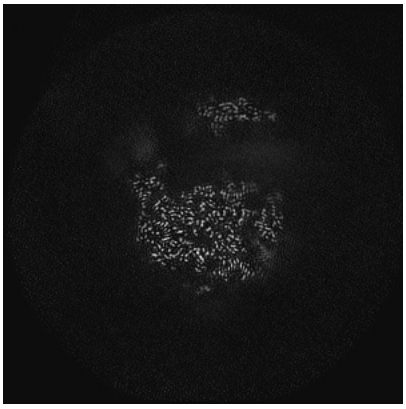
6.2.1 Primary map



X Index: 216



Y Index: 216

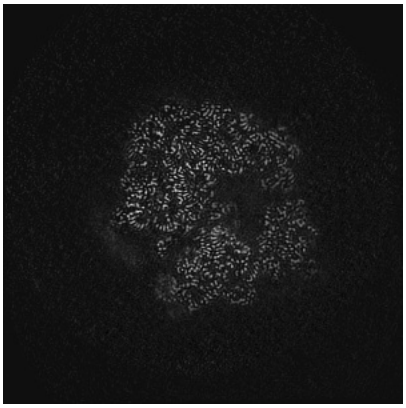


Z Index: 216

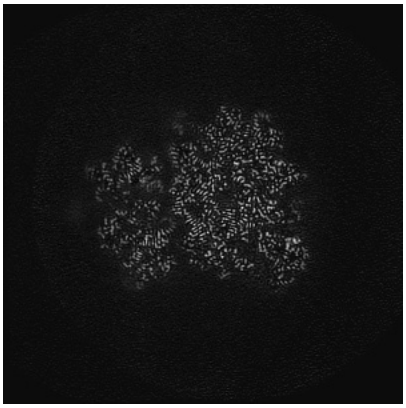
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

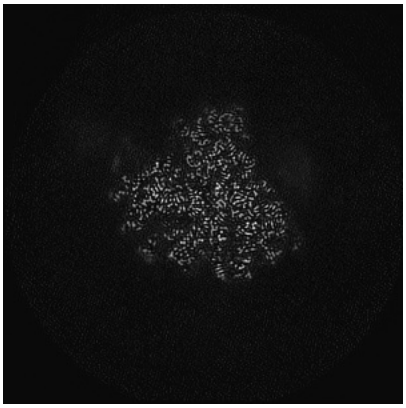
6.3.1 Primary map



X Index: 240



Y Index: 199

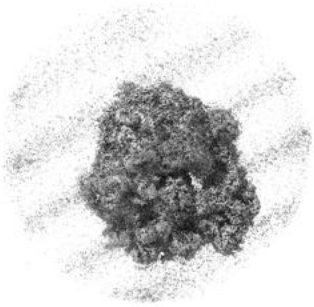


Z Index: 265

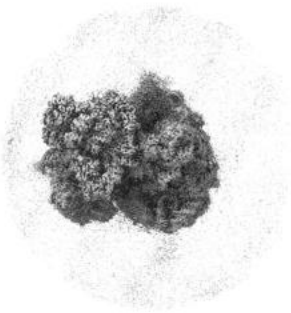
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

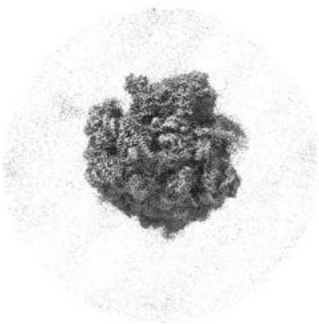
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

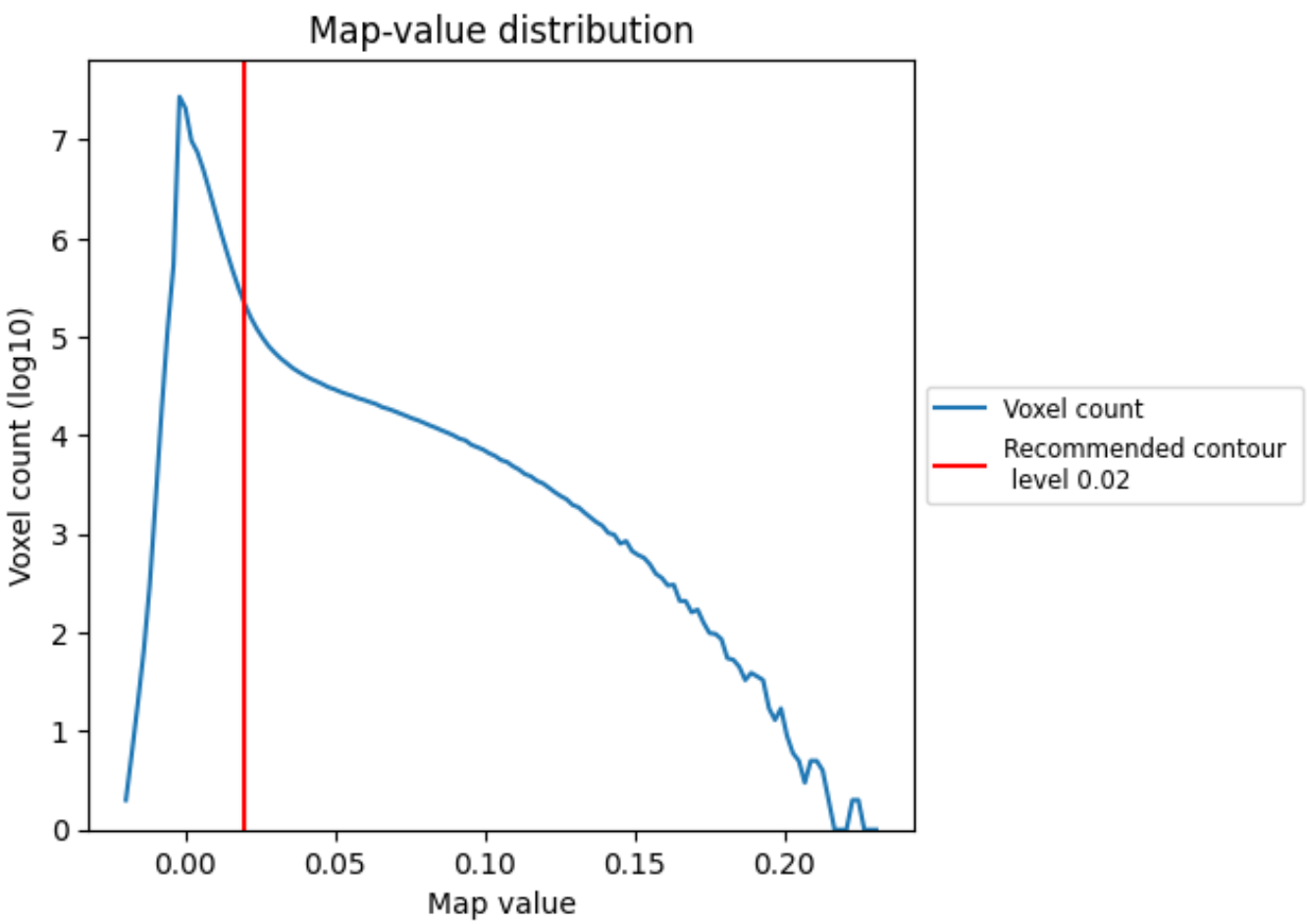
6.5 Mask visualisation (i)

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

7 Map analysis (i)

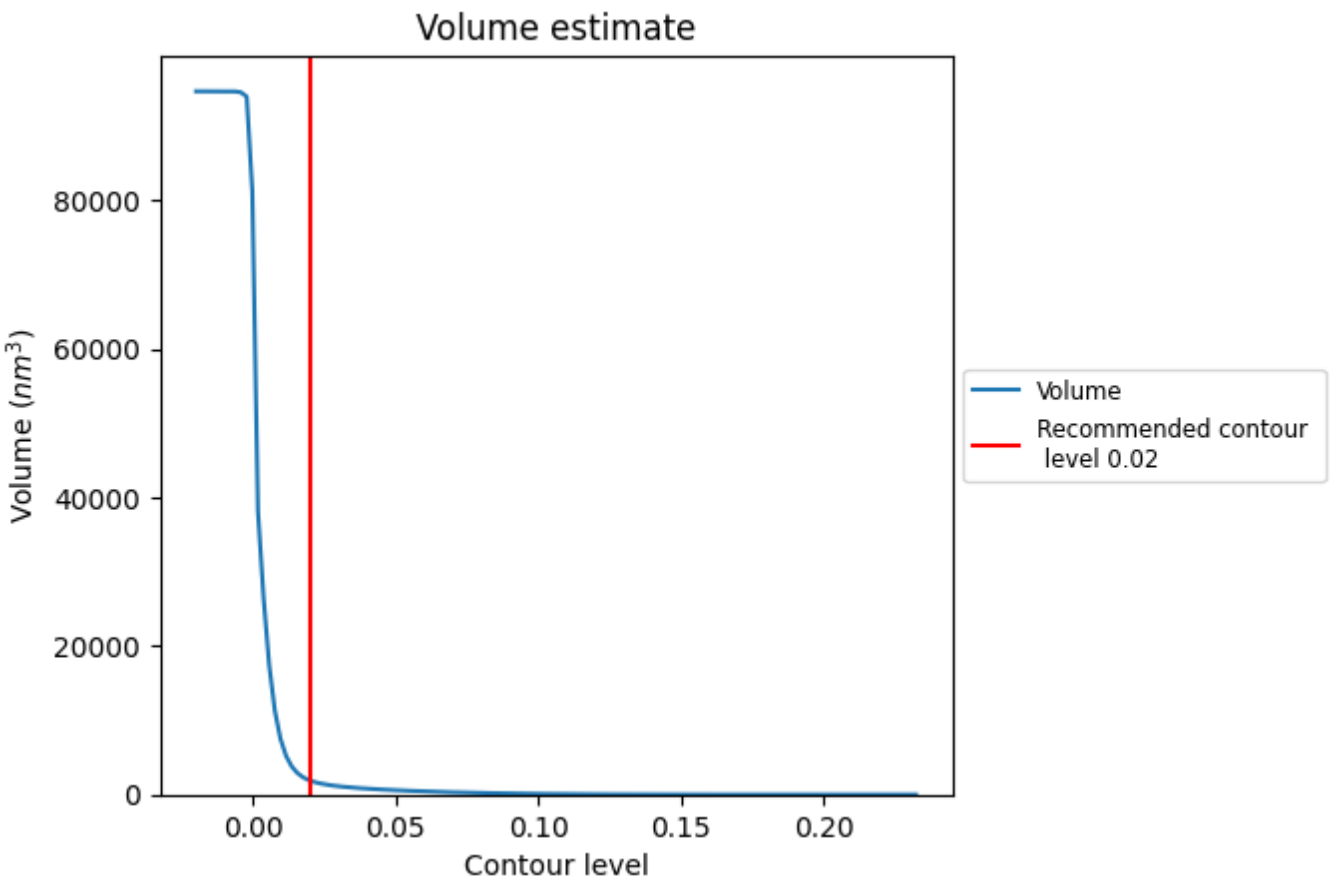
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

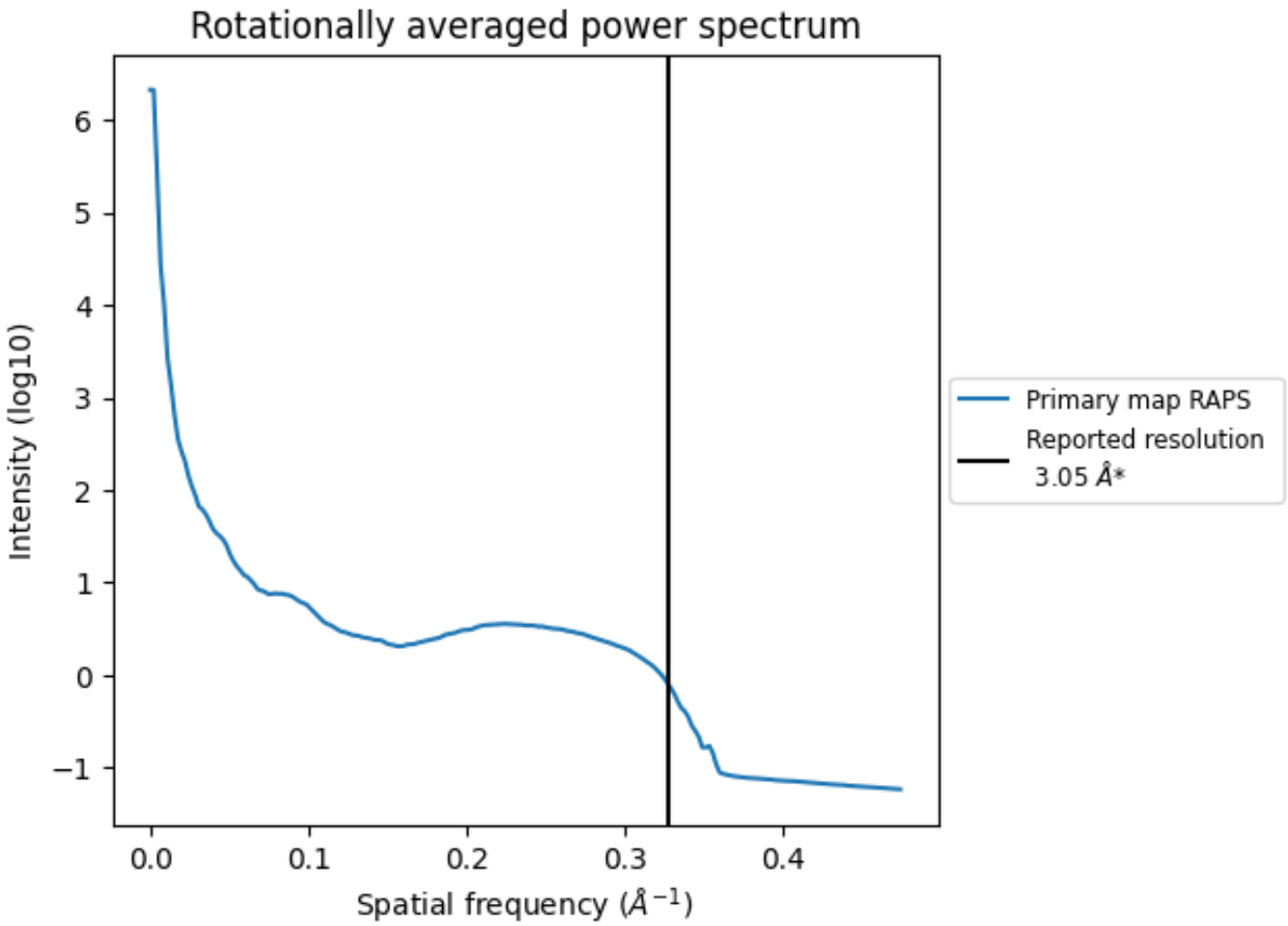
7.2 Volume estimate (i)



The volume at the recommended contour level is 1915 nm^3; this corresponds to an approximate mass of 1730 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 (i)



*Reported resolution corresponds to spatial frequency of 0.328 Å^{-1}

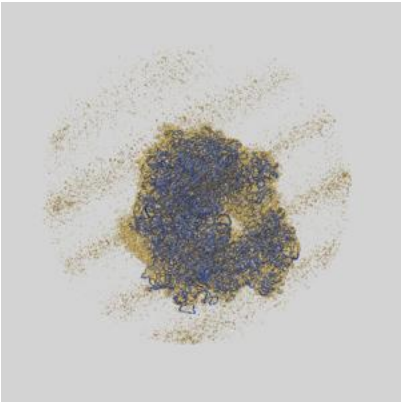
8 Fourier-Shell correlation (i)

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

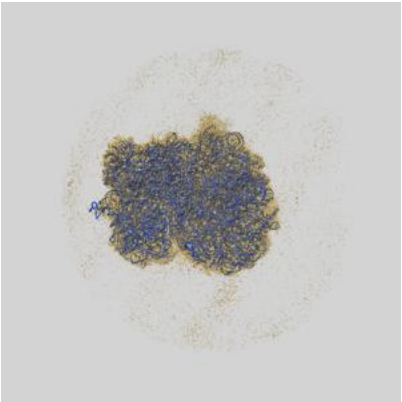
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24235 and PDB model 7N8B. Per-residue inclusion information can be found in section 3 on page 21.

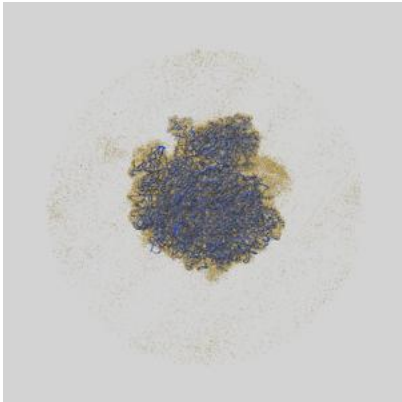
9.1 Map-model overlay (i)



X



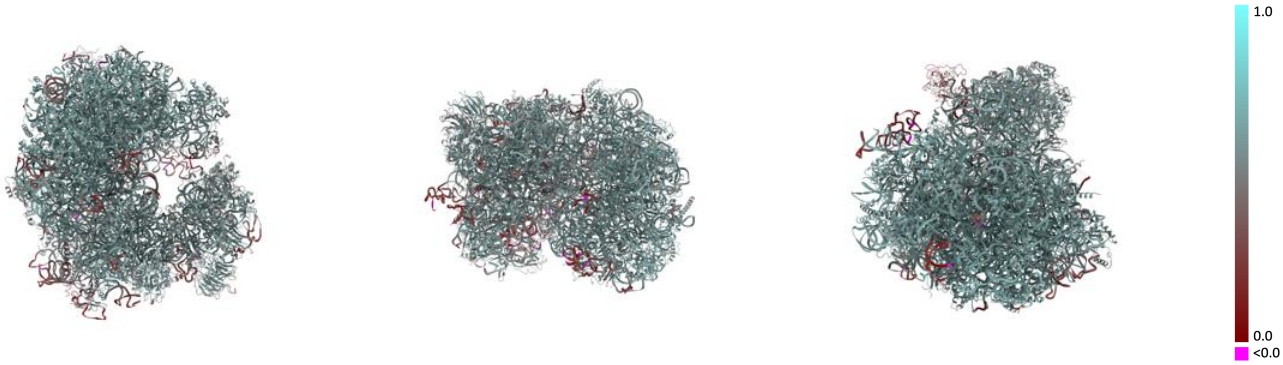
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

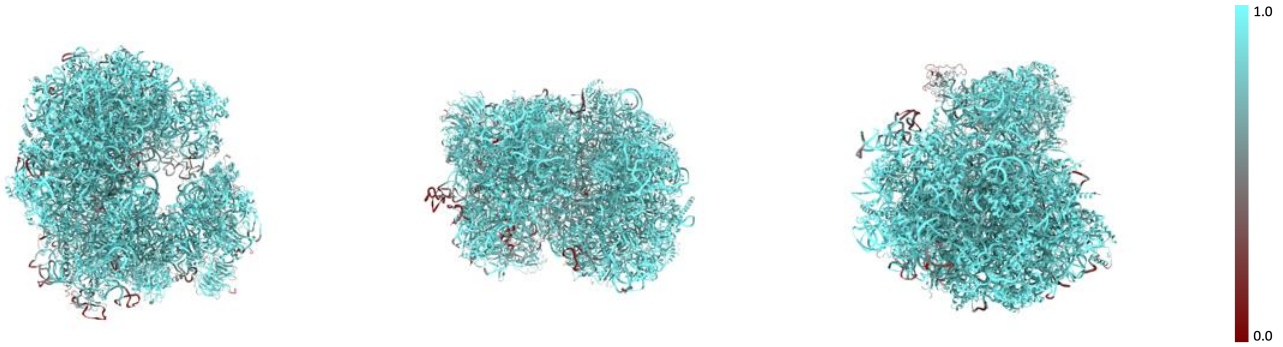
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

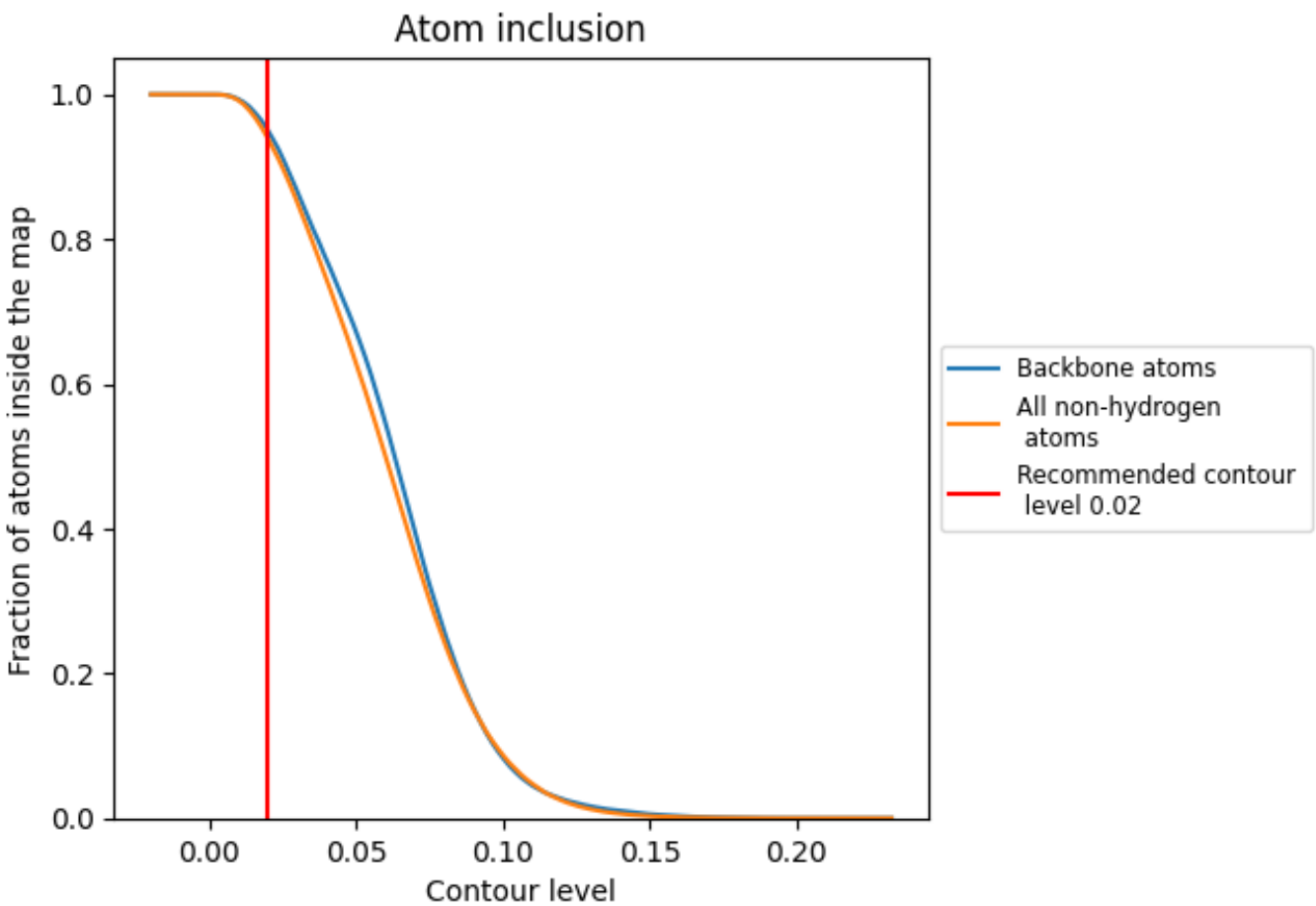
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9398	0.5700
A1	0.9630	0.5830
A3	0.9938	0.5940
A4	0.9881	0.6100
AA	0.9818	0.6150
AB	0.9800	0.6200
AC	0.9751	0.6080
AD	0.9271	0.5640
AE	0.9596	0.6000
AF	0.9690	0.6050
AG	0.9434	0.5870
AH	0.9595	0.5970
AI	0.9475	0.5810
AJ	0.8730	0.5080
AL	0.9537	0.6060
AM	0.9708	0.6100
AN	0.9902	0.6270
AO	0.9769	0.6120
AP	0.9754	0.6210
AQ	0.9828	0.6200
AR	0.8829	0.5390
AS	0.9729	0.6120
AT	0.9685	0.5970
AU	0.9450	0.5640
AV	0.9735	0.6090
AW	0.9960	0.6260
AX	0.9683	0.6080
AY	0.9648	0.6120
AZ	0.9636	0.5910
Aa	0.9641	0.6110
Ab	0.9469	0.5820
Ac	0.9549	0.5880
Ad	0.9294	0.6100
Ae	0.9799	0.6220
Af	0.9939	0.6330

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Chain	Atom inclusion	Q-score
Ag	0.9577	0.5980
Ah	0.9735	0.6150
Ai	0.9329	0.5620
Aj	0.9802	0.6190
Ak	0.9299	0.5730
Al	0.9807	0.6250
Am	0.9404	0.5890
An	0.8868	0.4910
Ao	0.9469	0.5910
Ap	0.9686	0.5960
B5	0.9188	0.5340
BA	0.9460	0.5750
BB	0.9166	0.5570
BC	0.9596	0.5870
BD	0.9041	0.5250
BE	0.9538	0.5950
BF	0.9147	0.5450
BG	0.9213	0.5630
BH	0.8099	0.5110
BI	0.9429	0.5740
BJ	0.9279	0.5730
BK	0.8263	0.4820
BL	0.8714	0.5500
BM	0.3915	0.2640
BN	0.9489	0.5790
BO	0.9221	0.5500
BP	0.8377	0.5160
BQ	0.9481	0.5790
BR	0.8427	0.5110
BS	0.8925	0.5350
BT	0.9323	0.5630
BU	0.8131	0.5050
BV	0.9428	0.5860
BW	0.9729	0.6070
BX	0.9689	0.5950
BY	0.9135	0.5750
BZ	0.8782	0.5410
Ba	0.9378	0.5700
Bb	0.9186	0.5710
Bc	0.8658	0.5190
Bd	0.9787	0.5790
Be	0.9085	0.5480

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Chain	Atom inclusion	Q-score
Bf	0.4527	0.2350
Bg	0.8663	0.5390
Bh	0.5366	0.3250