



Full wwPDB EM Validation Report ⓘ

Dec 2, 2024 – 02:29 PM EST

PDB ID : 8T3E
EMDB ID : EMD-41001
Title : Hypomethylated yeast 80S bound with Taura syndrome virus (TSV) internal ribosome entry site (IRES), eEF2, GDP, and sordarin, Structure IV
Authors : Zhao, Y.; Li, H.
Deposited on : 2023-06-07
Resolution : 3.04 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

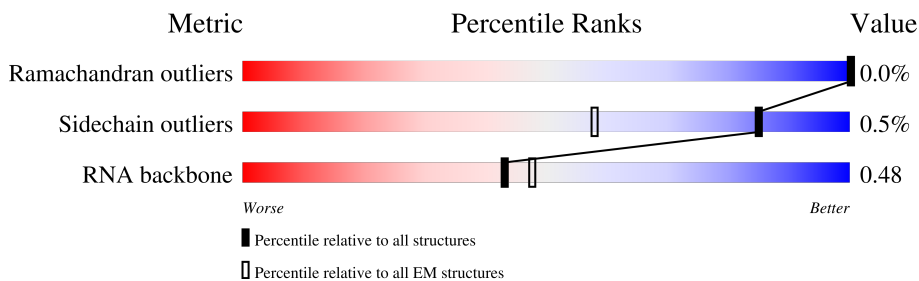
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 3.04 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.



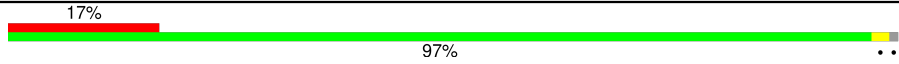
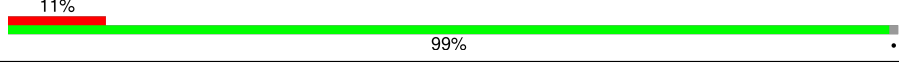
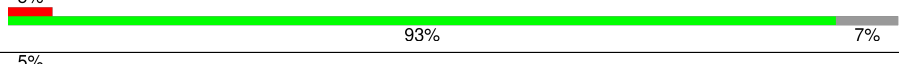
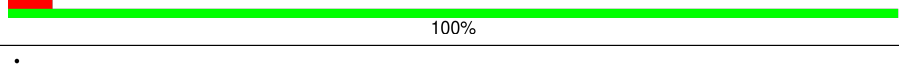
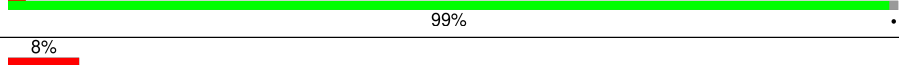
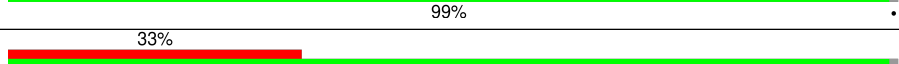
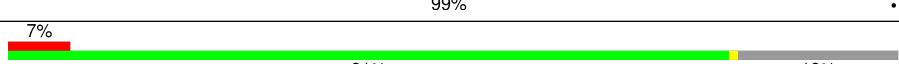
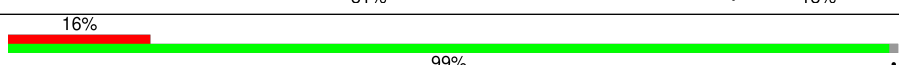
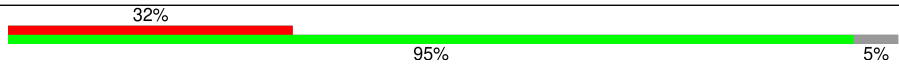
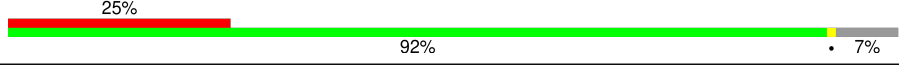
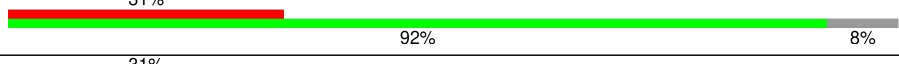
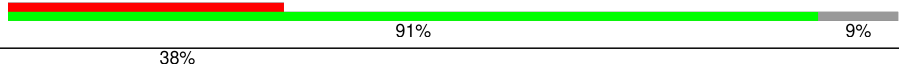
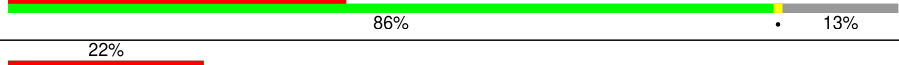
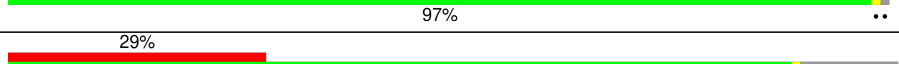
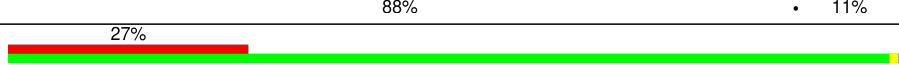
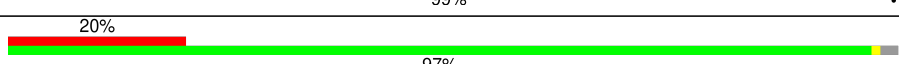


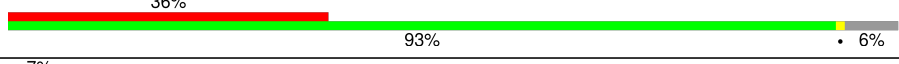
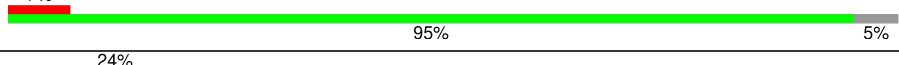
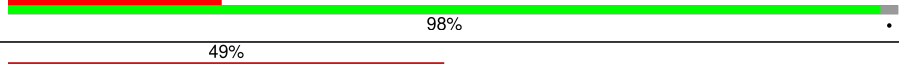




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	BA	252	
2	BB	255	
3	BC	254	
4	BE	261	
5	BG	236	
6	BH	190	
7	BI	200	
8	BJ	197	

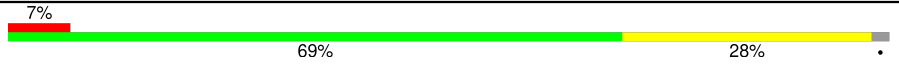
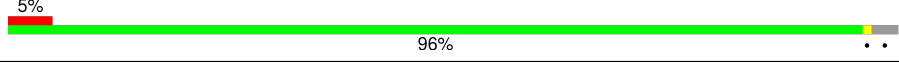
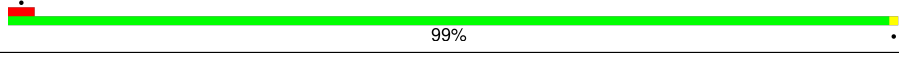
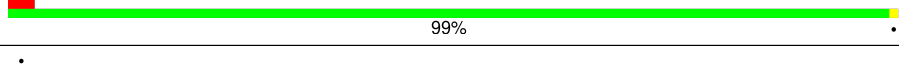

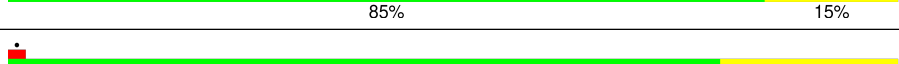
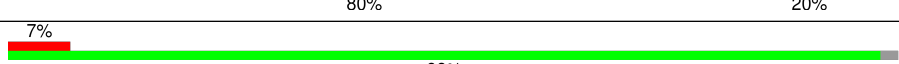
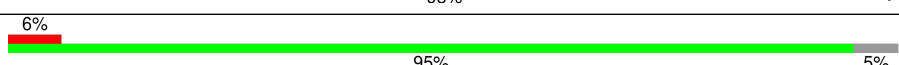
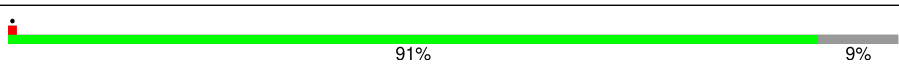

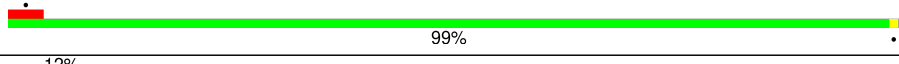
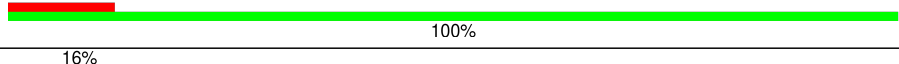
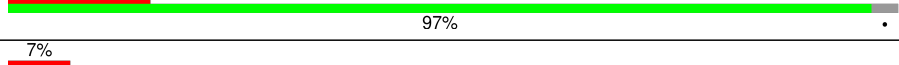
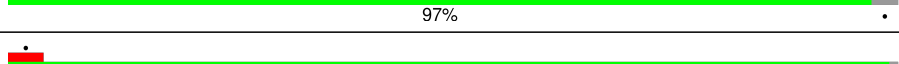
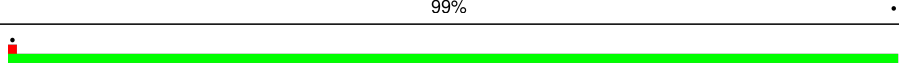
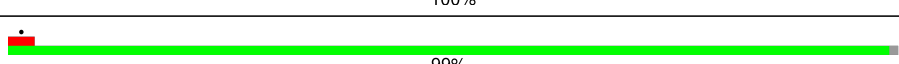
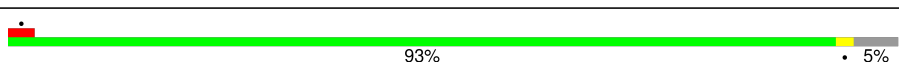
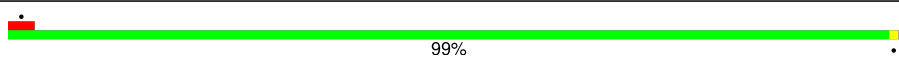
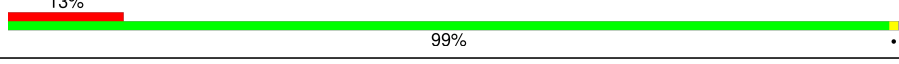
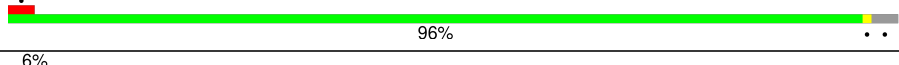
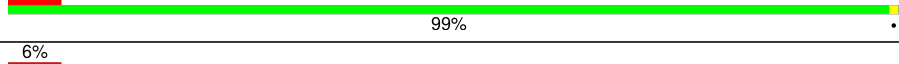

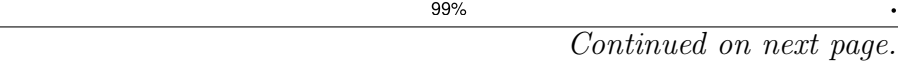


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Mol	Chain	Length	Quality of chain
9	BL	156	
10	BN	151	
11	BO	137	
12	BV	87	
13	BW	130	
14	BX	145	
15	BY	135	
16	Ba	119	
17	Bb	82	
18	Be	63	
19	BD	240	
20	BF	225	
21	BK	105	
22	BP	142	
23	BQ	143	
24	BR	136	
25	BS	146	
26	BT	144	
27	BU	121	
28	BZ	108	
29	Bc	67	
30	Bd	56	
31	Bg	319	
32	Bf	152	
33	BM	143	

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Mol	Chain	Length	Quality of chain
34	B5	1798	 7% 69% 28%
35	AA	254	 5% 96%
36	AB	387	 99%
37	AC	362	 99%
38	A1	3394	 73% 22% 5%
39	A3	121	 85% 15%
40	A4	158	 80% 20%
41	AD	297	 7% 98%
42	AE	176	 6% 95% 5%
43	AF	244	 91% 9%
44	AG	256	 5% 89% 10%
45	AH	191	 99%
46	AI	222	 12% 100%
47	AJ	174	 16% 97%
48	AL	199	 7% 97%
49	AM	138	 99%
50	AN	204	 100%
51	AO	199	 99%
52	AP	184	 93% 5%
53	AQ	186	 99%
54	AR	189	 13% 99%
55	AS	178	 96%
56	AT	160	 6% 99%
57	AU	121	 6% 83% 17%
58	AV	137	 11% 99%

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Mol	Chain	Length	Quality of chain
59	AW	155	
60	AX	142	
61	AY	127	
62	AZ	136	
63	Aa	149	
64	Ab	59	
65	Ac	105	
66	Ad	113	
67	Ae	130	
68	Af	107	
69	Ag	121	
70	Ah	120	
71	Ai	100	
72	Aj	88	
73	Ak	78	
74	Al	51	
75	Am	128	
76	An	25	
77	Ao	106	
78	Ap	92	
79	E	217	
80	DC	842	
81	EC	202	

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
85	SO1	DC	903	X	-	-	-

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 210978 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 2 is a protein called RPS1A isoform 1.

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

- Molecule 3 is a protein called RPS2 isoform 1.

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

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 5 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 6 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 7 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 8 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 9 is a protein called 40S ribosomal protein S11-A.

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

- Molecule 10 is a protein called 40S ribosomal protein S13.

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

- Molecule 11 is a protein called 40S ribosomal protein S14-A.

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

- Molecule 12 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 13 is a protein called RPS22A isoform 1.

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

- Molecule 14 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 15 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 16 is a protein called RPS26B isoform 1.

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

- Molecule 17 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 18 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 19 is a protein called RPS3 isoform 1.

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

- Molecule 20 is a protein called Rps5p.

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

- Molecule 21 is a protein called 40S ribosomal protein S10-A.

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

- Molecule 22 is a protein called RPS15 isoform 1.

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

- Molecule 23 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 24 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BR	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 25 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 26 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 27 is a protein called RPS20 isoform 1.

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

- Molecule 28 is a protein called RPS25A isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BZ	71	Total	C	N	O	0	0
			574	366	108	100		

- Molecule 29 is a protein called RPS28A isoform 1.

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

- Molecule 30 is a protein called RPS29A isoform 1.

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

- Molecule 31 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bf	75	Total	C	N	O	S	0	0
			605	386	116	99	4		

- Molecule 33 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BM	124	Total	C	N	O	S	0	0
			935	587	165	181	2		

- Molecule 34 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B5	1757	Total	C	N	O	P	1	0
			37463	16754	6635	12317	1757		

- Molecule 35 is a protein called 60S ribosomal protein L2-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AB	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 37 is a protein called RPL4A isoform 1.

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

- Molecule 38 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A1	3216	Total	C	N	O	P	0	0
			68786	30729	12387	22454	3216		

- Molecule 39 is a RNA chain called 5s rRNA.

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

- Molecule 40 is a RNA chain called 5.8 S rRNA.

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

- Molecule 41 is a protein called RPL5 isoform 1.

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

- Molecule 42 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	AE	167	1303	840	234	228	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	120	LYS	ASN	conflict	UNP Q02326

- Molecule 43 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 45 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 46 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	AI	222	1804	1147	339	310	8	0	0

- Molecule 47 is a protein called RPL11A isoform 1.

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

- Molecule 48 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 49 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 50 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 51 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 52 is a protein called 60S ribosomal protein L17-A.

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

- Molecule 53 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 54 is a protein called 60S ribosomal protein L19-A.

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

- Molecule 55 is a protein called 60S ribosomal protein L20.

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

- Molecule 56 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 57 is a protein called 60S ribosomal protein L22-A.

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

- Molecule 58 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 59 is a protein called RPL24A isoform 1.

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

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

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

- Molecule 61 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 62 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 63 is a protein called 60S ribosomal protein L28.

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

- Molecule 64 is a protein called RPL29 isoform 1.

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

- Molecule 65 is a protein called 60S ribosomal protein L30.

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

- Molecule 66 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 67 is a protein called RPL32 isoform 1.

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

- Molecule 68 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 69 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 70 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 71 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 72 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 73 is a protein called RPL38 isoform 1.

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

- Molecule 74 is a protein called 60S ribosomal protein L39.

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

- Molecule 75 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 76 is a protein called 60S ribosomal protein L41-A.

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

- Molecule 77 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 78 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 79 is a protein called RPL1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	E	217	1718	1097	299	312	10	0	0

- Molecule 80 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	DC	824	6419	4085	1096	1208	30	0	0

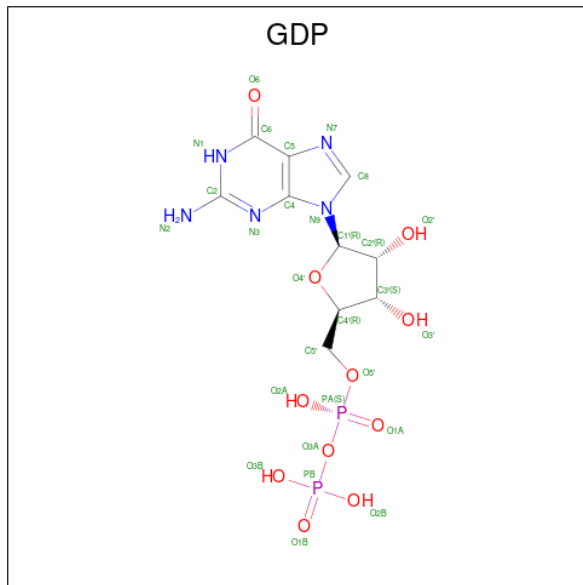
- Molecule 81 is a RNA chain called TSV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
81	EC	131	2764	1234	489	910	131	0	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

- Molecule 83 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

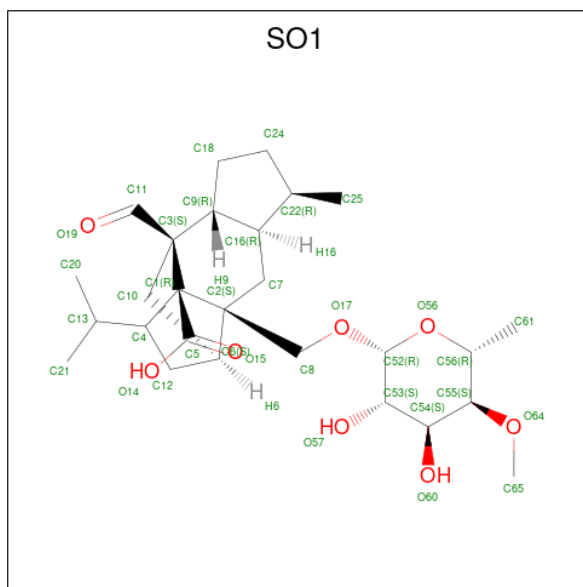


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
83	DC	1	28	10	5	11	2	0

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
84	DC	1	1	1	0

- Molecule 85 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.BETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (three-letter code: SO1) (formula: C₂₇H₄₂O₈).

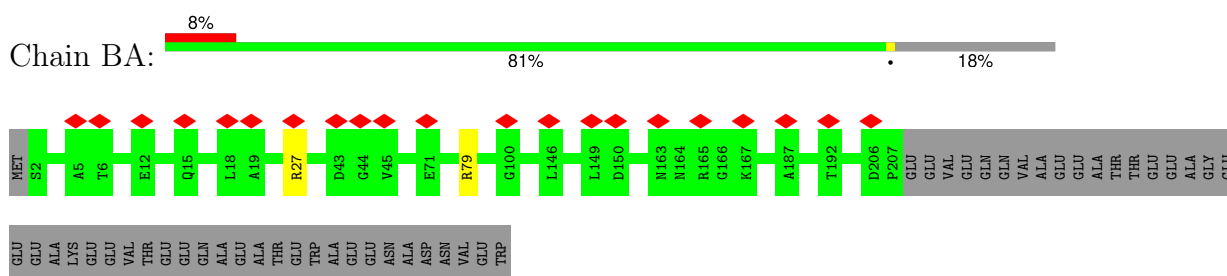


Mol	Chain	Residues	Atoms			AltConf
85	DC	1	Total	C	O	0
			35	27	8	

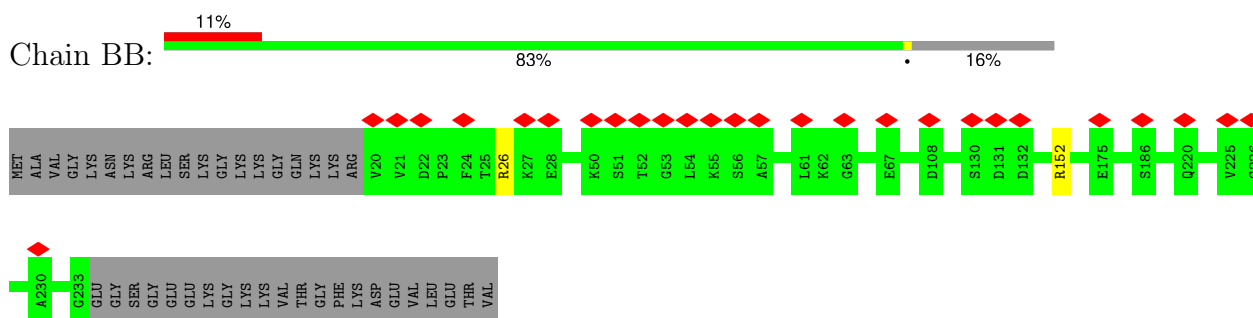
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

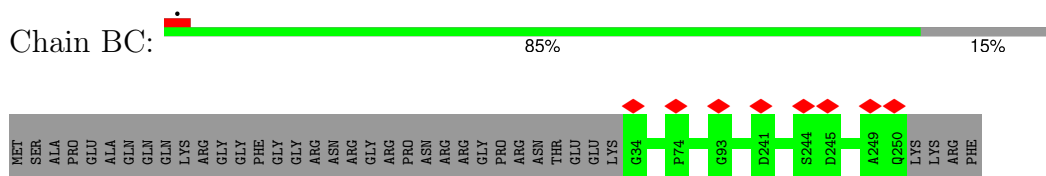
- Molecule 1: 40S ribosomal protein S0-A



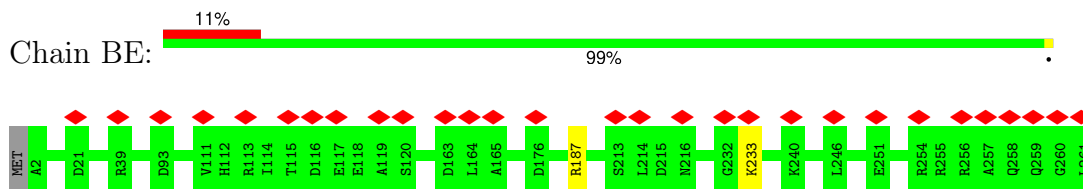
- Molecule 2: RPS1A isoform 1



- Molecule 3: RPS2 isoform 1

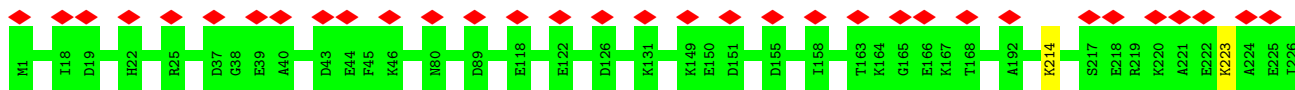


- Molecule 4: 40S ribosomal protein S4-A



- Molecule 5: 40S ribosomal protein S6-A

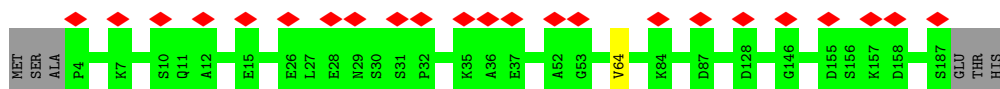
Chain BG: 



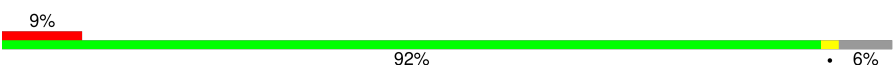
ARG
LYS
ARG
ARG
ALA
SER
SER
LEU
LYS
ALA

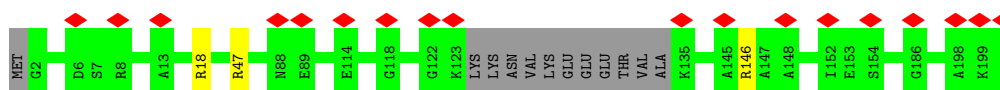
- Molecule 6: 40S ribosomal protein S7-A

Chain BH: 



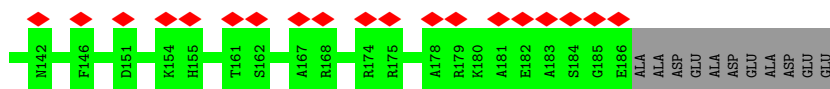
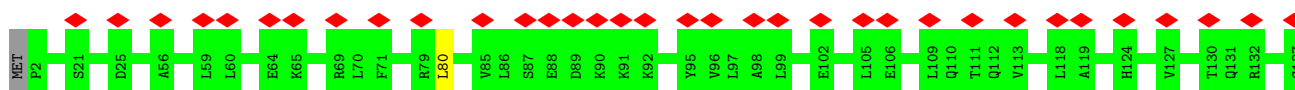
- Molecule 7: 40S ribosomal protein S8-A

Chain BI: 



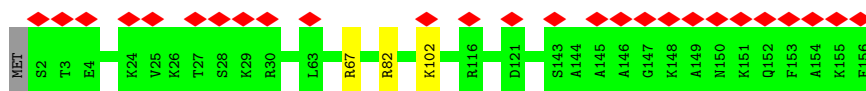
- Molecule 8: 40S ribosomal protein S9-A

Chain BJ: 



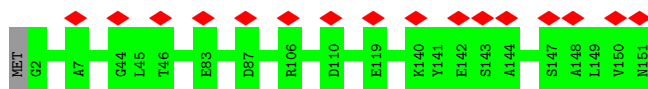
- Molecule 9: 40S ribosomal protein S11-A

Chain BL: 

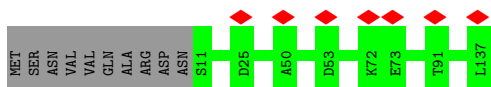


- Molecule 10: 40S ribosomal protein S13

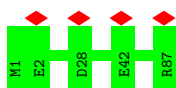
Chain BN: 



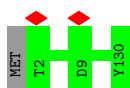
- Molecule 11: 40S ribosomal protein S14-A



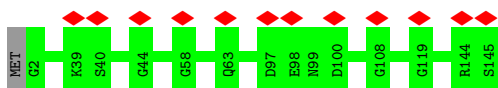
- Molecule 12: 40S ribosomal protein S21-A



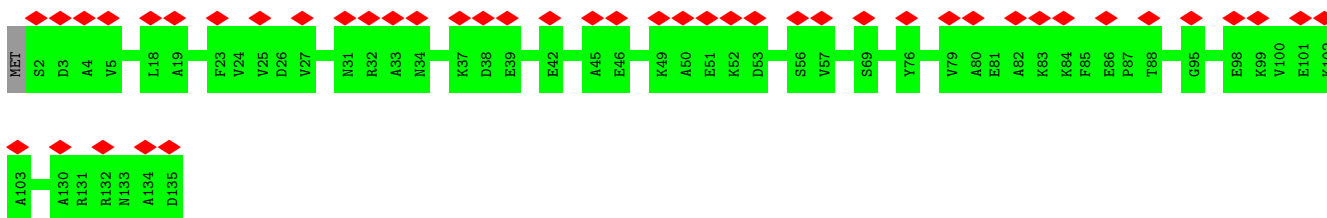
- Molecule 13: RPS22A isoform 1



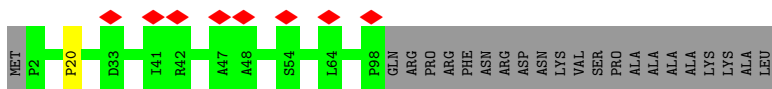
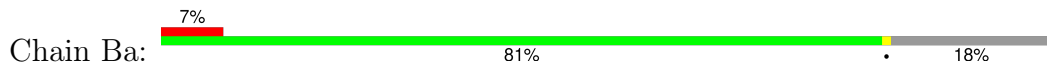
- Molecule 14: 40S ribosomal protein S23-A



- Molecule 15: 40S ribosomal protein S24-A

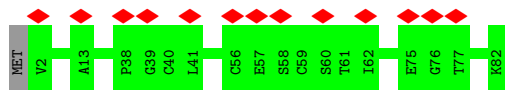


- Molecule 16: RPS26B isoform 1

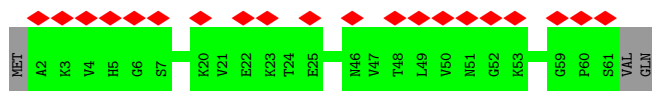


- Molecule 17: 40S ribosomal protein S27-A

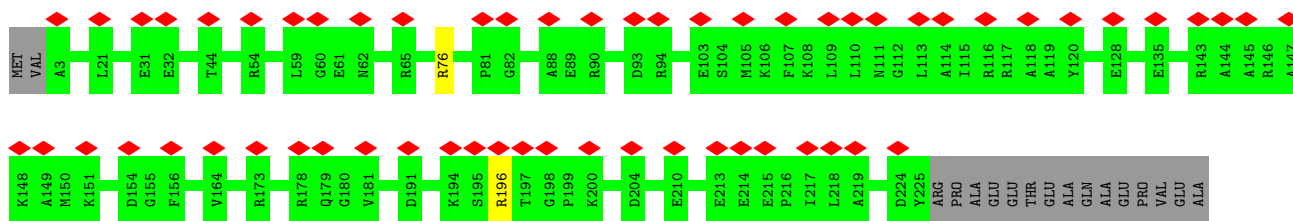




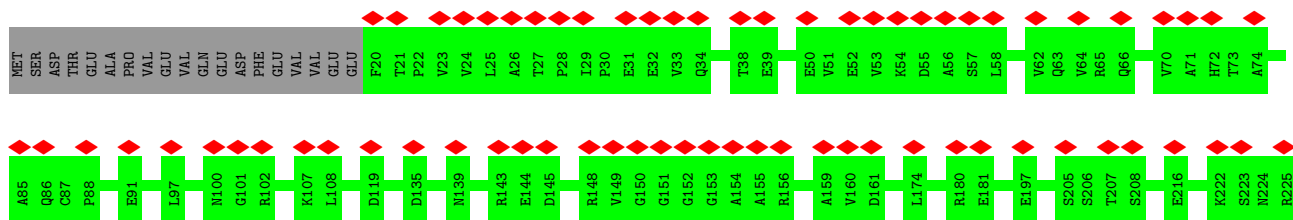
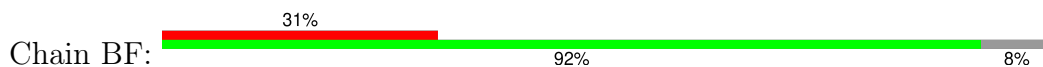
- Molecule 18: 40S ribosomal protein S30-A



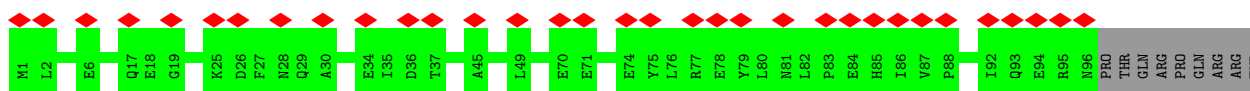
- Molecule 19: RPS3 isoform 1



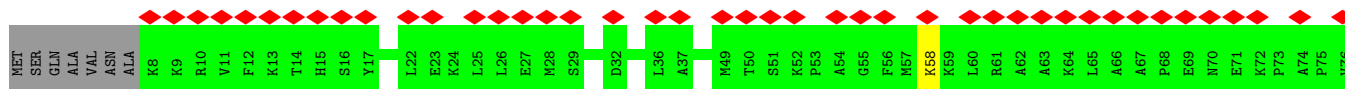
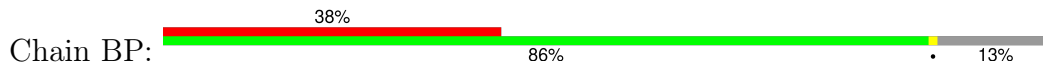
- Molecule 20: Rps5p

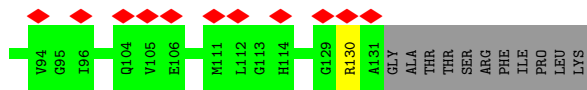


- Molecule 21: 40S ribosomal protein S10-A

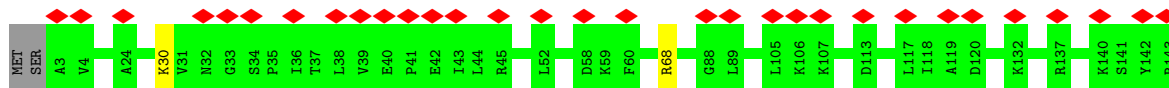


- Molecule 22: RPS15 isoform 1

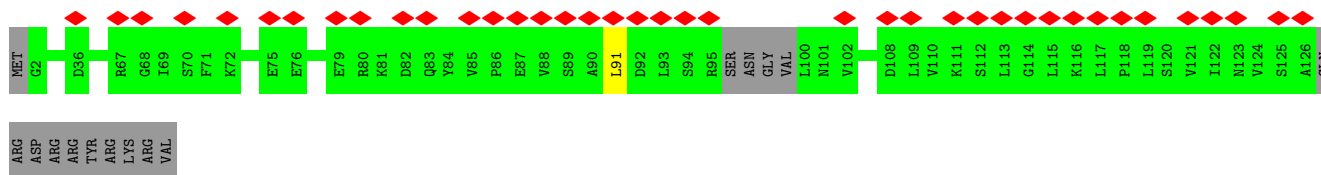
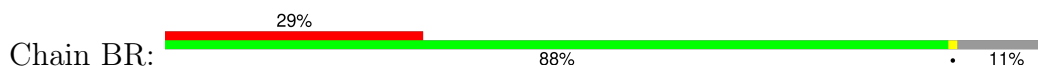




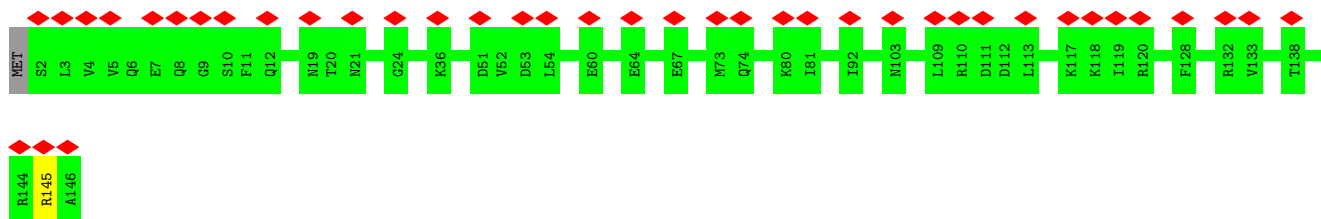
• Molecule 23: 40S ribosomal protein S16-A



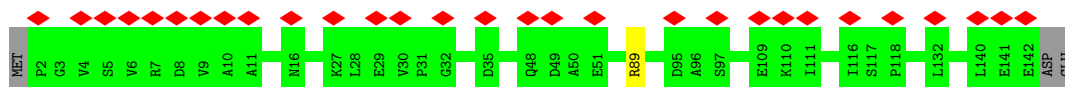
• Molecule 24: 40S ribosomal protein S17-A



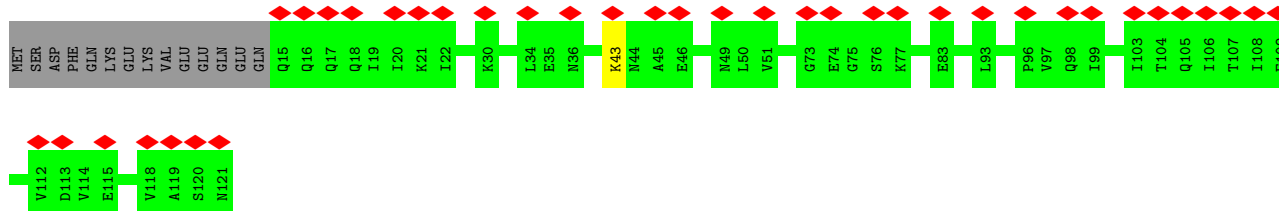
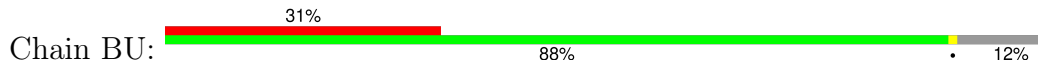
• Molecule 25: 40S ribosomal protein S18-A



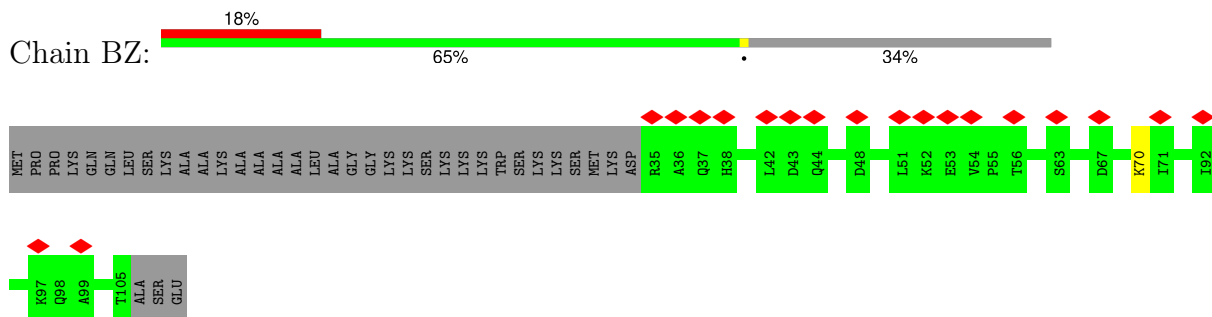
• Molecule 26: 40S ribosomal protein S19-A



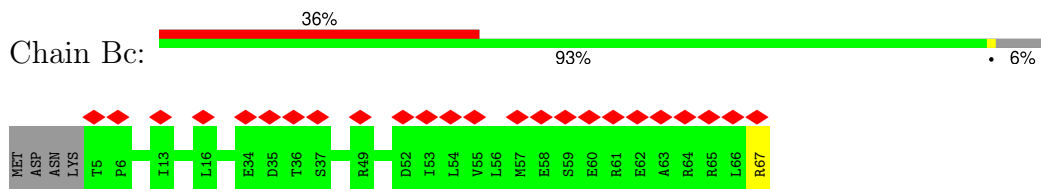
• Molecule 27: RPS20 isoform 1



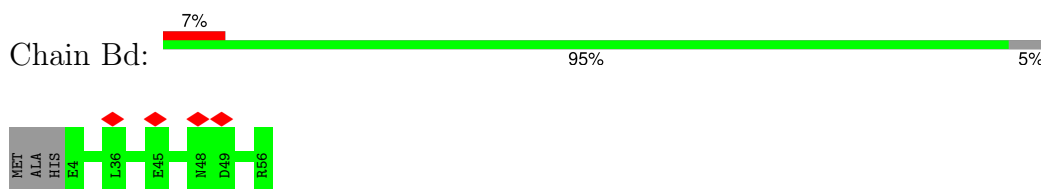
• Molecule 28: RPS25A isoform 1



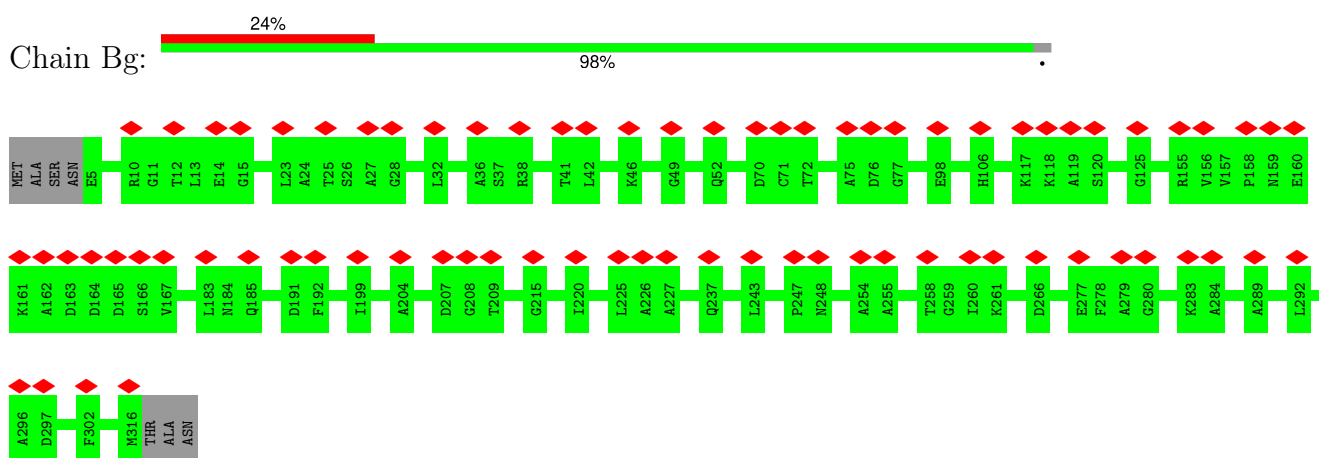
• Molecule 29: RPS28A isoform 1



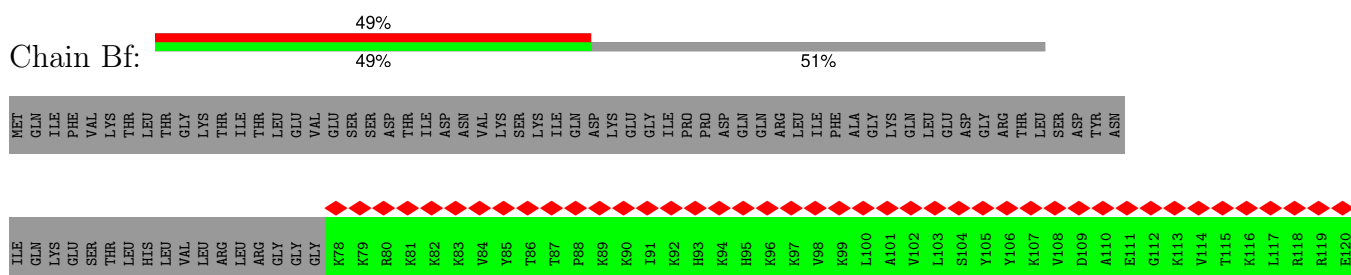
• Molecule 30: RPS29A isoform 1

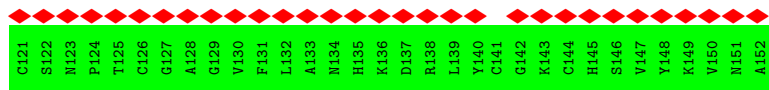


• Molecule 31: Guanine nucleotide-binding protein subunit beta-like protein

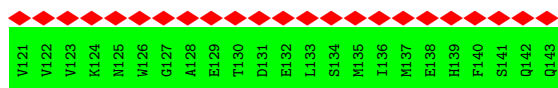
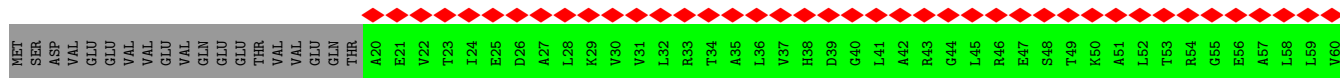
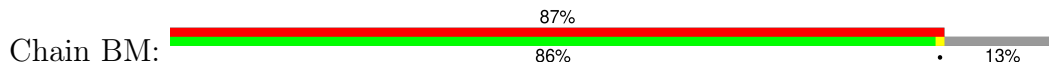


• Molecule 32: Ubiquitin-40S ribosomal protein S31

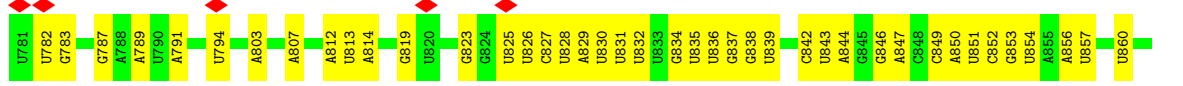
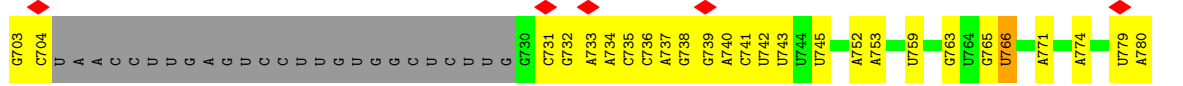
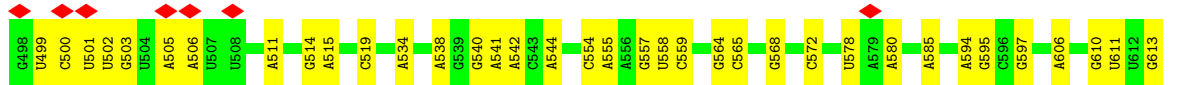


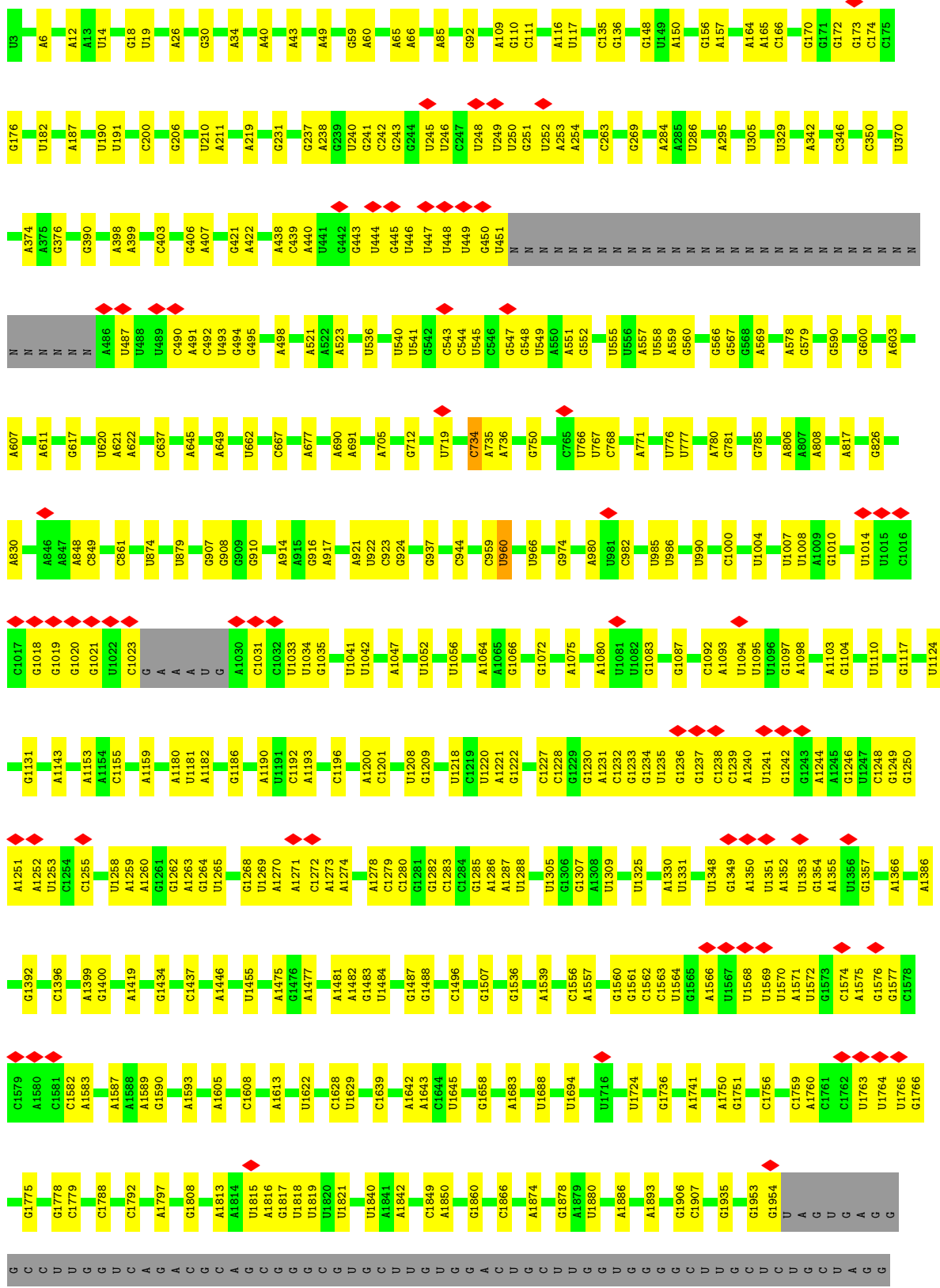


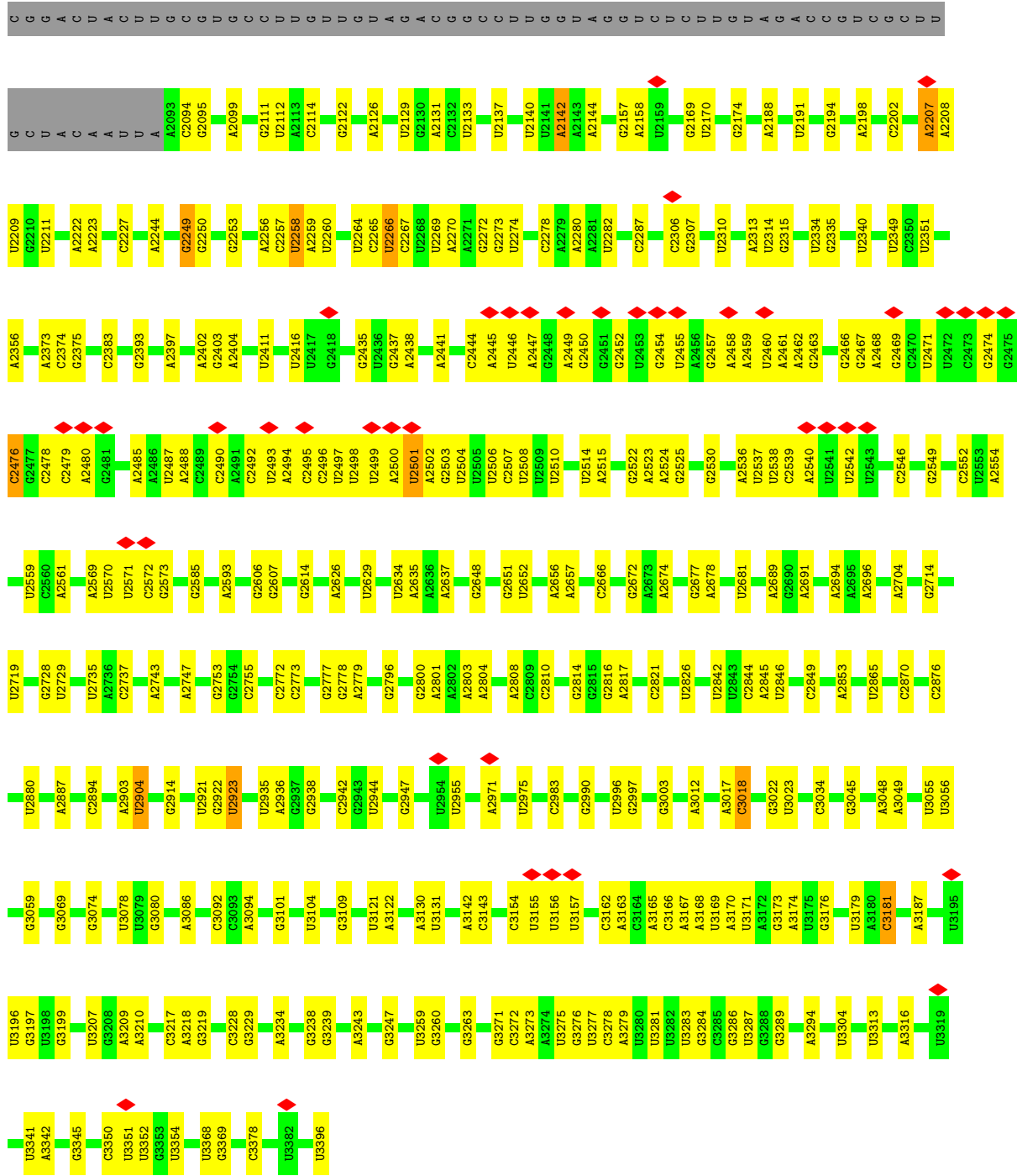
• Molecule 33: 40S ribosomal protein S12



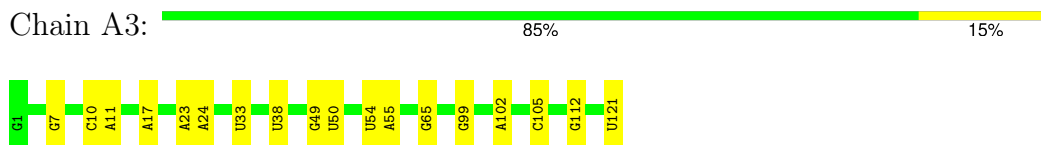
• Molecule 34: 18S rRNA



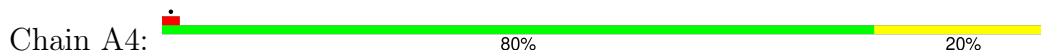


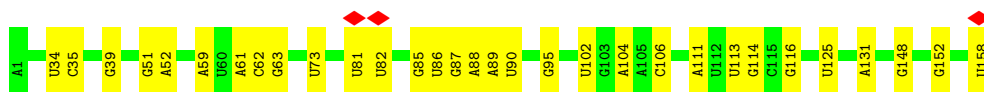


• Molecule 39: 5s rRNA

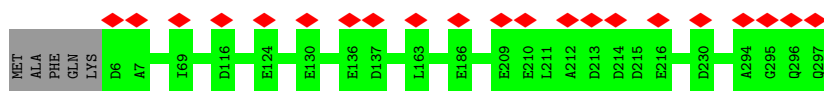


• Molecule 40: 5.8 S rRNA

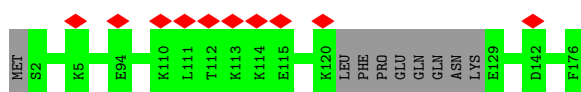




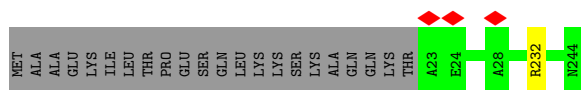
- Molecule 41: RPL5 isoform 1



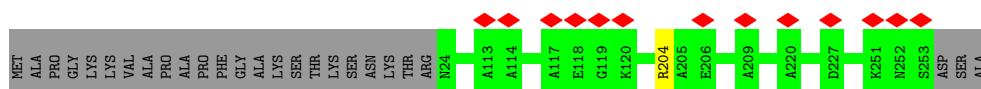
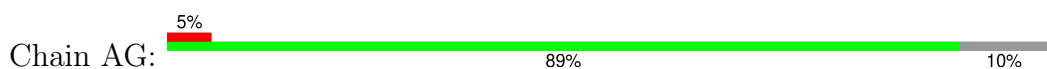
- Molecule 42: 60S ribosomal protein L6-A



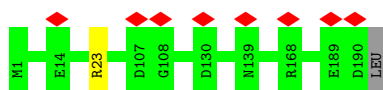
- Molecule 43: 60S ribosomal protein L7-A



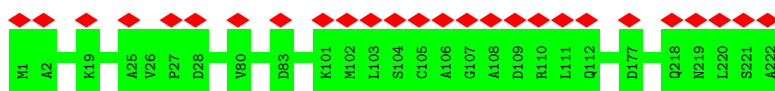
- Molecule 44: 60S ribosomal protein L8-A



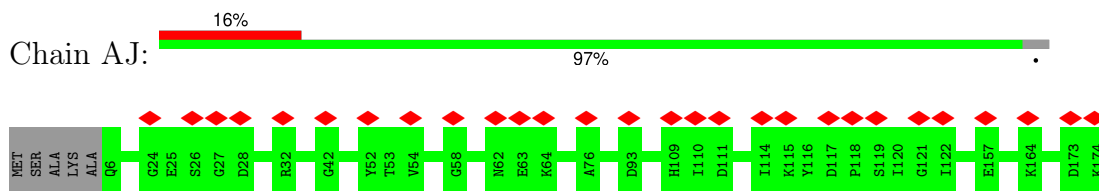
- Molecule 45: 60S ribosomal protein L9-A



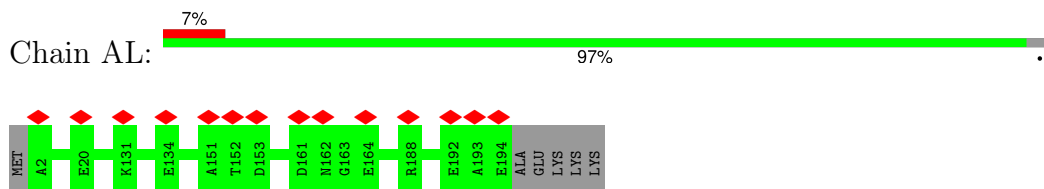
- Molecule 46: 60S ribosomal protein L10



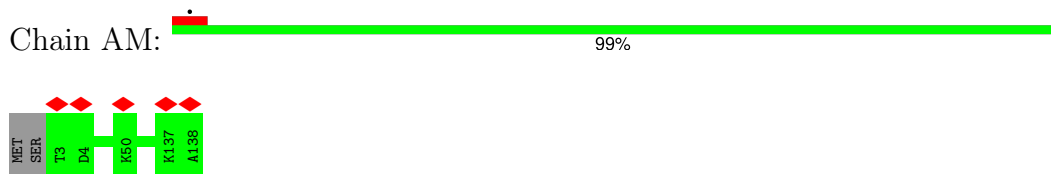
- Molecule 47: RPL11A isoform 1



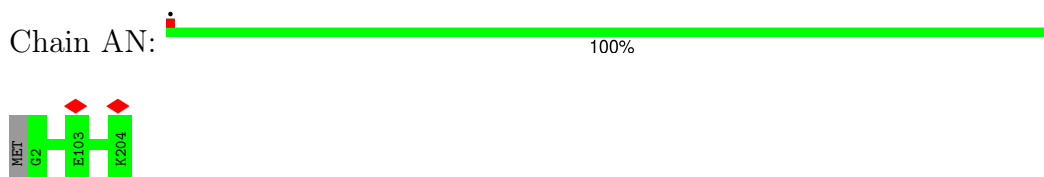
- Molecule 48: 60S ribosomal protein L13-A



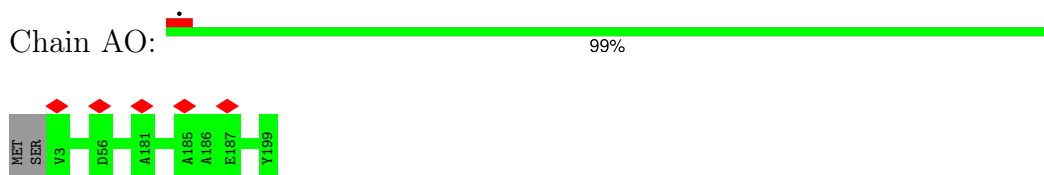
- Molecule 49: 60S ribosomal protein L14-A



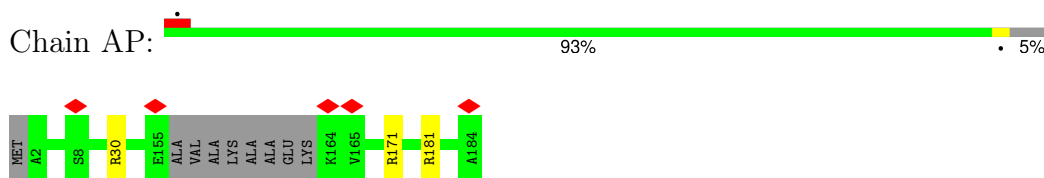
- Molecule 50: 60S ribosomal protein L15-A



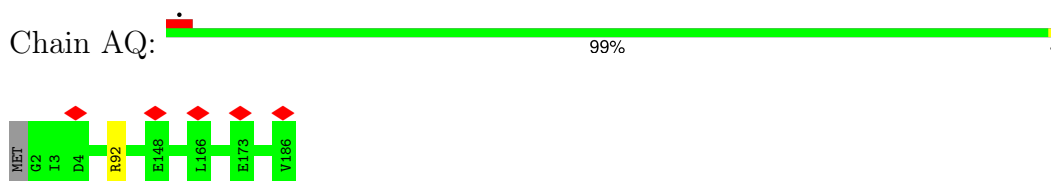
- Molecule 51: 60S ribosomal protein L16-A



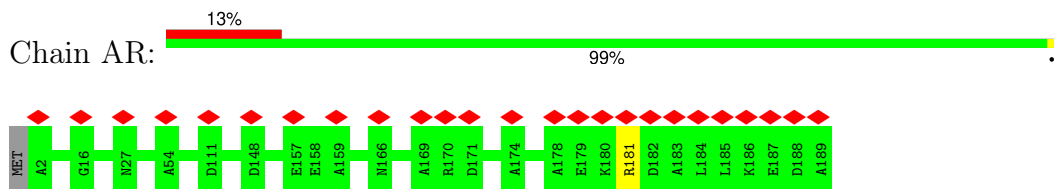
- Molecule 52: 60S ribosomal protein L17-A



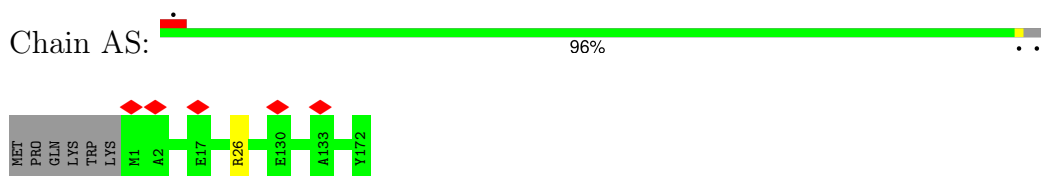
- Molecule 53: 60S ribosomal protein L18-A



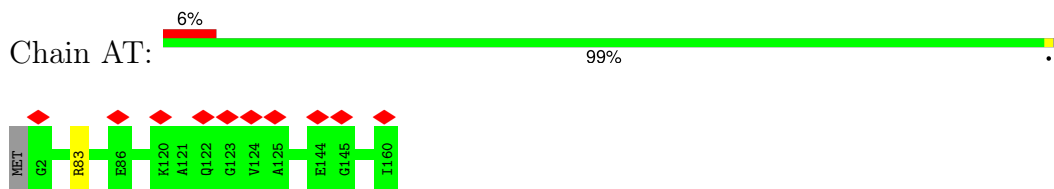
• Molecule 54: 60S ribosomal protein L19-A



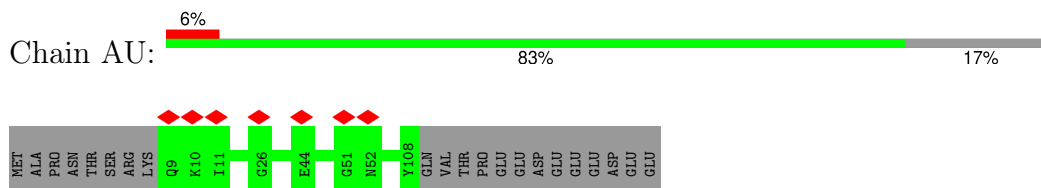
• Molecule 55: 60S ribosomal protein L20



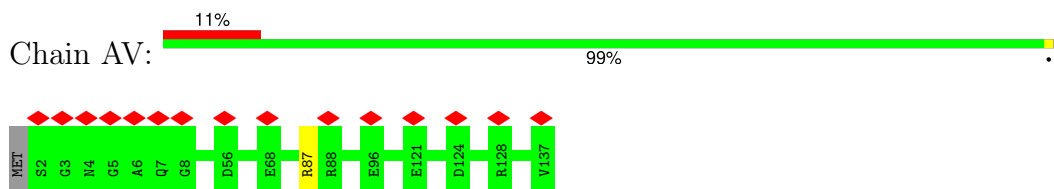
• Molecule 56: 60S ribosomal protein L21-A



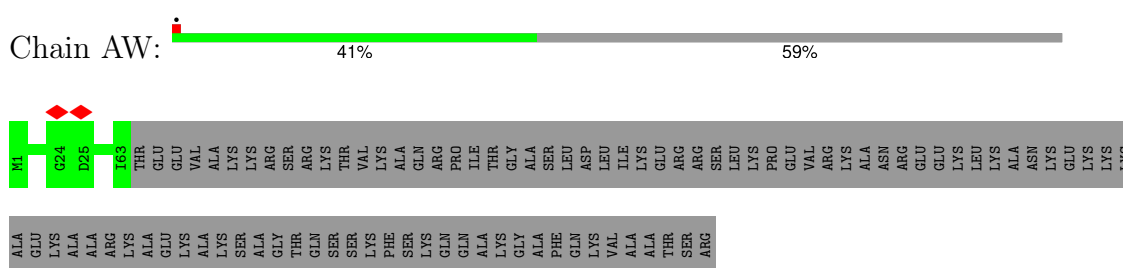
• Molecule 57: 60S ribosomal protein L22-A



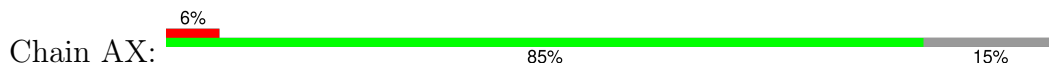
• Molecule 58: 60S ribosomal protein L23-A



• Molecule 59: RPL24A isoform 1



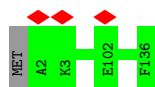
• Molecule 60: 60S ribosomal protein L25



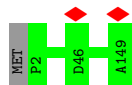
- Molecule 61: 60S ribosomal protein L26-A



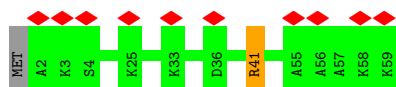
- Molecule 62: 60S ribosomal protein L27-A



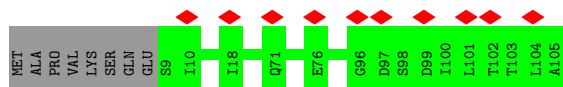
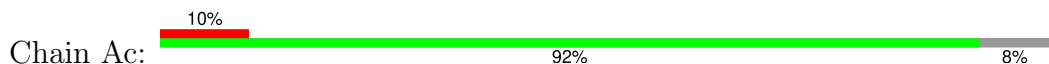
- Molecule 63: 60S ribosomal protein L28



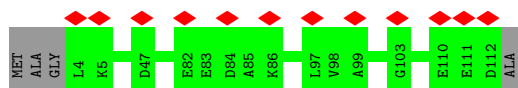
- Molecule 64: RPL29 isoform 1



- Molecule 65: 60S ribosomal protein L30

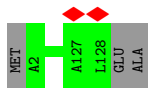


- Molecule 66: 60S ribosomal protein L31-A



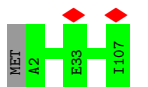
- Molecule 67: RPL32 isoform 1

Chain Ae:  98%



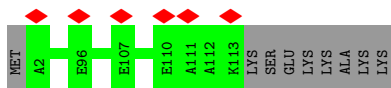
- Molecule 68: 60S ribosomal protein L33-A

Chain Af:  99%



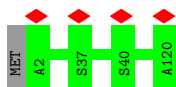
- Molecule 69: 60S ribosomal protein L34-A

Chain Ag:  5% 93% 7%



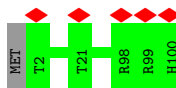
- Molecule 70: 60S ribosomal protein L35-A

Chain Ah:  99%



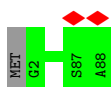
- Molecule 71: 60S ribosomal protein L36-A

Chain Ai:  5% 99%



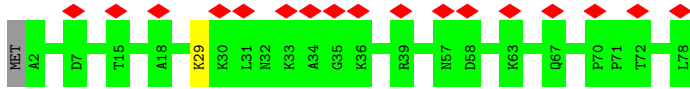
- Molecule 72: 60S ribosomal protein L37-A

Chain Aj:  99%



- Molecule 73: RPL38 isoform 1

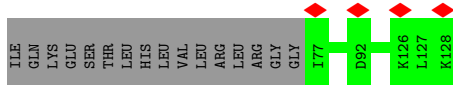
Chain Ak:  22% 97%



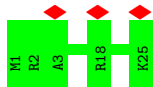
- Molecule 74: 60S ribosomal protein L39



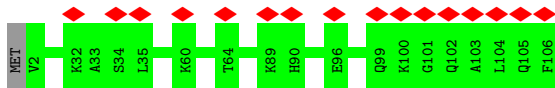
- Molecule 75: Ubiquitin-60S ribosomal protein L40



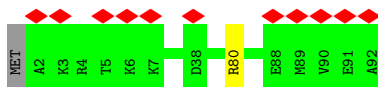
- Molecule 76: 60S ribosomal protein L41-A



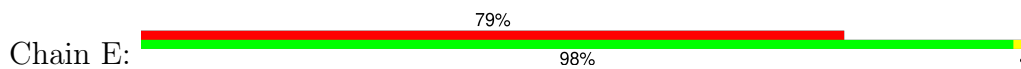
- Molecule 77: 60S ribosomal protein L42-A

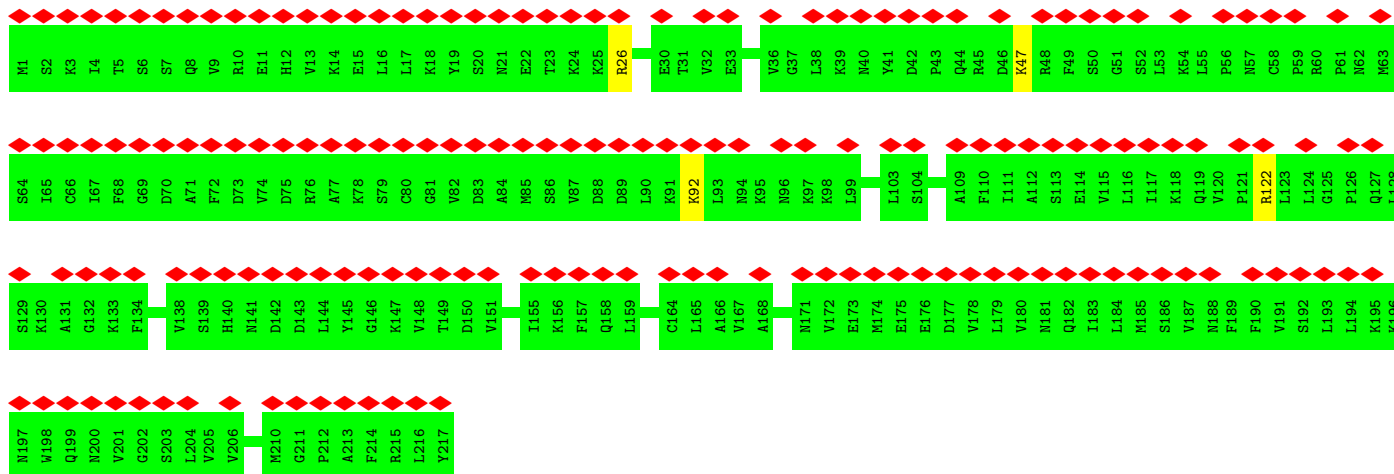


- Molecule 78: 60S ribosomal protein L43-A

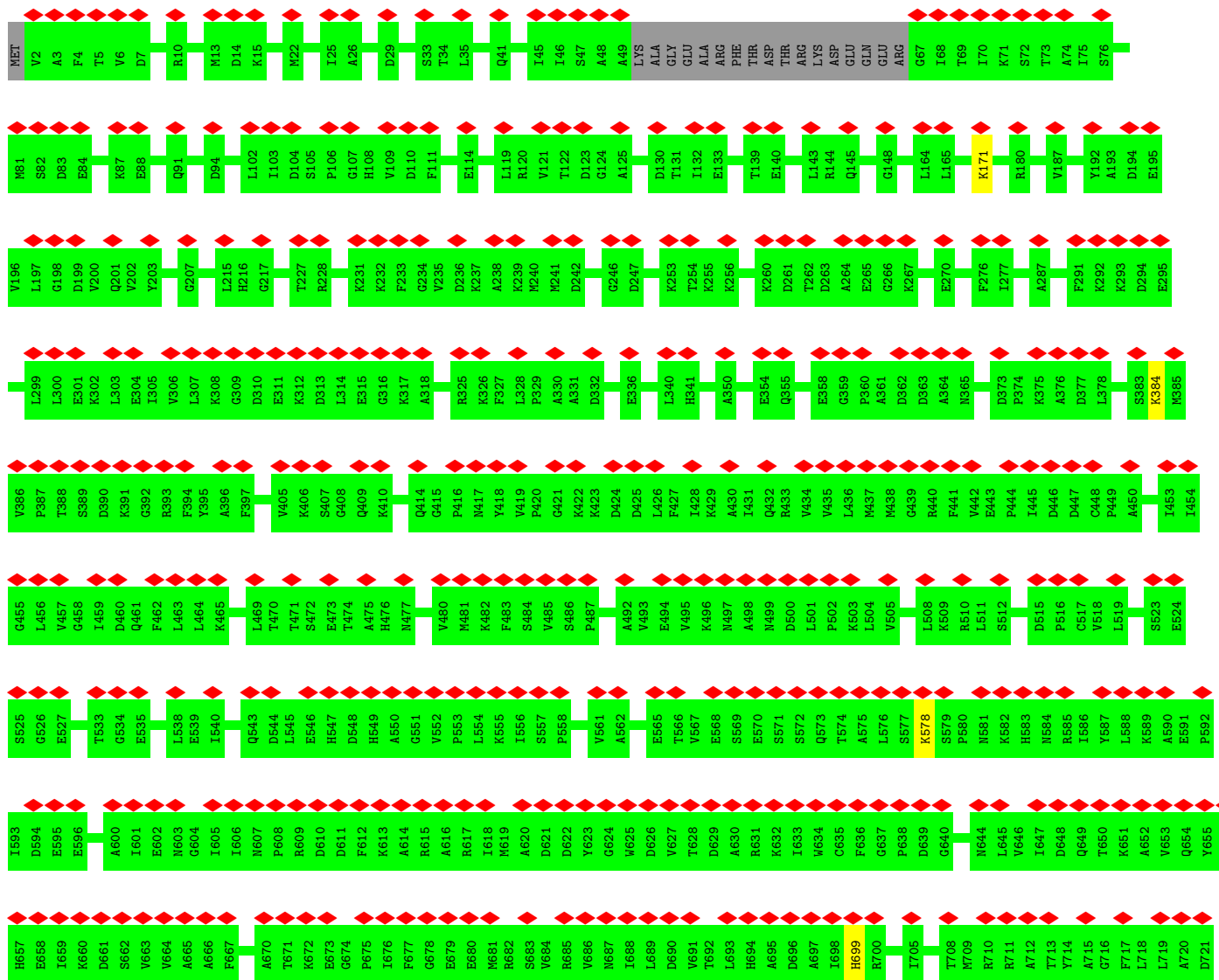


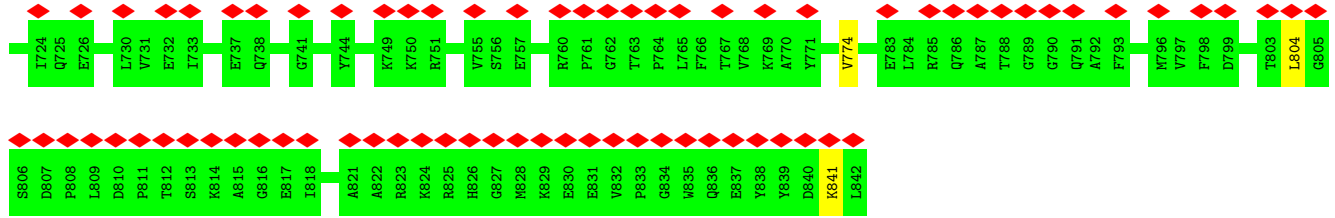
- Molecule 79: RPL1A isoform 1



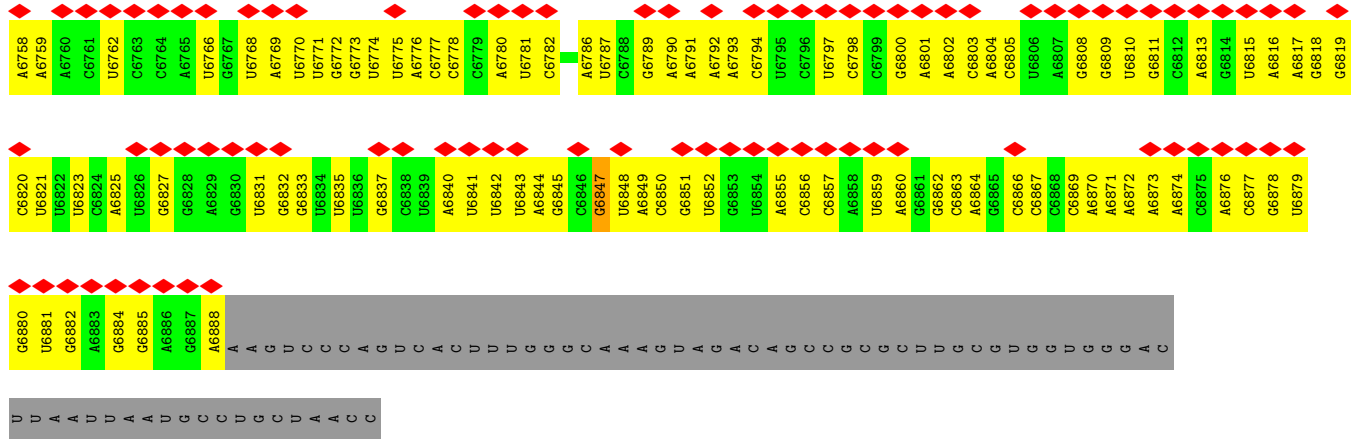
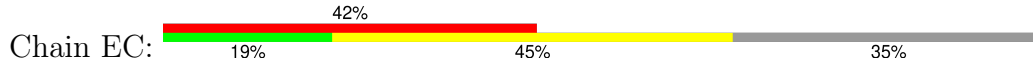


• Molecule 80: Elongation factor 2





• Molecule 81: TSV IRES



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75068	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.167	Depositor
Minimum map value	-1.037	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.104	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: 1MA, OMG, MG, B8N, UR3, GDP, ZN, DDE, HIC, MA6, OMU, G7M, 5MC, 4AC, SO1, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BA	0.35	0/1653	0.61	0/2261
2	BB	0.34	0/1735	0.59	0/2335
3	BC	0.35	0/1665	0.55	0/2263
4	BE	0.34	0/2109	0.61	0/2839
5	BG	0.30	0/1844	0.62	0/2464
6	BH	0.32	0/1506	0.60	0/2028
7	BI	0.36	0/1514	0.62	0/2021
8	BJ	0.34	0/1519	0.68	1/2035 (0.0%)
9	BL	0.37	0/1272	0.58	1/1712 (0.1%)
10	BN	0.37	0/1215	0.58	0/1638
11	BO	0.37	0/952	0.70	0/1279
12	BV	0.31	0/693	0.57	0/935
13	BW	0.40	0/1038	0.58	0/1395
14	BX	0.36	0/1139	0.58	0/1518
15	BY	0.32	0/1087	0.60	0/1449
16	Ba	0.41	0/782	0.79	3/1047 (0.3%)
17	Bb	0.32	0/620	0.60	0/838
18	Be	0.28	0/483	0.61	0/643
19	BD	0.31	0/1759	0.60	0/2368
20	BF	0.30	0/1629	0.58	0/2202
21	BK	0.33	0/837	0.65	0/1131
22	BP	0.29	0/1012	0.60	0/1356
23	BQ	0.30	0/1125	0.57	0/1510
24	BR	0.31	0/957	0.62	1/1283 (0.1%)
25	BS	0.32	0/1211	0.61	0/1628
26	BT	0.28	0/1113	0.55	0/1494
27	BU	0.33	0/865	0.59	0/1169
28	BZ	0.30	0/582	0.60	0/782
29	Bc	0.29	0/499	0.68	0/670
30	Bd	0.33	0/452	0.59	0/600
31	Bg	0.28	0/2454	0.57	0/3340
32	Bf	0.25	0/616	0.48	0/817

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BM	0.25	0/943	0.54	0/1274
34	B5	0.55	0/41450	0.85	18/64582 (0.0%)
35	AA	0.42	0/1912	0.64	2/2569 (0.1%)
36	AB	0.41	0/3139	0.58	0/4219
37	AC	0.38	0/2800	0.55	0/3790
38	A1	0.70	0/76160	0.85	26/118745 (0.0%)
39	A3	0.55	0/2861	0.80	0/4457
40	A4	0.71	0/3724	0.81	0/5798
41	AD	0.33	0/2390	0.54	0/3225
42	AE	0.35	0/1324	0.53	0/1782
43	AF	0.42	0/1821	0.56	0/2451
44	AG	0.37	0/1830	0.54	0/2469
45	AH	0.36	0/1531	0.59	0/2062
46	AI	0.34	0/1843	0.56	0/2471
47	AJ	0.32	0/1374	0.61	0/1842
48	AL	0.37	0/1568	0.59	0/2106
49	AM	0.36	0/1068	0.58	0/1438
50	AN	0.43	0/1757	0.63	0/2354
51	AO	0.40	0/1585	0.58	0/2128
52	AP	0.40	0/1410	0.61	0/1893
53	AQ	0.36	0/1465	0.59	0/1965
54	AR	0.36	0/1538	0.64	0/2050
55	AS	0.44	0/1481	0.63	0/1990
56	AT	0.38	0/1300	0.59	0/1743
57	AU	0.36	0/812	0.54	0/1099
58	AV	0.42	0/1018	0.62	0/1369
59	AW	0.42	0/533	0.65	0/707
60	AX	0.39	0/983	0.54	0/1325
61	AY	0.35	0/1004	0.58	0/1341
62	AZ	0.40	0/1118	0.57	0/1497
63	Aa	0.39	0/1204	0.56	0/1612
64	Ab	0.37	0/473	0.62	1/629 (0.2%)
65	Ac	0.38	0/751	0.52	0/1008
66	Ad	0.37	0/904	0.58	0/1213
67	Ae	0.38	0/1041	0.55	0/1394
68	Af	0.44	0/868	0.58	0/1168
69	Ag	0.40	0/890	0.61	0/1189
70	Ah	0.33	0/978	0.57	0/1301
71	Ai	0.33	0/778	0.62	0/1034
72	Aj	0.43	0/696	0.62	0/923
73	Ak	0.35	0/618	0.70	0/826
74	Al	0.39	0/443	0.70	0/588
75	Am	0.34	0/423	0.60	0/562

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	An	0.41	0/234	0.85	0/300
77	Ao	0.33	0/859	0.57	0/1133
78	Ap	0.40	0/701	0.65	0/934
79	E	0.28	0/1745	0.54	0/2342
80	DC	0.29	0/6521	0.55	1/8830 (0.0%)
81	EC	0.34	1/3088 (0.0%)	0.88	2/4805 (0.0%)
All	All	0.54	1/224894 (0.0%)	0.75	56/329582 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	BH	0	1
43	AF	0	1
64	Ab	0	1
79	E	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	EC	6758	A	OP3-P	-10.55	1.48	1.61

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Ba	20	PRO	N-CD-CG	-10.63	87.26	103.20
8	BJ	80	LEU	CA-CB-CG	9.86	137.98	115.30
38	A1	1227	C	C6-N1-C2	-9.29	116.58	120.30
34	B5	1389	C	C2-N1-C1'	7.65	127.22	118.80
16	Ba	20	PRO	CA-N-CD	-7.63	100.81	111.50
38	A1	1282	G	N3-C4-N9	-7.53	121.48	126.00
16	Ba	20	PRO	CA-CB-CG	-7.38	89.97	104.00
38	A1	734	C	C2-N1-C1'	6.77	126.24	118.80
38	A1	1282	G	N3-C4-C5	6.75	131.98	128.60
38	A1	922	U	C2-N1-C1'	6.68	125.72	117.70
34	B5	196	G	OP1-P-O3'	6.41	119.31	105.20
38	A1	3018	C	C2-N1-C1'	6.32	125.75	118.80
38	A1	734	C	N1-C2-O2	6.29	122.67	118.90
35	AA	150	LEU	CA-CB-CG	6.09	129.30	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	1227	C	C5-C6-N1	6.05	124.03	121.00
38	A1	2207	A	OP2-P-O3'	6.05	118.51	105.20
38	A1	1283	C	N1-C2-O2	5.98	122.49	118.90
38	A1	1282	G	C6-C5-N7	5.95	133.97	130.40
81	EC	6797	U	C2-N1-C1'	5.88	124.75	117.70
35	AA	150	LEU	CB-CG-CD2	-5.85	101.05	111.00
34	B5	860	U	N3-C2-O2	-5.76	118.17	122.20
34	B5	1458	G	C4-N9-C1'	5.66	133.86	126.50
38	A1	2249	G	C6-C5-N7	5.64	133.78	130.40
38	A1	1283	C	N3-C2-O2	-5.64	117.95	121.90
38	A1	2904	U	C2-N1-C1'	5.63	124.46	117.70
38	A1	2476	C	N1-C2-O2	5.54	122.23	118.90
38	A1	2501	U	C2-N1-C1'	5.54	124.35	117.70
38	A1	2476	C	N3-C2-O2	-5.52	118.03	121.90
34	B5	297	U	N3-C2-O2	-5.51	118.34	122.20
34	B5	1389	C	C5-C6-N1	5.50	123.75	121.00
38	A1	2249	G	N3-C4-N9	-5.50	122.70	126.00
34	B5	1389	C	C6-N1-C1'	-5.49	114.21	120.80
34	B5	860	U	N1-C2-O2	5.37	126.56	122.80
38	A1	406	G	O4'-C1'-N9	5.36	112.49	108.20
34	B5	252	U	N3-C2-O2	-5.33	118.47	122.20
38	A1	2846	U	C2-N1-C1'	5.29	124.05	117.70
38	A1	3181	C	N1-C2-O2	5.25	122.05	118.90
34	B5	1246	C	C2-N1-C1'	5.24	124.56	118.80
34	B5	1246	C	N1-C2-O2	5.23	122.04	118.90
38	A1	922	U	N1-C2-O2	5.23	126.46	122.80
81	EC	6847	G	P-O3'-C3'	5.23	125.98	119.70
34	B5	149	C	N1-C2-O2	5.23	122.04	118.90
38	A1	176	G	N3-C2-N2	5.23	123.56	119.90
34	B5	252	U	N1-C2-O2	5.22	126.45	122.80
34	B5	149	C	N3-C2-O2	-5.19	118.27	121.90
64	Ab	41	ARG	NE-CZ-NH2	-5.14	117.73	120.30
80	DC	804	LEU	CA-CB-CG	5.12	127.07	115.30
34	B5	1301	U	C2-N1-C1'	5.12	123.84	117.70
38	A1	2137	U	C2-N1-C1'	5.12	123.84	117.70
38	A1	1608	C	C2-N1-C1'	5.09	124.40	118.80
24	BR	91	LEU	CA-CB-CG	5.09	127.00	115.30
34	B5	196	G	P-O3'-C3'	5.08	125.79	119.70
9	BL	102	LYS	CD-CE-NZ	5.07	123.37	111.70
34	B5	1458	G	C8-N9-C1'	-5.07	120.41	127.00
34	B5	293	U	C2-N1-C1'	5.06	123.77	117.70
38	A1	1227	C	N3-C2-O2	-5.03	118.38	121.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	AF	232	ARG	Peptide
64	Ab	41	ARG	Sidechain
6	BH	64	VAL	Peptide
79	E	26	ARG	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	204/252 (81%)	185 (91%)	19 (9%)	0	100	100
2	BB	212/255 (83%)	185 (87%)	27 (13%)	0	100	100
3	BC	215/254 (85%)	208 (97%)	7 (3%)	0	100	100
4	BE	258/261 (99%)	235 (91%)	23 (9%)	0	100	100
5	BG	224/236 (95%)	209 (93%)	15 (7%)	0	100	100
6	BH	182/190 (96%)	168 (92%)	14 (8%)	0	100	100
7	BI	184/200 (92%)	162 (88%)	22 (12%)	0	100	100
8	BJ	183/197 (93%)	164 (90%)	19 (10%)	0	100	100
9	BL	153/156 (98%)	138 (90%)	15 (10%)	0	100	100
10	BN	148/151 (98%)	137 (93%)	11 (7%)	0	100	100
11	BO	125/137 (91%)	111 (89%)	14 (11%)	0	100	100
12	BV	85/87 (98%)	76 (89%)	9 (11%)	0	100	100
13	BW	127/130 (98%)	118 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	BX	142/145 (98%)	127 (89%)	15 (11%)	0	100	100
15	BY	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
16	Ba	95/119 (80%)	82 (86%)	13 (14%)	0	100	100
17	Bb	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
18	Be	58/63 (92%)	49 (84%)	9 (16%)	0	100	100
19	BD	221/240 (92%)	209 (95%)	12 (5%)	0	100	100
20	BF	204/225 (91%)	189 (93%)	15 (7%)	0	100	100
21	BK	94/105 (90%)	80 (85%)	14 (15%)	0	100	100
22	BP	122/142 (86%)	114 (93%)	8 (7%)	0	100	100
23	BQ	139/143 (97%)	131 (94%)	8 (6%)	0	100	100
24	BR	117/136 (86%)	109 (93%)	8 (7%)	0	100	100
25	BS	143/146 (98%)	129 (90%)	14 (10%)	0	100	100
26	BT	139/144 (96%)	125 (90%)	14 (10%)	0	100	100
27	BU	105/121 (87%)	99 (94%)	6 (6%)	0	100	100
28	BZ	69/108 (64%)	64 (93%)	5 (7%)	0	100	100
29	Bc	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
30	Bd	51/56 (91%)	49 (96%)	2 (4%)	0	100	100
31	Bg	310/319 (97%)	276 (89%)	34 (11%)	0	100	100
32	Bf	73/152 (48%)	65 (89%)	8 (11%)	0	100	100
33	BM	122/143 (85%)	114 (93%)	8 (7%)	0	100	100
35	AA	245/254 (96%)	231 (94%)	14 (6%)	0	100	100
36	AB	383/387 (99%)	355 (93%)	28 (7%)	0	100	100
37	AC	359/362 (99%)	332 (92%)	27 (8%)	0	100	100
41	AD	290/297 (98%)	271 (93%)	19 (7%)	0	100	100
42	AE	163/176 (93%)	146 (90%)	17 (10%)	0	100	100
43	AF	220/244 (90%)	208 (94%)	12 (6%)	0	100	100
44	AG	228/256 (89%)	213 (93%)	15 (7%)	0	100	100
45	AH	188/191 (98%)	175 (93%)	13 (7%)	0	100	100
46	AI	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
47	AJ	167/174 (96%)	154 (92%)	13 (8%)	0	100	100
48	AL	191/199 (96%)	178 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	AM	134/138 (97%)	128 (96%)	6 (4%)	0	100	100
50	AN	201/204 (98%)	186 (92%)	15 (8%)	0	100	100
51	AO	195/199 (98%)	188 (96%)	7 (4%)	0	100	100
52	AP	171/184 (93%)	165 (96%)	6 (4%)	0	100	100
53	AQ	183/186 (98%)	174 (95%)	9 (5%)	0	100	100
54	AR	186/189 (98%)	172 (92%)	14 (8%)	0	100	100
55	AS	170/178 (96%)	155 (91%)	15 (9%)	0	100	100
56	AT	157/160 (98%)	141 (90%)	16 (10%)	0	100	100
57	AU	98/121 (81%)	92 (94%)	6 (6%)	0	100	100
58	AV	134/137 (98%)	127 (95%)	7 (5%)	0	100	100
59	AW	61/155 (39%)	58 (95%)	3 (5%)	0	100	100
60	AX	119/142 (84%)	113 (95%)	6 (5%)	0	100	100
61	AY	124/127 (98%)	116 (94%)	8 (6%)	0	100	100
62	AZ	133/136 (98%)	121 (91%)	12 (9%)	0	100	100
63	Aa	146/149 (98%)	134 (92%)	12 (8%)	0	100	100
64	Ab	56/59 (95%)	49 (88%)	7 (12%)	0	100	100
65	Ac	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
66	Ad	107/113 (95%)	97 (91%)	10 (9%)	0	100	100
67	Ae	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
68	Af	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
69	Ag	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
70	Ah	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
71	Ai	97/100 (97%)	89 (92%)	8 (8%)	0	100	100
72	Aj	85/88 (97%)	80 (94%)	5 (6%)	0	100	100
73	Ak	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
74	Al	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
75	Am	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	102/106 (96%)	95 (93%)	7 (7%)	0	100	100
78	Ap	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
79	E	215/217 (99%)	190 (88%)	25 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	DC	819/842 (97%)	744 (91%)	73 (9%)	2 (0%)	44	74
All	All	11959/12946 (92%)	11051 (92%)	906 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
80	DC	171	LYS
80	DC	774	VAL

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	
1	BA	173/210 (82%)	171 (99%)	2 (1%)	67	84
2	BB	191/224 (85%)	189 (99%)	2 (1%)	73	87
3	BC	176/205 (86%)	176 (100%)	0	100	100
4	BE	221/222 (100%)	219 (99%)	2 (1%)	75	88
5	BG	193/201 (96%)	191 (99%)	2 (1%)	73	87
6	BH	165/170 (97%)	165 (100%)	0	100	100
7	BI	150/161 (93%)	147 (98%)	3 (2%)	50	75
8	BJ	158/166 (95%)	158 (100%)	0	100	100
9	BL	136/137 (99%)	134 (98%)	2 (2%)	60	80
10	BN	127/128 (99%)	127 (100%)	0	100	100
11	BO	96/105 (91%)	96 (100%)	0	100	100
12	BV	74/74 (100%)	74 (100%)	0	100	100
13	BW	110/111 (99%)	110 (100%)	0	100	100
14	BX	119/120 (99%)	119 (100%)	0	100	100
15	BY	112/113 (99%)	112 (100%)	0	100	100
16	Ba	83/100 (83%)	83 (100%)	0	100	100
17	Bb	70/71 (99%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Be	51/54 (94%)	51 (100%)	0	100	100
19	BD	182/195 (93%)	180 (99%)	2 (1%)	70	85
20	BF	173/191 (91%)	173 (100%)	0	100	100
21	BK	89/98 (91%)	89 (100%)	0	100	100
22	BP	104/118 (88%)	102 (98%)	2 (2%)	52	76
23	BQ	117/119 (98%)	115 (98%)	2 (2%)	56	78
24	BR	101/124 (82%)	101 (100%)	0	100	100
25	BS	128/129 (99%)	127 (99%)	1 (1%)	79	89
26	BT	113/116 (97%)	112 (99%)	1 (1%)	75	88
27	BU	100/114 (88%)	99 (99%)	1 (1%)	73	87
28	BZ	62/89 (70%)	61 (98%)	1 (2%)	58	79
29	Bc	56/60 (93%)	55 (98%)	1 (2%)	54	77
30	Bd	47/49 (96%)	47 (100%)	0	100	100
31	Bg	256/262 (98%)	256 (100%)	0	100	100
32	Bf	66/135 (49%)	66 (100%)	0	100	100
33	BM	100/119 (84%)	99 (99%)	1 (1%)	73	87
35	AA	189/196 (96%)	188 (100%)	1 (0%)	86	93
36	AB	321/322 (100%)	320 (100%)	1 (0%)	91	95
37	AC	288/289 (100%)	286 (99%)	2 (1%)	81	90
41	AD	241/245 (98%)	241 (100%)	0	100	100
42	AE	137/153 (90%)	137 (100%)	0	100	100
43	AF	186/205 (91%)	186 (100%)	0	100	100
44	AG	189/208 (91%)	188 (100%)	1 (0%)	86	93
45	AH	170/171 (99%)	169 (99%)	1 (1%)	84	92
46	AI	190/190 (100%)	190 (100%)	0	100	100
47	AJ	147/150 (98%)	147 (100%)	0	100	100
48	AL	154/159 (97%)	154 (100%)	0	100	100
49	AM	107/109 (98%)	107 (100%)	0	100	100
50	AN	175/176 (99%)	175 (100%)	0	100	100
51	AO	160/162 (99%)	160 (100%)	0	100	100
52	AP	141/146 (97%)	138 (98%)	3 (2%)	48	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	AQ	150/151 (99%)	149 (99%)	1 (1%)	81	90
54	AR	153/154 (99%)	152 (99%)	1 (1%)	81	90
55	AS	156/162 (96%)	155 (99%)	1 (1%)	84	92
56	AT	136/137 (99%)	135 (99%)	1 (1%)	81	90
57	AU	87/107 (81%)	87 (100%)	0	100	100
58	AV	104/105 (99%)	103 (99%)	1 (1%)	73	87
59	AW	55/129 (43%)	55 (100%)	0	100	100
60	AX	105/118 (89%)	105 (100%)	0	100	100
61	AY	109/110 (99%)	109 (100%)	0	100	100
62	AZ	115/116 (99%)	115 (100%)	0	100	100
63	Aa	118/119 (99%)	118 (100%)	0	100	100
64	Ab	46/47 (98%)	46 (100%)	0	100	100
65	Ac	81/88 (92%)	81 (100%)	0	100	100
66	Ad	96/97 (99%)	96 (100%)	0	100	100
67	Ae	109/111 (98%)	109 (100%)	0	100	100
68	Af	90/91 (99%)	90 (100%)	0	100	100
69	Ag	95/103 (92%)	95 (100%)	0	100	100
70	Ah	104/105 (99%)	104 (100%)	0	100	100
71	Ai	81/82 (99%)	81 (100%)	0	100	100
72	Aj	70/71 (99%)	70 (100%)	0	100	100
73	Ak	68/69 (99%)	67 (98%)	1 (2%)	60	80
74	Al	45/46 (98%)	45 (100%)	0	100	100
75	Am	47/116 (40%)	47 (100%)	0	100	100
76	An	23/23 (100%)	23 (100%)	0	100	100
77	Ao	90/91 (99%)	90 (100%)	0	100	100
78	Ap	71/72 (99%)	70 (99%)	1 (1%)	62	81
79	E	198/198 (100%)	195 (98%)	3 (2%)	60	80
80	DC	699/714 (98%)	696 (100%)	3 (0%)	89	94
All	All	10195/10903 (94%)	10148 (100%)	47 (0%)	85	93

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BA	27	ARG
1	BA	79	ARG
2	BB	26	ARG
2	BB	152	ARG
4	BE	187	ARG
4	BE	233	LYS
5	BG	214	LYS
5	BG	223	LYS
7	BI	18	ARG
7	BI	47	ARG
7	BI	146	ARG
9	BL	67	ARG
9	BL	82	ARG
19	BD	76	ARG
19	BD	196	ARG
22	BP	58	LYS
22	BP	130	ARG
23	BQ	30	LYS
23	BQ	68	ARG
25	BS	145	ARG
26	BT	89	ARG
27	BU	43	LYS
28	BZ	70	LYS
29	Bc	67	ARG
33	BM	73	LYS
35	AA	92	LYS
36	AB	332	ARG
37	AC	93	MET
37	AC	288	ARG
44	AG	204	ARG
45	AH	23	ARG
52	AP	30	ARG
52	AP	171	ARG
52	AP	181	ARG
53	AQ	92	ARG
54	AR	181	ARG
55	AS	26	ARG
56	AT	83	ARG
58	AV	87	ARG
73	Ak	29	LYS
78	Ap	80	ARG
79	E	47	LYS
79	E	92	LYS

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Mol	Chain	Res	Type
79	E	122	ARG
80	DC	384	LYS
80	DC	578	LYS
80	DC	841	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (172) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	21	ASN
1	BA	30	GLN
1	BA	49	ASN
1	BA	131	GLN
2	BB	79	HIS
2	BB	95	ASN
2	BB	118	GLN
2	BB	149	GLN
2	BB	211	HIS
2	BB	220	GLN
3	BC	110	HIS
3	BC	189	GLN
3	BC	233	GLN
4	BE	36	HIS
4	BE	96	ASN
4	BE	130	GLN
4	BE	157	ASN
5	BG	56	ASN
5	BG	59	GLN
5	BG	65	GLN
5	BG	139	ASN
6	BH	122	HIS
6	BH	174	ASN
7	BI	32	GLN
7	BI	84	HIS
7	BI	116	HIS
8	BJ	112	GLN
8	BJ	139	GLN
9	BL	81	HIS
9	BL	106	ASN
9	BL	138	ASN
9	BL	150	ASN
10	BN	5	HIS
10	BN	123	HIS

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Mol	Chain	Res	Type
12	BV	33	GLN
12	BV	74	GLN
13	BW	44	HIS
13	BW	70	ASN
13	BW	80	ASN
13	BW	120	HIS
15	BY	22	GLN
16	Ba	11	ASN
19	BD	101	GLN
19	BD	162	GLN
20	BF	35	GLN
20	BF	63	GLN
20	BF	103	ASN
20	BF	122	ASN
20	BF	170	GLN
20	BF	200	ASN
21	BK	9	ASN
21	BK	28	ASN
21	BK	32	HIS
21	BK	62	GLN
22	BP	15	HIS
22	BP	79	HIS
23	BQ	8	GLN
23	BQ	93	HIS
24	BR	31	ASN
25	BS	6	GLN
26	BT	12	GLN
26	BT	70	GLN
26	BT	77	ASN
26	BT	101	ASN
27	BU	17	GLN
27	BU	33	GLN
27	BU	48	HIS
27	BU	72	ASN
30	Bd	37	ASN
31	Bg	17	ASN
31	Bg	308	ASN
32	Bf	93	HIS
33	BM	38	HIS
33	BM	143	GLN
35	AA	50	HIS
35	AA	132	ASN

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Mol	Chain	Res	Type
36	AB	212	ASN
37	AC	9	HIS
37	AC	58	HIS
37	AC	110	ASN
37	AC	175	HIS
37	AC	196	ASN
37	AC	260	GLN
37	AC	279	HIS
37	AC	322	GLN
41	AD	39	GLN
41	AD	40	HIS
41	AD	63	GLN
41	AD	151	GLN
41	AD	175	HIS
41	AD	178	ASN
43	AF	81	HIS
43	AF	104	GLN
43	AF	186	HIS
43	AF	237	ASN
44	AG	38	GLN
45	AH	9	GLN
45	AH	169	ASN
46	AI	12	GLN
46	AI	59	GLN
46	AI	162	GLN
47	AJ	90	GLN
47	AJ	152	HIS
48	AL	6	ASN
48	AL	106	GLN
50	AN	86	ASN
50	AN	195	ASN
51	AO	29[A]	ASN
51	AO	122[A]	GLN
51	AO	193[A]	GLN
52	AP	34	GLN
52	AP	145	HIS
53	AQ	145	ASN
53	AQ	158	HIS
54	AR	118	HIS
54	AR	130	ASN
54	AR	134	HIS
54	AR	156	ASN

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Mol	Chain	Res	Type
55	AS	3	HIS
55	AS	89	ASN
56	AT	49	GLN
56	AT	95	HIS
56	AT	127	GLN
57	AU	87	ASN
58	AV	81	GLN
58	AV	98	ASN
59	AW	32	GLN
59	AW	58	HIS
59	AW	59	HIS
60	AX	53	HIS
60	AX	85	GLN
60	AX	111	ASN
61	AY	81	GLN
61	AY	120	GLN
62	AZ	127	ASN
63	Aa	120	ASN
64	Ab	43	HIS
64	Ab	48	HIS
65	Ac	71	GLN
66	Ad	21	HIS
66	Ad	57	GLN
67	Ae	35	GLN
67	Ae	52	GLN
69	Ag	61	GLN
70	Ah	34	GLN
70	Ah	59	ASN
71	Ai	92	ASN
72	Aj	79	GLN
73	Ak	67	GLN
74	Al	20	ASN
74	Al	50	ASN
75	Am	90	ASN
75	Am	117	HIS
77	Ao	22	GLN
77	Ao	47	GLN
77	Ao	59	HIS
77	Ao	82	GLN
77	Ao	102	GLN
80	DC	21	ASN
80	DC	91	GLN

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Mol	Chain	Res	Type
80	DC	101	ASN
80	DC	176	GLN
80	DC	251	ASN
80	DC	274	ASN
80	DC	365	ASN
80	DC	414	GLN
80	DC	432	GLN
80	DC	476	HIS
80	DC	603	ASN
80	DC	687	ASN
80	DC	738	GLN
80	DC	791	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1749/1798 (97%)	481 (27%)	11 (0%)
38	A1	3211/3394 (94%)	698 (21%)	22 (0%)
39	A3	120/121 (99%)	17 (14%)	1 (0%)
40	A4	157/158 (99%)	29 (18%)	1 (0%)
81	EC	128/202 (63%)	89 (69%)	7 (5%)
All	All	5365/5673 (94%)	1314 (24%)	42 (0%)

All (1314) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	2	A
34	B5	4	C
34	B5	25	C
34	B5	34	G
34	B5	42	G
34	B5	43	A
34	B5	47	A
34	B5	50	C
34	B5	57	G
34	B5	59	C
34	B5	60	U
34	B5	63	G
34	B5	68	A
34	B5	69	G
34	B5	73	U

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Mol	Chain	Res	Type
34	B5	74	U
34	B5	75	U
34	B5	76	A
34	B5	77	U
34	B5	78	A
34	B5	84	A
34	B5	104	A
34	B5	111	U
34	B5	114	C
34	B5	115	G
34	B5	118	U
34	B5	119	A
34	B5	121	U
34	B5	127	G
34	B5	130	C
34	B5	131	C
34	B5	133	U
34	B5	134	U
34	B5	135	A
34	B5	136	C
34	B5	137	U
34	B5	138	A
34	B5	141	U
34	B5	144	U
34	B5	145	A
34	B5	146	U
34	B5	150	U
34	B5	153	G
34	B5	156	A
34	B5	159	U
34	B5	161	U
34	B5	166	C
34	B5	169	A
34	B5	176	C
34	B5	178	U
34	B5	179	A
34	B5	188	A
34	B5	189	C
34	B5	191	C
34	B5	193	U
34	B5	194	U
34	B5	195	G

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Mol	Chain	Res	Type
34	B5	197	A
34	B5	210	A
34	B5	211	PSU
34	B5	215	A
34	B5	216	U
34	B5	217	A
34	B5	218	A
34	B5	224	C
34	B5	225	A
34	B5	226	A
34	B5	228	G
34	B5	229	U
34	B5	230	C
34	B5	231	U
34	B5	233	C
34	B5	234	G
34	B5	235	G
34	B5	238	U
34	B5	239	C
34	B5	240	U
34	B5	241	U
34	B5	242	U
34	B5	249	U
34	B5	250	C
34	B5	253	A
34	B5	257	A
34	B5	260	U
34	B5	261	U
34	B5	262	U
34	B5	265	A
34	B5	272	U
34	B5	273	G
34	B5	280	U
34	B5	299	A
34	B5	304	U
34	B5	309	C
34	B5	316	A
34	B5	320	U
34	B5	321	C
34	B5	322	G
34	B5	323	A
34	B5	333	A

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Mol	Chain	Res	Type
34	B5	337	G
34	B5	338	C
34	B5	350	U
34	B5	352	A
34	B5	359	A
34	B5	360	A
34	B5	361	C
34	B5	370	A
34	B5	380	U
34	B5	387	A
34	B5	388	G
34	B5	400	A
34	B5	401	A
34	B5	402	C
34	B5	404	G
34	B5	422	G
34	B5	423	G
34	B5	424	C
34	B5	425	A
34	B5	426	G
34	B5	428	A
34	B5	435	C
34	B5	439	U
34	B5	444	C
34	B5	454	U
34	B5	456	A
34	B5	460	A
34	B5	464	A
34	B5	468	A
34	B5	475	A
34	B5	480	G
34	B5	482	U
34	B5	483	A
34	B5	484	C
34	B5	486	G
34	B5	487	G
34	B5	488	G
34	B5	489	C
34	B5	490	C
34	B5	491	C
34	B5	492	A
34	B5	493	U

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Mol	Chain	Res	Type
34	B5	495	C
34	B5	496	G
34	B5	497	G
34	B5	499	U
34	B5	500	C
34	B5	501	U
34	B5	502	U
34	B5	503	G
34	B5	505	A
34	B5	506	A
34	B5	511	A
34	B5	514	G
34	B5	515	A
34	B5	519	C
34	B5	534	A
34	B5	538	A
34	B5	540	G
34	B5	541	A
34	B5	542	A
34	B5	544	A
34	B5	554	C
34	B5	555	A
34	B5	557	G
34	B5	558	U
34	B5	559	C
34	B5	564	G
34	B5	565	C
34	B5	568	G
34	B5	572	C
34	B5	578	U
34	B5	580	A
34	B5	585	A
34	B5	594	A
34	B5	595	G
34	B5	597	G
34	B5	606	A
34	B5	610	G
34	B5	611	U
34	B5	613	G
34	B5	619	A
34	B5	620	A
34	B5	623	A

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Mol	Chain	Res	Type
34	B5	624	G
34	B5	635	A
34	B5	648	G
34	B5	649	U
34	B5	650	U
34	B5	651	G
34	B5	652	G
34	B5	656	G
34	B5	657	U
34	B5	658	C
34	B5	677	G
34	B5	679	U
34	B5	681	U
34	B5	682	C
34	B5	684	A
34	B5	685	A
34	B5	691	C
34	B5	694	U
34	B5	696	C
34	B5	698	U
34	B5	699	U
34	B5	700	C
34	B5	701	U
34	B5	702	G
34	B5	703	G
34	B5	704	C
34	B5	731	C
34	B5	732	G
34	B5	733	A
34	B5	734	A
34	B5	735	C
34	B5	736	C
34	B5	737	A
34	B5	738	G
34	B5	739	G
34	B5	740	A
34	B5	741	C
34	B5	742	U
34	B5	743	U
34	B5	745	U
34	B5	753	A
34	B5	763	G

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Mol	Chain	Res	Type
34	B5	765	G
34	B5	766	PSU
34	B5	771	A
34	B5	774	A
34	B5	779	U
34	B5	780	A
34	B5	782	U
34	B5	783	G
34	B5	787	G
34	B5	789	A
34	B5	791	A
34	B5	794	U
34	B5	803	A
34	B5	807	A
34	B5	812	A
34	B5	813	U
34	B5	814	A
34	B5	819	G
34	B5	823	G
34	B5	825	U
34	B5	826	U
34	B5	827	C
34	B5	828	U
34	B5	829	A
34	B5	830	U
34	B5	831	U
34	B5	832	U
34	B5	834	G
34	B5	835	U
34	B5	836	U
34	B5	837	G
34	B5	838	G
34	B5	839	U
34	B5	842	C
34	B5	843	U
34	B5	844	A
34	B5	846	G
34	B5	847	A
34	B5	849	C
34	B5	850	A
34	B5	851	U
34	B5	852	C

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Mol	Chain	Res	Type
34	B5	853	G
34	B5	854	U
34	B5	856	A
34	B5	857	U
34	B5	863	A
34	B5	873	U
34	B5	883	C
34	B5	885	G
34	B5	890	C
34	B5	893	U
34	B5	895	G
34	B5	898	A
34	B5	899	G
34	B5	905	A
34	B5	914	G
34	B5	921	U
34	B5	927	C
34	B5	928	U
34	B5	933	A
34	B5	935	U
34	B5	945	U
34	B5	951	A
34	B5	959	U
34	B5	960	U
34	B5	966	A
34	B5	992	A
34	B5	1003	A
34	B5	1004	U
34	B5	1005	A
34	B5	1021	C
34	B5	1024	U
34	B5	1026	A
34	B5	1028	C
34	B5	1030	A
34	B5	1031	U
34	B5	1032	G
34	B5	1039	A
34	B5	1042	G
34	B5	1052	U
34	B5	1053	G
34	B5	1056	U
34	B5	1057	U

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Mol	Chain	Res	Type
34	B5	1059	U
34	B5	1060	U
34	B5	1061	A
34	B5	1062	A
34	B5	1063	U
34	B5	1064	G
34	B5	1076	A
34	B5	1081	A
34	B5	1082	C
34	B5	1083	G
34	B5	1092	A
34	B5	1098	U
34	B5	1100	G
34	B5	1113	A
34	B5	1115	U
34	B5	1126	G
34	B5	1138	A
34	B5	1150	G
34	B5	1158	C
34	B5	1182	U
34	B5	1183	A
34	B5	1185	U
34	B5	1186	U
34	B5	1194	A
34	B5	1196	A
34	B5	1199	G
34	B5	1200	G
34	B5	1201	G
34	B5	1202	A
34	B5	1207	C
34	B5	1212	G
34	B5	1217	A
34	B5	1218	G
34	B5	1228	G
34	B5	1229	G
34	B5	1230	A
34	B5	1243	G
34	B5	1244	A
34	B5	1245	G
34	B5	1246	C
34	B5	1250	U
34	B5	1251	U

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Mol	Chain	Res	Type
34	B5	1252	C
34	B5	1256	A
34	B5	1264	G
34	B5	1284	C
34	B5	1307	U
34	B5	1314	U
34	B5	1315	U
34	B5	1320	U
34	B5	1321	A
34	B5	1325	A
34	B5	1340	U
34	B5	1344	A
34	B5	1345	A
34	B5	1348	A
34	B5	1353	U
34	B5	1354	G
34	B5	1360	A
34	B5	1362	U
34	B5	1363	U
34	B5	1364	G
34	B5	1368	G
34	B5	1369	U
34	B5	1370	U
34	B5	1371	A
34	B5	1375	A
34	B5	1378	U
34	B5	1385	G
34	B5	1390	U
34	B5	1398	U
34	B5	1399	C
34	B5	1400	A
34	B5	1402	G
34	B5	1413	U
34	B5	1415	PSU
34	B5	1418	G
34	B5	1425	A
34	B5	1427	A
34	B5	1428	G
34	B5	1432	U
34	B5	1435	G
34	B5	1436	A
34	B5	1445	G

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Mol	Chain	Res	Type
34	B5	1447	C
34	B5	1450	U
34	B5	1459	C
34	B5	1460	A
34	B5	1469	A
34	B5	1471	A
34	B5	1486	G
34	B5	1490	C
34	B5	1491	U
34	B5	1492	A
34	B5	1493	A
34	B5	1496	U
34	B5	1506	G
34	B5	1514	U
34	B5	1515	A
34	B5	1516	A
34	B5	1521	G
34	B5	1523	G
34	B5	1524	A
34	B5	1526	A
34	B5	1529	C
34	B5	1534	G
34	B5	1537	C
34	B5	1539	G
34	B5	1540	G
34	B5	1542	G
34	B5	1543	A
34	B5	1557	U
34	B5	1559	A
34	B5	1560	U
34	B5	1565	C
34	B5	1567	U
34	B5	1573	A
34	B5	1584	G
34	B5	1596	C
34	B5	1601	G
34	B5	1607	G
34	B5	1611	A
34	B5	1616	G
34	B5	1634	C
34	B5	1635	A
34	B5	1658	G

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Mol	Chain	Res	Type
34	B5	1663	G
34	B5	1665	U
34	B5	1673	G
34	B5	1678	A
34	B5	1680	G
34	B5	1683	C
34	B5	1684	U
34	B5	1687	U
34	B5	1688	U
34	B5	1689	A
34	B5	1690	G
34	B5	1692	G
34	B5	1693	A
34	B5	1694	A
34	B5	1697	G
34	B5	1698	G
34	B5	1699	G
34	B5	1700	C
34	B5	1702	A
34	B5	1703	C
34	B5	1704	U
34	B5	1705	C
34	B5	1707	A
34	B5	1708	U
34	B5	1709	C
34	B5	1711	C
34	B5	1712	A
34	B5	1713	G
34	B5	1714	A
34	B5	1728	A
34	B5	1736	G
34	B5	1742	U
34	B5	1750	A
34	B5	1755	A
34	B5	1756[A]	A
34	B5	1757	G
34	B5	1760	G
34	B5	1766	A
34	B5	1769	U
34	B5	1780	G
34	B5	1792	G
34	B5	1793	G

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Mol	Chain	Res	Type
34	B5	1794	A
34	B5	1796	C
34	B5	1798	U
34	B5	1799	U
38	A1	6	A
38	A1	12	A
38	A1	14	U
38	A1	18	G
38	A1	19	U
38	A1	26	A
38	A1	30	G
38	A1	34	A
38	A1	40	A
38	A1	43	A
38	A1	49	A
38	A1	59	G
38	A1	60	A
38	A1	65	A
38	A1	66	A
38	A1	85	A
38	A1	92	G
38	A1	109	A
38	A1	110	G
38	A1	111	C
38	A1	116	A
38	A1	117	U
38	A1	135	C
38	A1	136	G
38	A1	148	G
38	A1	150	A
38	A1	156	G
38	A1	157	A
38	A1	164	A
38	A1	165	A
38	A1	166	C
38	A1	170	G
38	A1	172	G
38	A1	173	G
38	A1	174	C
38	A1	182	U
38	A1	187	A
38	A1	190	U

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Mol	Chain	Res	Type
38	A1	191	U
38	A1	200	C
38	A1	206	G
38	A1	210	U
38	A1	211	A
38	A1	219	A
38	A1	231	G
38	A1	237	G
38	A1	238	A
38	A1	241	G
38	A1	242	C
38	A1	243	G
38	A1	245	U
38	A1	246	U
38	A1	248	U
38	A1	249	U
38	A1	250	U
38	A1	251	G
38	A1	252	U
38	A1	253	A
38	A1	254	A
38	A1	263	C
38	A1	269	G
38	A1	284	A
38	A1	286	U
38	A1	295	A
38	A1	305	U
38	A1	329	U
38	A1	342	A
38	A1	346	C
38	A1	350	C
38	A1	370	U
38	A1	374	A
38	A1	376	G
38	A1	390	G
38	A1	398	A
38	A1	399	A
38	A1	403	C
38	A1	407	A
38	A1	421	G
38	A1	422	A
38	A1	438	A

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Mol	Chain	Res	Type
38	A1	439	C
38	A1	440	A
38	A1	443	G
38	A1	444	U
38	A1	445	G
38	A1	446	U
38	A1	447	U
38	A1	448	U
38	A1	449	U
38	A1	450	G
38	A1	451	U
38	A1	487	U
38	A1	490	C
38	A1	491	A
38	A1	492	C
38	A1	493	U
38	A1	494	G
38	A1	495	G
38	A1	498	A
38	A1	521	A
38	A1	523	A
38	A1	536	U
38	A1	540	U
38	A1	541	U
38	A1	543	C
38	A1	544	C
38	A1	545	U
38	A1	547	G
38	A1	548	G
38	A1	549	U
38	A1	551	A
38	A1	552	G
38	A1	555	U
38	A1	557	A
38	A1	558	U
38	A1	559	A
38	A1	560	G
38	A1	566	G
38	A1	567	G
38	A1	569	A
38	A1	578	A
38	A1	579	G

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Mol	Chain	Res	Type
38	A1	590	G
38	A1	600	G
38	A1	603	A
38	A1	607	A
38	A1	611	A
38	A1	617	G
38	A1	620	U
38	A1	621	A
38	A1	622	A
38	A1	637	C
38	A1	649	A
38	A1	662	U
38	A1	667	C
38	A1	677	A
38	A1	690	A
38	A1	691	A
38	A1	705	A
38	A1	712	G
38	A1	719	U
38	A1	734	C
38	A1	735	A
38	A1	736	A
38	A1	750	G
38	A1	766	U
38	A1	767	U
38	A1	768	C
38	A1	771	A
38	A1	777	U
38	A1	780	A
38	A1	781	G
38	A1	785	G
38	A1	806	A
38	A1	808	A
38	A1	817	A
38	A1	826	G
38	A1	830	A
38	A1	848	A
38	A1	849	C
38	A1	861	C
38	A1	874	U
38	A1	879	U
38	A1	907	G

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Mol	Chain	Res	Type
38	A1	908	G
38	A1	910	G
38	A1	914	A
38	A1	916	G
38	A1	917	A
38	A1	921	A
38	A1	923	C
38	A1	924	G
38	A1	937	G
38	A1	944	C
38	A1	959	C
38	A1	960	PSU
38	A1	974	G
38	A1	980	A
38	A1	982	C
38	A1	985	U
38	A1	1000	C
38	A1	1007	U
38	A1	1008	U
38	A1	1010	G
38	A1	1014	U
38	A1	1018	G
38	A1	1019	G
38	A1	1020	G
38	A1	1021	G
38	A1	1023	C
38	A1	1031	C
38	A1	1033	U
38	A1	1034	U
38	A1	1035	G
38	A1	1041	U
38	A1	1047	A
38	A1	1064	A
38	A1	1066	G
38	A1	1072	G
38	A1	1075	A
38	A1	1080	A
38	A1	1083	G
38	A1	1087	G
38	A1	1092	C
38	A1	1093	A
38	A1	1094	U

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Mol	Chain	Res	Type
38	A1	1095	U
38	A1	1097	G
38	A1	1098	A
38	A1	1103	A
38	A1	1104	G
38	A1	1117	G
38	A1	1131	G
38	A1	1143	A
38	A1	1153	A
38	A1	1155	C
38	A1	1159	A
38	A1	1180	A
38	A1	1181	U
38	A1	1182	A
38	A1	1186	G
38	A1	1190	A
38	A1	1192	C
38	A1	1193	A
38	A1	1196	C
38	A1	1200	A
38	A1	1201	C
38	A1	1208	U
38	A1	1209	G
38	A1	1218	U
38	A1	1220	U
38	A1	1221	A
38	A1	1222	G
38	A1	1228	C
38	A1	1230	G
38	A1	1231	A
38	A1	1232	C
38	A1	1233	G
38	A1	1234	G
38	A1	1235	U
38	A1	1236	G
38	A1	1237	G
38	A1	1238	C
38	A1	1239	C
38	A1	1240	A
38	A1	1241	U
38	A1	1242	G
38	A1	1244	A

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Mol	Chain	Res	Type
38	A1	1246	G
38	A1	1248	C
38	A1	1249	G
38	A1	1250	G
38	A1	1251	A
38	A1	1252	A
38	A1	1253	U
38	A1	1255	C
38	A1	1258	U
38	A1	1259	A
38	A1	1260	A
38	A1	1262	G
38	A1	1263	A
38	A1	1264	G
38	A1	1265	U
38	A1	1268	G
38	A1	1269	U
38	A1	1270	A
38	A1	1271	A
38	A1	1272	C
38	A1	1273	A
38	A1	1274	A
38	A1	1278	A
38	A1	1279	C
38	A1	1280	C
38	A1	1285	G
38	A1	1286	A
38	A1	1287	A
38	A1	1288	U
38	A1	1305	U
38	A1	1307	G
38	A1	1309	U
38	A1	1325	U
38	A1	1330	A
38	A1	1331	U
38	A1	1348	U
38	A1	1349	G
38	A1	1350	A
38	A1	1351	U
38	A1	1352	A
38	A1	1353	U
38	A1	1354	G

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Mol	Chain	Res	Type
38	A1	1355	A
38	A1	1357	G
38	A1	1366	A
38	A1	1386	A
38	A1	1392	G
38	A1	1396	C
38	A1	1399	A
38	A1	1400	G
38	A1	1419	A
38	A1	1434	G
38	A1	1437	C
38	A1	1446	A
38	A1	1455	U
38	A1	1475	A
38	A1	1477	A
38	A1	1481	A
38	A1	1482	A
38	A1	1483	G
38	A1	1484	U
38	A1	1487	G
38	A1	1488	G
38	A1	1496	C
38	A1	1507	G
38	A1	1536	G
38	A1	1539	A
38	A1	1556	C
38	A1	1557	A
38	A1	1561	G
38	A1	1562	C
38	A1	1563	C
38	A1	1564	U
38	A1	1566	A
38	A1	1568	U
38	A1	1569	U
38	A1	1570	U
38	A1	1571	A
38	A1	1572	U
38	A1	1574	C
38	A1	1575	A
38	A1	1576	G
38	A1	1577	G
38	A1	1582	C

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Mol	Chain	Res	Type
38	A1	1583	A
38	A1	1587	A
38	A1	1589	A
38	A1	1590	G
38	A1	1593	A
38	A1	1605	A
38	A1	1613	A
38	A1	1622	U
38	A1	1628	C
38	A1	1629	U
38	A1	1639	C
38	A1	1642	A
38	A1	1643	A
38	A1	1645	U
38	A1	1658	G
38	A1	1683	A
38	A1	1688	U
38	A1	1694	U
38	A1	1724	U
38	A1	1736	G
38	A1	1741	A
38	A1	1750	A
38	A1	1751	G
38	A1	1756	C
38	A1	1759	C
38	A1	1760	A
38	A1	1763	U
38	A1	1764	U
38	A1	1765	U
38	A1	1766	G
38	A1	1775	G
38	A1	1778	G
38	A1	1779	C
38	A1	1788	C
38	A1	1792	C
38	A1	1797	A
38	A1	1808	G
38	A1	1813	A
38	A1	1815	U
38	A1	1816	A
38	A1	1817	G
38	A1	1818	U

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Mol	Chain	Res	Type
38	A1	1819	U
38	A1	1821	U
38	A1	1840	U
38	A1	1842	A
38	A1	1849	C
38	A1	1850	A
38	A1	1860	G
38	A1	1866	C
38	A1	1874	A
38	A1	1878	G
38	A1	1880	U
38	A1	1886	A
38	A1	1893	A
38	A1	1906	G
38	A1	1907	C
38	A1	1935	G
38	A1	1953	G
38	A1	1954	G
38	A1	2094	C
38	A1	2095	G
38	A1	2099	A
38	A1	2111	G
38	A1	2112	U
38	A1	2114	C
38	A1	2122	G
38	A1	2126	A
38	A1	2131	A
38	A1	2140	U
38	A1	2142	1MA
38	A1	2144	A
38	A1	2157	G
38	A1	2158	A
38	A1	2169	G
38	A1	2170	U
38	A1	2174	G
38	A1	2188	A
38	A1	2194	G
38	A1	2198	A
38	A1	2202	C
38	A1	2207	A
38	A1	2208	A
38	A1	2209	U

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Mol	Chain	Res	Type
38	A1	2211	U
38	A1	2222	A
38	A1	2223	A
38	A1	2227	C
38	A1	2244	A
38	A1	2249	G
38	A1	2250	G
38	A1	2253	G
38	A1	2256	A
38	A1	2257	C
38	A1	2258	PSU
38	A1	2259	A
38	A1	2265	C
38	A1	2266	PSU
38	A1	2267	C
38	A1	2269	U
38	A1	2270	A
38	A1	2272	G
38	A1	2273	G
38	A1	2274	U
38	A1	2280	A
38	A1	2282	U
38	A1	2287	C
38	A1	2306	C
38	A1	2307	G
38	A1	2310	U
38	A1	2313	A
38	A1	2315	G
38	A1	2334	U
38	A1	2335	G
38	A1	2356	A
38	A1	2373	A
38	A1	2374	C
38	A1	2375	G
38	A1	2383	C
38	A1	2393	G
38	A1	2397	A
38	A1	2402	A
38	A1	2403	G
38	A1	2404	A
38	A1	2411	U
38	A1	2435	G

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Mol	Chain	Res	Type
38	A1	2438	A
38	A1	2441	A
38	A1	2444	C
38	A1	2445	A
38	A1	2446	U
38	A1	2447	A
38	A1	2449	A
38	A1	2450	G
38	A1	2452	G
38	A1	2454	G
38	A1	2455	U
38	A1	2457	G
38	A1	2458	A
38	A1	2459	A
38	A1	2460	U
38	A1	2461	A
38	A1	2462	A
38	A1	2463	G
38	A1	2466	G
38	A1	2467	G
38	A1	2468	A
38	A1	2469	G
38	A1	2471	U
38	A1	2474	G
38	A1	2476	C
38	A1	2478	C
38	A1	2479	C
38	A1	2480	A
38	A1	2485	A
38	A1	2487	U
38	A1	2488	A
38	A1	2490	C
38	A1	2492	C
38	A1	2493	U
38	A1	2494	A
38	A1	2495	C
38	A1	2496	C
38	A1	2497	U
38	A1	2498	U
38	A1	2499	U
38	A1	2500	A
38	A1	2501	U

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Mol	Chain	Res	Type
38	A1	2502	A
38	A1	2503	G
38	A1	2504	U
38	A1	2506	U
38	A1	2507	C
38	A1	2508	U
38	A1	2510	U
38	A1	2514	U
38	A1	2515	A
38	A1	2522	G
38	A1	2523	A
38	A1	2524	A
38	A1	2525	G
38	A1	2530	G
38	A1	2536	A
38	A1	2537	U
38	A1	2538	U
38	A1	2539	C
38	A1	2540	A
38	A1	2542	U
38	A1	2546	C
38	A1	2549	G
38	A1	2552	C
38	A1	2554	A
38	A1	2559	U
38	A1	2561	A
38	A1	2569	A
38	A1	2570	U
38	A1	2571	U
38	A1	2572	C
38	A1	2573	G
38	A1	2585	G
38	A1	2593	A
38	A1	2606	G
38	A1	2607	G
38	A1	2614	G
38	A1	2626	A
38	A1	2629	U
38	A1	2635	A
38	A1	2637	A
38	A1	2648	G
38	A1	2651	G

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Mol	Chain	Res	Type
38	A1	2652	U
38	A1	2656	A
38	A1	2657	A
38	A1	2666	C
38	A1	2672	G
38	A1	2674	A
38	A1	2677	G
38	A1	2678	A
38	A1	2681	U
38	A1	2689	A
38	A1	2691	A
38	A1	2694	A
38	A1	2696	A
38	A1	2704	A
38	A1	2714	G
38	A1	2719	U
38	A1	2728	G
38	A1	2729	U
38	A1	2737	C
38	A1	2743	A
38	A1	2747	A
38	A1	2753	G
38	A1	2755	C
38	A1	2772	C
38	A1	2773	C
38	A1	2777	G
38	A1	2778	G
38	A1	2779	A
38	A1	2796	G
38	A1	2800	G
38	A1	2801	A
38	A1	2803	A
38	A1	2804	A
38	A1	2808	A
38	A1	2810	C
38	A1	2814	G
38	A1	2816	G
38	A1	2817	A
38	A1	2821	C
38	A1	2842	U
38	A1	2844	C
38	A1	2845	A

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Mol	Chain	Res	Type
38	A1	2849	C
38	A1	2853	A
38	A1	2876	C
38	A1	2887	A
38	A1	2894	C
38	A1	2903	A
38	A1	2904	U
38	A1	2914	G
38	A1	2923	PSU
38	A1	2935	U
38	A1	2936	A
38	A1	2938	G
38	A1	2942	C
38	A1	2947	G
38	A1	2955	U
38	A1	2971	A
38	A1	2983	C
38	A1	2990	G
38	A1	2996	U
38	A1	2997	G
38	A1	3003	G
38	A1	3012	A
38	A1	3017	A
38	A1	3018	C
38	A1	3022	G
38	A1	3023	U
38	A1	3034	C
38	A1	3045	G
38	A1	3048	A
38	A1	3049	A
38	A1	3055	U
38	A1	3056	U
38	A1	3059	G
38	A1	3069	G
38	A1	3074	G
38	A1	3078	U
38	A1	3080	G
38	A1	3086	A
38	A1	3092	C
38	A1	3094	A
38	A1	3101	G
38	A1	3104	U

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Mol	Chain	Res	Type
38	A1	3109	G
38	A1	3122	A
38	A1	3130	A
38	A1	3131	U
38	A1	3142	A
38	A1	3143	C
38	A1	3155	U
38	A1	3156	U
38	A1	3157	U
38	A1	3162	C
38	A1	3163	A
38	A1	3165	A
38	A1	3166	C
38	A1	3167	A
38	A1	3168	A
38	A1	3169	U
38	A1	3170	A
38	A1	3171	U
38	A1	3173	G
38	A1	3174	A
38	A1	3176	G
38	A1	3179	U
38	A1	3181	C
38	A1	3187	A
38	A1	3196	U
38	A1	3197	G
38	A1	3199	G
38	A1	3207	U
38	A1	3209	A
38	A1	3210	A
38	A1	3217	C
38	A1	3218	A
38	A1	3219	G
38	A1	3228	C
38	A1	3229	G
38	A1	3234	A
38	A1	3238	G
38	A1	3239	G
38	A1	3243	A
38	A1	3247	G
38	A1	3259	U
38	A1	3260	G

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Mol	Chain	Res	Type
38	A1	3263	G
38	A1	3271	G
38	A1	3272	C
38	A1	3273	A
38	A1	3275	U
38	A1	3276	G
38	A1	3277	U
38	A1	3278	C
38	A1	3279	A
38	A1	3281	U
38	A1	3283	U
38	A1	3284	G
38	A1	3286	G
38	A1	3287	U
38	A1	3289	G
38	A1	3294	A
38	A1	3304	U
38	A1	3313	U
38	A1	3316	A
38	A1	3341	U
38	A1	3342	A
38	A1	3345	G
38	A1	3350	C
38	A1	3351	U
38	A1	3352	U
38	A1	3354	U
38	A1	3368	U
38	A1	3369	G
38	A1	3378	C
38	A1	3396	U
39	A3	7	G
39	A3	10	C
39	A3	11	A
39	A3	17	A
39	A3	23	A
39	A3	24	A
39	A3	33	U
39	A3	38	U
39	A3	49	G
39	A3	54	U
39	A3	55	A
39	A3	65	G

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Mol	Chain	Res	Type
39	A3	99	G
39	A3	102	A
39	A3	105	C
39	A3	112	G
39	A3	121	U
40	A4	34	U
40	A4	35	C
40	A4	39	G
40	A4	51	G
40	A4	52	A
40	A4	59	A
40	A4	61	A
40	A4	62	C
40	A4	63	G
40	A4	81	U
40	A4	82	U
40	A4	85	G
40	A4	86	U
40	A4	87	G
40	A4	89	A
40	A4	90	U
40	A4	95	G
40	A4	102	U
40	A4	104	A
40	A4	106	C
40	A4	111	A
40	A4	113	U
40	A4	114	G
40	A4	116	G
40	A4	125	U
40	A4	131	A
40	A4	148	G
40	A4	152	G
40	A4	158	U
81	EC	6759	A
81	EC	6762	U
81	EC	6766	U
81	EC	6768	U
81	EC	6769	A
81	EC	6770	U
81	EC	6771	U
81	EC	6772	G

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Mol	Chain	Res	Type
81	EC	6773	G
81	EC	6774	U
81	EC	6775	U
81	EC	6776	A
81	EC	6777	C
81	EC	6778	C
81	EC	6780	A
81	EC	6781	U
81	EC	6782	C
81	EC	6786	A
81	EC	6787	U
81	EC	6789	G
81	EC	6790	A
81	EC	6791	A
81	EC	6792	A
81	EC	6793	A
81	EC	6794	C
81	EC	6798	C
81	EC	6800	G
81	EC	6801	A
81	EC	6802	A
81	EC	6803	C
81	EC	6804	A
81	EC	6805	C
81	EC	6808	G
81	EC	6809	G
81	EC	6810	U
81	EC	6811	G
81	EC	6813	A
81	EC	6815	U
81	EC	6816	A
81	EC	6817	A
81	EC	6818	G
81	EC	6819	G
81	EC	6820	C
81	EC	6821	U
81	EC	6823	U
81	EC	6825	A
81	EC	6827	G
81	EC	6831	U
81	EC	6832	G
81	EC	6833	G

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Mol	Chain	Res	Type
81	EC	6835	U
81	EC	6837	G
81	EC	6840	A
81	EC	6841	U
81	EC	6842	U
81	EC	6843	U
81	EC	6844	A
81	EC	6845	G
81	EC	6847	G
81	EC	6848	U
81	EC	6849	A
81	EC	6850	C
81	EC	6852	U
81	EC	6855	A
81	EC	6856	C
81	EC	6857	C
81	EC	6859	U
81	EC	6860	A
81	EC	6862	G
81	EC	6863	C
81	EC	6864	A
81	EC	6866	C
81	EC	6867	C
81	EC	6869	C
81	EC	6870	A
81	EC	6871	A
81	EC	6872	A
81	EC	6873	A
81	EC	6874	A
81	EC	6876	A
81	EC	6877	C
81	EC	6878	G
81	EC	6879	U
81	EC	6880	G
81	EC	6881	U
81	EC	6882	G
81	EC	6884	G
81	EC	6885	G
81	EC	6888	A

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	B5	130	C
34	B5	196	G
34	B5	752	A
34	B5	889	U
34	B5	904	G
34	B5	1061	A
34	B5	1344	A
34	B5	1363	U
34	B5	1458	G
34	B5	1683	C
34	B5	1689	A
38	A1	116	A
38	A1	165	A
38	A1	240	U
38	A1	252	U
38	A1	916	G
38	A1	1287	A
38	A1	1560	G
38	A1	1818	U
38	A1	1953	G
38	A1	2094	C
38	A1	2207	A
38	A1	2222	A
38	A1	2437	G
38	A1	2468	A
38	A1	2493	U
38	A1	2497	U
38	A1	2506	U
38	A1	2772	C
38	A1	3022	G
38	A1	3121	U
38	A1	3154	C
38	A1	3169	U
39	A3	23	A
40	A4	88	A
81	EC	6789	G
81	EC	6802	A
81	EC	6818	G
81	EC	6819	G
81	EC	6847	G
81	EC	6851	G
81	EC	6877	C

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

60 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
34	PSU	B5	759	34	18,21,22	1.40	3 (16%)	21,30,33	2.12	4 (19%)
34	MA6	B5	1782	34	19,26,27	0.94	1 (5%)	18,38,41	1.92	4 (22%)
38	1MA	A1	645	38	17,25,26	1.41	2 (11%)	17,37,40	1.22	3 (17%)
38	PSU	A1	986	38	18,21,22	1.46	5 (27%)	21,30,33	2.18	5 (23%)
38	PSU	A1	2351	38	18,21,22	1.44	4 (22%)	21,30,33	2.10	4 (19%)
38	UR3	A1	2634	38	19,22,23	0.93	0	26,32,35	1.76	3 (11%)
38	PSU	A1	1056	38	18,21,22	1.43	4 (22%)	21,30,33	2.19	4 (19%)
38	PSU	A1	1110	38	18,21,22	1.43	4 (22%)	21,30,33	2.14	3 (14%)
34	PSU	B5	466	34	18,21,22	1.39	3 (16%)	21,30,33	2.07	4 (19%)
38	PSU	A1	2944	38	18,21,22	1.44	5 (27%)	21,30,33	2.23	5 (23%)
38	PSU	A1	1124	38	18,21,22	1.40	4 (22%)	21,30,33	2.09	4 (19%)
38	PSU	A1	2865	38	18,21,22	1.48	4 (22%)	21,30,33	2.15	4 (19%)
38	5MC	A1	2870	38	19,22,23	1.30	3 (15%)	26,32,35	1.12	2 (7%)
38	OMU	A1	2921	38	19,22,23	1.26	4 (21%)	25,31,34	1.89	6 (24%)
80	DDE	DC	699	-	15,20,21	0.97	1 (6%)	11,28,30	1.02	1 (9%)
34	PSU	B5	999	34	18,21,22	1.43	4 (22%)	21,30,33	2.17	4 (19%)
34	4AC	B5	1773	34	21,24,25	1.11	2 (9%)	28,34,37	2.10	5 (17%)
38	PSU	A1	2129	38	18,21,22	1.47	4 (22%)	21,30,33	2.18	4 (19%)
34	4AC	B5	1280	34	21,24,25	1.11	1 (4%)	28,34,37	0.98	1 (3%)
34	PSU	B5	302	34	18,21,22	1.44	4 (22%)	21,30,33	2.16	4 (19%)
38	PSU	A1	990	38	18,21,22	1.39	3 (16%)	21,30,33	2.07	4 (19%)
38	1MA	A1	2142	38	17,25,26	1.45	2 (11%)	17,37,40	1.17	3 (17%)
38	PSU	A1	2258	38	18,21,22	1.37	3 (16%)	21,30,33	2.16	4 (19%)
38	PSU	A1	2416	38	18,21,22	1.52	5 (27%)	21,30,33	2.13	4 (19%)
38	PSU	A1	2923	38	18,21,22	1.35	2 (11%)	21,30,33	2.10	3 (14%)
38	PSU	A1	2880	38	18,21,22	1.45	4 (22%)	21,30,33	2.19	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PSU	B5	632	34	18,21,22	1.47	4 (22%)	21,30,33	2.16	4 (19%)
38	5MC	A1	2278	38	19,22,23	1.37	3 (15%)	26,32,35	1.13	3 (11%)
34	PSU	B5	106	34	18,21,22	1.41	3 (16%)	21,30,33	2.01	3 (14%)
38	PSU	A1	776	38	18,21,22	1.29	3 (16%)	21,30,33	2.19	6 (28%)
34	PSU	B5	1415	34	18,21,22	1.35	3 (16%)	21,30,33	2.07	4 (19%)
34	PSU	B5	766	34	18,21,22	1.41	4 (22%)	21,30,33	2.22	5 (23%)
38	PSU	A1	960	38	18,21,22	1.45	3 (16%)	21,30,33	2.07	4 (19%)
34	MA6	B5	1781	34	19,26,27	0.90	1 (5%)	18,38,41	1.84	4 (22%)
38	PSU	A1	966	38	18,21,22	1.41	4 (22%)	21,30,33	2.10	4 (19%)
40	PSU	A4	73	40	18,21,22	1.36	3 (16%)	21,30,33	1.99	4 (19%)
38	PSU	A1	1042	38	18,21,22	1.36	3 (16%)	21,30,33	1.96	3 (14%)
38	PSU	A1	2191	38	18,21,22	1.43	4 (22%)	21,30,33	2.15	4 (19%)
38	PSU	A1	2975	38	18,21,22	1.46	4 (22%)	21,30,33	2.20	4 (19%)
38	PSU	A1	2133	38	18,21,22	1.55	4 (22%)	21,30,33	2.26	5 (23%)
34	B8N	B5	1191	34	25,29,30	1.38	3 (12%)	28,42,45	7.25	5 (17%)
38	PSU	A1	2826	38	18,21,22	1.42	5 (27%)	21,30,33	2.12	5 (23%)
38	PSU	A1	2314	38	18,21,22	1.37	3 (16%)	21,30,33	2.04	4 (19%)
38	PSU	A1	2260	38	18,21,22	1.38	2 (11%)	21,30,33	2.14	5 (23%)
34	PSU	B5	1187	34	18,21,22	1.38	3 (16%)	21,30,33	2.05	3 (14%)
38	OMG	A1	2922	38	19,26,27	0.88	1 (5%)	21,38,41	1.09	2 (9%)
38	PSU	A1	2266	38	18,21,22	1.46	5 (27%)	21,30,33	2.02	3 (14%)
34	G7M	B5	1575	34	20,26,27	2.23	5 (25%)	16,39,42	0.83	1 (6%)
38	PSU	A1	1004	38	18,21,22	1.43	4 (22%)	21,30,33	2.09	3 (14%)
34	PSU	B5	1290	34	18,21,22	1.39	3 (16%)	21,30,33	2.15	4 (19%)
38	PSU	A1	2264	38	18,21,22	1.42	3 (16%)	21,30,33	2.08	3 (14%)
38	PSU	A1	2340	38	18,21,22	1.47	4 (22%)	21,30,33	2.04	3 (14%)
36	HIC	AB	243	36	8,11,12	1.62	2 (25%)	5,14,16	0.97	0
34	PSU	B5	1181	34	18,21,22	1.39	2 (11%)	21,30,33	2.15	4 (19%)
34	PSU	B5	120	34	18,21,22	1.36	3 (16%)	21,30,33	2.03	4 (19%)
38	PSU	A1	2349	38	18,21,22	1.39	4 (22%)	21,30,33	2.07	3 (14%)
38	PSU	A1	1052	38	18,21,22	1.38	4 (22%)	21,30,33	2.10	4 (19%)
39	PSU	A3	50	39	18,21,22	1.39	2 (11%)	21,30,33	2.06	3 (14%)
38	PSU	A1	2735	38	18,21,22	1.40	4 (22%)	21,30,33	2.11	4 (19%)
34	PSU	B5	211	34	18,21,22	1.41	3 (16%)	21,30,33	2.01	3 (14%)

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
34	PSU	B5	759	34	-	0/7/25/26	0/2/2/2
34	MA6	B5	1782	34	-	4/7/29/30	0/3/3/3
38	1MA	A1	645	38	-	0/3/25/26	0/3/3/3
38	PSU	A1	986	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2351	38	-	0/7/25/26	0/2/2/2
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1056	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1110	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	466	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2944	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1124	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2865	38	-	0/7/25/26	0/2/2/2
38	5MC	A1	2870	38	-	4/7/25/26	0/2/2/2
38	OMU	A1	2921	38	-	0/9/27/28	0/2/2/2
80	DDE	DC	699	-	-	11/20/21/23	0/1/1/1
34	PSU	B5	999	34	-	0/7/25/26	0/2/2/2
34	4AC	B5	1773	34	-	3/11/29/30	0/2/2/2
38	PSU	A1	2129	38	-	0/7/25/26	0/2/2/2
34	4AC	B5	1280	34	-	2/11/29/30	0/2/2/2
34	PSU	B5	302	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	990	38	-	0/7/25/26	0/2/2/2
38	1MA	A1	2142	38	-	0/3/25/26	0/3/3/3
38	PSU	A1	2258	38	-	2/7/25/26	0/2/2/2
38	PSU	A1	2416	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2923	38	-	3/7/25/26	0/2/2/2
38	PSU	A1	2880	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	632	34	-	0/7/25/26	0/2/2/2
38	5MC	A1	2278	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	106	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	776	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	1415	34	-	1/7/25/26	0/2/2/2
34	PSU	B5	766	34	-	2/7/25/26	0/2/2/2
38	PSU	A1	960	38	-	1/7/25/26	0/2/2/2
34	MA6	B5	1781	34	-	1/7/29/30	0/3/3/3
38	PSU	A1	966	38	-	0/7/25/26	0/2/2/2
40	PSU	A4	73	40	-	0/7/25/26	0/2/2/2
38	PSU	A1	1042	38	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PSU	A1	2191	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2975	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2133	38	-	0/7/25/26	0/2/2/2
34	B8N	B5	1191	34	-	1/16/34/35	0/2/2/2
38	PSU	A1	2826	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2314	38	-	1/7/25/26	0/2/2/2
38	PSU	A1	2260	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	1187	34	-	2/7/25/26	0/2/2/2
38	OMG	A1	2922	38	-	0/5/27/28	0/3/3/3
38	PSU	A1	2266	38	-	3/7/25/26	0/2/2/2
34	G7M	B5	1575	34	-	2/3/25/26	0/3/3/3
38	PSU	A1	1004	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	1290	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2264	38	-	1/7/25/26	0/2/2/2
38	PSU	A1	2340	38	-	2/7/25/26	0/2/2/2
36	HIC	AB	243	36	-	2/5/6/8	0/1/1/1
34	PSU	B5	1181	34	-	1/7/25/26	0/2/2/2
34	PSU	B5	120	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2349	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1052	38	-	0/7/25/26	0/2/2/2
39	PSU	A3	50	39	-	0/7/25/26	0/2/2/2
38	PSU	A1	2735	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	211	34	-	2/7/25/26	0/2/2/2

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	O6-C6	5.89	1.37	1.23
34	B5	1575	G7M	C2-N2	5.74	1.47	1.34
38	A1	2142	1MA	C2-N3	4.48	1.34	1.28
38	A1	2278	5MC	C5-C4	4.42	1.47	1.44
38	A1	2870	5MC	C5-C4	4.20	1.47	1.44
38	A1	645	1MA	C2-N3	4.19	1.33	1.28
34	B5	1191	B8N	C4-C5	-3.83	1.38	1.47
38	A1	2133	PSU	C4-N3	-3.49	1.32	1.38
39	A3	50	PSU	C6-C5	3.49	1.39	1.35
36	AB	243	HIC	CD2-CG	3.27	1.41	1.36
34	B5	1280	4AC	C4-N4	-3.26	1.35	1.39
34	B5	632	PSU	C4-N3	-3.23	1.32	1.38
38	A1	2416	PSU	C4-N3	-3.23	1.32	1.38
38	A1	2129	PSU	C4-N3	-3.22	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1181	PSU	C6-C5	3.18	1.38	1.35
34	B5	1187	PSU	C6-C5	3.17	1.38	1.35
38	A1	2975	PSU	C4-N3	-3.17	1.32	1.38
38	A1	1056	PSU	C4-N3	-3.14	1.33	1.38
38	A1	2880	PSU	C4-N3	-3.14	1.33	1.38
38	A1	1004	PSU	C6-C5	3.14	1.38	1.35
38	A1	2944	PSU	C4-N3	-3.12	1.33	1.38
38	A1	960	PSU	C6-C5	3.11	1.38	1.35
38	A1	966	PSU	C4-N3	-3.11	1.33	1.38
38	A1	986	PSU	C4-N3	-3.11	1.33	1.38
38	A1	2266	PSU	C6-C5	3.10	1.38	1.35
34	B5	1191	B8N	C6-C5	3.08	1.39	1.35
34	B5	1575	G7M	C6-N1	-3.07	1.33	1.37
38	A1	2351	PSU	C4-N3	-3.07	1.33	1.38
34	B5	106	PSU	C6-C5	3.06	1.38	1.35
34	B5	1290	PSU	C4-N3	-3.04	1.33	1.38
34	B5	302	PSU	C4-N3	-3.04	1.33	1.38
34	B5	211	PSU	C6-C5	3.03	1.38	1.35
38	A1	2191	PSU	C4-N3	-3.03	1.33	1.38
34	B5	466	PSU	C6-C5	3.02	1.38	1.35
34	B5	759	PSU	C4-N3	-2.99	1.33	1.38
38	A1	2349	PSU	C4-N3	-2.98	1.33	1.38
34	B5	999	PSU	C4-N3	-2.98	1.33	1.38
38	A1	2264	PSU	C4-N3	-2.97	1.33	1.38
34	B5	759	PSU	C6-C5	2.95	1.38	1.35
38	A1	2340	PSU	C4-N3	-2.94	1.33	1.38
38	A1	1124	PSU	C4-N3	-2.94	1.33	1.38
38	A1	2258	PSU	C4-N3	-2.94	1.33	1.38
38	A1	990	PSU	C4-N3	-2.93	1.33	1.38
38	A1	2826	PSU	C4-N3	-2.92	1.33	1.38
38	A1	2923	PSU	C6-C5	2.91	1.38	1.35
34	B5	999	PSU	C6-C5	2.91	1.38	1.35
38	A1	2865	PSU	C6-C5	2.90	1.38	1.35
34	B5	211	PSU	C4-N3	-2.90	1.33	1.38
38	A1	2258	PSU	C6-C5	2.89	1.38	1.35
38	A1	2260	PSU	C6-C5	2.89	1.38	1.35
38	A1	1110	PSU	C4-N3	-2.89	1.33	1.38
38	A1	1004	PSU	C4-N3	-2.89	1.33	1.38
38	A1	1042	PSU	C4-N3	-2.88	1.33	1.38
38	A1	1052	PSU	C4-N3	-2.88	1.33	1.38
34	B5	1773	4AC	C4-N4	-2.88	1.35	1.39
38	A1	990	PSU	C6-C5	2.88	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2921	OMU	C4-N3	-2.87	1.33	1.38
38	A1	2314	PSU	C4-N3	-2.87	1.33	1.38
34	B5	466	PSU	C4-N3	-2.87	1.33	1.38
38	A1	2260	PSU	C4-N3	-2.86	1.33	1.38
38	A1	1124	PSU	C6-C5	2.86	1.38	1.35
40	A4	73	PSU	C4-N3	-2.85	1.33	1.38
34	B5	106	PSU	C4-N3	-2.85	1.33	1.38
38	A1	2735	PSU	C4-N3	-2.84	1.33	1.38
34	B5	1415	PSU	C6-C5	2.84	1.38	1.35
34	B5	120	PSU	C6-C5	2.84	1.38	1.35
34	B5	302	PSU	C6-C5	2.84	1.38	1.35
38	A1	2142	1MA	C6-N6	2.83	1.35	1.27
38	A1	2865	PSU	C4-N3	-2.83	1.33	1.38
34	B5	1181	PSU	C4-N3	-2.82	1.33	1.38
34	B5	766	PSU	C6-C5	2.82	1.38	1.35
34	B5	766	PSU	C4-N3	-2.81	1.33	1.38
38	A1	2264	PSU	C6-C5	2.81	1.38	1.35
38	A1	645	1MA	C6-N6	2.80	1.34	1.27
38	A1	960	PSU	C4-N3	-2.80	1.33	1.38
38	A1	2133	PSU	C2-N3	-2.80	1.32	1.37
38	A1	1052	PSU	C6-C5	2.80	1.38	1.35
34	B5	120	PSU	C4-N3	-2.79	1.33	1.38
34	B5	1415	PSU	C4-N3	-2.78	1.33	1.38
38	A1	2266	PSU	C4-N3	-2.77	1.33	1.38
38	A1	2314	PSU	C6-C5	2.77	1.38	1.35
38	A1	2340	PSU	C6-C5	2.74	1.38	1.35
34	B5	1290	PSU	C6-C5	2.73	1.38	1.35
38	A1	1042	PSU	C6-C5	2.72	1.38	1.35
38	A1	2923	PSU	C4-N3	-2.71	1.33	1.38
34	B5	1187	PSU	C4-N3	-2.71	1.33	1.38
40	A4	73	PSU	C6-C5	2.69	1.38	1.35
38	A1	2278	5MC	C6-N1	-2.69	1.33	1.38
38	A1	2191	PSU	C6-C5	2.67	1.38	1.35
38	A1	2416	PSU	C2-N3	-2.66	1.33	1.37
38	A1	2416	PSU	C2-N1	-2.65	1.33	1.36
39	A3	50	PSU	C4-N3	-2.64	1.33	1.38
38	A1	2921	OMU	C2-N3	-2.64	1.33	1.38
34	B5	632	PSU	C6-C5	2.60	1.38	1.35
38	A1	2880	PSU	C2-N3	-2.60	1.33	1.37
38	A1	776	PSU	C6-C5	2.59	1.38	1.35
38	A1	2870	5MC	C6-C5	2.58	1.38	1.34
38	A1	960	PSU	O4'-C1'	-2.58	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2865	PSU	O4'-C1'	-2.56	1.40	1.43
38	A1	2735	PSU	C6-C5	2.56	1.38	1.35
38	A1	2351	PSU	C6-C5	2.55	1.38	1.35
34	B5	632	PSU	C2-N3	-2.54	1.33	1.37
38	A1	2944	PSU	C6-C5	2.54	1.38	1.35
38	A1	2975	PSU	C2-N1	-2.52	1.33	1.36
38	A1	1110	PSU	C6-C5	2.51	1.38	1.35
38	A1	966	PSU	C6-C5	2.51	1.38	1.35
38	A1	1056	PSU	C6-C5	2.51	1.38	1.35
38	A1	2922	OMG	C6-N1	-2.49	1.34	1.37
38	A1	986	PSU	C6-C5	2.47	1.38	1.35
38	A1	2129	PSU	C2-N3	-2.44	1.33	1.37
38	A1	2826	PSU	C6-C5	2.43	1.38	1.35
38	A1	2351	PSU	C2-N3	-2.42	1.33	1.37
38	A1	1110	PSU	C2-N1	-2.41	1.33	1.36
38	A1	2351	PSU	C2-N1	-2.41	1.33	1.36
38	A1	2191	PSU	C2-N3	-2.36	1.33	1.37
38	A1	2278	5MC	C6-C5	2.35	1.38	1.34
38	A1	2129	PSU	C2-N1	-2.35	1.33	1.36
38	A1	2975	PSU	C2-N3	-2.34	1.33	1.37
38	A1	2870	5MC	C6-N1	-2.34	1.34	1.38
38	A1	2880	PSU	C6-C5	2.34	1.37	1.35
34	B5	1575	G7M	C2-N1	-2.33	1.31	1.37
38	A1	2133	PSU	C2-N1	-2.33	1.33	1.36
38	A1	2340	PSU	C2-N1	-2.33	1.33	1.36
34	B5	302	PSU	C2-N3	-2.31	1.33	1.37
34	B5	999	PSU	C2-N1	-2.31	1.33	1.36
38	A1	2129	PSU	C6-C5	2.31	1.37	1.35
38	A1	1056	PSU	C2-N3	-2.30	1.33	1.37
38	A1	2880	PSU	C2-N1	-2.29	1.33	1.36
36	AB	243	HIC	CZ-NE2	-2.28	1.42	1.48
38	A1	2349	PSU	C6-C5	2.28	1.37	1.35
38	A1	2133	PSU	C6-C5	2.27	1.37	1.35
38	A1	776	PSU	C2-N3	-2.27	1.33	1.37
34	B5	1773	4AC	C6-N1	-2.26	1.32	1.38
38	A1	2826	PSU	C2-N3	-2.26	1.33	1.37
38	A1	2735	PSU	C2-N1	-2.26	1.33	1.36
38	A1	2340	PSU	C2-N3	-2.24	1.33	1.37
38	A1	986	PSU	C2-N3	-2.22	1.33	1.37
38	A1	776	PSU	C4-N3	-2.22	1.34	1.38
38	A1	1042	PSU	C2-N3	-2.22	1.33	1.37
38	A1	2191	PSU	C2-N1	-2.21	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2735	PSU	C2-N3	-2.20	1.33	1.37
38	A1	2349	PSU	C2-N3	-2.20	1.33	1.37
38	A1	1056	PSU	C2-N1	-2.20	1.33	1.36
34	B5	1782	MA6	C6-C5	2.19	1.48	1.44
38	A1	2314	PSU	C2-N3	-2.19	1.33	1.37
34	B5	106	PSU	C2-N3	-2.19	1.33	1.37
38	A1	2349	PSU	C2-N1	-2.19	1.33	1.36
38	A1	2416	PSU	C6-C5	2.19	1.37	1.35
38	A1	2975	PSU	C6-C5	2.19	1.37	1.35
38	A1	966	PSU	C2-N3	-2.17	1.33	1.37
40	A4	73	PSU	C2-N3	-2.17	1.33	1.37
38	A1	2921	OMU	C5-C4	-2.17	1.39	1.43
34	B5	999	PSU	C2-N3	-2.17	1.33	1.37
38	A1	2944	PSU	O4'-C1'	-2.16	1.40	1.43
38	A1	1004	PSU	C2-N1	-2.16	1.33	1.36
38	A1	2826	PSU	O4'-C1'	-2.16	1.40	1.43
34	B5	1781	MA6	C6-C5	2.15	1.48	1.44
38	A1	1124	PSU	C2-N3	-2.15	1.33	1.37
34	B5	211	PSU	C2-N3	-2.13	1.34	1.37
34	B5	302	PSU	C2-N1	-2.13	1.33	1.36
34	B5	466	PSU	C2-N3	-2.13	1.34	1.37
38	A1	2266	PSU	O4'-C1'	-2.12	1.40	1.43
34	B5	1191	B8N	CN1-N1	2.12	1.50	1.46
38	A1	986	PSU	O4'-C1'	-2.11	1.40	1.43
34	B5	1290	PSU	C2-N3	-2.10	1.34	1.37
38	A1	2865	PSU	C2-N1	-2.09	1.33	1.36
34	B5	766	PSU	O4'-C1'	-2.08	1.41	1.43
38	A1	1110	PSU	C2-N3	-2.08	1.34	1.37
38	A1	1124	PSU	C2-N1	-2.08	1.33	1.36
38	A1	2944	PSU	C2-N1	-2.08	1.33	1.36
34	B5	759	PSU	C2-N3	-2.08	1.34	1.37
38	A1	990	PSU	C2-N3	-2.07	1.34	1.37
38	A1	2258	PSU	C2-N3	-2.07	1.34	1.37
34	B5	120	PSU	C2-N3	-2.07	1.34	1.37
38	A1	1004	PSU	C2-N3	-2.07	1.34	1.37
34	B5	1575	G7M	C5-C6	-2.06	1.40	1.45
80	DC	699	DDE	CD2-NE2	2.06	1.39	1.36
38	A1	986	PSU	C2-N1	-2.06	1.34	1.36
34	B5	1415	PSU	C2-N3	-2.06	1.34	1.37
38	A1	2266	PSU	C2-N3	-2.05	1.34	1.37
38	A1	1052	PSU	C2-N3	-2.04	1.34	1.37
38	A1	2264	PSU	C2-N3	-2.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2944	PSU	C2-N3	-2.04	1.34	1.37
38	A1	2826	PSU	C2-N1	-2.04	1.34	1.36
34	B5	632	PSU	C2-N1	-2.03	1.34	1.36
34	B5	1187	PSU	C2-N3	-2.03	1.34	1.37
34	B5	766	PSU	C2-N1	-2.03	1.34	1.36
38	A1	2921	OMU	C6-N1	-2.03	1.33	1.38
38	A1	2266	PSU	C2-N1	-2.02	1.34	1.36
38	A1	966	PSU	C2-N1	-2.02	1.34	1.36
38	A1	2416	PSU	O4'-C1'	-2.01	1.41	1.43
38	A1	1052	PSU	C2-N1	-2.01	1.34	1.36

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1191	B8N	C32-C31-N3	37.44	177.60	112.16
34	B5	1773	4AC	N4-C4-N3	7.81	126.55	113.87
38	A1	2133	PSU	N1-C2-N3	7.25	122.82	115.17
38	A1	2634	UR3	C4-N3-C2	-7.13	118.84	124.58
34	B5	766	PSU	N1-C2-N3	7.00	122.55	115.17
38	A1	2944	PSU	N1-C2-N3	6.98	122.53	115.17
38	A1	2258	PSU	N1-C2-N3	6.89	122.43	115.17
38	A1	2975	PSU	N1-C2-N3	6.80	122.34	115.17
38	A1	1056	PSU	N1-C2-N3	6.76	122.30	115.17
38	A1	986	PSU	N1-C2-N3	6.75	122.29	115.17
38	A1	2129	PSU	N1-C2-N3	6.75	122.29	115.17
34	B5	999	PSU	N1-C2-N3	6.75	122.29	115.17
38	A1	1110	PSU	N1-C2-N3	6.71	122.24	115.17
34	B5	302	PSU	N1-C2-N3	6.68	122.22	115.17
34	B5	1181	PSU	N1-C2-N3	6.66	122.20	115.17
38	A1	2865	PSU	N1-C2-N3	6.66	122.19	115.17
34	B5	632	PSU	N1-C2-N3	6.66	122.19	115.17
34	B5	1290	PSU	N1-C2-N3	6.65	122.18	115.17
38	A1	2264	PSU	N1-C2-N3	6.64	122.18	115.17
38	A1	2191	PSU	N1-C2-N3	6.64	122.18	115.17
38	A1	2880	PSU	N1-C2-N3	6.60	122.13	115.17
38	A1	2260	PSU	N1-C2-N3	6.58	122.11	115.17
34	B5	759	PSU	N1-C2-N3	6.56	122.09	115.17
34	B5	466	PSU	N1-C2-N3	6.53	122.06	115.17
34	B5	1415	PSU	N1-C2-N3	6.51	122.04	115.17
39	A3	50	PSU	N1-C2-N3	6.51	122.03	115.17
38	A1	2416	PSU	N1-C2-N3	6.50	122.02	115.17
34	B5	211	PSU	N1-C2-N3	6.48	122.00	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2923	PSU	N1-C2-N3	6.48	122.00	115.17
34	B5	1187	PSU	N1-C2-N3	6.47	122.00	115.17
38	A1	1052	PSU	N1-C2-N3	6.47	121.99	115.17
38	A1	1004	PSU	N1-C2-N3	6.45	121.97	115.17
38	A1	990	PSU	N1-C2-N3	6.44	121.96	115.17
38	A1	966	PSU	N1-C2-N3	6.43	121.95	115.17
38	A1	1124	PSU	N1-C2-N3	6.41	121.94	115.17
38	A1	2340	PSU	N1-C2-N3	6.40	121.92	115.17
38	A1	2351	PSU	N1-C2-N3	6.37	121.89	115.17
38	A1	2266	PSU	N1-C2-N3	6.37	121.88	115.17
38	A1	2826	PSU	N1-C2-N3	6.36	121.88	115.17
38	A1	960	PSU	N1-C2-N3	6.35	121.87	115.17
38	A1	2735	PSU	N1-C2-N3	6.33	121.85	115.17
38	A1	2314	PSU	N1-C2-N3	6.28	121.80	115.17
34	B5	120	PSU	N1-C2-N3	6.27	121.78	115.17
34	B5	106	PSU	N1-C2-N3	6.26	121.77	115.17
38	A1	2349	PSU	N1-C2-N3	6.26	121.77	115.17
38	A1	776	PSU	N1-C2-N3	6.22	121.73	115.17
40	A4	73	PSU	N1-C2-N3	6.10	121.60	115.17
38	A1	1042	PSU	N1-C2-N3	6.05	121.55	115.17
34	B5	1782	MA6	C2-N1-C6	5.50	122.23	116.84
34	B5	1781	MA6	C2-N1-C6	5.45	122.19	116.84
34	B5	1191	B8N	C4-N3-C2	-5.35	119.03	125.62
34	B5	1773	4AC	C5-C4-N4	-5.04	114.44	122.94
38	A1	2921	OMU	C4-N3-C2	-4.98	120.42	126.61
38	A1	2133	PSU	C4-N3-C2	-4.63	120.00	126.37
38	A1	2880	PSU	C4-N3-C2	-4.61	120.02	126.37
34	B5	632	PSU	C4-N3-C2	-4.59	120.05	126.37
34	B5	1290	PSU	C4-N3-C2	-4.51	120.16	126.37
34	B5	302	PSU	C4-N3-C2	-4.47	120.21	126.37
38	A1	2129	PSU	C4-N3-C2	-4.47	120.22	126.37
38	A1	1056	PSU	C4-N3-C2	-4.46	120.23	126.37
38	A1	2975	PSU	C4-N3-C2	-4.45	120.24	126.37
38	A1	986	PSU	C4-N3-C2	-4.44	120.25	126.37
38	A1	776	PSU	C6-C5-C4	-4.40	115.20	118.17
38	A1	2944	PSU	C4-N3-C2	-4.40	120.31	126.37
38	A1	2191	PSU	C4-N3-C2	-4.40	120.32	126.37
34	B5	759	PSU	C4-N3-C2	-4.39	120.33	126.37
38	A1	2258	PSU	C4-N3-C2	-4.37	120.35	126.37
38	A1	2826	PSU	C4-N3-C2	-4.36	120.36	126.37
38	A1	2351	PSU	C4-N3-C2	-4.35	120.38	126.37
34	B5	1181	PSU	C4-N3-C2	-4.34	120.39	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2349	PSU	C4-N3-C2	-4.34	120.39	126.37
38	A1	2735	PSU	C4-N3-C2	-4.34	120.39	126.37
38	A1	966	PSU	C4-N3-C2	-4.32	120.42	126.37
38	A1	2416	PSU	C4-N3-C2	-4.32	120.43	126.37
34	B5	766	PSU	C4-N3-C2	-4.30	120.44	126.37
38	A1	1052	PSU	C4-N3-C2	-4.30	120.45	126.37
34	B5	1415	PSU	C4-N3-C2	-4.30	120.45	126.37
38	A1	2921	OMU	N3-C2-N1	4.28	120.46	114.89
38	A1	1110	PSU	C4-N3-C2	-4.27	120.48	126.37
38	A1	2314	PSU	C4-N3-C2	-4.27	120.49	126.37
38	A1	2260	PSU	C4-N3-C2	-4.27	120.50	126.37
38	A1	990	PSU	C4-N3-C2	-4.25	120.51	126.37
34	B5	766	PSU	O2-C2-N1	-4.23	118.43	122.79
34	B5	999	PSU	C4-N3-C2	-4.23	120.55	126.37
38	A1	2923	PSU	C4-N3-C2	-4.23	120.55	126.37
38	A1	2260	PSU	O2-C2-N1	-4.23	118.43	122.79
34	B5	999	PSU	O2-C2-N1	-4.22	118.43	122.79
38	A1	1124	PSU	C4-N3-C2	-4.21	120.57	126.37
38	A1	2865	PSU	O2-C2-N1	-4.19	118.47	122.79
38	A1	776	PSU	C4-N3-C2	-4.17	120.62	126.37
34	B5	466	PSU	C4-N3-C2	-4.17	120.62	126.37
38	A1	2975	PSU	O2-C2-N1	-4.17	118.49	122.79
38	A1	960	PSU	C4-N3-C2	-4.16	120.64	126.37
40	A4	73	PSU	C4-N3-C2	-4.15	120.65	126.37
38	A1	2944	PSU	O2-C2-N1	-4.09	118.57	122.79
34	B5	120	PSU	C4-N3-C2	-4.08	120.74	126.37
38	A1	1056	PSU	O2-C2-N1	-4.08	118.58	122.79
38	A1	2264	PSU	C4-N3-C2	-4.08	120.75	126.37
38	A1	1004	PSU	C4-N3-C2	-4.07	120.77	126.37
38	A1	1004	PSU	O2-C2-N1	-4.07	118.60	122.79
38	A1	1110	PSU	O2-C2-N1	-4.05	118.61	122.79
38	A1	2735	PSU	O2-C2-N1	-4.05	118.61	122.79
38	A1	2865	PSU	C4-N3-C2	-4.04	120.80	126.37
34	B5	106	PSU	C4-N3-C2	-4.04	120.81	126.37
34	B5	1187	PSU	C4-N3-C2	-4.02	120.83	126.37
38	A1	1042	PSU	C4-N3-C2	-3.96	120.92	126.37
38	A1	2826	PSU	O2-C2-N1	-3.94	118.72	122.79
38	A1	2340	PSU	C4-N3-C2	-3.94	120.95	126.37
39	A3	50	PSU	C4-N3-C2	-3.90	121.00	126.37
34	B5	211	PSU	C4-N3-C2	-3.90	121.00	126.37
38	A1	2921	OMU	C5-C4-N3	3.89	120.25	114.80
38	A1	1052	PSU	O2-C2-N1	-3.88	118.78	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2923	PSU	O2-C2-N1	-3.87	118.80	122.79
38	A1	2349	PSU	O2-C2-N1	-3.87	118.80	122.79
38	A1	2880	PSU	O2-C2-N1	-3.86	118.80	122.79
34	B5	1181	PSU	O2-C2-N1	-3.86	118.81	122.79
38	A1	2416	PSU	O2-C2-N1	-3.86	118.81	122.79
38	A1	2129	PSU	O2-C2-N1	-3.83	118.84	122.79
38	A1	1124	PSU	O2-C2-N1	-3.82	118.85	122.79
38	A1	966	PSU	O2-C2-N1	-3.80	118.87	122.79
39	A3	50	PSU	O2-C2-N1	-3.76	118.91	122.79
38	A1	2264	PSU	O2-C2-N1	-3.75	118.92	122.79
38	A1	2266	PSU	C4-N3-C2	-3.75	121.20	126.37
38	A1	960	PSU	O2-C2-N1	-3.75	118.92	122.79
38	A1	986	PSU	O2-C2-N1	-3.75	118.92	122.79
38	A1	2266	PSU	O2-C2-N1	-3.73	118.94	122.79
38	A1	2340	PSU	O2-C2-N1	-3.71	118.96	122.79
34	B5	1187	PSU	O2-C2-N1	-3.71	118.97	122.79
38	A1	2258	PSU	O2-C2-N1	-3.71	118.97	122.79
38	A1	2351	PSU	O2-C2-N1	-3.68	118.99	122.79
34	B5	759	PSU	O2-C2-N1	-3.68	118.99	122.79
34	B5	1290	PSU	O2-C2-N1	-3.68	119.00	122.79
34	B5	1781	MA6	N3-C2-N1	-3.64	123.73	128.67
34	B5	302	PSU	O2-C2-N1	-3.62	119.06	122.79
34	B5	1782	MA6	N3-C2-N1	-3.60	123.78	128.67
34	B5	466	PSU	O2-C2-N1	-3.59	119.09	122.79
38	A1	990	PSU	O2-C2-N1	-3.54	119.14	122.79
34	B5	120	PSU	O2-C2-N1	-3.51	119.17	122.79
38	A1	2191	PSU	O2-C2-N1	-3.51	119.17	122.79
34	B5	106	PSU	O2-C2-N1	-3.48	119.20	122.79
34	B5	1415	PSU	O2-C2-N1	-3.46	119.22	122.79
38	A1	2314	PSU	O2-C2-N1	-3.43	119.25	122.79
38	A1	2870	5MC	C5-C6-N1	-3.43	119.59	123.31
38	A1	2278	5MC	C5-C6-N1	-3.38	119.64	123.31
38	A1	2634	UR3	C5-C4-N3	3.32	119.42	115.04
34	B5	632	PSU	O2-C2-N1	-3.31	119.38	122.79
34	B5	1280	4AC	N4-C4-N3	3.25	119.15	113.87
34	B5	1773	4AC	CM7-C7-N4	3.25	120.51	115.27
40	A4	73	PSU	O2-C2-N1	-3.23	119.45	122.79
34	B5	1191	B8N	N3-C2-N1	3.20	120.63	116.72
38	A1	2133	PSU	O2-C2-N1	-3.20	119.49	122.79
34	B5	211	PSU	O2-C2-N1	-3.18	119.51	122.79
38	A1	1042	PSU	O2-C2-N1	-3.08	119.61	122.79
38	A1	2921	OMU	O4-C4-C5	-3.04	119.92	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1782	MA6	C4-C5-N7	-2.95	106.22	109.34
38	A1	645	1MA	C8-N7-C5	2.89	107.47	102.55
34	B5	1781	MA6	C4-C5-N7	-2.89	106.29	109.34
38	A1	2922	OMG	C8-N7-C5	2.89	107.46	102.55
34	B5	1782	MA6	N1-C6-N6	2.76	120.02	116.83
34	B5	1773	4AC	C6-C5-C4	2.75	120.32	117.00
34	B5	1191	B8N	C31-N3-C2	2.75	121.70	117.64
38	A1	2133	PSU	C5-C6-N1	-2.71	118.39	122.14
38	A1	2921	OMU	O2-C2-N1	-2.67	119.32	122.80
38	A1	2142	1MA	C8-N7-C5	2.64	107.05	102.55
38	A1	2870	5MC	C5-C4-N3	-2.59	119.10	121.75
34	B5	632	PSU	C5-C6-N1	-2.57	118.57	122.14
34	B5	1290	PSU	C5-C6-N1	-2.56	118.59	122.14
38	A1	986	PSU	C5-C6-N1	-2.52	118.64	122.14
38	A1	2826	PSU	C5-C6-N1	-2.48	118.69	122.14
38	A1	2278	5MC	C5-C4-N3	-2.48	119.21	121.75
38	A1	645	1MA	C5-C6-N1	2.43	117.45	113.95
38	A1	2142	1MA	C5-C6-N1	2.38	117.37	113.95
38	A1	776	PSU	O2-C2-N1	-2.38	120.34	122.79
38	A1	2314	PSU	C5-C6-N1	-2.37	118.86	122.14
38	A1	2133	PSU	O2-C2-N3	-2.35	117.69	121.86
34	B5	1415	PSU	C5-C6-N1	-2.33	118.90	122.14
34	B5	759	PSU	C5-C6-N1	-2.32	118.93	122.14
38	A1	2975	PSU	C5-C6-N1	-2.31	118.94	122.14
38	A1	2129	PSU	C5-C6-N1	-2.30	118.94	122.14
38	A1	2258	PSU	C5-C6-N1	-2.30	118.95	122.14
34	B5	1773	4AC	C5-C4-N3	-2.29	119.01	122.60
34	B5	1781	MA6	N1-C6-N6	2.29	119.48	116.83
34	B5	1575	G7M	C2-N1-C6	-2.29	120.92	125.11
38	A1	990	PSU	C5-C6-N1	-2.27	118.99	122.14
38	A1	2634	UR3	C3U-N3-C2	2.26	121.27	117.33
38	A1	645	1MA	N1-C2-N3	-2.25	123.08	125.90
38	A1	2922	OMG	C5-C6-N1	2.24	118.34	114.07
34	B5	302	PSU	C5-C6-N1	-2.24	119.03	122.14
38	A1	776	PSU	O2-C2-N3	-2.21	117.94	121.86
38	A1	2880	PSU	C5-C6-N1	-2.20	119.08	122.14
38	A1	2865	PSU	O4 ¹ -C1 ¹ -C2 ¹	2.20	108.20	105.15
38	A1	2944	PSU	C5-C6-N1	-2.20	119.09	122.14
38	A1	966	PSU	C5-C6-N1	-2.19	119.10	122.14
34	B5	999	PSU	O4 ¹ -C1 ¹ -C2 ¹	2.15	108.13	105.15
34	B5	1181	PSU	C5-C6-N1	-2.15	119.15	122.14
34	B5	766	PSU	O4 ¹ -C1 ¹ -C2 ¹	2.15	108.13	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2191	PSU	O4'-C1'-C2'	2.15	108.13	105.15
38	A1	2351	PSU	C5-C6-N1	-2.14	119.17	122.14
38	A1	960	PSU	C5-C6-N1	-2.13	119.18	122.14
34	B5	766	PSU	C5-C6-N1	-2.10	119.23	122.14
38	A1	1056	PSU	C5-C6-N1	-2.10	119.23	122.14
34	B5	1191	B8N	O4'-C1'-C2'	2.10	108.05	105.15
38	A1	2826	PSU	O4'-C1'-C2'	2.10	108.05	105.15
38	A1	2278	5MC	O2-C2-N3	-2.10	119.02	122.33
38	A1	2921	OMU	CM2-O2'-C2'	-2.09	109.10	114.47
80	DC	699	DDE	CAU-CBW-CBI	-2.09	107.13	111.22
38	A1	2260	PSU	C5-C6-N1	-2.09	119.25	122.14
38	A1	2260	PSU	O4'-C1'-C2'	2.09	108.04	105.15
38	A1	1124	PSU	C5-C6-N1	-2.08	119.26	122.14
34	B5	466	PSU	C5-C6-N1	-2.07	119.26	122.14
38	A1	776	PSU	O4'-C1'-C2'	2.06	108.01	105.15
34	B5	120	PSU	C5-C6-N1	-2.06	119.28	122.14
38	A1	1052	PSU	C5-C6-N1	-2.05	119.29	122.14
40	A4	73	PSU	C5-C6-N1	-2.05	119.30	122.14
38	A1	2142	1MA	N1-C2-N3	-2.04	123.34	125.90
38	A1	2944	PSU	O4'-C1'-C2'	2.03	107.96	105.15
38	A1	2735	PSU	C5-C6-N1	-2.03	119.33	122.14
38	A1	986	PSU	O4'-C1'-C2'	2.02	107.95	105.15
38	A1	2416	PSU	C5-C6-N1	-2.02	119.33	122.14

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	AB	243	HIC	CA-CB-CG-ND1
36	AB	243	HIC	CA-CB-CG-CD2
80	DC	699	DDE	O-C-CA-CB
80	DC	699	DDE	N-CA-CB-CG
80	DC	699	DDE	C-CA-CB-CG
80	DC	699	DDE	CAU-CAT-CE1-NE2
80	DC	699	DDE	CBI-CBW-NCB-CAB
80	DC	699	DDE	CAT-CAU-CBW-NCB
34	B5	1280	4AC	N3-C4-N4-C7
34	B5	1280	4AC	C5-C4-N4-C7
34	B5	1773	4AC	N3-C4-N4-C7
34	B5	1773	4AC	O7-C7-N4-C4
34	B5	1773	4AC	CM7-C7-N4-C4
34	B5	1782	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
38	A1	1042	PSU	O4'-C1'-C5-C4
38	A1	1042	PSU	O4'-C1'-C5-C6
38	A1	2258	PSU	O4'-C4'-C5'-O5'
38	A1	2266	PSU	C2'-C1'-C5-C4
38	A1	2870	5MC	C2'-C1'-N1-C2
38	A1	2870	5MC	C2'-C1'-N1-C6
34	B5	211	PSU	C3'-C4'-C5'-O5'
34	B5	1187	PSU	O4'-C4'-C5'-O5'
38	A1	2923	PSU	C3'-C4'-C5'-O5'
80	DC	699	DDE	CAT-CAU-CBW-CBI
38	A1	2923	PSU	O4'-C4'-C5'-O5'
34	B5	1782	MA6	N1-C6-N6-C9
34	B5	1782	MA6	C3'-C4'-C5'-O5'
38	A1	2258	PSU	C3'-C4'-C5'-O5'
34	B5	1781	MA6	N1-C6-N6-C9
34	B5	211	PSU	O4'-C4'-C5'-O5'
34	B5	1187	PSU	C3'-C4'-C5'-O5'
80	DC	699	DDE	CBI-CBW-NCB-CAC
80	DC	699	DDE	CAU-CBW-NCB-CAB
80	DC	699	DDE	CAU-CBW-NCB-CAC
34	B5	766	PSU	C3'-C4'-C5'-O5'
34	B5	1575	G7M	O4'-C4'-C5'-O5'
38	A1	2923	PSU	C4'-C5'-O5'-P
34	B5	1575	G7M	C3'-C4'-C5'-O5'
38	A1	2870	5MC	O4'-C1'-N1-C6
34	B5	1782	MA6	C5-C6-N6-C9
80	DC	699	DDE	CE1-CAT-CAU-CBW
38	A1	2340	PSU	C4'-C5'-O5'-P
34	B5	1181	PSU	O4'-C1'-C5-C4
34	B5	1191	B8N	O4'-C1'-C5-C4
38	A1	2340	PSU	C3'-C4'-C5'-O5'
38	A1	2266	PSU	C4'-C5'-O5'-P
38	A1	2870	5MC	O4'-C1'-N1-C2
38	A1	2264	PSU	C3'-C4'-C5'-O5'
38	A1	2314	PSU	C4'-C5'-O5'-P
34	B5	766	PSU	O4'-C4'-C5'-O5'
38	A1	960	PSU	O4'-C1'-C5-C6
34	B5	1415	PSU	C3'-C4'-C5'-O5'
38	A1	2266	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
85	SO1	DC	903	-	34,39,39	0.68	1 (2%)	38,64,64	1.23	5 (13%)
83	GDP	DC	901	84	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)

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
85	SO1	DC	903	-	1/1/15/16	4/21/104/104	0/7/5/5
83	GDP	DC	901	84	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	DC	903	SO1	O14-C5	-2.95	1.19	1.30
83	DC	901	GDP	C6-N1	-2.10	1.34	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	DC	903	SO1	C12-C6-C2	-4.51	98.10	105.09
83	DC	901	GDP	C8-N7-C5	2.83	107.37	102.55
85	DC	903	SO1	C7-C2-C6	2.37	116.58	112.05
85	DC	903	SO1	O57-C53-C54	-2.29	104.98	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	DC	903	SO1	C21-C13-C4	2.28	118.49	112.41
85	DC	903	SO1	C18-C9-C16	-2.11	100.84	103.72
83	DC	901	GDP	C4'-O4'-C1'	2.02	111.78	109.92

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
85	DC	903	SO1	C4

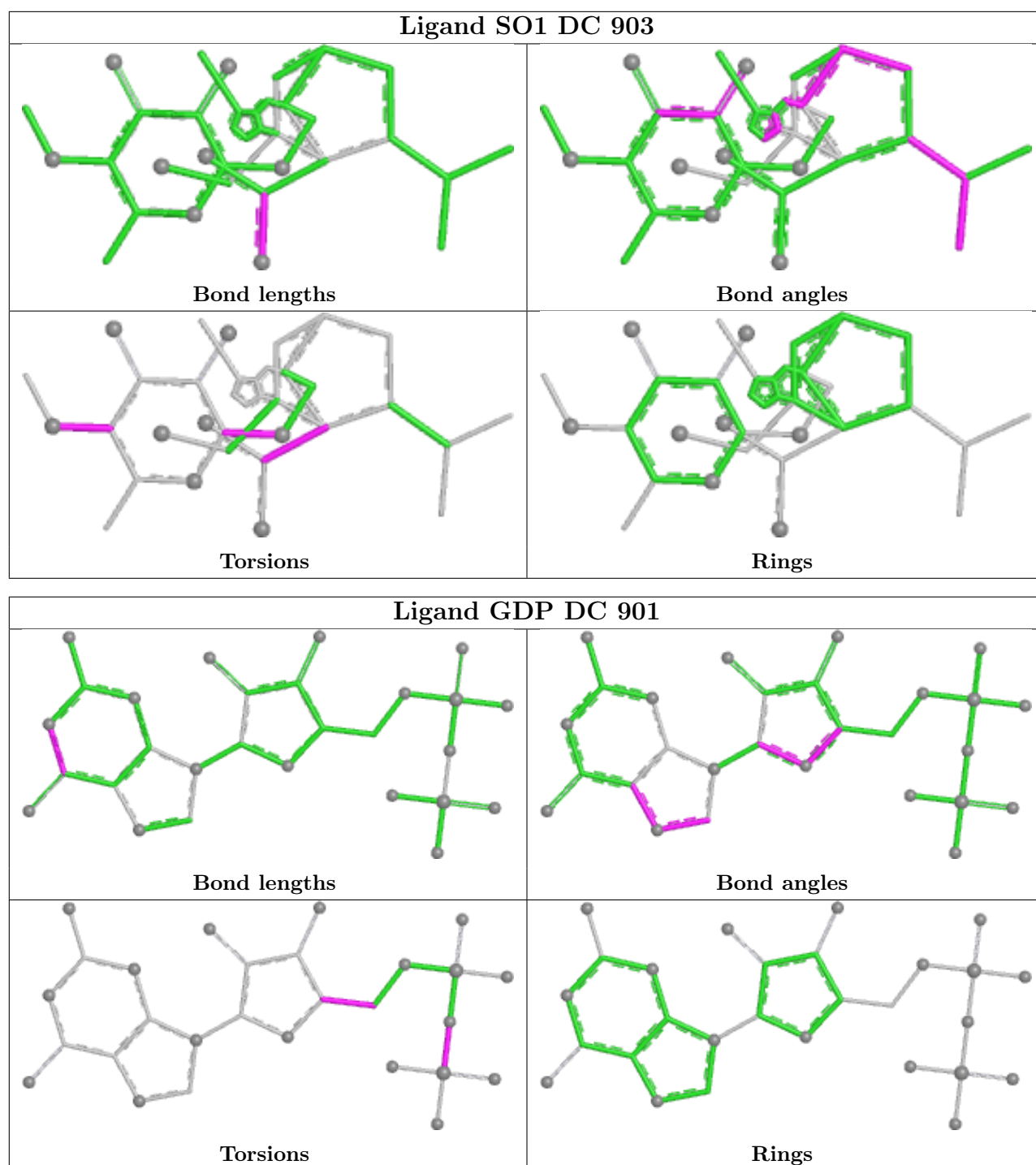
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	DC	903	SO1	C2-C1-C5-O14
85	DC	903	SO1	C2-C1-C5-O15
85	DC	903	SO1	O56-C52-O17-C8
85	DC	903	SO1	C54-C55-O64-C65
83	DC	901	GDP	PA-O3A-PB-O2B
83	DC	901	GDP	C3'-C4'-C5'-O5'
83	DC	901	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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
38	A1	1
77	Ao	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	1282:G	O3'	1283:C	P	4.95
1	Ao	105:GLN	C	106:PHE	N	3.24

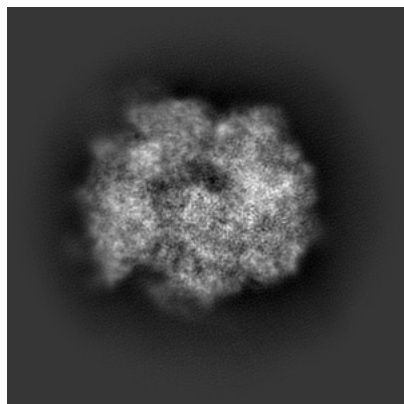
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41001. These allow visual inspection of the internal detail of the map and identification of artifacts.

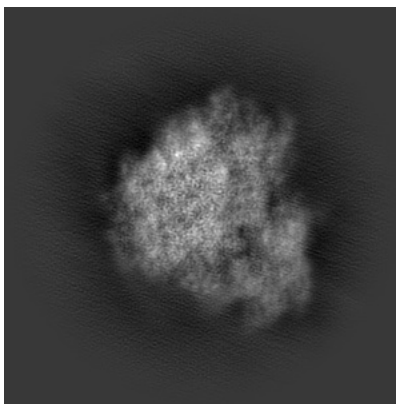
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

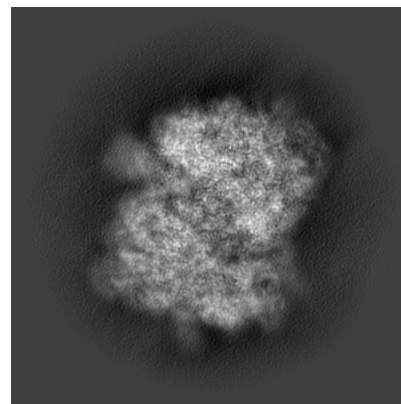
6.1.1 Primary map



X

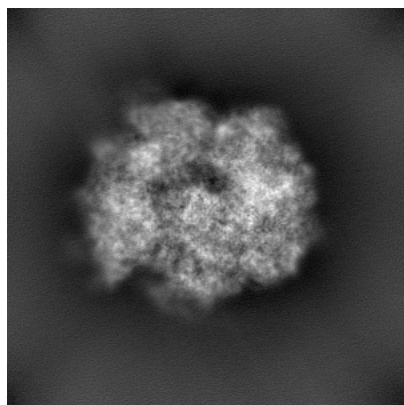


Y

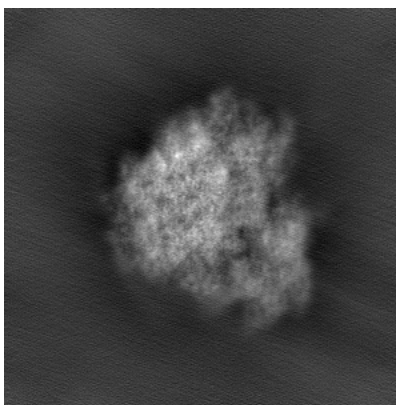


Z

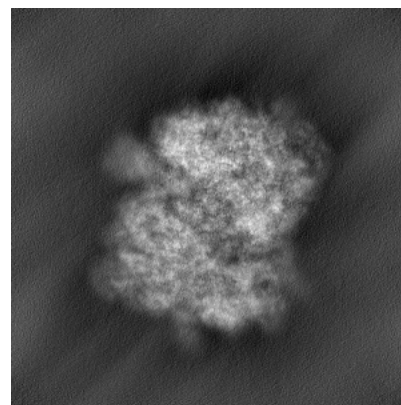
6.1.2 Raw map



X



Y

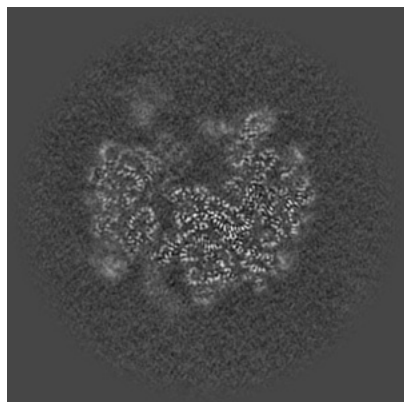


Z

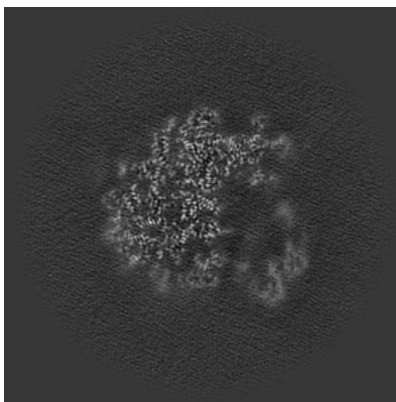
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

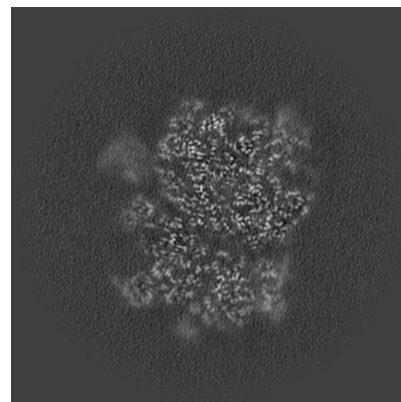
6.2.1 Primary map



X Index: 200

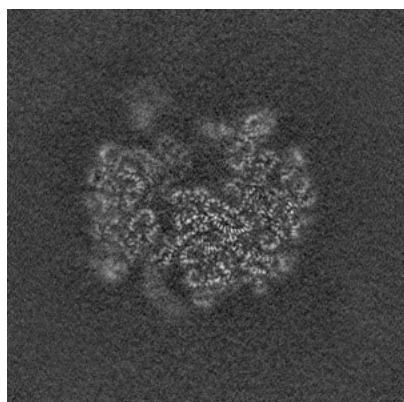


Y Index: 200

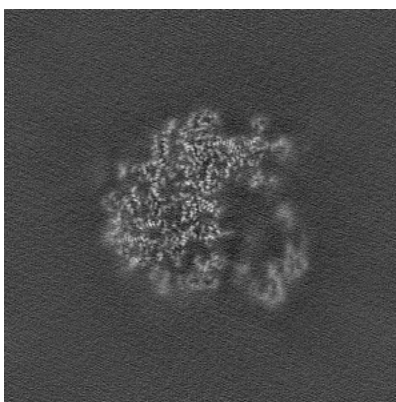


Z Index: 200

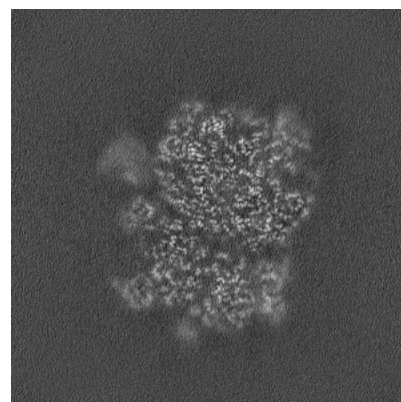
6.2.2 Raw map



X Index: 200



Y Index: 200

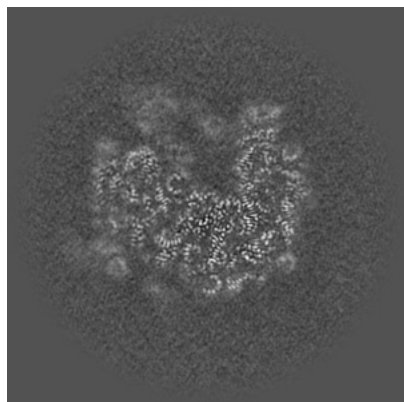


Z Index: 200

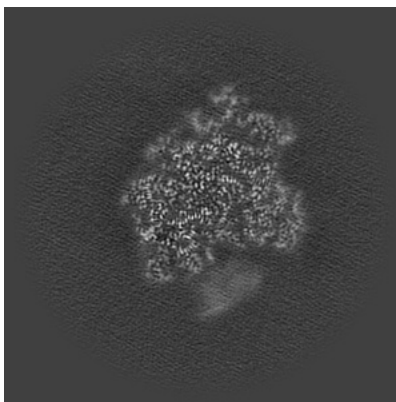
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

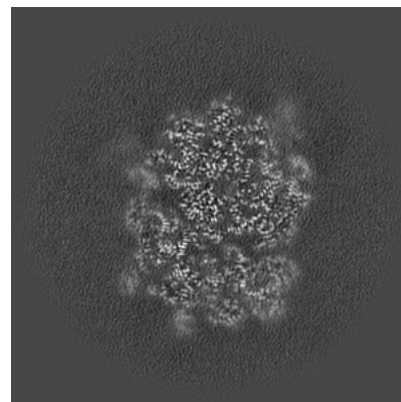
6.3.1 Primary map



X Index: 192

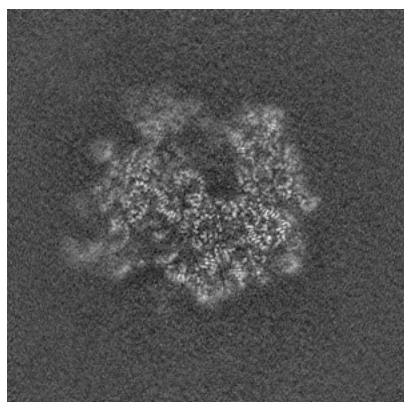


Y Index: 245

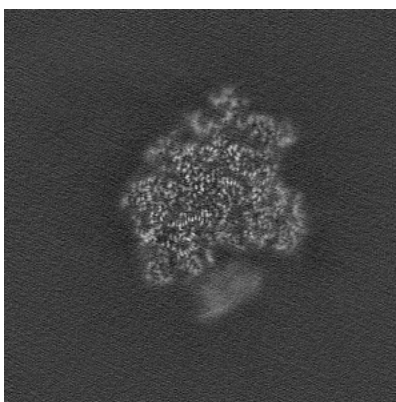


Z Index: 190

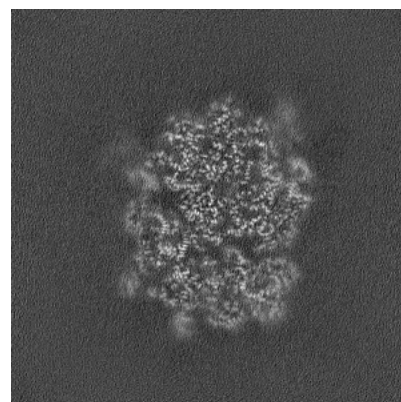
6.3.2 Raw map



X Index: 185



Y Index: 245

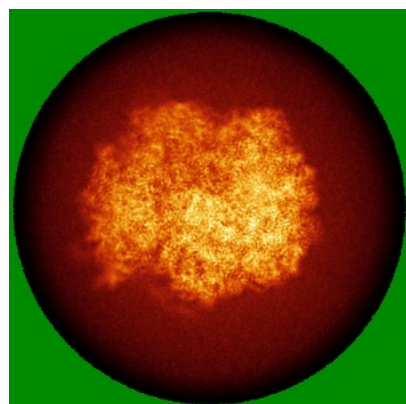


Z Index: 190

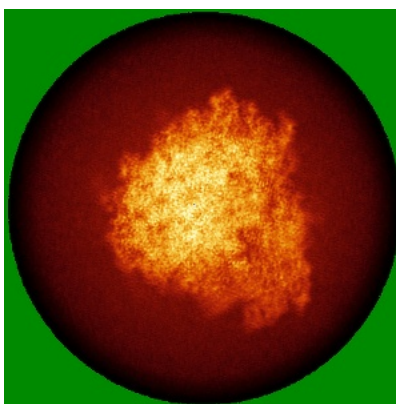
The images above show the largest variance slices of the map in three orthogonal directions.

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

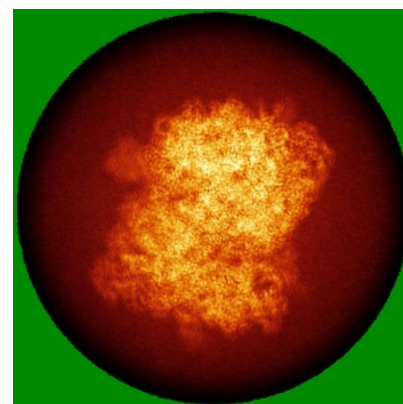
6.4.1 Primary map



X

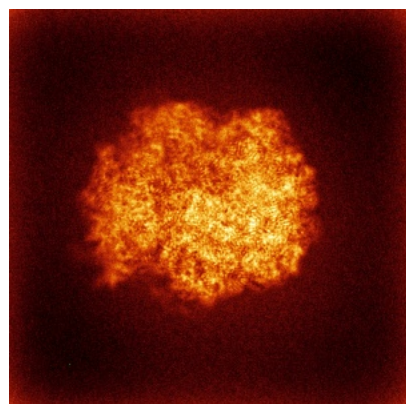


Y

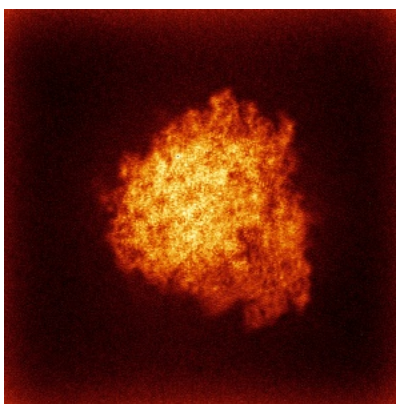


Z

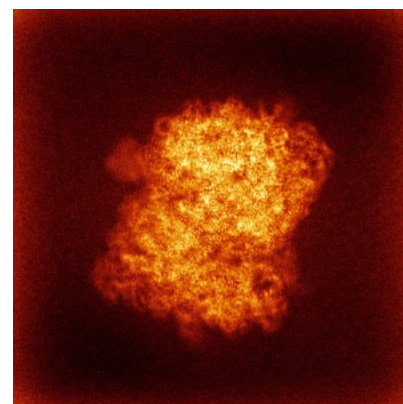
6.4.2 Raw map



X



Y

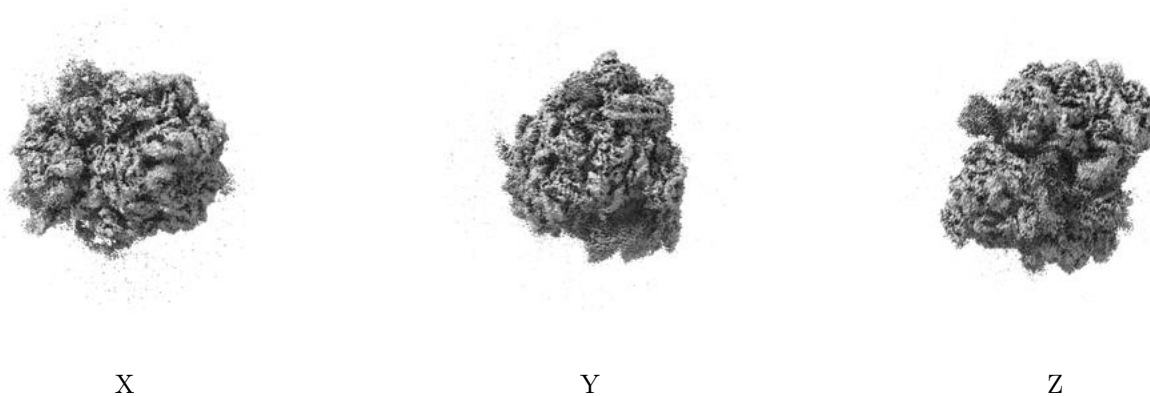


Z

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

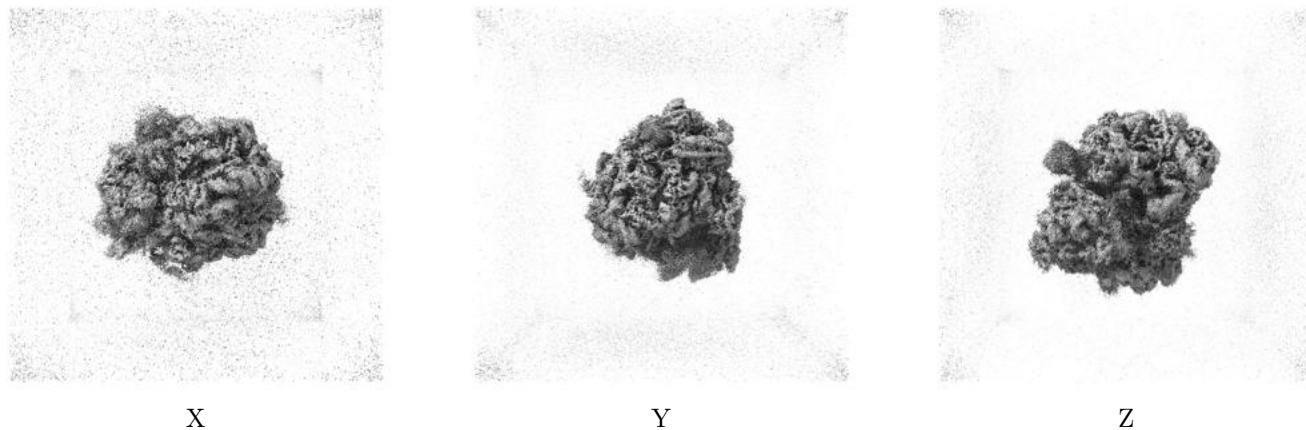
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

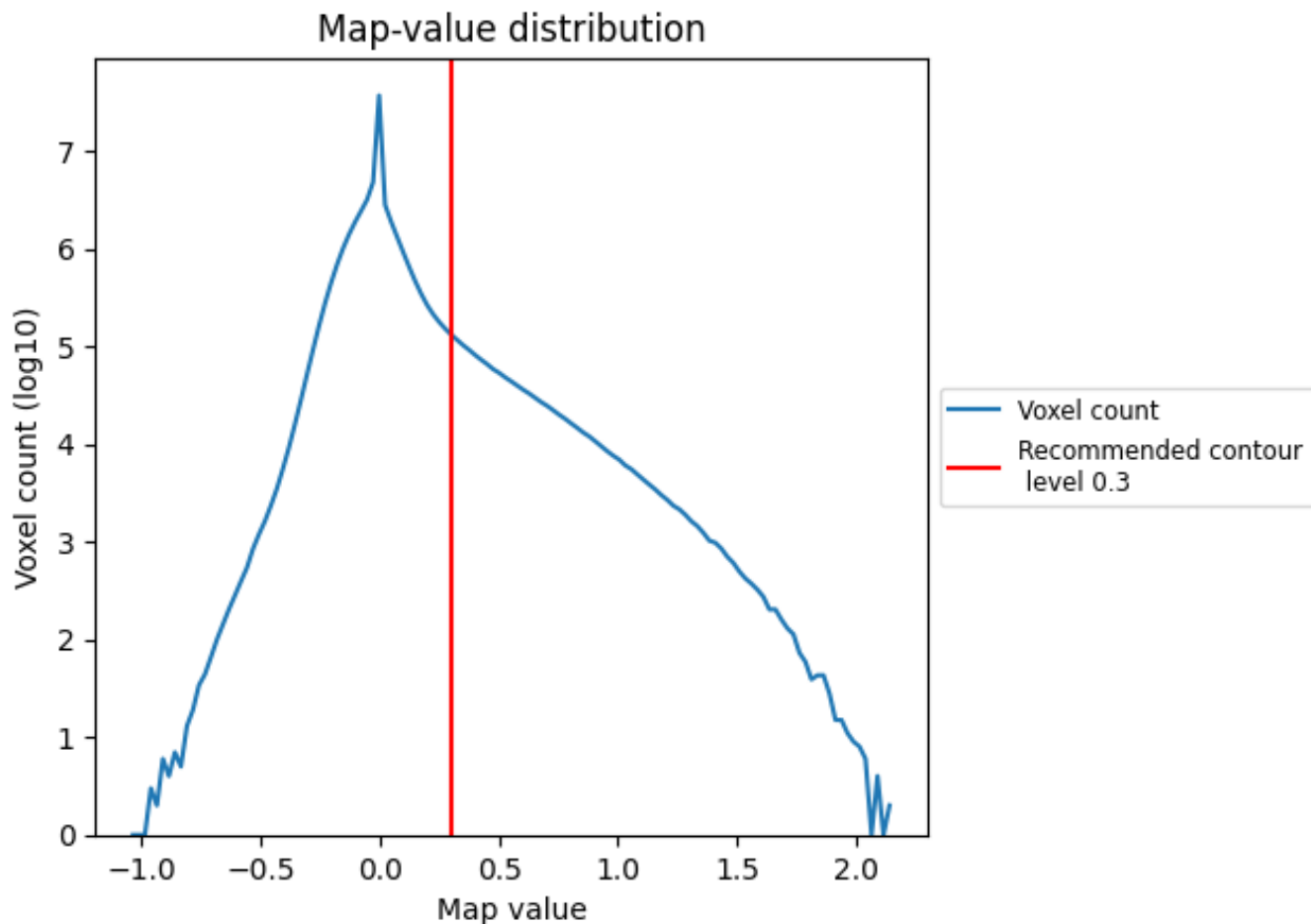
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

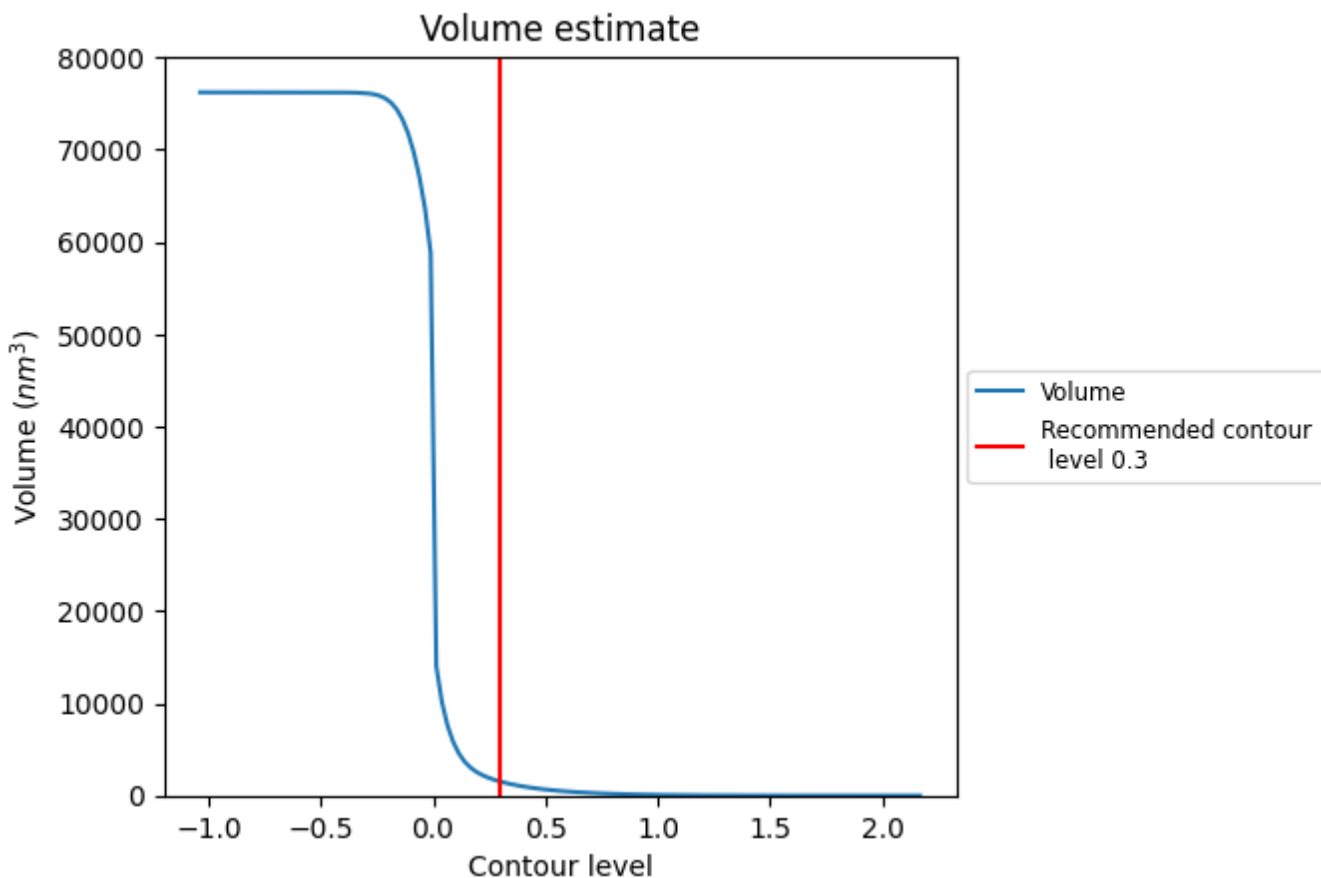
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

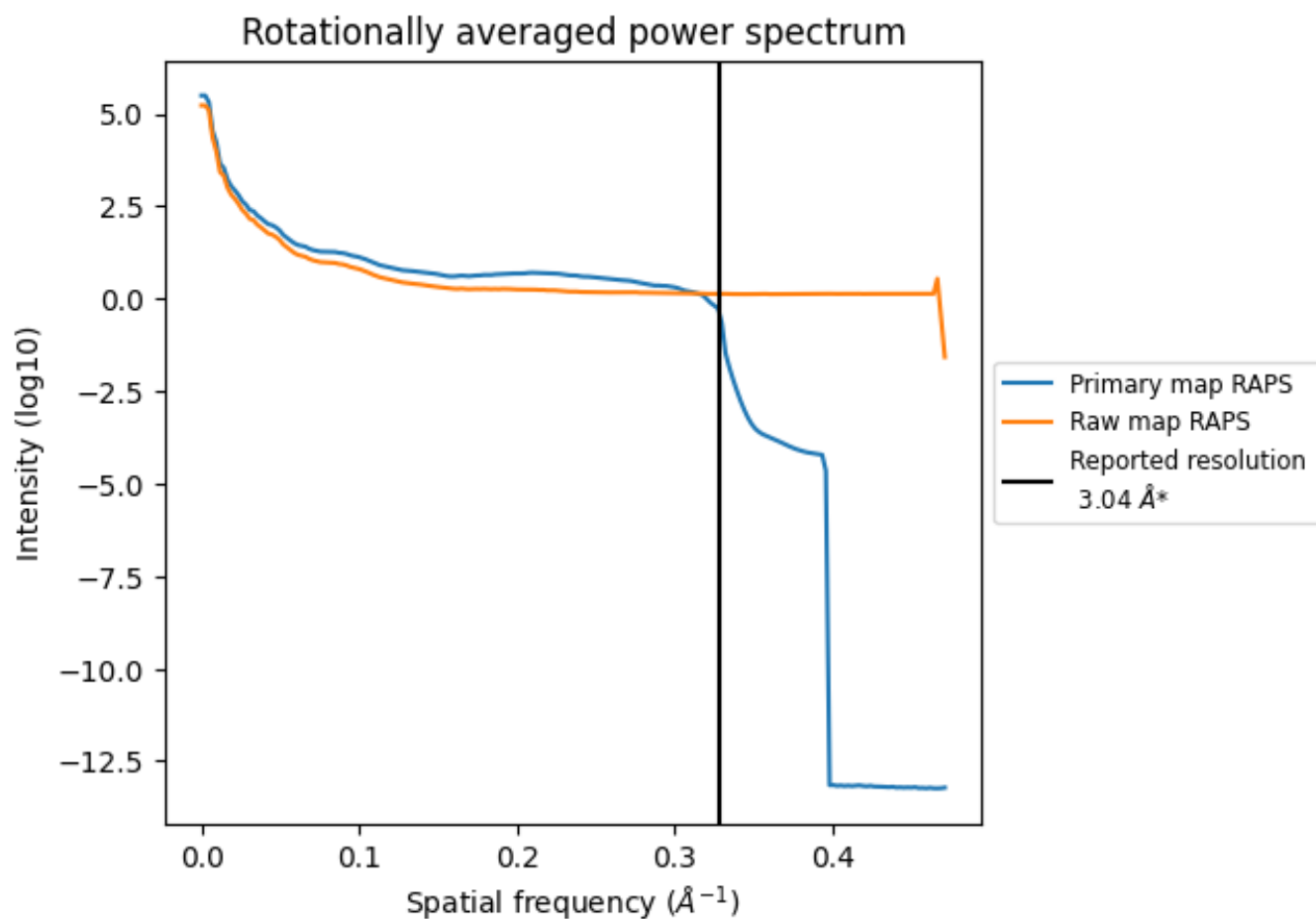
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1514 nm³; this corresponds to an approximate mass of 1367 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

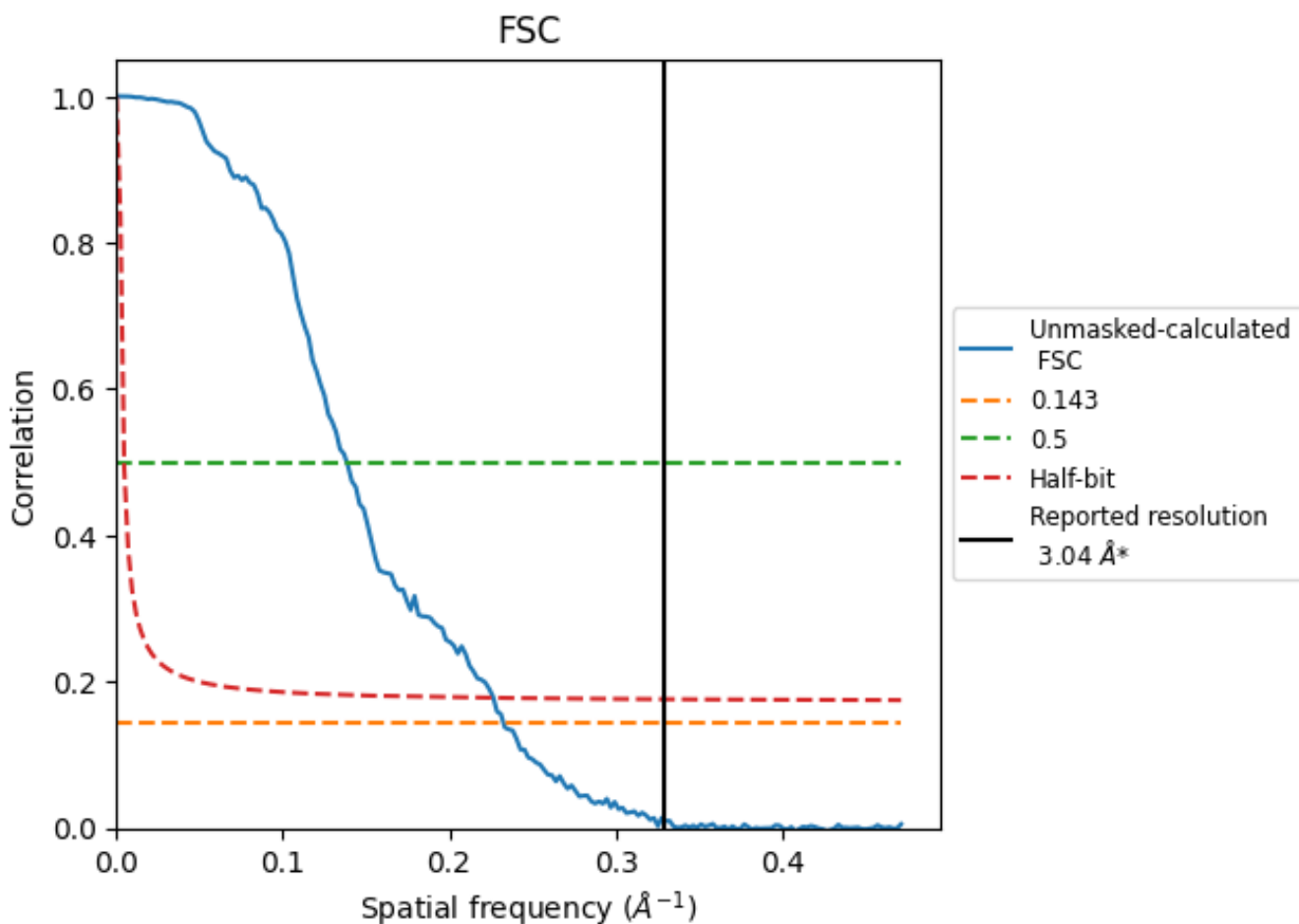


*Reported resolution corresponds to spatial frequency of 0.329 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.329 \AA^{-1}

8.2 Resolution estimates [i](#)

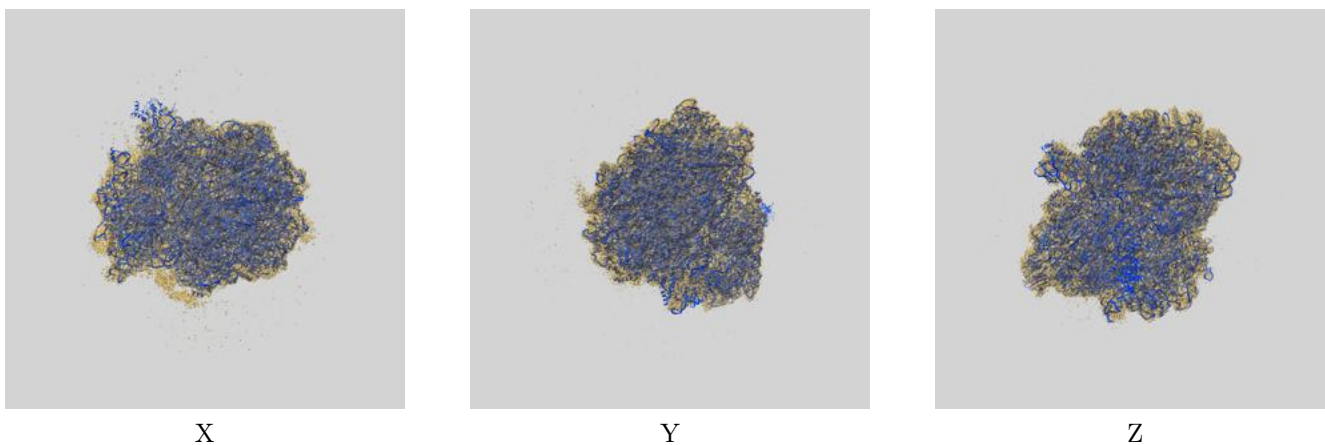
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.30	7.23	4.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

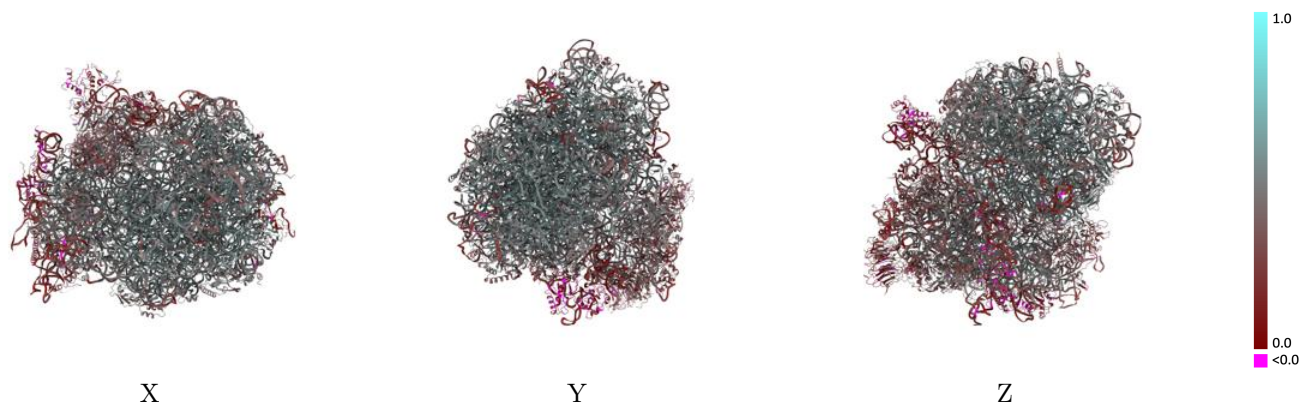
This section contains information regarding the fit between EMDB map EMD-41001 and PDB model 8T3E. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



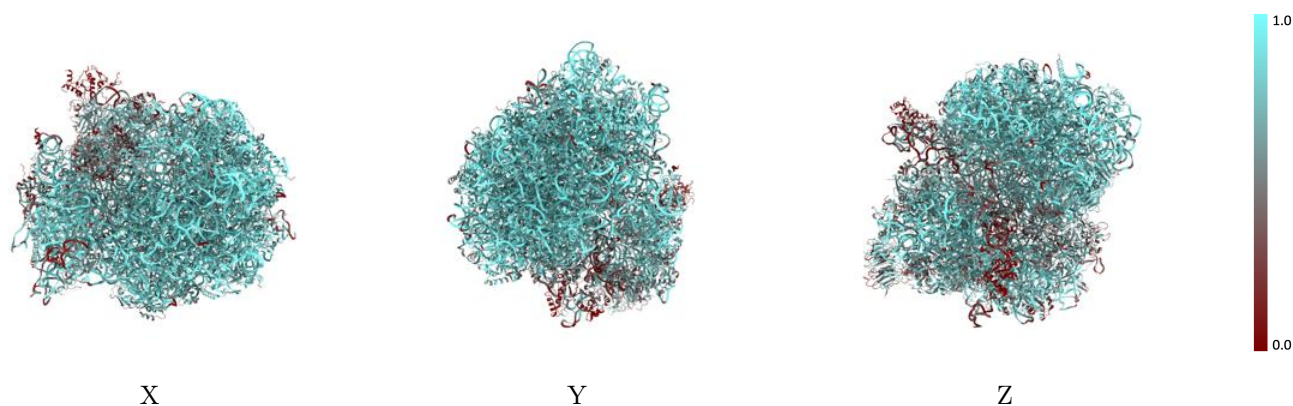
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



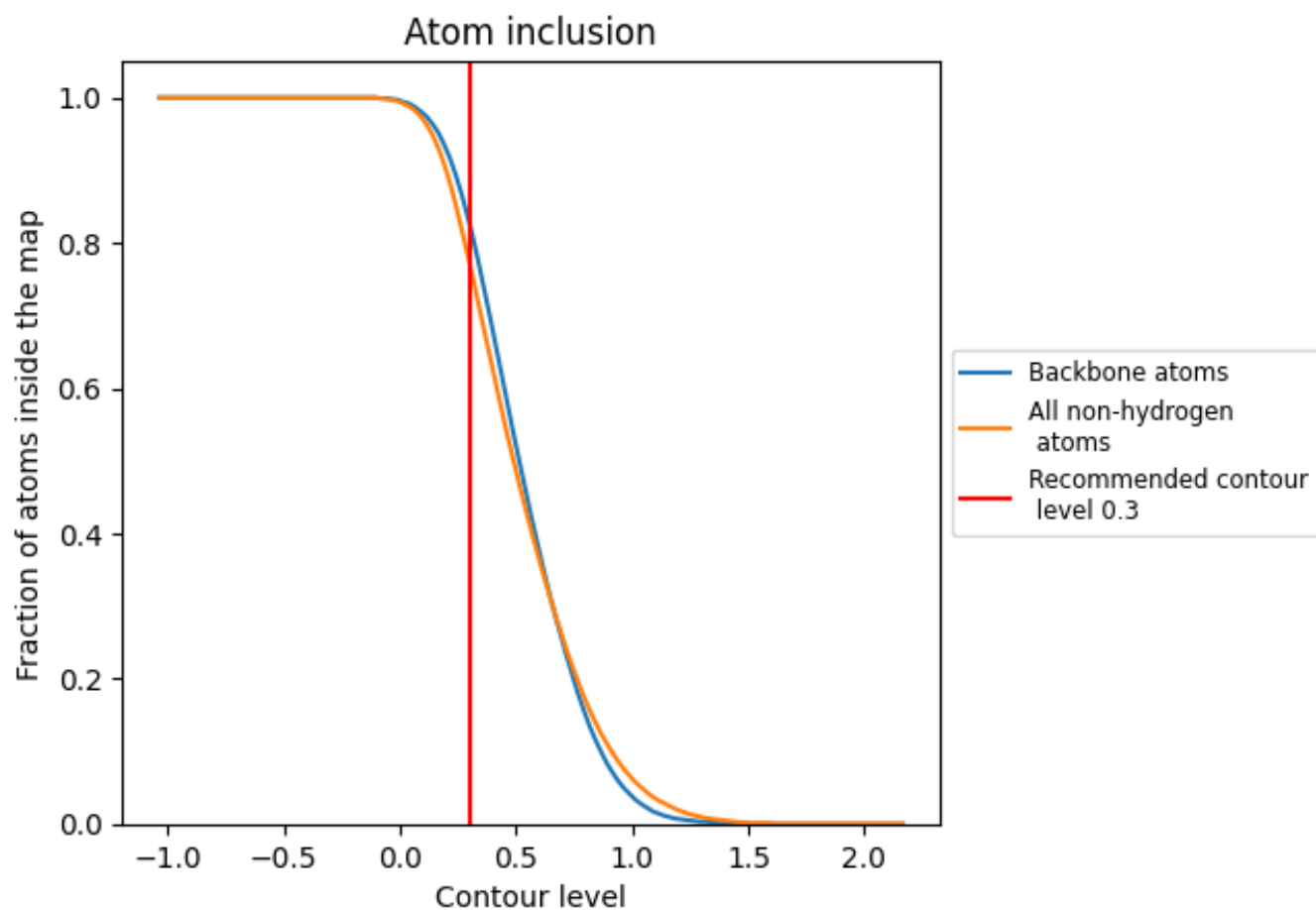
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.4370
A1	0.8870	0.4840
A3	0.9390	0.4710
A4	0.9290	0.5070
AA	0.7400	0.5350
AB	0.8200	0.5040
AC	0.8130	0.5060
AD	0.7520	0.4110
AE	0.8030	0.4450
AF	0.8400	0.5040
AG	0.7820	0.4580
AH	0.7600	0.4780
AI	0.7100	0.4540
AJ	0.6210	0.3900
AL	0.8200	0.4960
AM	0.7890	0.4660
AN	0.8170	0.5300
AO	0.7960	0.4990
AP	0.8200	0.5080
AQ	0.7840	0.5120
AR	0.6920	0.4560
AS	0.8240	0.4970
AT	0.7640	0.4940
AU	0.7350	0.4280
AV	0.7140	0.4980
AW	0.8080	0.4940
AX	0.7470	0.4860
AY	0.8180	0.4920
AZ	0.8260	0.4790
Aa	0.8350	0.5110
Ab	0.6440	0.4660
Ac	0.6840	0.4830
Ad	0.7750	0.4700
Ae	0.8060	0.5190
Af	0.8660	0.5360













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Chain	Atom inclusion	Q-score
Ag	 0.7560	 0.5020
Ah	 0.7980	 0.4800
Ai	 0.7600	 0.4590
Aj	 0.8630	 0.5480
Ak	 0.5930	 0.4110
Al	 0.7900	 0.5240
Am	 0.7490	 0.5000
An	 0.7080	 0.5070
Ao	 0.6250	 0.4820
Ap	 0.6790	 0.4890
B5	 0.8200	 0.4070
BA	 0.6870	 0.4000
BB	 0.6770	 0.4040
BC	 0.7450	 0.4620
BD	 0.5620	 0.3630
BE	 0.6930	 0.4060
BF	 0.5080	 0.3340
BG	 0.6830	 0.3420
BH	 0.6710	 0.3880
BI	 0.7230	 0.4390
BJ	 0.5830	 0.2440
BK	 0.5220	 0.2880
BL	 0.6860	 0.4610
BM	 0.0210	 0.1830
BN	 0.7090	 0.4750
BO	 0.7140	 0.4630
BP	 0.4510	 0.2980
BQ	 0.5850	 0.3350
BR	 0.5480	 0.3170
BS	 0.5690	 0.3310
BT	 0.6330	 0.3160
BU	 0.5120	 0.3430
BV	 0.7400	 0.4430
BW	 0.8030	 0.5010
BX	 0.6710	 0.4880
BY	 0.5470	 0.2320
BZ	 0.5580	 0.2970
Ba	 0.7280	 0.4830
Bb	 0.6960	 0.4340
Bc	 0.4650	 0.3270
Bd	 0.7590	 0.4110
Be	 0.5250	 0.3320

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Chain	Atom inclusion	Q-score
Bf	 0.0350	 0.1960
Bg	 0.5830	 0.2470
DC	 0.3660	 0.3210
E	 0.2200	 0.1130
EC	 0.3200	 0.2000